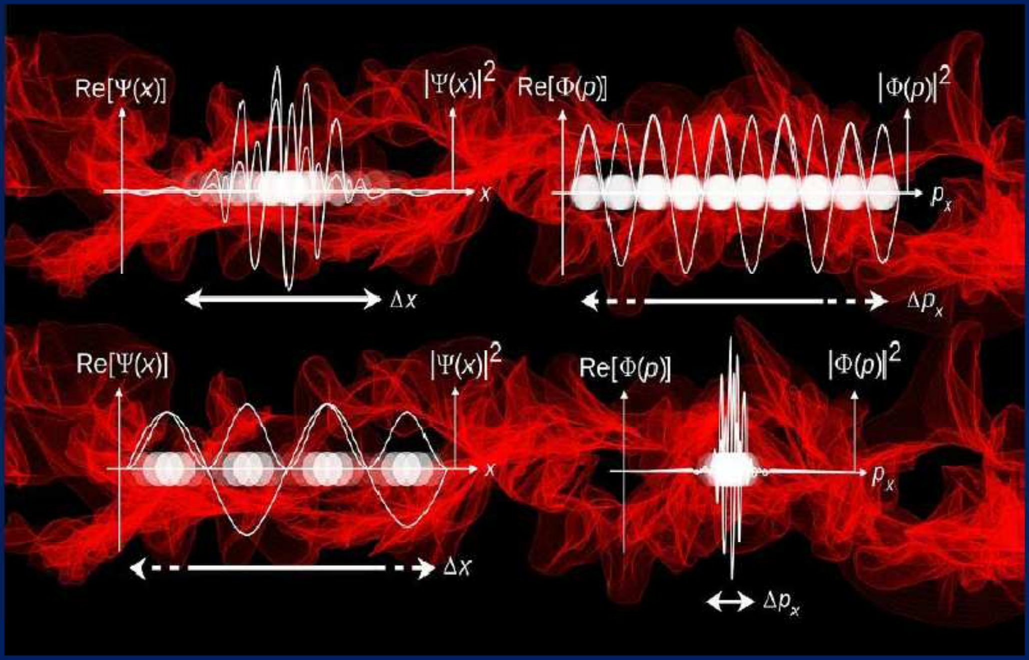
BSCPH-301

B. Sc. III YEAR

Elements of quantum mechanics and relativity



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Elements of Quantum mechanics and Relativity

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Course 9: Elements of Quantum mechanics and Relativity Course code: BSCPH201 Credit: 3

UNIT-1 ORIGIN OF QUANTUM MECHANICS

Structure

1.1 Introduction

Classical mechanics was utilized to explain dynamics of material bodies and matter-radiation interaction together with Maxwell electromagnetic theory. It seemed that all known physical phenomena could be explained by using these theories. At the turn of the twentieth century, classical physics fails miserably in providing the proper explanation for several new discoveries based on experimental observations. The failure of classical physics to explain several microscopic phenomena such as blackbody radiation, the photoelectric effect, Compton Effect had made the way for new theories. With the introduction of the concept of the quantum of energy by Max Planck in 1900, new direction of thinking was culminated. An accurate explanation of blackbody radiation was put forward by Planck by using his new idea of energy quantization. Later on in 1905 Einstein used the Planck’s postulates to explain photoelectric effect. Then in 1923 A.H. Compton made an important discovery of x-rays scattering by electrons, thus finally confirming the corpuscular nature of light having momentum hʋ/c, where ʋ is the frequency of x-rays.

1.2 Objectives

The objective of this unit is to provide insight, through the experimental findings, the need of quantum mechanics. Following are the experimental observations

- Black-body radiation spectral distribution
- Photoelectric effect
- Compton effect
- Specific heat capacity

Which could not be satisfactorily explained by classical theory, therefore, lay down the foundation of quantum mechanics, staring from the idea of Planck’s hypothesis, which are later used by the Einstein to explain many observed phenomena.

1.3 Black Body Radiation

Blackbody is an object which gives the maximum amount of energy radiated from its surface at any temperature and wavelength and absorbs all the radiation that falls on it. Model a blackbody is a small cavity. A black body is an ideal body which allows the whole of the incident radiation to pass into it (without reflecting the energy) and absorbs within itself this whole incident radiation (without passing on the energy). This is permissible for all radiations falling on at all angels. Therefore, the black body is an ideal absorber and emitter of incident radiation.

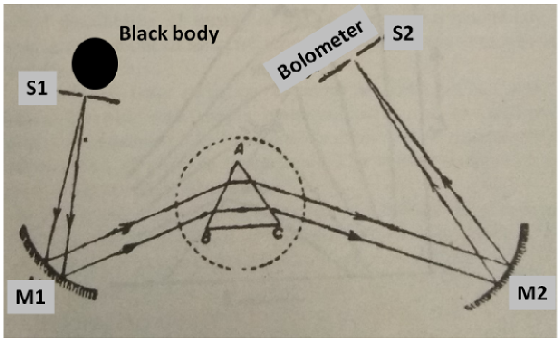

Figure1.1. Schematic of Lummer-Pringsheim experiment to measure spectral distribution of energy from back-body

Lummer and Pringsheim investigated the distribution of energy among the radiation emitted by black body at different temperatures. The experimental arrangement is shown in figure 1. In this case the black-body is electrically heated and temperature was monitored by thermocouple. As shown in figure 1, the radiations from black body pass through the slit S1 and fall on the mirror M1, which reflects radiations towards a prism (ABC) placed on rotating table. It worth to remember that the prism ABC is made of either rock salt or fluorspar. The radiations emergent from prism ABC are focussed by the concave reflector M2 towards slit S2. Behind slit S2, a bolometer is placed, which is connected to a sensitive galvanometer. If the rotating table is rotated slightly is such a manner that different part of spectrum successively falls on the bolometer and so that galvanometer can be read. The intensity of corresponding to each wavelength is found to the proportional to the deflection in the galvanometer. From Intensity versus wavelength curves, at different temperatures of black body, are drawn as shown in figure 1. On the basis of these experimental curves following conclusions can be made;

1. As the shapes of the curves at any particular temperatures are not symmetric, therefore, the energy is not uniformly distributed in the radiation spectrum of a black body.

2. At a given temperature, the intensity of the radiations increases with the increase in wavelength, reaches maximum value at a particular wavelength (λ_m), (as shown by dotted line) and afterwards decreases with further increase in wavelength.

3. As clear from the dotted line, the value of $\lambda_m$decreases with the increase in temperature. According to Wien's law;

$$\lambda_m . T = constant = 0.2896 \times 10^{-2}\, mK \ldots\ldots\ldots\ldots\ldots\ldots\ldots..(1.1)$$

4. With the increase in temperature, intensity corresponding to each wavelength increases thereby indicating increase in energy emission for all wavelengths.

5. The area under the each curve represents the total energy emitted by the black body at a particular temperature for the range of wavelengths considered. The area under the curve increases with the increase in temperature. It is found by Stefan's that the area under the curve (E) is directly proportional to the fourth power of absolute temperature (T^4). Thus Stefan's law can be written as;

$$E \propto T^4 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \qquad (1.2)$$

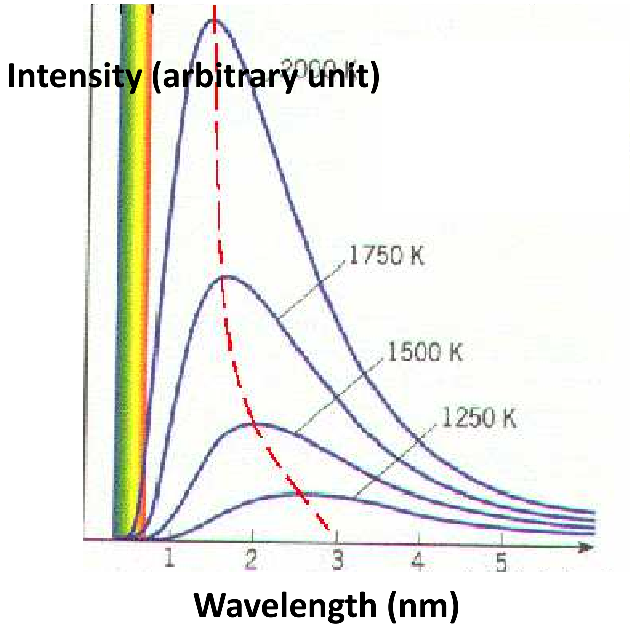

Figure1.2 Intensity versus wavelength plots as measured from black-body radiation at different temperatures

1.4 Rayleigh-Jeans law of Spectral Distribution of Energy

Rayleigh formula for the distribution of energy in the normal spectrum is based on the principle of equipartition of the energy for all the possible modes of free vibrations which might be assigned to radiation. According to him the radiation to consist of standing waves having a temperature T with nodes at the metallic surfaces. These standing waves are equivalent to harmonic oscillators. Classically average energy of an oscillator can be written as,

$$\bar{E} = kT \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \qquad (1.3)$$

The number of modes of vibration per unit volume in the frequency range υ and $\upsilon + d\upsilon$ is given by,

$$N_v d_v = \frac{8\pi v^2}{c^3} dv \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1.4)$$

The energy density within the frequency range υ and υ + dυ can be written as,

$$E_v dv = \frac{8\pi v^2}{c^3} dv \times kT \ldots\ldots\ldots\ldots\ldots\ldots\ldots. (1.5)$$

In terms of wavelength, Rayleigh-Jeans law may be written as,

$$E_\lambda d\lambda = \frac{8\pi}{c^3}\left(\frac{c^2}{\lambda^2}\right)\left|-\frac{c}{\lambda^2}d\lambda\right| kT = \frac{8\pi kT}{\lambda^4} d\lambda \ldots\ldots\ldots\ldots\ldots (1.6)$$

The Rayleigh –Jeans law explains the experimental measurements of the energy-distribution as mention in Figure 1.2 at long wavelength at higher temperatures only. It does not fit well for shorter wavelengths.

Moreover, according to above mentioned formula, the energy density should continuously increase with the decrease in wavelength and approach infinite when wavelength reduces to zero. Thus the total energy corresponding to wavelength range 0 to ∞ can be written as,

$$E = \int_0^\infty E_\lambda \, d\,\lambda = \int_0^\infty \frac{8\pi kT}{\lambda^4} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (1.7)$$

$$= 8\pi kT \left[-\frac{1}{3\lambda^3}\right]_0^\infty = \infty \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots. (1.8)$$

This indicates that almost all the energy should be confined in the vibrations of very small wavelengths, which is contrary to experimental results, and known as ultraviolet catastrophe.

1.5 Planck's Radiation law

Planck found an empirical formula to explain theexperimentally observed distribution of energy in the spectrum of a black-body. The formula may be deduced by using the following assumptions which are known as Planck's hypothesis;

1. A black-body chamber is filled up not only with the radiations but also simple harmonic oscillators or resonators of molecular dimensions known as Planck's oscillators or Planck's resonators. These oscillators vibrate with all possible frequencies having one degree of freedom.

2. The oscillators can absorbs or emit radiations in the quantized manner, i.e. an oscillator of frequency υ can only radiate or absorb energy in the units of nhυ (h is known as Planck's constant, its value being equal to 6.62×10^{-34} Joules/second) and n varies as 0,1,2,3,4,..... so on

Hence, we can say that the exchanges of energy between radiation and matter cannot take place continuously, but limited to discrete set of values 0, hυ, 2hυ, 3hυ, 4hυ...... nhυ in the multiple of some unit called the quantum.

Self Assessment Question (SAQ) 1.1: Define black body radiation. How does back body radiation varies with temperature?

Self Assessment Question (SAQ) 1.2: State Wien's law of back body radiation.

Self Assessment Question (SAQ) 1.3: What is the relation between the total energy of black body radiation and temperature?

Self Assessment Question (SAQ) 1.4: What isultraviolet catastrophe?

Self Assessment Question (SAQ) 1.5: State Planck's radiation law?

1.5.1 Derivation

For an electromagnetic (or light) wave travelling at the speed of light in some arbitary direction, e.g., in the direction of the vector r. If the wave has wavelength λ, at some instant the amplitude of the wave in the r-direction is,

$$A(r) = A_0 sin\frac{2\pi r}{\lambda} \dots\dots\dots\dots\dots\dots\dots\dots\dots..(1.9)$$

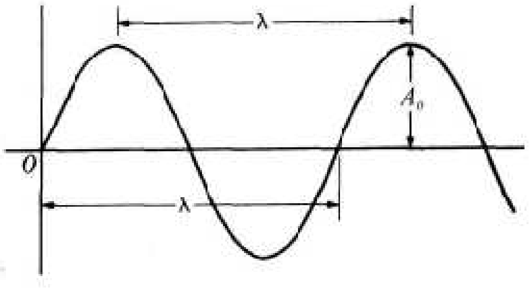

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Figure 1.3 representation of wave of moving in the direction of r.

In terms of the wave vector k,

$$A(r) = A_0 \sin(k.r) = A_0 sinkr \dots\dots\dots\dots\dots\dots\dots(1.10)$$

Where, |k| = 2π/λ. Wave vectors will prove to be very important quantities in what follows. The wave travels at the speed of light c in the r-direction and so, after time t, the whole wave pattern is shifted a distance ct in the positive r-direction and the pattern is A_0sin kr′, where we have shifted the origin to the point ct along the r-axis such that $r = r' + ct$. Thus, the expression for the wave after time t is

$$A(r,t) = A_0 sinkr' = A_0 \sin(kr - kct) \dots\dots\dots\dots\dots\dots (1.11)$$

But, if we observe the wave at a fixed value of r, we observe the amplitude to oscillate at frequency ν. Therefore, the time dependence of the wave amplitude is sin(2πt/T) where $T = \nu^{-1}$ is the period of oscillation of the wave. Therefore, the time dependence of the wave at any point is sinωt, where w= 2πυ, is the angular frequency of the wave. Therefore, the expression of wave

$$A(r,t) = A_0 \sin(kr - \omega t) \dots\dots\dots\dots\dots\dots (1.12)$$

and the speed of the wave is c = ω/k.

Consider a cubical box of side L, as shown in figure 4 below and imagine waves bouncing back and forth inside it. The box has fixed, rigid, perfectly conducting walls. Therefore, the electric field of the electromagnetic wave must be zero at the walls of the box and so we can only fit waves into the box which are multiples of half a wavelength.

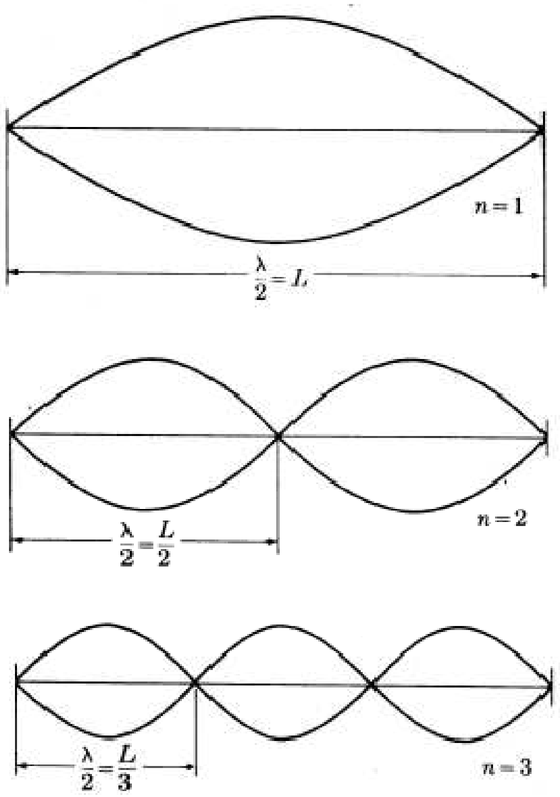


Figure 1.4 Schematic representation of wave formation inside a box of length L.

In the *x*-direction, the wavelengths of the waves which can be fitted into the box (as shown above) are those for which,

$$\frac{l\lambda_x}{2} = L \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(1.13)$$

Similarly, for the y- and z- directions

$$\frac{l\lambda_y}{2} = L \; and \; \frac{l\lambda_x}{2} = L \ldots\ldots\ldots\ldots\ldots\ldots.(1.14)$$

where l, m, n takes any positive integral value, 1, 2, 3, ...

The expression for the waves which fit in the box in the *x*-direction is,

$$A(x) = A_0 sink_x x \ldots\ldots\ldots\ldots\ldots\ldots\ldots(1.15)$$

where k_x is the component of the wave-vector of the mode of oscillation in the *x*-direction.

$$k_x = \frac{2\pi}{\lambda_x} \; and \; k_x = \frac{2\pi l}{2L} = \frac{\pi l}{L} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1.16)$$

Similarly

$$k_y = \frac{\pi m}{L}, k_z = \frac{\pi n}{L} \ldots\ldots\ldots\ldots\ldots\ldots.(1.17)$$

Let us now plot a three-dimensional diagram with axes k_x, k_y and k_z showing the allowed values of k_x, k_y and k_z. These form a regular cubical array of points, each of them defined by the three integers, *l, m, n*. The waves can oscillate in three dimensions but the components of their *k*-vectors, k_x, k_y and k_z, must be such that they are associated with one of the points of the lattice in *k*-space. A wave oscillating in three dimensions with any of the allowed values of *l, m, n* satisfies the boundary conditions and so every point in the lattice represents a possible mode of oscillation of the waves within the box, consistent with the boundary conditions. Thus, in three-dimensions, the modes of oscillation can be written as,

$$A(x, y, z) = A_0 \sin(k_x x) \sin(k_y y) \sin(k_z z) \ldots\ldots\ldots\ldots\ldots..(1.18)$$

Consider this is a trial solution into the three-dimensional wave equation, The time dependence of the wave is also sinusoidal, $A = A_0 \sin\omega t$ and so we can find the dispersion relation for the waves, that is, the relation between w and k_x, k_y, k_z,

$$\frac{\partial^2 A}{\partial x^2} + \frac{\partial^2 A}{\partial y^2} + \frac{\partial^2 A}{\partial z^2} = \frac{1}{c^2}\frac{\partial^2 A}{\partial t^2} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1.19)$$

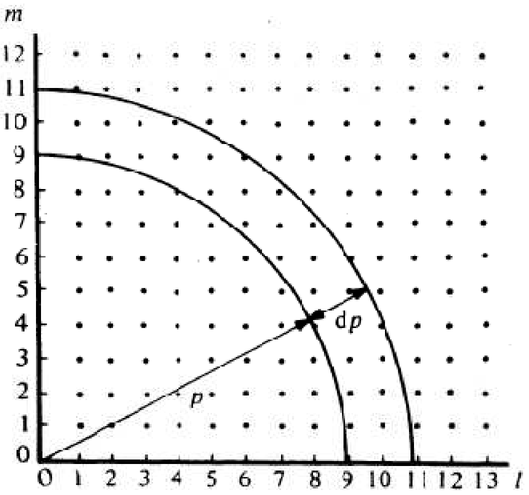


Figure 1.5 Possible values of l (along x-axis) and m (along y-axis) are drawn in x-y plane.

Then we find that

$$|k|^2 = \left(k_x^2 + k_y^2 + k_z^2\right) = \frac{\omega^2}{c^2}$$

$$k^2 = k_x^2 + k_y^2 + k_z^2 = \frac{\pi^2}{L^2}(l^2 + m^2 + n^2),$$

$$\frac{\omega^2}{c^2} = \frac{\pi^2}{L^2}(l^2 + m^2 + n^2) = \frac{\pi^2 p^2}{L^2}, \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1.20)$$

where $p^2 = (l^2 + m^2 + n^2) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1.21)$

To find out number of modes of oscillation in the frequency interval υ to υ + dυ, we need only count up the number of lattice points in the interval of k-space k to k + dk corresponding to υ to υ + dυ. We carried out a similar calculation in converting from $dv_x dv_y dv_z$ to $4\pi v^2 dv$.

Considering only positive values of *l*, *m* and *n* and so we need only one-eighth of the sphere of radius *p*. The volume of a spherical shell of radius *p* and thickness d*p* is $4\pi p^2 dp$ and so the number of modes in the octant is,

$$dN(p) = N(p)dp = \left(\frac{1}{8}\right) 4\pi p^2 dp \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1.22)$$

$$k = \frac{\pi p}{L} \text{ and } dk = \frac{\pi \, dp}{L}$$

$$dN(p) = \frac{L^3}{2\pi^2} k^2 dk,$$

Therefore, $dN(p) = \frac{V}{2\pi^2} k^2 \, dk = \frac{V}{2\pi^2} . \frac{8\pi^3 v^2}{c^3} dv = \frac{4\pi v^2 V}{c^3} dv \ldots\ldots\ldots\ldots\ldots..(1.23)$

Finally, for electromagnetic waves, we are always Note on the Polarisation of Electro-magnetic Waves Illustrating the electric and magnetic fields of an electromagnetic wave. The *E* and *B* fields of the wave are perpendicular to each other and to the direction of propagation of the wave. There is an independent mode of propagation in which *E* and *B* are rotated through 90± with respect to the direction of propagation *C*. Any polarisation of the wave can be formed by the sum of these two independent modes of propagation, allowed two independent modes, or polarisations, per state and so we have to multiply the result by two. Because of the nature of light waves, there are two independent states associated with each lattice point (*l; m; n*). The final result is that the number of modes of oscillation in the frequency interval υ to υ + dυ is,

$$dN = \frac{8\pi v^2 V}{c^3} dv \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(1.24)$$

Thus, number of states per unit state is

$$dN = \frac{8\pi v^2}{c^3} dv \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(1.25)$$

The quantisation of electromagnetic radiation means that the energy of a particular mode of frequency υ cannot have any arbitrary value but only those energies which are multiples of hυ, in other words the energy of the mode is E(υ) = nhυ, where we associate n photons with this mode. We now consider all the modes (and photons) to be in thermal equilibrium at temperature T. In order to establish equilibrium, there must be ways of exchanging energy between the modes (and photons) and this can occur through interactions with any particles or oscillators within the volume or with the walls of the enclosure. We now use the Boltzmann distribution to determine the expected occupancy of the modes in thermal equilibrium. The probability that a single mode has energy $E_n = nhv$ is given by the usual Boltzmann factor,

$$p(n) = \frac{\exp\left(-\frac{E_n}{kT}\right)}{\sum_{n=0}^{\infty} \exp\left(-\frac{E_n}{kT}\right)} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1.26)$$

This is the probability that the state contains n photons of frequency υ. The mean energy of the mode of frequency υ is therefore,

$$\overline{E_v} = \sum_{n=0}^{\infty} E_n p(n) = \frac{\sum_{n=0}^{\infty} E_n \exp\left(-\frac{E_n}{kT}\right)}{\sum_{n=0}^{\infty} \exp\left(-\frac{E_n}{kT}\right)}$$

$$= \frac{\sum_{n=0}^{\infty} nhv\, exp\,(-\frac{nhv}{kT})}{\sum_{n=0}^{\infty} exp\,(-\frac{nhv}{kT})} \text{ ……………..} (1.27)$$

To simplify the calculation, let us substitute $x = \exp\left(-\frac{hv}{kT}\right)$ then equation (1.26) becomes,

$$\overline{E_v} = hv\frac{\sum_{n=0}^{\infty} nx^n}{\sum_{n=0}^{\infty} x^n} = hv\frac{(x + 2x^2 + 3x^3 + \cdots)}{(1 + x + x^2 + \cdots)},$$

$$hv.x\frac{(x + 2x^2 + 3x^3 + \cdots)}{(1 + x + x^2 + \cdots)}.$$

As you know the following series expansions,

$$\frac{1}{(1-x)} = 1 + x + x^2 + x^3 + \cdots$$

$$\frac{1}{(1-x)^2} = 1 + 2x + 3x^2 + \cdots$$

$$\bar{E} = \frac{hvx}{1-x} = \frac{hv}{x^{-1}-1} = \frac{hv}{e^{\frac{hv}{kT}}-1}$$

To find the classical limit, we allow the energy quanta *hυ* to tend to zero. Expanding $e^{h\upsilon/kT}$ -1 for small values of *hυ/kT*,

$$e^{hv/_{kT}} - 1 = \left(1 + \frac{hv}{kT} + \frac{1}{2!}\left(\frac{hv}{kT}\right)^2 + \cdots\right) - 1$$

$$e^{hv/_{kT}} - 1 = \frac{hv}{kT}$$

Then

$$\bar{E} = \frac{hv}{e^{hv/kT}-1} = \frac{hv}{\epsilon/_{kT}} = kT \text{ ………………….} (1.28)$$

Thus, if we take the classical limit, we get exactly the expression for the average energy of a harmonic oscillator in thermal equilibrium,$\bar{E}$= *kT*.

The energy density of radiation in the frequency range υ and υ+dυ is,

$$u(v)dv = \frac{8\pi v^2}{c^3}\overline{E_v}dv$$

$$= \frac{8\pi h v^3}{c^3}.\frac{1}{\exp\left({}^{hv}/_{kT}\right) - 1} \dots\dots\dots\dots(1.29)$$

This formula is Planck's distribution formula. This formula can be written in terms of wavelength by using the relation υ = c/λ so

$$\left| dv = \left| -\frac{c}{\lambda^2} d\lambda \right| \right|$$

$$u(\lambda)d\lambda = \frac{8\pi hc}{\lambda^5}.\frac{d\lambda}{e^{\frac{hc}{\lambda kT}} - 1} \dots\dots\dots\dots\dots\dots\dots\dots\dots(1.30)$$

Total energy density of radiation,

$$u = \int_0^\infty u(v)dv$$

$$= \frac{8\pi h}{c^3}\int_0^\infty \frac{v^3 dv}{e^{{}^{hv}/_{kT}} - 1}$$

Let us replace $x = \frac{hv}{kT}$ and $dx = \frac{h}{kT}dv$ then energy density of radiation,

$$u = \frac{8\pi h}{c^3}\left(\frac{kT}{h}\right)^4 \int_0^\infty \frac{x^3}{e^x - 1}dx$$

The integral $\int_0^\infty \frac{x^3 dx}{e^x - 1}$is an standard integral value of which is equal to $\frac{\pi^4}{15}$, therefore,

$$u = \left(\frac{8\pi^5 k^4}{15c^3h^3}\right)T^4 = aT^4 \dots\dots\dots\dots\dots\dots(1.31)$$

The calculated value of $a = 7.566 \times 10^{-16} Jm^{-3}K^{-4}$. This relationship is known as Stefan-Boltzmann law for the energy density of black body radiation.

We can now relate this energy density to the energy emitted per second from the surface of a black body maintained at temperature *T*. Because the enclosure is in thermal equilibrium, we can use the relations derived from kinetic theory to work out the rate of arrival of photons per unit area. The flux of photons is ${}^{1}/_{4Nv} = {}^{1}/_{4Nc}$, since all the photons travel at the speed of light, where *N* is their number density. Therefore, the rate at which energy arrives at the walls per second, and consequently the rate at which the energy must be re-radiated from them,

$$^{1}/_{4Nh\nu c} = {}^{1}/_{4uc} \quad since\ u = Nh\nu$$

Therefore,

$$I = \frac{1}{4}uc = \frac{ac}{4}T^4 = \sigma T^4 = \left(\frac{2\pi^5 k^4}{15c^2h^3}\right)T^4 \qquad (1.32)$$

$$\sigma = \frac{ac}{4} = \left(\frac{2\pi^5 k^4}{15c^2h^3}\right) = 5.67 \times 10^{-8} Wm^{-2}K^{-4} \ldots\ldots\ldots\ldots\ldots..(1.33)$$

Equation (1.32) is referred as Stefan-Boltzmann Law. Again Planck's radiation formula in terms of wavelength (λ)

$$u(\lambda)d\lambda = \frac{8\pi hc}{\lambda^5}.\frac{1}{e^{\frac{hc}{\lambda kT}}-1}d\lambda \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(34)$$

Differentiating partially with respect to λ we get

$$= \frac{1}{e^{hc/_{\lambda kT}}-1} \times \frac{-5(8\pi hc)}{\lambda^6} + \frac{8\pi hc}{\lambda^5} + \frac{\frac{hc}{\lambda^2 kT}e^{hc/_{\lambda kT}}}{\left(e^{hc/_{\lambda kT}}-1\right)^2}$$

$$= -\frac{40\pi hc}{\lambda^6}.\frac{1}{e^{hc/_{\lambda kT}}-1} + \frac{8\pi hc}{\lambda^5} \times \frac{hc}{\lambda^2 kT}\frac{e^{hc/_{\lambda kT}}}{\left(e^{hc/_{\lambda kT}}-1\right)^2}$$

For maximum value of above expression, it must be equal to zero. Then,

$$-\frac{40\pi hc}{\lambda^6}.\frac{1}{e^{hc/_{\lambda kT}}-1} + \frac{8\pi hc}{\lambda^5} \times \frac{hc}{\lambda^2 kT}\frac{e^{hc/_{\lambda kT}}}{\left(e^{hc/_{\lambda kT}}-1\right)^2} = 0$$

$$\frac{8\pi hc}{(e^{hc/_{\lambda kT}}-1)\lambda^6}\left[-5 + \frac{hc}{\lambda kT} \times \frac{e^{hc/_{\lambda kT}}}{(e^{hc/_{\lambda kT}}-1)}\right] = 0$$

$$\left[-5 + \frac{hc}{\lambda kT} \times \frac{e^{hc/_{\lambda kT}}}{(e^{hc/_{\lambda kT}}-1)}\right] = 0$$

Let us assume $\frac{hc}{\lambda kT} = x$ then above equation becomes,

$$-5 + \frac{xe^x}{e^x - 1} = 0$$

$$5 = \frac{xe^x}{e^x - 1} = \frac{x}{1 - e^{-x}}$$

$$\frac{x}{5} + e^{-x} = 1$$

By the method of approximation, the exact value of x can be calculated to be equal to 4.965, then

$$x = \frac{hc}{\lambda kT} = 4.965 \ldots\ldots\ldots\ldots\ldots\ldots\ldots.(1.35)$$

Thus, the wavelength λ_m at which the energy per unit range of wavelength u_λ has its maximum value is given by,

$$\lambda_m . T = \frac{hc}{4.965k} = constant \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1.36)$$

Equation (1.36) is known as Wien's displacement law.

SAQ 1.6: How both the laws, Wien's and Rayleigh-Jean's are incorporated in the Planck's law.

1.6 Photoelectric Effect

1.6.1 Experimental observations

In 1887, Heinrich Hertz discovered that when electromagnetic radiation falls on a clean, metal surface, electrons are emitted from the surface. This phenomenon is called the photoelectric effect. Photo-emission depends upon the metal used. In case of alkali metals and alkaline earth metals, the emission of photo electrons can occurs even by ordinary visible light. The number of electrons emitted per unit time (called the photocurrent) depends on the intensity (i.e. brightness) and frequency (i.e. color) of the light that shines on the metal surface.

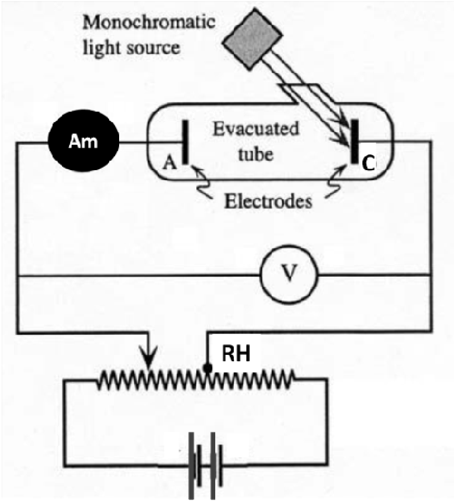


Figure1.6 Experimental setup to observe photoelectric effect.

The photoelectric effect is experimentally studied with the help of setup as shown in Figure 1.6. It consists of an evacuated glass tube that contains two metal electrodes A (anode) and C (cathode). The tube is connected to a power supply with a variable resistor that controls the potential difference V between the two electrodes. Light shines on one electrode which emits electrons called as cathode (C). The current due to the emitted electrons is measured by an ameter (Am). The purpose of the variable resistor and power supply is to measure the energy of the electrons emitted from the metal plate. If there is no potential difference (and therefore no electric field), electrons will be able to travel across the evacuated tube and reach the other end. However, if the potential is applied so that there is an electric force opposing the motion of each electron, only electrons with sufficient energy will be able to cross the tube. By increasing the potential until there is no photocurrent (and measuring that potential) the maximum kinetic energy of electrons leaving the metal surface can be determined. When light falls on the surface of the metal, it is absorbed. The photo-electrons are emitted by the surface. These photo-electrons short-circuit the gap between A and C and then current flows in the external circuit. The flow of photo-electrons stops as soon as the source of light is removed. The photo electric effect depends on the following factors;

(a) The potential difference between two electrodes

(b) The intensity of incident radiations

(c) The frequency of incident radiations

(d) The property of metal used to eject photo-electrons.

The effect of each of the above mentioned factors are explained below,

(a) The effect of potential difference

If the potential difference (V) between A and C is increased while keeping the intensity and frequency of radiation constant, the photo-current in the external circuit increases and becomes constant afterwards, know as saturation, as shown on figure 7 below. With the further increase in potential difference photo-current remains same. However, as clear from the figure that a small current flows even when the potential between A and C is zero. This happens because the emitted electrons have finite velocity and able to reach the plate A by overcoming a small repulsive force. When all the emitted photoelectrons are able to reach A, then it is called as a saturation. When the negative potential is applied (now A and C are connected to negative and positive terminals of battery, respectively) even then current flows and becomes zero at certain value of applied potential called as a stopping potential or cut off potential (V_0).

Therefore, the stopping potential of cut off potential is defined as the retarding potential for which no photo-current flows. It means the kinetic energy of emitted photo-electrons is not enough the reach the anode (A). If emitted photo-electron of mass *m* emitted with velocity *v* then the stopping potential is just equal to the kinetic energy of emitted photo-electrons. Therefore, we can write,

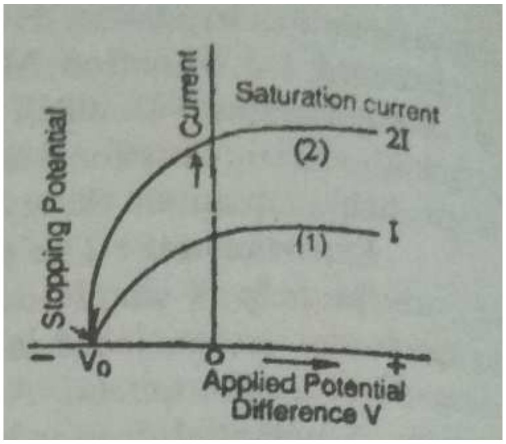


Figure 1.7 Effect of applied potential difference between A and C, while incident frequency is kept constant.

Kinetic energy of photoelectron = electrostatic potential energy`

$$\frac{1}{2}\, mv^2 = eV_0$$

The value of stopping potential (V_0) depends on the frequency of radiation incident on the cathode.

(b) The Effect of Intensity of Radiation

Value of saturation current depends on the intensity of radiation. As intensity of radiation increases the saturation current also increases, as shown in figure 8. Intensity of radiation means number of radiation falling on the surface per second. If the number of radiation falling on surface per second increase number of emitted photo-electrons also increases. Curves 1 and 2 are corresponding to intensities I and 2I, respectively. On increasing the intensity of radiation twice from the previous value, saturation current found to increase, as clear from figure.

(c) The Effect of frequency of Radiation

On increasing the frequency of radiation, it was found that higher stopping potential is required to reduce the photo-current to zero, as clear from the figure. In these measurements, the intensity of radiation and cathode material are kept same. If the frequency of the incident radiation is plotted against the corresponding stopping potential, a straight line is obtained. The frequency υ_0, the value of stopping potential corresponding to this is zero, is known as threshold frequency for the particular photo-metal used.

Threshold frequency is defined as the minimum value of frequency of incident radiation below which the photo-electric emission stops completely, irrespective the radiation intensity. The value of threshold frequency depends on the metal used. The kinetic energy of emitted photo-electrons is directly proportional to the frequency of incident radiation, and at threshold frequency its value is zero.

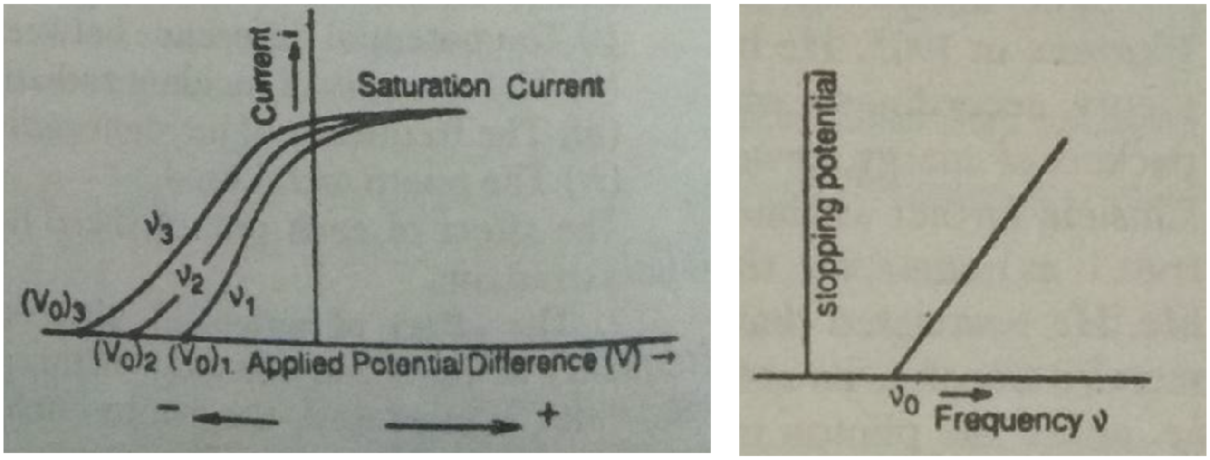


Figure 1.8 Effect of applied potential difference between A and C at different incident frequency of radiation

(b) The Effect of cathode metal

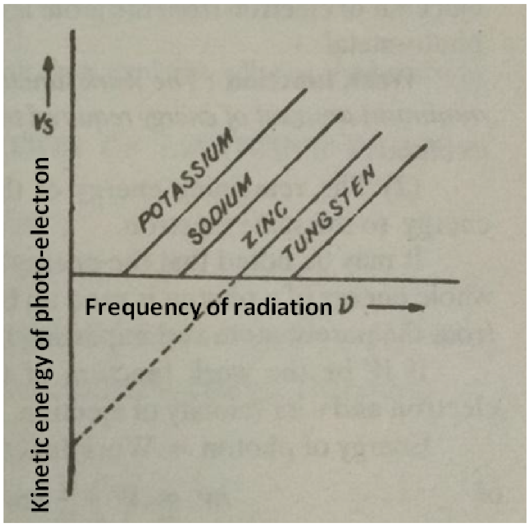


Figure 1.9 Effect of cathode metal to emit photo-electron

As clear from the figure 1.9 the kinetic energy is emitted photo-electrons depends on the metal used as a cathode. The curves corresponding potassium, sodium zinc and tungsten intersect the frequency axis at different values, indicating that the threshold potential corresponding to these metals are different.

From the above mentioned experimental observations on photo-electric effect can be summarized as the fundamental laws of photo-electric effect.

1. The rate at which photo-electrons emit is directly proportional to the intensity of the incident radiations.

2. The kinetic energy of emitted photo-electrons is independent of the intensity of incident radiation.

3. The kinetic energy of emitted photo-electrons is directly proportional to the frequency of the incident radiations and only takes above the certain frequency known as threshold frequency characteristic of metal surface used.

4. There is no delay between the incidence of radiation and emission of photo-electrons.

1.6.2 Einstein's Theory for Photoelectric Effect

Planck's gave explanation of the blackbody spectrum in 1900. In 1905, Einstein explained the photoelectric effect by using Planck's idea of quanta of radiation. He considered that the emission of radiation takes place in small packet of energy known as quanta of photons rather than continuously. The radiation can be defined as a ray of photons of energy hυ, moving with the speed of light (c), where h is Planck's constant and υ is the frequency of radiation. Photons move without dividing that is photon preserves their identity throughout their life and these can only be produced and absorbed as complete units. When a photon of energy hυ collides with an electron of the metal, it transfers its energy to the electron either completely of the electron or no energy at all. When a photon of energy hυ, is incident on the metal surface, its energy can be used up in two ways;

1. A part of energy is used up to eject out the electrons from the binding forces of the nucleus. This is metal dependent and known as work function (W) of the metal.

2. The remaining energy of the photon is used to impart kinetic energy to the same electron.

Thus we can write

Incident photon energy= work function + kinetic energy of electron

$$hv = W + \frac{1}{2}mv^2 \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (1.38)$$

Now, as mentioned before at threshold frequency υ_0 the kinetic energy of electron is zero. Therefore,

$$hv_0 = W \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (1.39)$$

So we can write

$$hv = hv_0 + \frac{1}{2}mv^2 \dots\dots\dots\dots\dots\dots\dots\dots\dots (1.40)$$

$$\frac{1}{2}mv^2 = h(v - v_0) \dots\dots\dots\dots\dots\dots\dots\dots (1.41)$$

This is known as Einstein photo-electric equation. On the basis of this equation Einstein put forward the following explanation regarding the laws of photo-electric effect.

1. If the intensity of light of a particulate frequency υ increases then the photons of energy hυ falling on the metal surface will increase that will cause emission of more photo-electrons.

2. As the energy of photons hυ is fixed then for a given metal, which has a particular value of work function then emitted electrons energy will remain unchanged as clear from above equation.

3. However the kinetic energy of emitted electrons depends on the energy of incident photons and work function of metal. If $\upsilon < \upsilon_0$ then the kinetic energy of electrons will become negative, which is not possible, therefore it means that in this condition emission of electrons is not possible.

4. As soon as a photon falls on the metal surface it is immediately absorbed by some electron and with no time gap ejected out.

Additionally, if we plot the photon frequency versus applied potential curve for a particular metal, then we can calculate work function of the metal, as shown in figure 10 below.

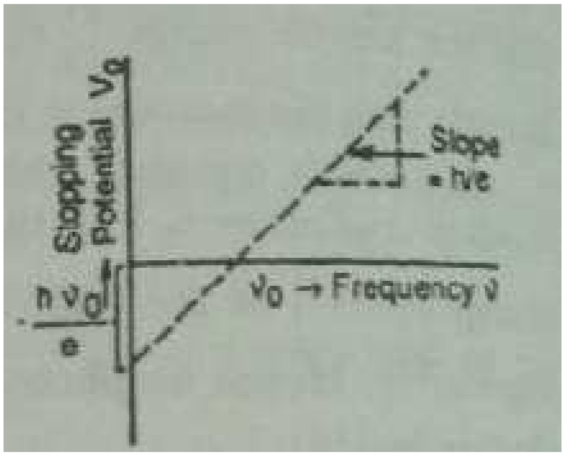


Figure 10 Plot to find out the work-function of metal

As mentioned in the figure the slope of straight line = $\frac{h}{e}$

and intercept on the potential axis is = $-\frac{h\upsilon_0}{e}$ … … … … … … … … … (1.42)

Then we calculate work function $W = h\upsilon_0 = -imtercept\ \times e$ … … … … (1.43)

SAQ 1.7 State photoelectric effect.

SAQ 1.8: State Einstein postulates to explain photoelectric effect.

1.7 Compton Effect

Compton scattering was discovered in 1922 by Arthur H. Compton (1892-1962) while conducting research on the scattering of X-rays by light elements. In 1922 he subsequently reported his experimental and theoretical results and received the Nobel Prize in 1927 for this discovery. His theoretical explanation of what is now known as Compton scattering deviated from classical theory and required the use of special relativity and quantum mechanics, both of which were hardly understood at the time.

When a beam of monochromatic high frequency radiation (for example x-rays or gamma rays) is scattered by light elements such as carbon, the scattered radiations contain radiations of lower frequencies along with the incident frequency. The scattered radiations with incident frequency are called the unmodified radiations while the scattered radiations with changed frequency are known as the modified radiations. This effect is known as Compton Effect. It was observed that the difference in the frequencies of these scattered radiations increases with the angle of scattering and it is independent of frequency of incident radiation. It is also not dependent on the scattering material.

To realise Compton scattering, high frequency photons are to be used. When high frequency photon collides with an atom, it knocks out its electrons and then photon is scattered with lower frequency. The theory of Compton scattering takes into account relativistic mechanics for two reasons.

(i) It involves the scattering of photons that are mass-less

(ii) The energy transferred to the electron is comparable to its rest energy.

As a result the energy and momentum of the photons and electrons must be expressed using their relativistic values. The laws of conservation of energy and conservation of momentum are used along with these relativistic values to develop the theory of Compton scattering.

Let a photon of energy hυ collide with light materials consisting of huge number of atoms. The energy of incident photon is very large as compared to work function of the materials so electron can be treated as a free. As a result of photons by an electron which is at rest initially, the electron recoils at an angle θ with the direction of incident photon as shown in figure 11. At the same time photon of lesser energy hυ′ scattered with an angle ϕ.

The energy of incident photon = $h\upsilon$

The energy of scattered photon = $h\upsilon' < h\upsilon$

The kinetic energy of the recoiled electron = $\frac{1}{2}mv^2$ where m is the mass of electron at velocity v.

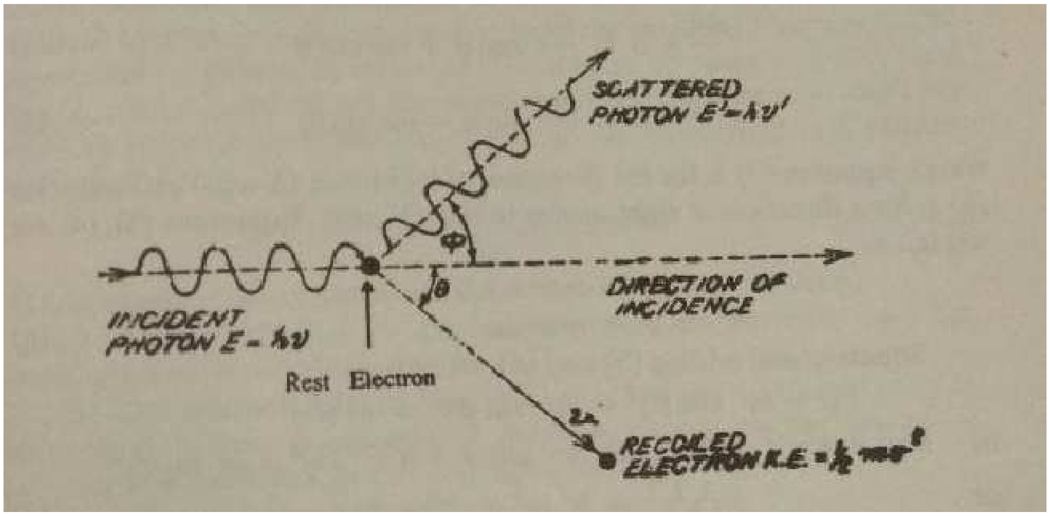


Figure 1.11 Schematic representation of scattering of incident photons by electron at rest

Now, before collision,

1. The energy of incident photon = hv

2. Rest mass energy of electron = $m_0\ c^2$, where m$_0$ is the rest mass of electron and c is the velocity of light.

3. The momentum of incident photons $p = \frac{energy}{c} = \frac{hv}{c}$

4. The momentum of the rest electron = 0

Now, after collision,

1. The energy of the scattered = hv'

2. Rest mass energy of electron = mc^2, where m is the mass of electron with recoil velocity v_e.

3. The momentum of incident photons $p = \frac{energy}{c} = \frac{hv'}{c}$

4. The momentum of the rest electron = mv

From the special theory of relativity, an object whose rest mass is $m_0$and is moving at a velocity $v_e$will have a relativistic mass m given by

$$m = \frac{m_0}{\sqrt{1 - \left({}^{v_e}/_{c}\right)^2}} \dots\dots\dots\dots\dots\dots (1.44)$$

Now according to conservation of energy,

Energy before collision = energy after collision

$h\upsilon + m_0\ c^2 = h\upsilon' + mc^2$.......................... (1.45)

Now according to conservation of momentum, momentum should remain same along x- and y-directions

Along x-direction,

$$\frac{h\upsilon}{c} + 0 = \frac{h\upsilon'}{c} cos\phi + m v cos\theta$$

$$\frac{h\upsilon}{c} - \frac{h\upsilon'}{c} cos\phi = m v cos\theta \ldots\ldots\ldots\ldots\ldots\ldots. (1.46)$$

Along y-direction,

$$0 + 0 = \frac{h\upsilon'}{c} sin\phi - m v sin\theta$$

$$\frac{h\upsilon'}{c} sin\phi = m v sin\theta \ldots\ldots\ldots\ldots\ldots\ldots. (1.47)$$

Squaring and adding equations (46) and (47),

$$(\frac{h\upsilon}{c} - \frac{h\upsilon'}{c} cos\phi)^2 + (\frac{h\upsilon'}{c} sin\phi)^2 = (m v sin\theta)^2 + (m v cos\theta)^2$$

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

$$m^2c^4 = h^2(\upsilon^2 + \upsilon'^2 - 2\upsilon\upsilon') + 2hm_0c^2(\upsilon - \upsilon') + m_0^2c^4$$

$$m^2c^4 - m^2v^2c^2 = (2h^2\upsilon\upsilon'\ (cos\phi - 1) + 2hm_0c^2(\upsilon - \upsilon') + m_0^2c^4$$

$$m^2c^4 - m^2v^2c^2 = \frac{m_0}{1-\frac{v^2}{c^2}} . c^4 - \frac{m_0}{1-\frac{v^2}{c^2}} . v^2c^4$$

$$= m_0 . c^4 \left[\frac{1-\frac{v^2}{c^2}}{1-\frac{v^2}{c^2}}\right] = m_0 . c^4$$

Therefore,

$$m^2c^4 = h^2(\upsilon^2 + \upsilon'^2 - 2\upsilon\upsilon') + 2hm_0c^2(\upsilon - \upsilon') + m_0^2c^4 \dots\dots\dots\dots\dots.(1.48)$$

Becomes

$$(2h^2\upsilon\upsilon'\,(1 - cos\phi) = 2hm_0c^2(\upsilon - \upsilon')$$

So

$$\frac{(\upsilon - \upsilon')}{\upsilon\upsilon'} = \frac{h}{m_0c^2}\,(1 - cos\phi)$$

$$\frac{1}{\upsilon'} - \frac{1}{\upsilon} = \frac{h}{m_0c^2}(1 - cos\phi) \dots\dots\dots\dots\dots\dots.(1.49)$$

In this equation (49) the right hand side is positive quantity therefore in left hand side must be positive therefore we get, $\upsilon' < \upsilon$. In terms of wavelength using the relation $\lambda = c/\upsilon$ and $\lambda' = c/\upsilon'$, we get

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_0c}(1 - cos\phi) \dots\dots\dots\dots\dots..(1.50)$$

The change in wavelength (Δλ) is known as Compton shift. This equation shows some important points to be remembered.

1. $scattered\ wavelength\ \lambda' > \lambda\ incident\ wavelength$

2. Δλ only depends on angle of scattering and independent of incident wavelength λ and materials used.

3. When $\phi = 0$ then $\cos\phi = 1$ and then $\Delta\lambda = \lambda' - \lambda = 0$, indicating no scattering along the direction of incident photons.

4. When $\phi = \pi/2$ then $\cos\phi = 0$ then

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_0c} = 0.0242\ \text{Å} \dots\dots\dots\dots\dots\dots\dots(51)$$

Expression given in equation (1.51) is known as Compton wavelength (λ_c).

5. When $\phi = \pi$ then $\cos\phi = -1$ then

$$\Delta\lambda = \lambda' - \lambda = \frac{2h}{m_0c} = 0.0484\ \text{Å} \dots\dots\dots\dots\dots\dots.(1.52)$$

Maximum shift in the wavelength of the scattered electron occurs. Although this maximum shift is only 0.001% of the initial light for λ = 6000 Å, while 4.84% when λ = 1 Å corresponding to x-rays. Therefore in X-rays and gamma rays this effect is easily observable.

$$tan\theta = \frac{hv'sin\phi}{h(v - v'cos\phi)} = \frac{v'sin\phi}{(v - v'cos\phi)}$$

$$\frac{1}{v'} = \frac{1}{v} + \frac{h}{m_0c^2}(1 - cos\phi) = \frac{1}{v} + \frac{h}{m_0c^2}\ 2sin^2\frac{\phi}{2}$$

$$\frac{(1 + \frac{h}{m_0c^2}\ 2sin^2\frac{\phi}{2})}{v}$$

$$v' = \frac{v}{(1 + \frac{hv}{m_0c^2}\ 2sin^2\frac{\phi}{2})}$$

Therefore,

$$tan\theta = \frac{cot\frac{\phi}{2}}{1 + \frac{hv}{m_0c^2}} \dots\dots\dots\dots\dots\dots\dots\dots (1.53)$$

This equation shows that the direction of electron recoil depends on the scattering angle ϕ. As ϕ changes from 0° to 180°, θ varies from 90° to 0°, thereby indicating that the electron can get recoiled only in the forward direction at angles less than 90°. On the other hand, photons can scatter in all directions as is ϕ can take values ranging from 0° to 180°.

Kinetic energy of the recoil electron can be calculated as

$$K.E. = hv - hv'$$

$$K.E. = hv - \frac{hv}{(1 + \frac{h}{m_0c^2}\ 2sin^2\frac{\phi}{2})}$$

$$K.E. = hv(\frac{\frac{2hv}{m_0c^2}sin^2\frac{\phi}{2}}{\left(1 + \frac{2hv}{m_0c^2}sin^2\frac{\phi}{2}\right)} \dots\dots\dots\dots\dots\dots.. (1.54)$$

When photons strikes with the bound electrons then the electron itself does not get detached by the impact but remains firmly bound so that the atom as a whole recoils. As the mass of recoiled atom is thousand times more than the recoil electrons, therefore, Compton shift Δλ becomes too small to be detected. Thus we can conclude that when a photon collides with a free electron its wavelength modify whereas when collides with a bound electron due to weak modification can consider it as unmodified radiation.

Experimental Verification of Compton Effect

A beam of monochromatic x-rays after passing through slits S1 and S2 falls on a graphite crystal, which acts as a scatter for x-rays. To record scattering of x-rays, a Bragg's spectrometer is placed at different scattering angles ϕ, as shown below in figure.

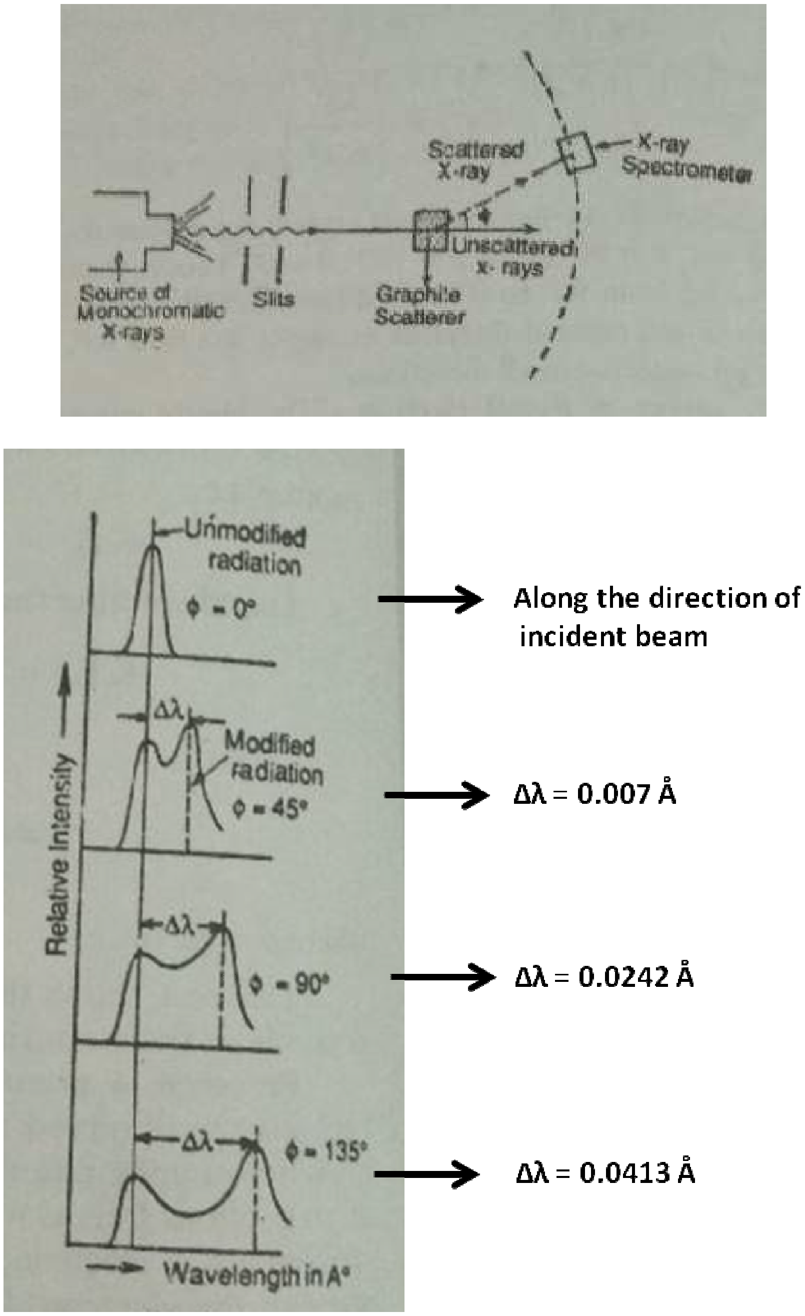


Figure 12 Setup to verify Compton shift at different angles of scattering

At different scattering angles, the scattered wavelength is recorded. The observational values were found according to the predicted Compton shifts.

SAQ 1.9: Explain Compton Effect.

SAQ 1.10: Why Compton Effect is not observable with visible light?

1.8 Classical Theory of Heat Capacity of Solids

The atoms in a solid are executing oscillations about their equilibrium positions with energy governed by the temperature of the solid .Such oscillations in crystals are called lattice vibrations. The lattice vibrations are responsible for the characteristic properties of matter such as specific heat, thermal conductivity, electrical conductivity, optical and dielectric properties, diffusion mechanism, phase change phenomena etc.

Atoms in a crystal are considered to be residing at particular lattice sites. But, in reality they undergo continuous fluctuations in the neighborhood of their regular positions in the lattice. These fluctuations arise from the heat or thermal energy in the lattice, and become more pronounced at higher temperatures.

When certain amount of heat (dQ) is added to the in order to change the temperature (dT) under the conditions either constant volume or constant pressure, then the quantity dQ/dT defines the heat capacity of solids.

At constant volume the change in temperature only change the internal energy of the solid, therefore we can write the expression for the heat capacity at constant volume as,

$$C = \left(\frac{dQ}{dT}\right)_V = \left(\frac{dE}{dT}\right)_V \dots\dots\dots\dots\dots\dots\dots..(1.55)$$

The specific heat has two contributions, one from the lattice vibrations i.e., lattice specific heat capacity and the other from the thermal motion of the electrons i.e., electron heat capacity. When temperatures are not too low, the contributions of electrons towards the specific heat can be neglected as it is smaller than that of the lattice specific heat capacity. If the lattice vibrations behave classically then, according to the equipartition theorem each normal mode of oscillation has an associated mean energy in equilibrium at temperature T= k_BT, half of it resides in the kinetic energy of the oscillation, and rest resides in the potential energy.

If there are N atoms in a solid, there will be 3N harmonic vibrations then the average energy can be given as,

$$\bar{E} = 3N\, k_B T \ldots\ldots\ldots\ldots\ldots\ldots\ldots. (1.56)$$

The specific heat thus obtained (by using equation 1.55) is given as,

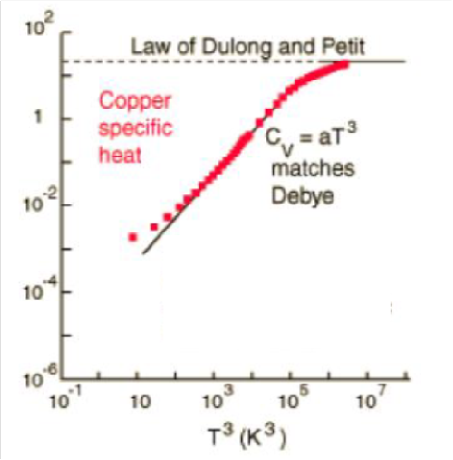
$$C_V = \left(\frac{dQ}{dT}\right)_V = \left(\frac{dE}{dT}\right)_V = 3Nk_B = 3R \ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (1.57)$$

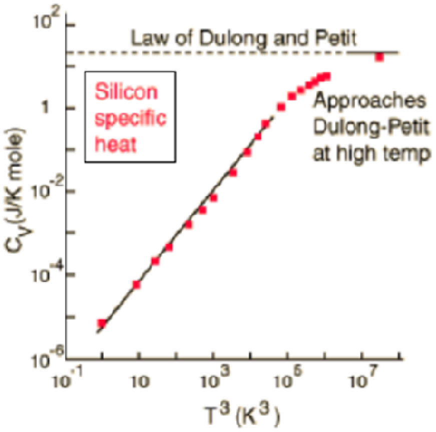
It follows that the molar heat capacity at constant volume is equal to 24.9 joules/mole/degree. In fact, at room temperature most solids (in particular, metals) have heat capacities which lie remarkably close to this value. This fact was discovered experimentally by Dulong and Petit at the beginning of the nineteenth century, and was used to make some of the first crude estimates of the molecular weights of solids. The heat capacity at constant volume (C_V) is somewhat less than the constant pressure (C_P) value, but not by much, because solids are fairly incompressible.

Thus according to Dulong and Petit law, the lattice specific heat capacity is independent of material properties and temperature. This holds good for higher temperatures but, for lower temperatures C_v is no longer a constant and decreases with temperature. The molar heat capacity cannot remain a constant as the temperature approaches absolute zero, which violates the third law of thermodynamics. Following experimental facts are observed regarding the heat capacity;

1. The Dulong and Petit law holds at very high temperature, just below the melting points of solid.

2. At low temperature, the heat capacity drops remarkably and approaches zero following T^3-law and T-law in insulators and metals, respectively, as T goes to zero, as shown in figure below.





$$C_V = \underset{\substack{\uparrow \\ \text{due to} \\ \text{electron gas}}}{bT} + \underset{\substack{\uparrow \\ \text{due to} \\ \text{atomic lattice}}}{aT^3}$$

3. In magnetic soilds, there is a large contribution to the heat capacity near the temperature at which magnetic moments become ordered.

1.9 Einstein Theory of Specific Heat of solids

According to Einstein theory, the crystal can be regarded as an aggregate of atomic oscillators, all of which vibrating independently with some natural frequency ω. The quantum mechanical oscillators can take values as,

$$\epsilon_n = n\hbar\omega \ldots\ldots\ldots\ldots..(1.58) \; where \;\; n = 0, 1,2,3 \ldots.$$

The thermal properties of the vibration of a lattice of N atoms can be represented a set of 3N one dimensional independent harmonic oscillators. Then the average energy can be written as,

$$\bar{E} = \frac{\sum_0^\infty \epsilon_n.\exp\left(-n\hbar\omega/k_B\ T\right)}{\sum_0^\infty exp\left(-n\hbar\omega/k_B\ T\right)}$$

Let us consider, $x = -\frac{\hbar\omega}{k_B T}$

Then the above expression can be expanded as

$$\bar{E} = \frac{\hbar\omega\left(e^x + 2e^{2x} + 3e^{3x} + \cdots\ldots\ldots\ldots\right)}{\left(1 + e^x + 2e^{2x} + 3e^{3x} + \cdots\ldots\ldots\ldots\right)}$$

$$\bar{E} = \hbar\omega \frac{d}{dx}\left\{\log\left(\frac{1}{1-e^{x}}\right)\right\}$$

$$\bar{E} = \frac{\hbar\omega}{e^{-x}-1}$$

On substituting the value of x

$$\bar{E} = \frac{\hbar\omega}{e^{\frac{\hbar\omega}{k_BT}}-1}$$

By including the zero point energy of the oscillators, total energy of 3N oscillators can be written as;

$$E = \frac{3N\hbar\omega}{2} + \frac{3N\hbar\omega}{e^{\frac{\hbar\omega}{k_BT}}-1}$$

The molar heat capacity is defined as,

$$C_V = \left(\frac{dE}{dT}\right)_V = 3N\frac{\hbar^2\omega^2}{k_BT^2}\frac{1}{\left(\exp\left(\frac{\hbar\omega}{k_BT}\right)-1\right)^2}\exp\left(\frac{\hbar\omega}{k_BT}\right)$$

Now $\hbar\omega = k_B\,\theta_E$

Therefore, above equation can be written as,

$$C_V = 3Nk_B\left(\frac{\theta_E}{T}\right)^2\frac{1}{\left(\exp\left(\frac{\theta_E}{T}\right)-1\right)^2}\exp\left(\frac{\theta_E}{T}\right) \ldots\ldots\ldots\ldots\ldots\ldots.(1.59)$$

(i) For very low temperatures, $T \ll \theta_E$ then $\exp(\theta_E/T) \gg 1$, therefore above equation can be written as,

$$C_V = 3Nk_B\left(\frac{\theta_E}{T}\right)^2\exp\left(-\frac{\theta_E}{T}\right) \ldots\ldots\ldots\ldots\ldots\ldots(1.60)$$

Thus, C_V tends to zero as T approaches zero exponentially. Although it has been found that the

$$C_V \,\alpha\, T^3$$

The reason for this discrepancy is the crude approximation that all normal modes have the same frequency. In fact, long wavelength modes have lower frequencies than short wavelength modes. A more realistic model of lattice vibrations was developed by the Dutch physicist Peter Debye in

1912. In the Debye model, the frequencies of the normal modes of vibration are estimated by treating the solid as an isotropic continuous medium. This approach is reasonable because the only modes which really matter at low temperatures are the long wavelength modes: *i.e.*, those whose wavelengths greatly exceed the interatomic spacing. It is plausible that these modes are not particularly sensitive to the discrete nature of the solid: *i.e.*, the fact that it is made up of atoms rather than being continuous.

(ii) For very high temperatures, T >> θ_E then $\exp(\theta_E/T) = 1 + \theta_E/T$, therefore above equation changes to,

$$C_V = 3Nk_B\left(\frac{\theta_E}{T}\right)^2 \frac{1+\frac{\theta_E}{T}}{\left(\frac{\theta_E}{T}\right)^2} \ldots\ldots\ldots\ldots\ldots (1.61)$$

$$C_V \cong 3Nk_B, \text{ classical limit}$$

Example 1.1. Calculate the momentum of a photon of energy 5 ergs.

Solution: For photon, $h\nu = mc^2$ *or we can write,* $mc^2 = h\nu = E$

Momentum is defined as, $p = mass \times velocity = mc$

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

$$\text{Given } E = 5\ ergs$$

$$\because 1\ ergs = 1 \times 10^{-7} Joule$$

$$\therefore 5\ ergs = 5 \times 1 \times 10^{-7} Joule$$

$$\therefore\ p = \frac{5 \times 1 \times 10^{-7}}{3 \times 10^8} = 1.67 \times 10^{-15} kg.m/sec$$

Example1.2. Calculate the number of photons emitted per second by a 3 Kilo watt monochromatic source of wavelength 2Å.

Solution: we know that energy of photon,

$$E = h\nu = \frac{hc}{\lambda}$$

Given, power of incident photons =3 Kilo watt = 3×10^3 watt= 3×10^3 Joule/sec

$$\because power = number\ of\ photons\ incident\ per\ second$$

Suppose "n"photons incident per second then,

$$power = nh\nu = \frac{nhc}{\lambda}$$

Therefore,

$$n = \frac{power\ \times \lambda}{hc}$$

$$\therefore n = \frac{3 \times 10^{3}\ \times 2 \times 10^{-10}}{6.6 \times 10^{-34} \times 3 \times 10^{8}} = 3.03 \times 10^{18}$$

Example 1.3: The work function of potassium is 2 eV. When a ultraviolet light of wavelength 3500 Å falls on the potassium surface, calculate the maximum kinetic energy of the emitted photoelectrons.

Solution: Energy of incident light, $E = hv = \frac{hc}{\lambda}$

Given, incident wavelength λ= 3500 Å=3500×10^{-10} m

h= 6.626 ×10^{-34} Joule.sec, c= 3.0 ×10^{8} m/sec

$$\therefore E = \frac{6.626 \times 10^{-34} \times 3 \times 10^{8}}{3500 \times 10^{-10}} Joule$$

$$= \frac{6.626 \times 10^{-34} \times 3 \times 10^{8}}{3500 \times 10^{-10} \times 1.6 \times 10^{-19}} eV = 3.57\ eV$$

Maximum kinetic energy $K_{max} = E - W\ (work\ function)$

$$= 3.57 - 2.0 = 1.57\ eV$$

Example 1.4 The work function of a metal is 1.24 eV.Find the velocity of ejected photo-electrons by the light of wavelength 4000 Å.

Solution: Energy of incident photons $E = hv = \frac{hc}{\lambda}$

$$= \frac{6.6\ \times 10^{-34} \times 3 \times 10^{8}}{4000 \times 10^{-10}} Joule$$

$$= \frac{6.6\ \times 10^{-34} \times 3 \times 10^{8}}{4000 \times 10^{-10} \times 1.6 \times 10^{-19}} = 3.09\ eV$$

Therefore, kinetic energy of ejected photo-electrons $\frac{1}{2}mu^{2} = E - W$

$$\frac{1}{2}mu^2 = 3.09 - 1.24 = 1.85\ eV$$

Therefore, velocity of ejected photo-electrons,

$$u = \sqrt{\frac{2 \times 1.85\ eV}{m}}$$

$$= \sqrt{\frac{2 \times 1.85 \times 1.6 \times 10^{-19}}{9.1 \times 10^{-31}}} = 8.06 \times 10^5 m/sec$$

1.10 Summary

In this unit, we have learned about black body radiation and then the requirement of the quantum approach to explain the observational facts. Furthermore the photo-electric effect and characteristics of photo-electric effects are understood. The hypotheses by Einstein to explain photo-electric effect are well described in this unit. Compton Effect is also explained in the later section. Therefore, we can conclude that the experimental observations of black body radiation, photo-electric effect and Compton Effect are historic in drawing the basis of quantum concept.

- Rayleigh- Jeans law,

$$E_\lambda d\lambda = \frac{8\pi}{c^3}\left(\frac{c^2}{\lambda^2}\right)\left|-\frac{c}{\lambda^2}d\lambda\right| kT = \frac{8\pi kT}{\lambda^4}d\lambda$$

- Planck's radiation law, the energy density of radiation per unit frequency interval,

$$u(v)dv = \frac{8\pi hv^3}{c^3} . \frac{1}{\exp\left({}^{hv}/_{kT}\right) - 1}dv$$

- Wien's displacement law,

$$\lambda_m . T = \frac{hc}{4.965k} = constant$$

- Stefan's Boltzmann Law,

$$u = \left(\frac{8\pi^5 k^4}{15c^3h^3}\right)T^4 = aT^4$$

$$a = 7.566 \times 10^{-16} Jm^{-3}K^{-4}$$

$$I = \sigma T^4 = \left(\frac{2\pi^5 k^4}{15c^2h^3}\right)T^4$$

$$\sigma = \frac{ac}{4} = \left(\frac{2\pi^5 k^4}{15c^2h^3}\right) = 5.67 \times 10^{-8} Wm^{-2}K^{-4}$$

- Einstein photoelectric equation

$$\frac{1}{2}mv^2 = h(\upsilon - \upsilon_0)$$

- Compton Shift

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

- Einstein equation of heat capacity

$$C_V = 3Nk_B\left(\frac{\theta_E}{T}\right)^2 \frac{1}{(\exp\left(\frac{\theta_E}{T}\right) - 1)^2}\exp\left(\frac{\theta_E}{T}\right)$$

1.11 Glossary

Black body - An object which gives the maximum amount of energy radiated from its and wavelength and absorbs all the radiation that falls on it.

Radiation – Transmission of energy in the form of wave through space or medium

Quanta – The minimum amount of any physical entity like energy involved in interaction.

Photoelectric effect: - Emission of electrons from a metallic surface when electromagnetic radiation falls on it.

1.12 References:

1. Quantum Mechanics: Concepts and Applications, Nouredine Zettili, A John Wiley and Sons, Ltd., Publication

2. Quantum Mechanics of atoms, molecules solids, nuclei and particles, Robert Eisberg and Robert Resnick, A John Wiley and Sons, Ltd., Publication

3. QUANTUM PHYSICS of Atoms, Molecules, Solids, Nuclei, and Particles, Robert Eisberg, A John Wiley and Sons, Ltd., Publication

10.13 Suggested Readings:

1. Fundamentals of Modern Physics, J.P. Agarwal and Amit Agarwal, Pragati Prakhasnan, Meerut

1.14 Terminal Questions:

Objective Questions:

a) The total energy emitted by black body depends on-

(i) T^4

(ii) T^2

(iii) T^{-4}

(iv) $1/T$

b) According to Wien's displacement law-

(i) $\lambda_m T^2$ = constant

(ii) $\lambda_m T^{-1}$= constant

(iii) $\lambda_m T$ = constant

(iv) $\lambda_m T = 0$

c) Kinetic energy of emitted photo-electron is independent of-

(i) Intensity of incident radiation

(ii) Work-function of emitting surface

(iii) Frequency of incident radiation

(iv) None of the above mentioned

d) The value of Compton wavelength (λ_c) is equal to-

(i) 0.242 Å

(ii) 0.0121 Å

(iii) 0.0484 Å

(iv) 0.0242 Å

e) The value of Compton shift $\Delta\lambda$ depends on-

(i) Angle of scattering

(ii) Incident wavelength

(iii) Incident frequency

(iv) Materials used

f) Maximum Compton shift in the wavelength of the scattered electron occurs when-

(i) $\phi = 0$

(ii) $\phi = 90°$

(iii) $\phi = 180°$

(iv) $\phi = 45°$

Short Answer Type Questions:

1.1 Explain the terms, Work function, cut off frequency, threshold potential and stopping potential.

1.2 Explain how Einstein postulates explain the observations of photo electric effect

1.3 State Wien's displacement law.

1.4 Explain the importance of photoelectric effect.

Long Answer type questions

1.1. Show that Planck's law reduces to Wien's law for shorter wavelengths and Rayleigh-Jean's law for longer wavelength.

1.2. Calculate the average energy E of an oscillator of frequency 6.0×10^{13} Hz at T= 1800 K, considering it as a (i) classical oscillator and (ii) Planck's oscillator

1.3. The photo-electric threshold wavelength of metal is 5000 Å. Find the following;

(i) the value of work function in electron volts

(ii) the kinetic energy of photo-electron in electron volts ejected on incident of radiations of 4000 Å and 3000 Å.

1.4. Calculate the velocity of a photo-electron, if the work function of metal surface is 1.24 eV and wavelength of the incident radiation is 4360 Å. What will be the magnitude of retarding potential?

1.5. X-rays of wavelength 1.00 Å are scattered by a carbon block. The scattered radiations are viewed at an angle of 90° to the direction of incidence. Calculate (i) Compton Shift and (ii) the energy of recoiled electron. [rest mass of electron $m_0 = 9.1 \times 10^{-31}$ kg, velocity of light $c= 3.0 \times 10^8$ m/sec, Planck's constant $h = 6.62 \times 10^{-34}$ joule.sec]

1.6. X-rays of wavelength 1 Å are scattered at such an angle that the recoil electron has a maximum kinetic energy, Calculate wavelength of the scattered wave.

1.7. If the Compton shift for a scattered x-ray beam at an angle 90° be 0.024 Å. Find out incident x-ray wavelength.

1.15: Answers of Terminal Questions:

Answer of objective questions: a) (i) **b)** (iii) **c)** (i) **d)** (iv) **e)** (i) **f)** (iii)

Answer of Long answer type:

1.2. (i) 2.48×10^{-20} J, **(ii)** 1.01×10^{-20} J

1.3.(i) 2.475 eV, **(ii)** 0.62 eV and 1.65 eV

1.4. 1.57 eV

1.5. (i) 0.02417 Å (ii) 293 eV

1.6. 1.0485Å

1.7. 2Å

Unit-2 Origin of Quantum Mechanics (Classical Theories)

Structure

1.1 Introduction

Atomic model was proposed initially by Thompson followed by Rutherford based on classical theories. Both the theories were found incapable to explain the observed experimental results, thus suffered serious drawbacks. However, both models provided the direction, which need improvements and modifications in order to offer the correct picture of atomic model so that experimental results could be explained satisfactorily. In this unit, we will learn about different models which describe the atomic structures by applying the concept of quantization of energy and photons, as discussed in the unit 1.

1.2 Objective

The objective of this unit is to introduce various approaches to describe the atomic structures and thus the experimentally observed spectra. Various models including their hypotheses, results and limitations are described. The following topics are incorporated in this unit;

- Bohr's Atomic Model
- Atomic spectra of hydrogen atom
- Franck-Hertz experiment

- Sommerfeld atomic model
- Shortcoming of classical and old quantum theories
- Foundation of quantum mechanics or wave mechanics

1.3 Bohr's Atomic model

To overcome the difficulty associated with the classical collapse of the electron into the nucleus, in 1913, Niels Bohr proposed a model for the hydrogen atom by using the following postulates to explain the electron motion in an atom and the observed spectral lines:

1. An electron in an atom moves in a circular orbit around the nucleus under the influence of Coulomb force of attraction between the electron and nucleus. The Coulombian force of attraction is balanced by Newtonian centrifugal force. Thus we have,

$$\frac{(Ze)(e)}{4\pi\varepsilon_0 r^2} = \frac{mu^2}{r} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots. (2.1)$$

2. An electron cannot revolve round the nucleus in all possible orbits as suggested by the classical theory. It can revolve only in a few widely separated permitted orbits. While moving along these orbits round the nucleus, an electron does not radiate energy. These non-radiating orbits are called stationary orbits.

3. The permissible orbits of an electron revolving round a nucleus are those for which the angular momentum of the electron is an integral multiple of *h*/2π, where *h* is *Planck's constant.* Thus for any permitted orbit,

$$I\omega = n\left(\frac{h}{2\pi}\right)$$

$$(mr_n^2)\frac{u_n}{r_n} = n\left(\frac{h}{2\pi}\right)$$

$$mr_n u_n = n\left(\frac{h}{2\pi}\right) \dots\dots\dots\dots\dots\dots\dots\dots (2.2)$$

where m and $u_n$are the mass and velocity of the electron, $r_n$the radius of the orbit and n is a positive integer, called the quantum number. The above equation (2.2) is called Bohr's quantum condition.

4. An atom radiates energy only when an electron jumps from a stationary orbit of higher energy to another of lower energy. Thus, if the electron jumps from an initial orbit of energy *Ei* to a final orbit of energy $E_f(E_i>E_f)$, the frequency υ of the radiation emitted is given by the relationship,

$$hv = E_i - E_f \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2.3)$$

This equation is called Bohr's frequency condition. Now let us consider the case of hydrogen atom, in which an electron of mass m is moving with velocity v_n around nucleus (Ze, proton) in circular nth orbit of radius r_n, as shown in figure 2.1.

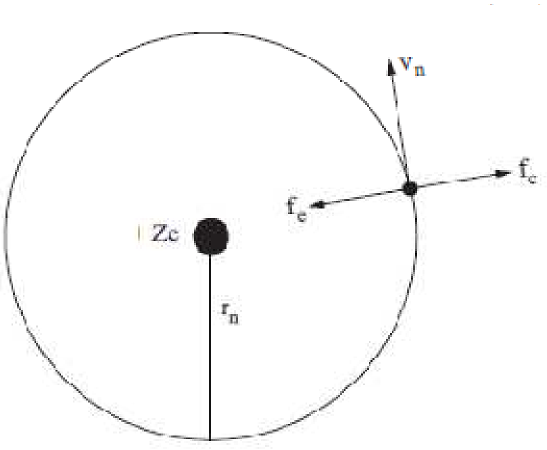


Figure 2.1 Bohr's model for hydrogen atom

From Bohr's first postulate, we have

$$\frac{mu_n^2}{r_n} = \frac{(Ze)(e)}{4\pi\varepsilon_0 r_n^2}$$

$$mr_n u_n^2 = \frac{Ze^2}{4\pi\varepsilon_0} \ldots\ldots\ldots\ldots\ldots\ldots. (2.4)$$

Z=1 for hydrogen atom. According to Bohr's third postulate, the angular momentum of the electron in a permitted orbit must be an integral multiple of *h/*2π, i.e.

$$mr_n u_n = n\left(\frac{h}{2\pi}\right)$$

$$u_n = n\left(\frac{h}{2\pi}\right)\left(\frac{1}{mr_n}\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (2.5)$$

Then equation (2.4) takes the form

$$(mr_n)\left[\frac{nh}{2\pi mr_n}\right]^2 = \frac{Ze^2}{4\pi\varepsilon_0}$$

$$\frac{n^2h^2}{4\pi^2 m r_n} = \frac{Ze^2}{4\pi\varepsilon_0}$$

Thus, the radius of n^{th} permissible orbit for electron in hydrogen atom is given by,

$$r_n = \left(\frac{n^2h^2\varepsilon_0}{\pi m Z e^2}\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(2.6)$$

Hence, the radii of different stationary orbits are directly proportional to the square of n, principal quantum number. Velocity u_n of electron in the stationary orbits can be obtained by substituting this value of r_n in equation,

$$u_n = \left(\frac{nh}{2\pi m}\right)\left[\frac{\pi m Z e^2}{n^2h^2\varepsilon_0}\right]$$

$$u_n = \frac{Ze^2}{2nh\varepsilon_0} \ldots\ldots\ldots\ldots\ldots\ldots..(2.7)$$

Therefore, the velocity of the electron is inversely proportional to the principal quantum number *n*. Thus, electron moves at a lower speed in higher orbits and vice versa. The orbital frequency (f_n) of an electron in the stationary orbits is also inversely proportional to third power of principle quantum number, as calculated below.

$$\omega_n = \frac{2\pi}{T_n} = 2\pi f_n = \frac{u_n}{r_n}$$

$$f_n = \left(\frac{1}{2\pi}\right)\left[\frac{Ze^2}{2nh\varepsilon_0}\right]\left[\frac{\pi m Z e^2}{n^2h^2\varepsilon_0}\right]$$

$$f_n = \frac{mZ^2e^4}{4\varepsilon_0^2 n^3 h^3} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(2.8)$$

The electron revolving round the nucleus has both potential energy, due to its position with respect to the nucleus and kinetic energy. The potential energy of the electron is considered to be zero when it is at infinite distance from the nucleus. Potential energy of an electron in an orbit is given by the work done in taking the electron from the distance *r* to infinity against the electrostatic attraction between the nucleus and the electron. This is obtained by integrating the electrostatic force of attraction between the nucleus and the electron from the limit ∞ to r_n. Thus potential energy can be written as,

$$P.E. = -\int_{r_n}^{\infty} F(r)dr$$

$$= \int_0^{r_n} \frac{Ze^2 dr}{4\pi\varepsilon_0 r_n^2}$$

$$= -\frac{Ze^2}{4\pi\varepsilon_0 r_n} \ldots\ldots\ldots\ldots\ldots\ldots..(2.9)$$

Similarly, Kinetic energy of the electron $K.E. = \frac{1}{2}mu_n^2$

Using the vlue of u_n from above equation,

$$K.E. = \frac{Ze^2}{8\pi\varepsilon_0 r_n} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(2.10)$$

Then the total energy of electron in nth orbit can be written as,

$$E_n = P.E. + K.E.$$

$$= -\frac{Ze^2}{4\pi\varepsilon_0 r_n} + \frac{Ze^2}{8\pi\varepsilon_0 r_n} = -\frac{Ze^2}{8\pi\varepsilon_0 r_n}$$

On substitution of value of r_n we can get,

$$E_n = -\frac{mZ^2e^4}{8\varepsilon_0^2 n^2 h^2} \ldots\ldots\ldots\ldots\ldots\ldots\ldots.(2.11)$$

The negative sign of the energy expression shows that the electron is bound to the nucleus and work must be done to pull out electron from its orbit. Total energy E_n decreases as n increases.

Now for hydron atom Z=1 then

$$r_n = \frac{n^2h^2\varepsilon_0}{\pi m Z e^2} \; with\, Z = 1$$

On substituting the values of $h=6.6262 \times 10^{-34}$, $\varepsilon_0 = 8.854 \times 10^{-12}$, $m = 9.109\times 10^{-31}$kg and $e = 1.602 \times 10^{-19}$ Coulomb, we get,

$$r_n = (0.529 \times 10^{-10}).n^2 \; metre \ldots\ldots\ldots\ldots\ldots\ldots\ldots(2.12)$$

Thus, radius of first orbit $r_1 = (0.529 \times 10^{-10})\; metre$ known as Bohr radius.

Siminlarly energy of electron can be expressed as after substituting the values in the equation (2.11)

$$E_n = -\frac{13.6}{n^2}\; eV \ldots\ldots\ldots\ldots\ldots\ldots\ldots(2.13)$$

The value of E corresponding to n =1 is known as the ground state energy of the atom, and is called the ionisation potential of hydrogen atom.

SAQ 2.1: What do you mean by ionization potential? Calculate the ionization potential of hydrogen atom.

SAQ 2.2: What is the energy of photon emitted when electron jumps from n=1 to n=2.

SAQ 2.3: Calculate the radius offirst Bohr orbit in hydrogen atom.Calculate the time taken by electron to transverse the first orbit in Hydrogen atom.

1.3.1 Bohr: Hydrogen spectra

If an electron jumps from an outer orbit n_2 of higher energy to an inner orbit n_1 of lower energy, emitted energy is, $hv = (E_{n2} - E_{n1})$

$$= \left[-\frac{mZ^2e^4}{8\varepsilon_0^2h^2n_2^2}\right] - \left[-\frac{mZ^2e^4}{8\varepsilon_0^2h^2n_1^2}\right]$$

Then emitted radiation frequency can be written as,

$$v = \frac{mZ^2e^4}{8\varepsilon_0^2h^3}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

Then as,

$$v = \frac{c}{\lambda} = \frac{mZ^2e^4}{8\varepsilon_0^2h^3}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] \ldots\ldots\ldots\ldots\ldots\ldots\ldots..(2.15)$$

Then the wavelength of emitted radiation,

$$\frac{1}{\lambda} = \frac{mZ^2e^4}{8\varepsilon_0^2ch^3}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.\ldots..(2.16)$$

Wavenumber (ῡ) is defined as inverse of wavelength therefore,

$$\bar{v} = \frac{1}{\lambda} = \frac{mZ^2e^4}{8\varepsilon_0^2ch^3}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right] \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(2.17)$$

$R_H = \frac{mZ^2e^4}{8\varepsilon_0^2ch^3}\ with\ Z = 1,$ is called Rydberg constant for hydrogen atom. The value of which can be calculates on substituting values and is equal to 1.0961 $\times 10^7$ m^{-1}.

An atom is said to be excited, if the electron is raised to an orbit of higher energy. The electron can be completely freed from the influence of the nucleus by supplying sufficient energy and the minimum energy needed for this is called ionisation energy.

$$E_I = E_\infty - E_1 = \frac{me^4}{8\varepsilon_0^2 ch^2} \cdot \left[\frac{1}{1} - \frac{1}{\infty}\right] = 13.6\ eV$$

As long as the electron remains in its orbit, no energy is radiated, but whenever an electron jumps from an outer orbit to an inner orbit, energy is emitted in the form of radiation. When the hydrogen atom is subjected to an external source to energy, the electron jumps from lower energy state to higher energy state. The atom is said to be excited. The excited state is not stable and hence the electron returns to its ground state in about 10^{-8} second. The excess of energy is now emitted in the form of radiations of different wavelengths. In a hydrogen discharge tube there are very large numbers of hydrogen atoms which are excited, and radiate energy. In some atoms the electrons may jump from the second orbit to the first orbit, in some others from the third to the second or first and so on. The different wavelengths due to different transitions of the electrons constitute spectral series which are characteristics of the atom emitting them.

1.3.2 Hydrogen Spectral Series

Lyman Series

When electrons jump from n_2 = 2, 3, 4, ... etc. orbits to the first orbit n_1 = 1, the spectral lines are in the ultraviolet region and called Lyman series. The wave-number (ῡ) corresponding to emitted radiation can be expressed as,

$$\bar{\upsilon} = \frac{1}{\lambda} = R_H \left[\frac{1}{1^2} - \frac{1}{n_2^2}\right] \dots\dots\dots\dots\dots\dots\dots\dots (2.18)$$

Balmer series

When electrons jump from outer orbits to the second orbit (n_1 = 2, n_2 = 3, 4, 5, ...), we get lines of Balmer series and lies in the visible region of the spectrum.

$$\bar{\upsilon} = \frac{1}{\lambda} = R_H \left[\frac{1}{2^2} - \frac{1}{n_2^2}\right] \dots\dots\dots\dots\dots\dots (2.19)$$

The first line in the series (n_2 = 3) is called H_α *line* then wave-number can be expressed as,

$$\bar{\upsilon}\,(H_\alpha) = \frac{1}{\lambda} = R_H \left[\frac{1}{2^2} - \frac{1}{3^2}\right]$$

the second line ($n_2 = 4$) is called H_β

$$\bar{\upsilon}\,(H_\beta) = \frac{1}{\lambda} = R_H\left[\frac{1}{2^2} - \frac{1}{4^2}\right]$$

Paschen series

Theselines in the infrared region are due to the transition of electrons from outer orbits ($n_2 = 4, 5, 6$............) to the third orbit ($n_1=3$).

$$\bar{\upsilon} = \frac{1}{\lambda} = R_H\left[\frac{1}{3^2} - \frac{1}{n_2^2}\right] \dots\dots\dots\dots\dots\dots\dots.(2.20)$$

Brackett Series

On transition from $n_1 = 4$ and $n_2 = 5, 6, 7, \dots$, we get Brackett series lines.

$$\bar{\upsilon} = \frac{1}{\lambda} = R_H\left[\frac{1}{4^2} - \frac{1}{n_2^2}\right] \dots\dots\dots\dots\dots\dots\dots.(2.21)$$

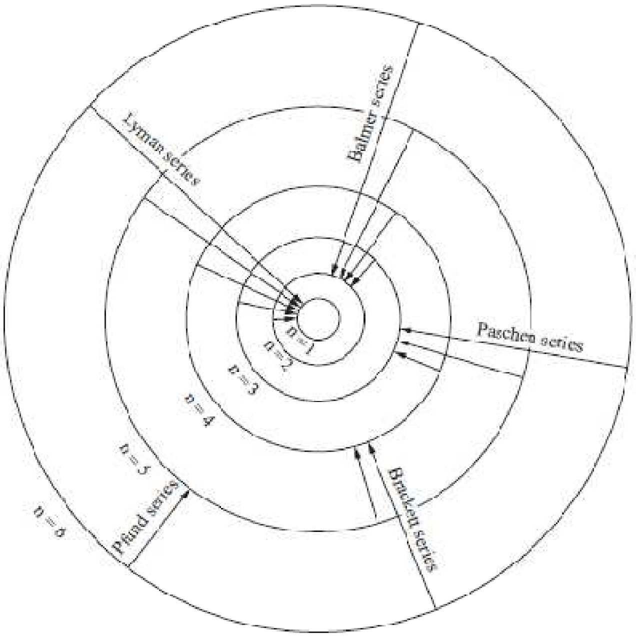


Figure 2.2. Different transition Series for hydrogen atom.

Pfund Series

If $n_1 = 5$ and $n_2 = 6, 7, 8, \ldots$, we get the Pfund series lines. For this series,

$$\bar{\upsilon} = \frac{1}{\lambda} = R_H\left[\frac{1}{5^2} - \frac{1}{n_2^2}\right] \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2.22)$$

Brackett and Pfund series lie in the far infrared region of the hydrogen spectrum.

The graphical representation and energy band diagram of transition corresponding to above mentioned series are given in figure 2 and 3, respectively.

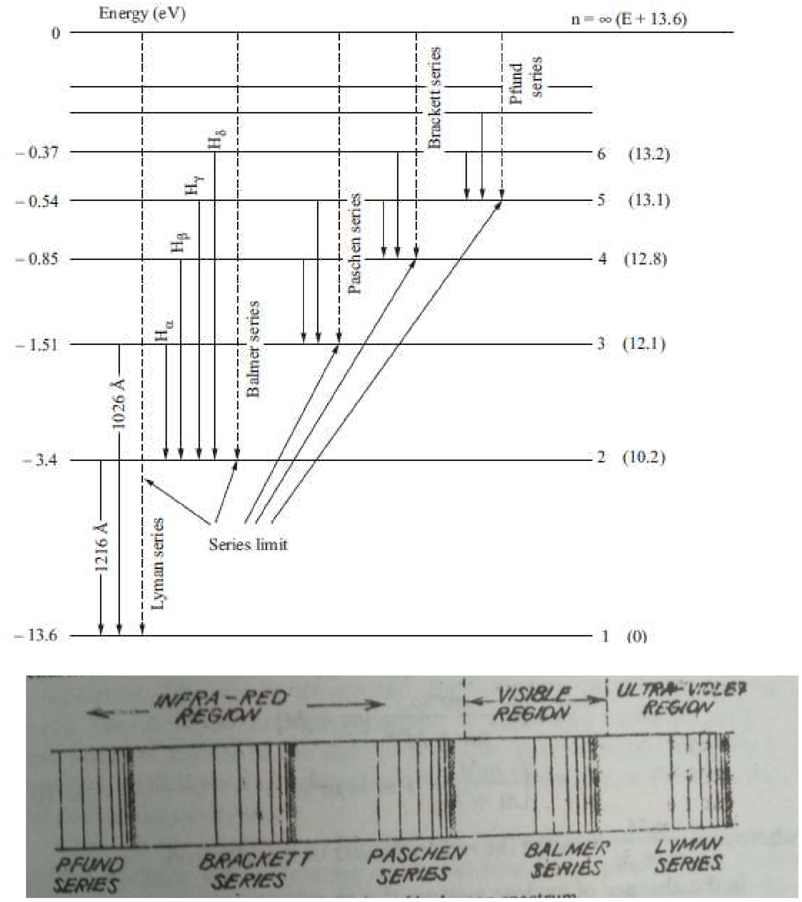


Figure 2.3. Energy level diagram and spectral series at different parts of electromagnetic spectrum of hydrogen atom.

1.3.3 Limitations of Bohr's Theory

Bohr's theory, based on circular electron orbits, was able to explain successfully a number of experimentally observed facts and has correctly predicted the spectral lines of neutral hydrogen atom and singly ionised helium atom in terms of the principal quantum number n. However, the theory fails to explain the following facts;

(i) Spectra of atoms more complex than hydrogen

(ii) Distribution and arrangement of electrons in atoms

(iii) Experimentally observed variations in intensity of the spectral lines of an element

(iv) Selection rules for the transitions of electrons from one level to another

(v) Fine structure of spectral lines

(vi) Quantitative study of chemical bonding.

(vii) Splitting of spectral lines in the presence of electric field (Stark effect) or magnetic field (Zeeman Effect).

SAQ 2.4: Calculate the wavelength of the first member of Balmer series of hydrogen atom. Given Rydberg constant for hydrogen $R = 1.097 \times 10^7 m^{-1}$

SAQ 2.5: Calculate the wavelength of the first member of Lyman series of hydrogen atom. Given Rydberg constant for hydrogen $R = 1.097 \times 10^7 m^{-1}$

1.4 Franck-Hertz Experiment

The Franck-Hertz experiment, first undertaken shortly after Bohr's theory of the atom was presented, and provided indications that atoms had discrete energy levels. Remarkable results of this elegant experiment led foundation of early developments of quantum theory.In 1914 Franck and Hertz performed a simple experiment to directly confirm that the internal energy states of an atom are quantized. Figure 4 schematically shows the experimental setup. When cathode (C) is heated then low energy electrons are thermally emitted from the cathode surface. On applying, potential V between the two anode (A) and cathode (C), electrons are accelerated. Some of the electrons pass through holes in *A* and reach to plate *P,* if they carry enough kinetic energy upon leaving *A* to overcome a small retarding potential V_r,applied between *P* and A. These electrodes C, A and P are enclosed inside the tube and the entire tube is filled at a low pressure with a gas or vapor of the atoms to be investigated. The experiment involves measuring the electron current (I) on reaching P as a function of the applied voltage *V.* The first experiment was performed with the tube containing Hg vapor. The observed variation in current value I as a function of applied voltage is depicted in Figure 5. On increasing voltage *V*, the current *I* is observed to increase at low accelerating voltage. When *V* reaches 4.9 V, the current abruptly drops, indicating that when the electrons gain a kinetic energy of 4.9 eV, some interaction between the electrons and the Hg atoms suddenly begins. A significant fraction of the electrons having energy ~4.9 eV excite the

Hg atoms and afterwards lose their entirely kinetic energy. If *V* is increased further, the electrons can gain enough kinetic energy after the excitation process to overcome V_r, and reach *P*. The sharpness of the break in the curve indicates that if electrons possess energy less than 4.9 eV then they are not able to transfer their energy to an Hg atom. This indicates the existence of discrete energy states for the Hg atom. So it can be said that the first excited state of Hg is 4.9 eV higher in energy than the ground state. Hg atom can not to accept energy from the electrons on collision if it is less than 4.9 eV.

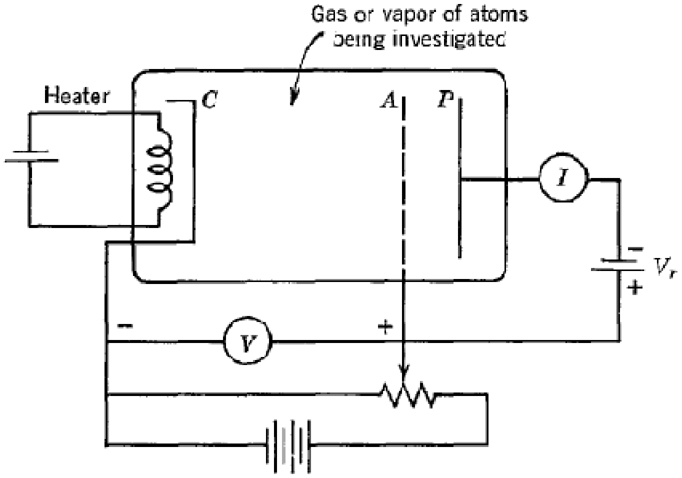


Figure 2.4. Schematic diagram of Franck-Hertz experiment.

Now, if the separation between the ground state and the first excited state is actually 4.9 eV, there should be a line in the Hg emission spectrum corresponding to the atom's loss of 4.9 eV in undergoing a transition from the first excited state to the ground state. Franck and Hertz found that when the energy of the bombarding electrons is less than 4.9 eV no spectral lines at all are emitted from the Hg vapor in the tube, and when the energy is not more than a few electron volts greater than this value only a single line is seen in the spectrum. This line is of wavelength 2536 A, which corresponds exactly to a photon energy of 4.9 eV.

The Franck-Hertz experiment provided striking evidence for the quantization of the energy of atoms. It also provided a method for the direct measurement of the energy differences between the quantum states of an atom. When the curve of *I* versus *V* is extended to higher voltages, additional breaks are found. Some are due to electrons exciting the first excited state of the atoms on several separate occasions in their trip from *C* to *A;* but some are due to excitation of the higher excited states and, from the position of these breaks, the energy differences between the higher excited states and the ground state can be directly measured.

Another experimental method of determining the separations between the energy states of an atom, is to measure its atomic spectrum and then empirically to construct a set of energy states which would lead to such a spectrum. In practice this is often quite difficult to do since the set of lines constituting the spectrum, as well as the set of energy states, is often very complicated; however, in common with all spectroscopic techniques, it is a very accurate method. In all cases in which determinations of the separations between the energy states of a certain atom have been made, using both this technique and the Franck-Hertz technique, the results have been found to be in excellent agreement. Figure 6 is a simplified representation of the energy states of Hg in terms of an energy level diagram. The separations between the ground state and the first and second excited states are known, from the Franck-Hertz experiment, to be 4.9 eV and 6.7 eV.

These numbers can be confirmed, and in fact determined with much higher accuracy, by measuring the wavelengths of the two spectral lines corresponding to transitions of an electron in the Hg atom from these two states to the ground state. The energy E=10.4 eV, of the ground state relative to a state of zero total energy, is not determined by the Franck-Hertz experiment. However, it can be found by measuring the wavelength of the line corresponding to a transition of an atomic electron from a state of zero total energy to the ground state. This is the series limit of the series terminating on the ground state. The energy (can also be measured by measuring the energy which must be supplied to an Hg atom in order to send one of its electrons from the ground state to a state of zero total energy. Since an electron of zero total energy is no longer bound to the atom, this is the energy required to ionize the atom and is therefore called the ionization energy. Lying above the highest discrete state at E = 0 are the energy states of the system consisting of an unbound electron plus an ionized Hg atom. The total energy of an unbound electron (a free electron with E > 0) is not quantized. Thus any energy E > 0 is possible for the electron, and the energy states form a continuum. The electron can be excited from its ground state to a continuum state if the Hg atom receives an energy greater than 10.4 eV. Conversely, it is possible for an ionized Hg atom to capture a free electron into one of the quantized energy states of the neutral atom. In this process, radiation of frequency greater than the series limit corresponding to that state will be emitted. The exact value of the frequency depends on the initial energy E of the free electron. Since E can have any value, the spectrum of Hg should have a continuum extending beyond every series limit in the direction of increasing frequency. This can actually be seen experimentally, although with some difficulty. These comments concerning the continuum of energy states for E > 0, and its consequences, have been made in reference to the Hg atom, but they are equally true for all atoms.

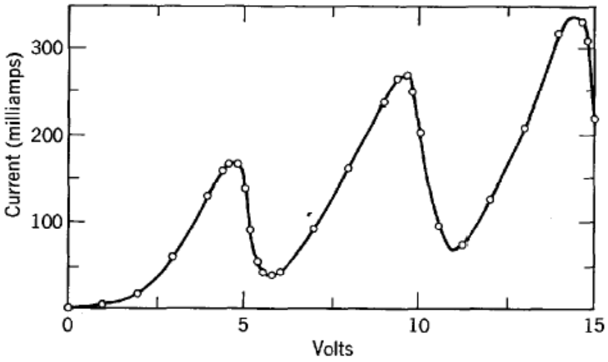


Figure 2.5. Measured current as a function of applied voltage.

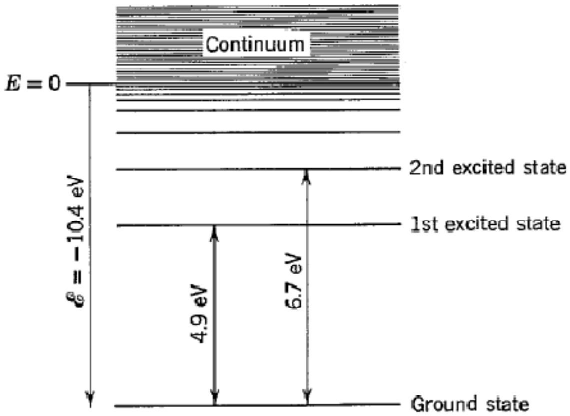


Figure 2.6. Simplified energy level diagram of Hg, above E> 0 the levels are continuous.

SAQ 2.6: The excited states of sodium are 2.1 and 3.7 eV. Find the corresponding wavelength in spectra.

1.5 Sommerfeld's Atomic Model

Sommerfeld succeeded partially in explaining the observed fine structure of spectral lines by introducing the following main modifications in Bohr's theory;

(*i*) Sommerfeld suggested that the path of an electron around the nucleus, in general, is an ellipse with the nucleus at one of the foci. The circular orbits of Bohr are a special case of this.

(*ii*) The velocity of the electron moving in an elliptical orbit varies considerably at different parts of the orbit. This causes relativistic variation in the mass of the moving electron. Therefore, Sommerfeld took into account the relativistic variation of the mass of the electron with velocity. Hence this model of the atom is called the relativistic atom model.

1.5.1 Elliptical orbit for electrons

An electron moving in the field of the nucleus describes elliptical orbits, with the nucleus at one focus. Circular orbits are only special cases of ellipses. When the electron moves along a circular orbit, the angular coordinate is sufficient to describe its motion. In an elliptical orbit, the position of the electron at any time instant is fixed by two coordinates namely the angular coordinate (φ) and the radial coordinate (r). Here r is the radius vector and φ is the angle which the radius vector makes with the major axis of the ellipse.

Consider an electron of mass *m* and linear tangential velocity *v* revolving in the elliptical orbit. This tangential velocity of the electron can be resolved into two components: One along the radius vector called radial velocity and the other perpendicular to the radius vector called the transverse velocity. Corresponding to these velocities, the electron has two momenta: One along the radius vector called radial momentum and the other perpendicular to the radius vector known as azimuthal momentum or angular momentum. So in the case of elliptic motion, both the angle φ and the radius vector r vary periodically, as shown in Figure 7.

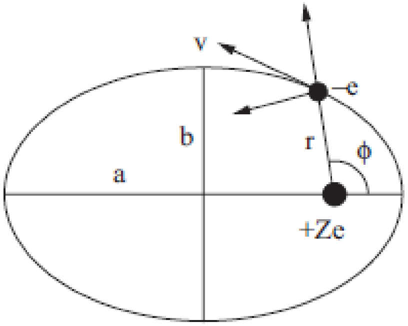


Figure 2.7. Sommerfeld model of hydrogen atom showing radial and transverse component of velocity.

Thus, the momenta associated with both these coordinates (φ and *r*) may be quantised in accordance with Bohr's quantum condition. Now, we have two quantization conditions related to the momenta associated with both the angular and radial coordinates.

$$\oint p_\phi d\phi = n_\phi h \ldots\ldots\ldots\ldots\ldots (2.23\,a)$$

$$\oint p_r dr = n_r h \ldots\ldots\ldots\ldots\ldots\ldots (2.23b)$$

where n_ϕ and n_r are the two quantum numbers introduced by Sommerfeld. Since they stand for one periodic system, therefore, $n_r + n_\phi = n$. Where n_r is defined as radial quantum number, n_ϕ as angular or azimuthal quantum number and n is known as principal quantum number. As, the force on the electron is due to the electrostatic attraction to the nucleus which acts along the radius vector, therefore, no force at right angles to this radius vector, so the transverse component of the acceleration is zero throughout the atom. Hence,

$$\frac{1}{r^2}\frac{d}{dt}\left[r^2\frac{d\phi}{dt}\right] = 0 \ldots\ldots\ldots\ldots\ldots\ldots..(2.24)$$

Therefore, $r^2\frac{d\phi}{dt}$ so $mr^2\frac{d\phi}{dt}$ must be constant. Then

$$p_\phi\int_0^{2\pi} d\phi = n_\phi h$$

$$p_\phi = n_\phi\left(\frac{h}{2\pi}\right)\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(2.25)$$

This equation shows that the angular momentum of the electron is an integral multiple of $h/2\pi$. It is considerably difficult to evaluate the integral in equation (2.18). However, an attempt is made here. The polar equationto the ellipse is,

$$\frac{1}{r} = \frac{1+\varepsilon cos\phi}{a(1-\varepsilon^2)}\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(2.26)$$

where a is the semi-major axis and ε is the eccentricity. Thus differentiating this equation with respect to ϕ, we get,

$$\left(\frac{1}{r^2}\right)\left(\frac{dr}{d\phi}\right) = \frac{\varepsilon cos\phi}{a(1-\varepsilon^2)}$$

$$\left(\frac{1}{r}\right)\left(\frac{dr}{d\phi}\right) = \frac{r\varepsilon cos\phi}{a(1-\varepsilon^2)}$$

$$\left(\frac{1}{r}\right)\left(\frac{dr}{d\phi}\right) = \frac{\varepsilon cos\phi}{a(1-\varepsilon^2)}\left[\frac{a(1-\varepsilon^2)}{(1+\varepsilon cos\phi)}\right]$$

$$\left(\frac{1}{r}\right)\left(\frac{dr}{d\phi}\right) = \frac{\varepsilon cos\phi}{(1+\varepsilon cos\phi)}$$

$$As\ mentioned\ before\ that \oint p_r dr = n_r h$$

$$\therefore \qquad \oint m\left(\frac{dr}{dt}\right)dr = n_r h$$

$$\therefore \qquad \oint m\left(\frac{dr}{d\phi}\right)\left(\frac{d\phi}{dt}\right)\left(\frac{dr}{d\phi}\right)d\phi = n_r h$$

$$\therefore \qquad \oint mr^2\frac{d\phi}{dt}\left[\frac{1}{r^2}\left(\frac{dr}{d\phi}\right)\left(\frac{dr}{d\phi}\right)\right]d\phi = n_r h$$

Now putting,

$$mr^2\frac{d\phi}{dt} = p_\phi$$

$$\frac{1}{r}\frac{d\phi}{dt} = \frac{\varepsilon sin\theta}{a(1-\varepsilon^2)}$$

Therefore, we get

$$\oint p_\phi\left[\frac{\varepsilon sin\phi}{(1+\varepsilon cos\phi)}\right]^2 d\phi = n_r h$$

Now using value of p_ϕ from equation (2.25) then we get,

$$n_\phi\frac{h}{2\pi}\oint\left[\frac{\varepsilon sin\phi}{(1+\varepsilon cos\phi)}\right]^2 d\phi = n_r h$$

$$\frac{n_\phi}{2\pi}\oint\left[\frac{\varepsilon sin\phi}{(1+\varepsilon cos\phi)}\right]^2 d\phi = n_r$$

$$u = \varepsilon sin\phi \; and \; v = \frac{1}{1+\varepsilon cos\phi}$$

Then above equation can be written as,

$$\frac{n_\phi}{2\pi}\oint udv = \left(\frac{n_\phi}{2\pi}\right)\left[[uv]_0^{2\pi} - \int_0^{2\pi} vdu\right]$$

$$= 0 - \left(\frac{n_\phi}{2\pi}\right)\int_0^{2\pi}\frac{(\varepsilon cos\phi)d\phi}{1+\varepsilon cos\phi} = n_r$$

$$= -\left(\frac{n_\phi}{2\pi}\right)\int_0^{2\pi}\frac{(\varepsilon cos\phi)d\phi}{1+\varepsilon cos\phi} = n_r$$

$$= \left(\frac{n_\phi}{2\pi}\right)\int_0^{2\pi}\left[\frac{1}{1+\varepsilon cos\phi} - 1\right]d\phi = n_r \ldots\ldots\ldots\ldots (2.27)$$

Solution of the integral:

$$\int_0^{2\pi} \frac{d\phi}{1+\varepsilon cos\phi}$$

Property of definite integral,

$$\int_0^{2\pi} f(x)dx = 2\int_0^{a} f(x)dx, if\ f(2a-x) = f(x)$$

$$= 0, if\ f(2a-x) = -f(x)$$

Therefore in the integral,

$$\int_0^{2\pi} \frac{d\phi}{1+\varepsilon cos\phi}$$

Let us consider,

$$f(\emptyset) = \frac{1}{1+\varepsilon cos\emptyset}$$

$$f(2\pi-\emptyset) = \frac{1}{1+\varepsilon\cos(2\pi-\emptyset)} = \frac{1}{1+\varepsilon cos\emptyset}$$

Thus,

$$\int_0^{2\pi} \frac{d\phi}{1+\varepsilon cos\phi} = 2\int_0^{\pi} \frac{d\phi}{1+\varepsilon cos\phi}$$

Let us consider, $t = tan\frac{\emptyset}{2}$

$$\emptyset = 0, t = 0 \colon when\ \emptyset = \pi, t = \infty$$

$$then, dt = \left[\sec^2\frac{\emptyset}{2}\right]\frac{d\emptyset}{2}$$

$$\therefore d\emptyset = \frac{2dt}{\sec^2\frac{\emptyset}{2}} = \frac{2dt}{1+\tan^2\frac{\emptyset}{2}} = \frac{2dt}{1+t^2}$$

$$and \qquad cos\emptyset = \frac{1-\tan^2\frac{\emptyset}{2}}{1+tan^2\frac{\emptyset}{2}} = \frac{1-t^2}{1+t^2}$$

Substituting these values, the integral becomes,

$$2\int_0^{\pi}\frac{d\phi}{1+\varepsilon cos\phi}=2\int_0^{\infty}\left(\frac{2dt}{1+t^2}\right)\frac{1}{1+\frac{\varepsilon(1-t^2)}{1+t^2}}$$

$$=2\int_0^{\infty}\left(\frac{2dt}{1+t^2}\right)\frac{(1+t^2)}{1+t^2+\varepsilon-\varepsilon t^2}$$

$$=4\int_0^{\infty}\frac{dt}{(1+\varepsilon)+\ t^2(1-\varepsilon)}$$

$$=\frac{4}{(1-\varepsilon)}\int_0^{\infty}\frac{dt}{t^2+\frac{(1+\varepsilon)}{(1-\varepsilon)}}$$

$$=\frac{4}{(1-\varepsilon)}\int_0^{\infty}\frac{dt}{t^2+\left[\sqrt{\frac{(1+\varepsilon)}{(1-\varepsilon)}}\right]^2}$$

$$=\frac{4}{(1-\varepsilon)}\left[\frac{1}{\sqrt{\frac{(1+\varepsilon)}{(1-\varepsilon)}}}\right]\left[\tan^{-1}\frac{t}{\left[\sqrt{\frac{(1+\varepsilon)}{(1-\varepsilon)}}\right]}\right]_0^{\infty}=\ \frac{4}{\sqrt{1-\varepsilon^2}}\left[\frac{\pi}{2}\right]=\frac{2\pi}{\sqrt{1-\varepsilon^2}}$$

Then equation (27) becomes,

$$\frac{n_\emptyset}{2\pi}\left[\frac{2\pi}{\sqrt{1-\varepsilon^2}}-2\pi\right]=n_r$$

$$n_\emptyset\left[\frac{1}{\sqrt{1-\varepsilon^2}}-1\right]=n_r$$

$$\frac{1}{\sqrt{1-\varepsilon^2}}=1+\frac{n_r}{n_\emptyset}=\frac{n_\emptyset+n_r}{n_\emptyset}$$

$$\sqrt{1-\varepsilon^2}=\frac{n_\emptyset}{n_\emptyset+n_r}=\frac{n_\emptyset}{n}$$

$$1-\varepsilon^2\ =\frac{{n_\emptyset}^2}{n^2}$$

$$\varepsilon^2\ =1-\frac{{n_\emptyset}^2}{n^2}=\frac{n^2-n_\emptyset^2}{n^2}$$

$$\varepsilon=\left[1-\frac{{n_\emptyset}^2}{n^2}\right]^{1/2}\ \dots\dots\dots\dots\dots\dots(2.28)$$

For an ellipse $(1-\varepsilon^2)=\frac{b^2}{a^2}$, where a and b are the semi-major and semi-minor axes, respectively.

$$\frac{b^2}{a^2}=\frac{{n_\emptyset}^2}{n^2}\dots\dots\dots\dots\dots\dots\dots..(2.29)$$

When $n_\phi = n$, $b = a$ and $\varepsilon = 0$, the orbit becomes circular. n_ϕ cannot be zero, since the ellipse would then degenerate into a straight line passing through the nucleus. Also n_ϕ cannot be greater than n, since b is always less than a. Hence for a given value of n, n_ϕ can take only n different values, so there can be only n elliptical orbits of different eccentricities. The tangential velocity of the electron at any time can be resolved into two component; radial $\frac{dr}{dt}$and transverse$r\frac{d\phi}{dt}$.

Therefore, radial momentum $p_r=m\frac{dr}{dt}\dots\dots\dots\dots\dots\dots\dots\dots.(2.30a)$

and the orbital angular momentum $p_\phi=mr^2\frac{d\phi}{dt}\dots\dots\dots\dots\dots\dots\dots\dots(2.30b)$

The kinetic energy of the circulating electron can be written as,

$$K.E.=\frac{1}{2}mu^2=\frac{1}{2}m\left[\left(\frac{dr}{dt}\right)^2+\left(r\frac{d\emptyset}{dt}\right)^2\right]$$

$$K.E.=\frac{p_r^2}{2m}+\frac{p_\emptyset^2}{2mr^2}\dots\dots\dots\dots\dots\dots\dots\dots\dots.(2.31)$$

We can write,

$$\frac{dr}{dt}=\frac{dr}{d\phi}.\frac{d\phi}{dt}$$

Then,

$$\frac{dr}{dt}=\left(\frac{dr}{d\emptyset}\right)\left(\frac{p_\emptyset}{mr^2}\right)$$

$$p_\emptyset^2=m^2r^4\left(\frac{d\emptyset}{dt}\right)^2$$

$$r^2\left[\frac{d\emptyset}{dt}\right]^2=\frac{p_\emptyset^2}{m^2r^2}$$

Then kinetic energy expression can be written as;

$$K.E.=\frac{1}{2}m\left[\frac{p_\emptyset^2}{m^2r^4}\left(\frac{dr}{d\emptyset}\right)^2+\frac{p_\emptyset^2}{m^2r^2}\right]\dots\dots\dots\dots\dots(2.32)$$

$$\frac{1}{2}\frac{p_{\emptyset}^{2}}{mr^{2}}\left[\left(\frac{1}{r}\frac{dr}{d\emptyset}\right)^{2}+1\right]$$

and potential energy can be written as;

$$P.E.=-\frac{Ze^{2}}{4\pi\varepsilon_{0}r}\ldots\ldots\ldots\ldots\ldots\ldots..(3.33)$$

Thus, the total energy of the system,

$$E_{n}=\frac{1}{2}\frac{p_{\emptyset}^{2}}{mr^{2}}\left[\left(\frac{1}{r}\frac{dr}{d\emptyset}\right)^{2}+1\right]-\frac{Ze^{2}}{4\pi\varepsilon_{0}r}\ldots\ldots\ldots\ldots\ldots\ldots(3.34)$$

$$\frac{1}{2}\frac{p_{\emptyset}^{2}}{mr^{2}}\left[\left(\frac{1}{r}\frac{dr}{d\emptyset}\right)^{2}+1\right]=E_{n}+\frac{Ze^{2}}{4\pi\varepsilon_{0}r}$$

$$\left[\frac{1}{r}\frac{dr}{d\emptyset}\right]^{2}=\frac{2mr^{2}E_{n}}{p_{\emptyset}^{2}}+\frac{mrZe^{2}}{2\pi\varepsilon_{0}p_{\emptyset}^{2}}-1$$

Now using the values of dr/dϕ value in terms of eccentricity, then

$$\frac{1}{r^{2}}\left[\frac{dr}{d\emptyset}\right]^{2}=\frac{\varepsilon^{2}r^{2}\sin^{2}\emptyset}{[a(1-\varepsilon^{2})]^{2}}=\frac{\varepsilon^{2}r^{2}(1-cos^{2}\emptyset)}{[a(1-\varepsilon^{2})]^{2}}$$

$$\frac{1}{r^{2}}\left[\frac{dr}{d\emptyset}\right]^{2}=\left[\frac{r}{a(1-\varepsilon^{2})}\right]^{2}(\varepsilon^{2}-\varepsilon^{2}cos^{2}\emptyset)$$

Now by the following relations,

$$(1+\varepsilon cos\emptyset)=\frac{a(1-\varepsilon^{2})}{r}$$

$$\varepsilon cos\emptyset=\frac{a(1-\varepsilon^{2})}{r}-1$$

$$(\varepsilon cos\emptyset)^{2}=\left[\frac{a(1-\varepsilon^{2})}{r}-1\right]^{2}$$

We get,

$$\frac{1}{r^{2}}\left[\frac{dr}{d\emptyset}\right]^{2}=\left[\frac{r}{a(1-\varepsilon^{2})}\right]^{2}\left[(\varepsilon^{2}-\left\{\frac{a(1-\varepsilon^{2})}{r}-1\right\}^{2}\right]$$

$$=\left[\frac{r}{a(1-\varepsilon^{2})}\right]^{2}\left[(\varepsilon^{2}-\left\{\frac{a^{2}(1-\varepsilon^{2})^{2}}{r^{2}}+1-\frac{2a(1-\varepsilon^{2})}{r}\right\}\right]$$

$$= \frac{r^2\varepsilon^2}{a^2(1-\varepsilon^2)^2} - 1 - \frac{r^2}{a^2(1-\varepsilon^2)^2} + \frac{2r}{a(1-\varepsilon^2)}$$

$$= \frac{r^2\varepsilon^2 - r^2}{a^2(1-\varepsilon^2)^2} + \frac{2r}{a(1-\varepsilon^2)} - 1$$

$$= -\frac{r^2(1-\varepsilon^2)}{a^2(1-\varepsilon^2)^2} + \frac{2r}{a(1-\varepsilon^2)} - 1 \ldots\ldots\ldots.(2.35)$$

Now, equating the coefficient of r^2 and r in equations (2.34) and (2.35), we get;

$$\frac{2mE_n}{p_\emptyset^2} = \frac{1}{a^2(1-\varepsilon^2)}$$

$$\frac{mZe^2}{2\pi\varepsilon_0 p_\emptyset^2} = \frac{2}{a(1-\varepsilon^2)}$$

Then,

$$E_n = -\frac{p_\emptyset^2}{2ma^2(1-\varepsilon^2)}$$

Now on substituting the value of $(1-\varepsilon^2)$ we get,

$$E_n = -\frac{p_\emptyset^2}{2ma^2}\left[\frac{amZe^2}{4\pi\varepsilon_0 p_\emptyset^2}\right]$$

$$E_n = -\frac{Ze^2}{8\pi a\varepsilon_0}$$

Again putting the value of a, we get;

$$E_n = -\left(\frac{Ze^2}{8\pi\varepsilon_0}\right)\left(\frac{mZe^2}{2\pi\varepsilon_0 p_\emptyset^2}\right)\left(\frac{1-\varepsilon^2}{2}\right)$$

$$E_n = -\left(\frac{mZ^2e^4}{32\pi^2\varepsilon_0^2}\right)\left(\frac{1-\varepsilon^2}{p_\emptyset^2}\right)$$

Substituting the value of $(1-\varepsilon^2)$ and p_ϕ, we obtain the expression of total energy as;

$$E_n = -\left(\frac{mZ^2e^4}{32\pi^2\varepsilon_0^2}\right)\left(\frac{n_\emptyset}{n}\right)^2\left(\frac{2\pi}{n_\emptyset h}\right)^2$$

$$E_n = -\left(\frac{mZ^2e^4}{8\varepsilon_0^2h^2n^2}\right) = -\frac{mZ^2e^4}{8\varepsilon_0^2h^2}\left[\frac{1}{n_r + n_\emptyset}\right]^2 \dots\dots\dots\dots.(2.36)$$

This is expression for the energy of the electron depending on only principle quantum number *n.* The magnitude of the semi-major axis *a* is obtained from equation (36) as follows:

$$E_n = -\frac{Ze^2}{8\pi\varepsilon_0 a} \quad \therefore a = -\frac{Ze^2}{8\pi\varepsilon_0 E_n}$$

Substituting the value of E_n then;

$$a = -\left[\frac{Ze^2}{8\pi\varepsilon_0}\right]\left[\frac{8\varepsilon_0^2h^2n^2}{mZ^2e^4}\right]$$

$$= \frac{\varepsilon_0 h^2 n^2}{\pi m Z e^2}$$

$$= \frac{n^2 r_B}{Z} \dots\dots\dots\dots\dots\dots.(2.37)$$

Where, r_B is the Bohr radius and defined as;

$$r_B = \frac{\varepsilon_0 h^2}{\pi m e^2} = 0.0529\, nm$$

In case of ellipse we know,

$$(1 - \varepsilon^2) = \frac{b^2}{a^2}$$

$$b = a\sqrt{1-\varepsilon^2} = a\left(\frac{n_\emptyset}{n}\right) = \left(\frac{n^2 r_B}{Z}\right)\left(\frac{n_\emptyset}{n}\right) \dots\dots\dots\dots\dots\dots(2.38)$$

Equations (2.37) and (2.38) show that the length of the semi-major axis is determined solely by the principal quantum number *n,* while the length of the semi-minor axis depends upon the azimuthal quantum number n_ϕ (l) as well as *n*.

For a given value of *n*, the possible values of

n_ϕ = 0, 1, 2, ..., *n*

n_r= *n*, (*n* – 1), ..., ...0

When n_ϕ = 0, the ellipse reduces to a straight line and the electron then passes through the nucleus traversing the orbit. This leads to the collapse of the atom. Therefore, the value of n_ϕ = 0 is forbidden and for a given value *n*,

$$n_\phi = 1, 2, 3, \ldots\ldots\ldots\ldots\ldots\ldots\ldots, n$$

$$n_r = (n-1), (n-2), \ldots\ldots\ldots\ldots, 0$$

For the first orbit $n = 1$,

$(n_r + n_\phi) = 1$ and $n_\phi \neq 0 \Rightarrow n_\phi = 1$ and $n_r = 0$, therefore, first orbit is a circle

For the first orbit $n = 2$,

Possible values of $n_\phi = 1, 2$ with identical energy

So for $n = 2$ and $n_\phi = 1$, orbit an ellipse

So for $n = 2$ and $n_\phi = 1$, orbit is a circle

Similarly with $n = 3$,

Possible values of $n_\phi = 1, 2$ with identical energy

So for $n = 3$ and $n_\phi = 1$, orbit an ellipse

So for $n = 3$ and $n_\phi = 2$, orbit an ellipse

So for $n = 3$ and $n_\phi = 3$, orbit a circle

The orbit corresponding to n = 1, 2, 3 are depicted in figure 8.

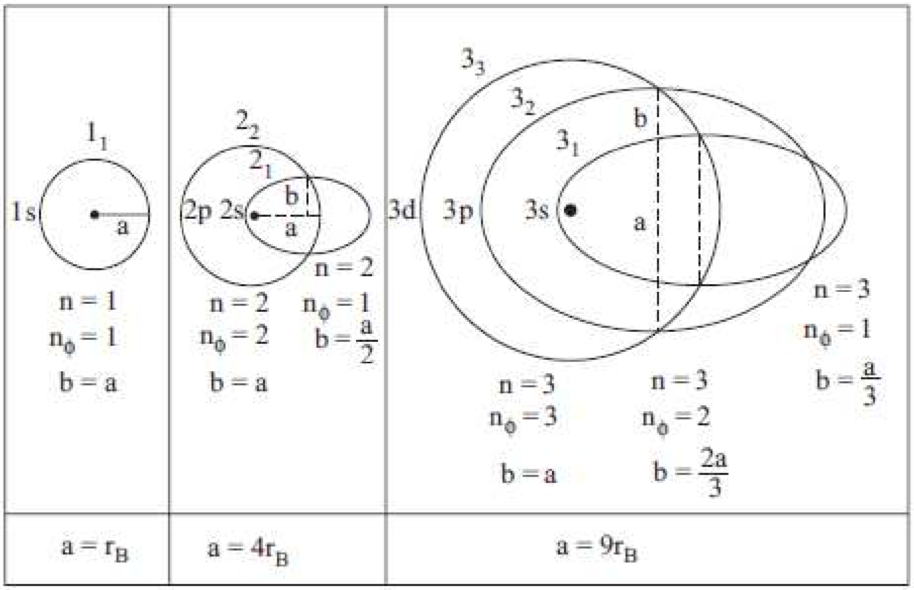


Figure 2.8. Shapes of the Sommerfeld orbits in hydrogen atom.

Thus, the introduction of elliptical orbits does not lead to create new energy terms only multiplicity of orbits; hence no new spectral lines cannot be predicted. Hence Sommerfeld's elliptical orbit model could not explain the fine structure of spectral lines in the hydrogen atom. Although, experimental results and quantum mechanical predictions confirm that n_ϕ also assumes a value of zero. So corresponding to n, n_ϕ can have values 0, 1, 2, ..., $(n - 1)$, In wave mechanics, azimuthal quantum number n_ϕ is denoted by l. On the other hand, on the basis of variation of mass of the electron with velocity, Sommerfeld was able to find a solution to the problem of fine structure of spectral lines.

1.5.2 Sommerfeld relativistic correction

In an elliptical orbit, the velocity of an electron varies, which is maximum at the shortest distance from the nucleus and minimum at farther away from the nucleus. It was found that the value of this velocity is quite large c/137. According to the theory of relativity, mass of the electron depends on the velocity. Therefore, Sommerfeld included the relativistic correction in the treatment of elliptical orbits, showed that path of the electron of the form of equation (2.39)

$$\frac{1}{r} = \frac{1 + \varepsilon cos\psi\emptyset}{a(1 - \varepsilon^2)} \ldots\ldots\ldots\ldots\ldots\ldots\ldots..(2.39)$$

Where is denoted by the equation (2.40)

$$\psi^2 = 1 - \left[\frac{Ze^2}{4\pi\varepsilon_0 pc}\right]^2 \ldots\ldots\ldots\ldots\ldots\ldots..(2.40)$$

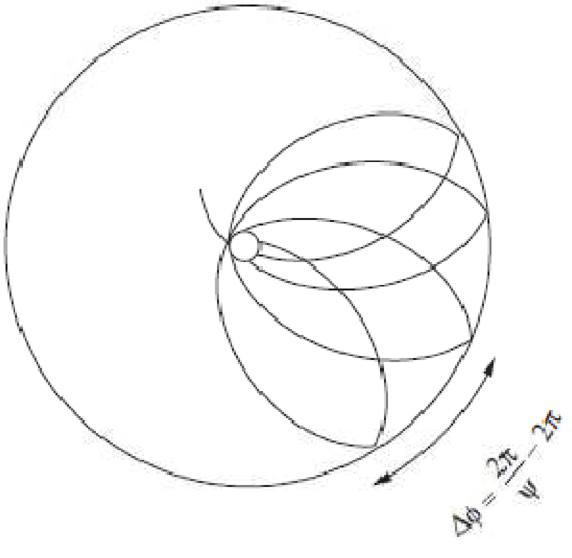


Figure2.9. Rosette path of electron about the nucleus.

This the equation of ellipse which precesses means the major axis turns slowly about the nucleus in the plane of ellipse. Therefore, electron is moving in rosette path, as shown in figure 9. Then on taking relativistic theory of electron motion the total energy with a principal quantum number n can be written as,

$$E_{n,n_\phi} = -\frac{mZ^2e^4}{8\varepsilon_0^2h^2n^2} - \frac{mZ^2e^4\alpha^2}{8\varepsilon_0^2h^2}\left[\frac{n}{n_\phi} - \frac{3}{4}\right]\frac{1}{n^4} \ldots\ldots\ldots\ldots\ldots..(2.41)$$

Where, $\alpha = \frac{e^2}{2\varepsilon_0 ch} = \frac{1}{137}$ is a dimensionless constant and is known as the fine structure constant. The dependency of total energy value on n_ϕ values leads to splitting of energy levels in the atom and hence multiplicity in the spectral lines can be explained.

1.5.3 Fine Structure of H_α line in hydrogen atom

H_α line in the hydrogen atom is due to the transition from n=3 to n=2.

Now for $n = 3$, so possible values of n_ϕ =1, 2, 3. The notation of energy levels can be written as,

n=3, n_ϕ =1 as 3_1

n=3, n_ϕ =2 as 3_2

n=3, n_ϕ =3 as 3_3

For $n = 2$, the possible values of n_ϕ =1, 2. So energy levels can be defined as,

n=2, n_ϕ =1 as 2_1

n=2, n_ϕ =2 as 2_2

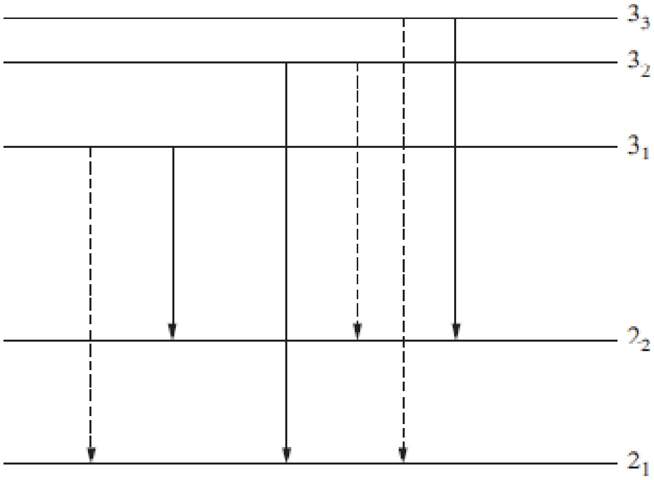


Figure 10. Allowed and forbidden transitions from n=3 to n=2, corresponding to H_α lines in the hydrogen fine structure.

So there are six possible transition of different energy from n=3 to n=2. However, H_α line has three components. So transition must be based on some selection rule. The selection rule is that $\Delta n_\phi = \pm 1$. Then allowed transitions are, $3_1 \rightarrow 2_2$, $3_2 \rightarrow 2_1$ and $3_3 \rightarrow 2_2$, as shown schematic in figure10 by solid lines. The other transitions are forbidden transitions as shown by dotted lines.

1.5.4 Limitations of Sommerfeld Model

(i) Bohr's theory could not explain the fine structure of spectral lines even in the simplest hydrogen atom.

(ii) Bohr-Sommerfeld theory failed to calculate the energy levels and hence frequencies of radiation emitted for complex atoms having more than one electron.

(iii) Sommerfeld's model could not explain the correct number of observed fine structure lines. However, provided a theoretical background of the splitting of individual spectral lines of hydrogen,

(iv) The model could not explain the distribution and arrangement of electrons in atoms.

(v) Intensities of the spectral lines could not be explained.

(vi) Explanation regarding the Anomalous Zeeman effect and Stark effect was not given by Sommerfeld model.

Later on, the vector model of the atom was formulated to provide a satisfactory explanation of observational findings.

SAQ 2.7: State Sommerfeld hypothesis of atomic model.

SAQ 2.8: What is Sommerfeld's quantisation conditions?

SAQ 2.9: What are the limitations of Sommerfeld atomic model?

SAQ 2.10: What is Sommerfeld's relativistic correction?

1.6 Shortcomings of classical theories and old quantum mechanics

1.6.1 Classical models of atoms: Thompson's model

Chemical elements differ by the number Z of electrons in their atoms. Atoms are electrically neutral, so that the negative charge Ze of all electrons in an atom must be compensated by additional positive charge Ze. Therefore, Thompson modeled an atom as a sphere of radius ~1Å filled uniformly by a cloud of positive charge Ze. Inside this cloud there are Z point-like electrons which sit still at their equilibrium positions determined by Coulomb forces. Under various circumstances, for example at by raising temperature, electrons can be excited into vibrating or orbiting motion. Such accelerated motion of charge leads to emission of electromagnetic radiation according to Maxwell equations, which can qualitatively explain why atoms radiate. The model can also describe ejection of electrons from atoms. However, this kind of an atom is not stable according to the laws of electrodynamics. Some unknown forces must rigidly maintain the spatial distribution of the positive charge. Furthermore, Rutherford's experiment, which experimentally observed discrete atomic radiation spectra, proved that Thomson assumptions are not correct.

1.6.2 Classical models of atoms: Rutherford's model

Rutherford conducted the first scattering experiment to probe the internal structure of atoms. A beam of α particles was collimated by a pair of diaphragms and let to pass through a thin foil of metal substance. Since α particles are energetic Helium nuclei produced by radioactive decay of some materials, they have positive charge $2e$ and mass much larger than the electron mass. Therefore, αparticles can scatter from the positive charge in atoms due to Coulomb forces, while scattering from electrons can be neglected.In principle, α particles can interact electrostatically with many atoms as they pass through the foil and scatter in various directions. The incoming collimated beam becomes divergent upon incidence on the foil. A fluorescent screen can be placed some distance away from the foil to detect deflected α particles at an arbitrary angle towith respect to the direction of the incident beam. This allows the measurement of the number of αparticles which get deflected at any given angle. A significant number of αparticles found to scatter at large angles observed, even particles by 180°(bounced back). This implied large electric fields inside the solid, created by highly concentrated positive charge attached to non-negligible mass. Furthermore, the number of αparticles scattered by large angles was found to be proportional to the thickness of the solid, consistent with rare large angle scattering events which randomly occur at only one atom on the path of an alpha particle. Rutherford's experiment discovered atomic nucleus: a highly concentrated positive charge of appreciable mass. Therefore, Rutherford models an atom as a small massive core (nucleus) carrying positive charge *Ze* with *Z* light electrons of charge *Ze* orbiting around it (in analogy of planets orbiting around the Sun). Detailed measurements of the numbers of αparticles deflected by different angles can be use in estimating the size of a nucleus. These estimates yielded a radius ~ 10^{-14}m, whereas the size of an atom is of the order of 10^{-10}m = 1Å (obtained from the density of a typical solid, atomic weight and Avogadro's number). Most of an atom's mass is inside its nucleus, roughly the number of protons and neutrons times the atomic mass unit $u = 1.66 \times 10^{-27}$Kg. Mass of an electron is roughly 9.1×10^{-31}Kg, which is about 1836 times smaller than the mass of a proton. The size of an atom is determined by the size of electron orbitals around the nucleus.

Rutherford's model is much better than Thompson's, but still not adequate. Classical electrodynamics predicts that a Rutherford's atom cannot be stable. Electrons orbiting around a nucleus must radiate electromagnetic waves because their motion is accelerated. In this manner they must loose energy and eventually slow down and fall on the nucleus (in about 10^{-12}s). A stable atom would be rather similar to the Thompson's atom, but of much smaller size (10^{-14} m) than observed.

1.6.3 Old Quantum Theories

The first real breakthrough came in 1900 when Max Planck introduced the concept of the quantum of energy in quest to explain the phenomenon of blackbody radiation. He postulates that the energy exchange between radiation and its surroundings takes place in discrete, or quantized, amounts. He argued that the energy exchange between an electromagnetic wave of frequency υ and matter occurs only in integer multiples of hυ, called as the energy of a quantum, where h is a fundamental constant called Planck's constant. This idea of the quantization of electromagnetic radiation proved to be landmark in providing an accurate explanation of blackbody radiation and hence provoked new direction of thinking that give way solutions to the most outstanding problems or discoveries of that time.

In 1905 Einstein used Planck's quantum concept to understand the photoelectric effect, Einstein recognized that Planck's idea of the quantization of the electromagnetic waves must be valid for light as well. Therefore, light itself is made of discrete bits of energy (or tiny particles), called photons, each of energy hυ, υ being the frequency of the light. By introducing the photon concept Einstein provided an elegantly accurate explanation to the photoelectric problem, long after its first experimental observation by Hertz in 1887.

Another essential breakthrough came from Niels Bohr in explaining atomic model. By combining Rutherford's atomic model, Planck's quantum concept, and Einstein's photons, Bohr introduced in 1913 his model of the hydrogen atom. He postulates that atoms can be found only in discrete states of energy and that the interaction of atoms with radiation, i.e., the emission or absorption of radiation by atoms, takes place only in discrete amounts of hυ because it results from transitions of the atom between its various discrete energy states. This work provided a satisfactory explanation to several outstanding problems. Further modifications in the Bohr models are incorporates by Sommerfeld by using elliptical orbit and relativistic approach. Then in 1923 Compton made an important discovery that gave the most conclusive confirmation for the corpuscular aspect of light. By scattering X-rays with electrons, he confirmed that the X-ray photons behave like particles with momenta *hυ/c*; υ is the frequency of the X-rays. This series of breakthroughs—due to Planck, Einstein, Bohr, and Compton gave both the theoretical foundations as well as the conclusive experimental confirmation for the particle aspect of waves; that is, the concept that waves exhibit particle behaviour at the microscopic scale.

in 1923 de Broglie introduced another powerful new concept that classical physics could not resolve. According to de Broglie postulate that not only does radiation exhibit particle-like behavior but, conversely, material particles themselves display wave-like behaviour. This concept was confirmed experimentally in 1927 by Davisson and Germer as interference patterns, a property of waves, can be obtained with material particles such as electrons.

Maurice de Broglie was a French experimental physicist who, from the outset, had supported Compton's view of the particle nature of radiation. In his doctoral thesis, presented in 1924 to the Faculty of Science at the University of Paris, Louis de Broglie proposed the existence of matter waves. The thoroughness and originality of his thesis was recognized at once but, because of the apparent lack of experimental evidence, de Broglie's ideas were not considered to have any physical reality. It was Albert Einstein who recognized their importance and validity and in turn called them to the attention of other physicists. Five years later de Broglie won the Nobel Prize in physics, after experimental confirmation. The hypothesis of de Broglie was that the dual nature that is wave-particle, of radiation holds equally well to matter. A material particle (e.g., an electron) has an associated matter wave that governs its motion like a photon. According to de Broglie, for matter *and* for radiation alike the total energy E of an entity is related to the frequency υ of the wave associated with its motion by the equation,

$$E = h\upsilon \dots\dots\dots\dots\dots\dots..(2.42)$$

and the momentum p of the entity is related to the wavelength λof the associated wave by the equation,

$$p = \frac{h}{\lambda} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots..(2.43)$$

de Broglie predicts the wavelength λ of a matter wave associated with the motion of a material particle having a momentum p.

$$\lambda = \frac{h}{p} = \frac{h}{mv} \dots\dots\dots\dots\dots\dots\dots\dots\dots.(2.44)$$

Now, kinetic energy can be written as,

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

$$p = (2mK)^{\frac{1}{2}} \dots\dots\dots\dots\dots\dots\dots\dots..(2.45)$$

When a charged particle, carrying a charge q, is accelerated through a potential difference of V volts, then kinetic energy,

$$K = qV$$

$$\lambda = \frac{h}{\sqrt{2mqV}} \dots\dots\dots\dots\dots\dots\dots.(2.46)$$

If the material particles are in thermal equilibrium at associated temperature T, then kinetic energy is,

$$K = \frac{3}{2}k_BT$$

1.7 Foundation of Quantum Mechanics or Wave Mechanics

The theory had dominated by the ideas of Planck and Bohr from 1900–1925 and known as the old quantum theory. The attempt was made by Heisenberg and Schrödinger for the theoretical foundation underlying these new ideas so that a consistent theory can be developed. Both skillfully linked the various experimental findings as well as Bohr’s postulates into a refined theory known as quantum mechanics. This not only provided an accurate reproduction of the existing experimental data, but also astonishingly reliable predictions to explore and unravel many unexplored areas of the microphysical world.

Historically, there were two independent formulations of quantum mechanics. The first formulation was developed by Heisenberg (1925) to describe atomic structure starting from the observed spectral lines and known as matrix mechanics. Heisenberg used Planck’s quantization of waves and by Bohr’s model of the hydrogen atom, Heisenberg expressed dynamical quantities such as energy, position, momentum and angular momentum in terms of matrices and he obtained an eigenvalue problem to describe the dynamics of microscopic systems. Moreover, discrete energy exchange between microphysical systems in terms of quanta was taken as the only allowed values. The diagonalization of the Hamiltonian matrix yields the energy spectrum and the state vectors of the system. Matrix mechanics was very successful in accounting for the discrete quanta of light emitted and absorbed by atoms.

The second formulation was put forward by Schrödinger in 1926 and called as wave mechanics. This is a generalization of the de Broglie postulate and describes the dynamics of microscopic matter by means of a wave equation, called the Schrödinger equation. This approach Schrödinger obtained a differential equation was found more intuitive than matrix mechanics. The solutions of differential equations yield the energy spectrum and the wave function of the system under consideration. Based on probabilistic interpretation, Max Born in 1927 proposed that solutions to the Schrödinger wave equation, square moduli of the wave functions, are probability densities.

$$\lambda = \frac{h}{\sqrt{2mk_BT}} \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2.47)$$

Example 2.1: What is the de Broglie wavelength of a baseball moving at a speed v = 10 m/sec? Assuming the mass of baseball is 1.0 kg.

Solution: $\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.62\times 10^{-34}}{1.0\times 10} = 6.62\times\ 10^{-35}m$

Example 2.2: What is the de Broglie wavelength of an electron whose kinetic energy is 100 eV?

Solution: $\lambda = \frac{h}{\sqrt{2meV}} = \frac{6.62\times 10^{-34}}{\sqrt{2\times 9.1\times 10^{-31}\times 1.6\times 10^{-19}\times 100}} = 1.2\ \times 10^{-10} = 1.2\text{Å}$

Example 2.3 Energy in a Bohr orbit is given to be $-\frac{A}{n^2}$, where A= 2.197 × 10^{-18} Joules. Calculate the frequency of radiation and also the wave number when the electron jumps from second to first orbit. Given h= 6.62× 10^{-34} Joule-sec.

Solution: Energy of nth Bohr orbit is given by,

$$E_n = -\frac{A}{n^2} = -\frac{2.197\times 10^{-18}}{n^2}\ Joules$$

For the second orbit, n=2

$$E_2 = -\frac{2.197\times 10^{-18}}{2^2} = -0.54475\times 10^{-18}\,Joules$$

$$E_1 = -\frac{2.197 \times 10^{-18}}{1^2} = -2.197 \times 10^{-18}\, Joules$$

Therefore, $E_2 - E_1 = \big(-0.54475 - (2.197)\big) \times 10^{-18} = 1.65227 \times 10^{-18}\, Joules$

Hence, frequency of radiation when electron jumps from n=2 to n=1,

$$\upsilon = \frac{E_2 - E_1}{h} = \frac{1.65227 \times 10^{-18}}{6.62 \times 10^{-34}} = 0.2496 \times 10^{16}$$

$$= 2.496 \times 10^{15} sec^{-1}$$

The corresponding wavenumber when electron jumps from n=2 to n=1,

$$\bar{\nu} = \frac{1}{\lambda} = \frac{\nu}{c} = \frac{2.496 \times 10^{15}}{3 \times 10^8}$$

$$= 0.832\ \times 10^7 m^{-1}$$

Example 2.4. The series limit wavelength of Balmer series in hydrogen spectrum is experimentally found to be 3646 Å. Find the wavelength of the first member of this series.

Solution: The wavelengthsof Balmer series are given by,

$$\bar{\nu} = \frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{p^2}\right)\ where\ p = 3, 4, 5 \ldots \ldots \infty$$

For series limit p=∞, then

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

$$= R\left(\frac{1}{2^2} - 0\right)$$

$$\frac{1}{\lambda} = \left(\frac{R}{4}\right)\ therefore\ R = \frac{4}{\lambda}$$

Given, λ =3646 Å, therefore, $R = \frac{4}{\lambda} \ldots \ldots \ldots \ldots \ldots (a)$

For the first member of the Balmer series, p=3, then

$$\bar{\nu} = \frac{1}{\lambda_1} = R\left(\frac{1}{2^2} - \frac{1}{3^2}\right) = \frac{5R}{36}$$

Using the value of R from equation(a), we get

$$\lambda_1 = \frac{36}{5R} = \frac{36\lambda}{5 \times 4} = \frac{36 \times 3646}{5 \times 4}$$

$$\lambda_1 = 6562.8\,\text{Å}$$

1.8 Summary

- the radius of n^{th} permissible Bohr orbit for electron in hydrogen atom is,

$$r_n = \left(\frac{n^2 h^2 \varepsilon_0}{\pi m Z e^2}\right)$$

- Bohr radius is defined as $r_B = (0.529 \times 10^{-10})\ metre.$
- Total energy of the orbit according to Bohr model,

$$E_n = -\frac{13.6}{n^2}\ eV$$

- Wavenumber of emitted radiation,

$$\bar{\nu} = \frac{1}{\lambda} = \frac{mZ^2e^4}{8\varepsilon_0^2 ch^3}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

- Rydberg constant $R_H = \frac{mZ^2e^4}{8\epsilon_0^2 ch^3}$

- Sommerfeld Model

(i) Quantization conditions for elliptical orbit,

$$\oint p_\phi d\phi = n_\phi h$$

$$\oint p_r dr = n_r h$$

(ii) Ratio of semi-minor to semi-major axis

$$\frac{b^2}{a^2} = \frac{n_\emptyset{}^2}{n^2}$$

(iii) total energy of the electron in nth orbit

$$E_n = -\left(\frac{mZ^2e^4}{32\pi^2\varepsilon_0^2}\right)\left(\frac{n_\emptyset}{n}\right)^2\left(\frac{2\pi}{n_\emptyset h}\right)^2$$

$$E_n = -\left(\frac{mZ^2e^4}{8\varepsilon_0^2h^2n^2}\right) = -\frac{mZ^2e^4}{8\varepsilon_0^2h^2}\left[\frac{1}{n_r + n_\emptyset}\right]^2$$

(iv) in relativistic approach total energy of an electron

$$E_{n,n_\phi} = -\frac{mZ^2e^4}{8\varepsilon_0^2h^2n^2} - \frac{mZ^2e^4\alpha^2}{8\varepsilon_0^2h^2}\left[\frac{n}{n_\phi} - \frac{3}{4}\right]\frac{1}{n^4}$$

- de Broglie relationship

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

1.9 Glossary

- Postulate: a statement that is accepted to be true and forms a basis for theory.
- Energy level diagram: is a sort of one-dimensional scale of energy along which each electron according to its energy state can be located.
- Ground state: lowest energy state of an electron is called as known as ground state.
- Excited state: any state other than ground state is known as excited state.
- Excitation: of an atoms and molecules is a process in which the electron of the system absorbs energy and pass on to higher energy states.
- Ionization: minimum energy required to ionize atom or molecule.
- Relativistic: moving at a velocity such that there is a significant change in properties such as mass.
- Ellipse: is oval like a circle that has been pressed in from two sides.
- Quantization: is a process of using discrete values rather than continuous

1.10 References

1. Quantum Mechanics Concepts and Applications, Nouredine Zettili, A John Wiley and Sons, Ltd., Publication

2. Fundamentals of Modern Physics, J.P. Agarwal and Amit Agarwal, Pragati Prakhasnan, Meerut

3. QUANTUM PHYSICS of Atoms, Molecules, Solids, Nuclei, and Particles, Robert Eisberg, A John Wiley and Sons, Ltd., Publication

10.11 Suggested Readings:

1. Fundamentals of Modern Physics, J.P. Agarwal and Amit Agarwal, Pragati Prakhasnan, Meerut

1.12 Terminate questions.

Objective questions:

a) According to Bohr, only those orbitals are permissible for electrons in which the total angular momentum of the electron is equal to an integral multiple of;

i) $\frac{h}{2\pi}$

ii) $\frac{h}{\pi}$

iii) $\frac{h}{4\pi}$

iv) h

b) In case of elliptical orbit, the Wilson-Sommerfeld's qunatisation condition is

i) $p.q = h$

ii) $\oint p.dq = nh$

iii) $\oint p.dq = h$

iv) $\oint q.dp = nh$

c) For hydrogen atom, first Bohr radius is equal to,

i) 0.526 Å

ii) 1 Å

iii) 2 Å

iv) 0.226 Å

d) According to Louis de Broglie, an electron of mass m, moving with a velocity υ was equivalent to a wave of wavelength,

i) $\lambda = \frac{h}{2mv}$

ii) $\lambda = \frac{hm}{v}$

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

iv) $\lambda = \frac{1}{mv}$

Short Answer type questions:

2.1. Write down Bohr's postulates of atomic model.

2.2. What are the shortcomings of Bohr's atomic model?

2.3. State corrections proposed by Sommerfeld in Bohr atomic model.

2.4. What do you mean by excitation and ionization potentials?

Long answer type questions:

2.1. Calculate for hydrogen atom;

(i) velocity of an electron in the ground state

(ii) radius of Bohr orbit in the ground state

(iii) Rydberg constant

Given $e = 1.6 \times 10^{-19}$ coulomb, $m_e = 9.1 \times 10^{-31}$ kg and $h = 6.62 \times 10^{-34}$ Joule-sec.

2.2. Energy in a Bohr orbit is given by $-A/n^2$, where $A = 2.179 \times 10^{-18}$ Joules and n is the number of orbit. Calculate the frequency of radiation and also the wavenumber when the electron jumps from the third orbit to second orbit. (given $h = 6.62 \times 10^{-34}$ Joule-sec)

2.3. Calculate the ionization potential of hydrogen atom from the followings, e= 1.6×10^{-19} coulomb,

$m_e = 9.1 \times 10^{-31}$ kg and

$h = 6.62 \times 10^{-34}$ Joule-sec.

2.4. In a Franck-Hertz experiment the first dip in the current vs voltage graph for hydrogen was observed at 10.2 Volts. Calculate the wavelength of light emitted by hydrogen when excited to the first excitation level.

2.5. A given atom shows two excitation potentials at 4.85 and 9.67 volts. Show these on an energy diagram and calculate the wavelengths of possible emission transitions.

2.6. A proton moves with a speed of 7.45×10^5 m/s directly towards a free proton originally at rest. Find the distance of closest approach for the two protons.

2.7. For Lyman series, calculate the wavelength of the second member and the series limit.

1.13 Answer of terminal questions

Self Assessment Questions

2.2. Energy of emitted photon 10.21 eV

2.3. 0.529 Å, 1.51×10^{-10} Secs

2.4. 6563 Å

2.5. 1212 Å

2.6. 5910 Å, 3354 Å

Objective type:

a) (i), **b)** (ii), **c)** (i), **d)** (iii)

Long answer type questions:

2.1. (i) 2.19×10^6 m/sec. (ii) 0.526 Å and (iii) 1.096×10^7 m^{-1}

2.2. 0.30265×10^{-18} Joules and (ii) 1.52×10^6 m^{-1}

2.3.13.6 eV

2.4. 1216.9 Å

2.5 1859 Å, 2551 Å, 6852 Å

Unit-3 : Basics of Wave Mechanics

Structure

3.1. Introduction

3.2. Objectives

3.3. de Broglie Matter Wave

3.4. Derivation of deBroglie's Relation.

  3.4.1 deBroglie wavelength of High Energy Electrons

  3.4.2 Properties of deBroglie Waves (Matter Waves)

3.5. Experimental Evidence of Matter Wave : Proof of deBroglie's Hypothesis.

3.1 Introduction

We have seen that radiation exhibits wave behaviour in the phenomena of interference, diffraction etc. These are the result of interaction of radiation with radiation. At the same time in some phenomena like black body radiation, photo electric effect and Compton effect, radiation behaves as a set of discrete particles called 'photons'. These phenomena are the result of interaction of radiation with matter. Radiation was thus regarded having a dual wave-particle character but both characters, -wave and particle, are never exhibited simultaneously in any experiment. Scientists made use of either the wave or particle nature of light (radiation) to explain experimental phenomena as per requirements. In 1924-25 French Physicist Louis de Broglie made a suggestion that "if the light which is known to consist of waves can assume the aspect of a particle (matter), then from symmetry concept, the material particles e.g. proton, electron, etc. should also possess a wave like nature". The waves associated with these particles are known as deBroglie waves or matter waves". This suggestion about the wave nature of particles were later verified experimentally by Davisson andGermar in 1927 and by G.P.Thomson in 1928. The wave properties of matter can be reconciled with particle properties by the superposition of waves of different wavelengths to form a group of waves or a wave packet. A wave packet can represent a particle in motion as a moving particle at any instant is confined to a small region of space. We shall discuss about it in detail later on.

3.2 Objectives

After studying this unit you should be able to –

- Understand the basis on which de Broglie suggested the concept of 'matter wave'.
- Derive an expression for the wavelength of matter wave.
- Examine why matter waves cannot be observed with a macroscopic bodies whereas it can be observed with microscopic bodies like electrons protons, neutrons etc. only.
- Know about the experimental evidences of matter waves as proof of deBroglie's hypothesis.
- Know about group, wave and particle velocities and their interrelations.
- Understand the concept of 'wave packet'.
- Solve simple numerical problems based on matter wave, group velocity, wave velocity and particle velocity etc.

3.3 deBroglie's Matter Wave

According to deBroglie a moving particle, having any nature, has wave properties associated with it and its wavelength is given by

$$\lambda = \frac{h}{mv} \tag{3.1}$$

Where h is Planck's constant having value 6.6256×10^{-34} J-s, m is the mass and v is the velocity of the particle with which it is moving. From the above relation it is clear that the wavelength associated with a moving particle is inversely proportional to its momentum.

3.4 Derivation of deBroglie's Relation

Let us first consider the case of photon. If the photon is considered as a wave of frequency ν, then its energy is given by

$$E = h\nu \tag{3.2}$$

If the photon is considered to be a particle of mass m, then its energy is given by

$$E = mc^2 \tag{3.3}$$

Where c is the velocity of light. Thus from eqns. (3.1) and (3.2) we get,

$$h\nu = mc^2 \tag{3.4}$$

As the photon travels in free space with velocity of light c, its momentum is given by

$$p = mc \tag{3.5}$$

Dividing eqns. (3.4) by (3.5) we have

$$\frac{hv}{p} = \frac{mc^2}{mc} = c$$

or
$$p = \frac{hv}{c} = \frac{h}{\lambda} \; (\because \frac{c}{v} = \lambda \text{ the wavelength of radiation})$$

∴
$$\lambda = \frac{h}{p} \tag{3.6}$$

deBroglie assumed that this equation should be equally applicable to both the photons of radiation and material particles like electrons. Hence, if m is the mass of the particle moving with velocity v, then its momentum $p = mv$. The wavelength of the wave associated with material particle is then

$$\lambda = \frac{h}{p} = \frac{h}{mv} \tag{3.7}$$

This equation is known as deBroglie's wave equation and λ is called deBroglie wavelength.

This relation can also be derived by considering a material particle as a standing wave system and the theory of relativity.

Consider a material particle e.g. electron or proton, as a standing wave system in the vicinity of the particle. Let the standing wave at any instant t_0 at the point (x_0, y_0, z_0) be represented by the function

$$\psi = \psi_0 \sin 2\pi\nu_0 t_0 \tag{3.8}$$

Whereν_0 is the frequency of the wave and ψ_0 its amplitude at (x_0, y_0, z_0).

If the particleis given a velocity v along the positive x-direction, then according to inverse Lorentz transformation.

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

and the variation of ψ is given by

$$\psi = \psi_0 \sin 2\pi\nu_0 \left[\frac{\left(t + \frac{v}{c^2}x \right)}{\sqrt{1 - \frac{v^2}{c^2}}} \right] \tag{3.9}$$

The standard equation of wave motion is given by

$$\psi = \psi_0 \sin \left\{ \frac{2\pi}{T} \left(t + \frac{x}{u} \right) \right\} \tag{3.10}$$

whereψ_0 is the amplitude, T the periodic time and u the phase velocity of the wave along x-axis.

Comparing equations (3.9) and (3.10) we get

$$u = \frac{c^2}{v} \tag{3.11}$$

and

$$\frac{1}{T} = \nu = \frac{\nu_0}{\sqrt{1-\frac{v^2}{c^2}}} \tag{3.12}$$

From Einstein's mass-energy relation

$$E = m_0c^2 = h\nu_0$$

or

$$\nu_0 = \frac{m_0c^2}{h}$$

Putting this in equation (3.12), we get

$$= \frac{\frac{m_0c^2}{h}}{\sqrt{1-\frac{v^2}{c^2}}}$$

or

$$\nu = \frac{mc^2}{h} \tag{3.13}$$

As

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

The wavelength of the material particle is given by

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

∴

$$\lambda = \frac{h}{mv} \tag{3.14}$$

which is the same as given by eqn. (3.7). This relation connects the wave property of light i.e. □, to the particle property of photon i.e. photon momentum p. If E_k is the kinetic energy of material particle then

$$p = \sqrt{2mE_k} \qquad \text{(provided } v \ll c\text{)}$$

Thus the de-Broglie wave length is given by

$$\lambda = \frac{h}{\sqrt{2mE_k}} \tag{3.15}$$

If a charged particle of charge q is accelerated through a potential difference V volts then $E_k = qV$. The de-Broglie wavelength for such a particle is given by

$$\lambda = \frac{h}{\sqrt{2meV}} \tag{3.16}$$

If a particle, say an electron, of charge $e = 1.6\times10^{-19}C$, is accelerated through 100 volts then

$$\lambda = \frac{6.63\times10^{-34}}{\sqrt{2\times9.1\times10^{-31}\times100\times1.6\times10^{-19}}} = 1.226 \text{ Å}$$

Such wavelengths are of the same order of magnitude as those of x-rays. It would therefore, appear that the regular array of atoms in a crystal, which have a spacing of several Å between them, might well provide a conventional diffraction grating for electron waves. Experiments on the scattering of electron beam by the atoms at the surface of the crystal, by Davisson and Germer, were in fact the proof of the existence of matter waves.

Introducing the wavenumber $k = \frac{2\pi}{\lambda}$ and the angular frequency $\omega = 2\pi\nu$, the de-Broglie relation can be written as

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

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

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

and similarly the energy $$E = h\nu = h\frac{\omega}{2\pi}$$

or $$E = \hbar\omega \qquad (3.17) \text{ (where } \hbar = h/2\pi\text{)}$$

Some of de-Broglie's ideas were used by Schrodinger, Dirac, Born, Heisenberg and other physicists which developed into the modern theory of Quantum mechanics.

It can be concluded from eqn. (3.7) that the smaller is the velocity of the particle, greater is the wavelength associated with it and vice-versa. Further lighter the particle, greater is the wavelength associated with it. The velocity of the matter wave depends on the velocity of material particle. Waves are produced by the motion of the particle and are independent of the charge.

From equation (3.14) we note that $\lambda \propto 1/m$ when$v$ is constant. For macroscopic bodies,$m\to\infty$, so $\lambda\to 0$. For example, consider the case of a cricket ball of mass 500 g flying with a velocity of 13.9 m/s, its de Broglie wavelength is

$$\lambda = \frac{h}{mv} = \frac{6.62\times10^{-34}Js}{0.5\,kg\times13.9\,m/s} \approx 10^{-34}\,m = 10^{-24}\,\text{Å}$$

which is insignificant compared to the size of the ball. As a result we are unable to observe the wave character of such object nor we can detect the associated waves.

On the other hand, for microscopic objects □ is large and significant. For example an electron of mass 9.1×10^{-31} kg moving with velocity 4.47×10^{6} m/s, its de Broglie wavelength is

$$\lambda = \frac{h}{mv} = \frac{6.62\times10^{-34}Js}{9.1\times10^{-31}\,kg\times4.47\times10^{6}\,m/s} = 9.3\times10^{-34}\,m = 9.3\,\text{Å}$$

which is large compared to the size of the electron and are well within the limit of measurement. It may, therefore, be treated as a wave than a particle.

3.4.1 de-Broglie Wavelength of High Energy Electrons

If the energy of the electron is so high that mass of the electron varies with velocity, then the simple expression of de Broglie wavelength of the electron $\left(\lambda = \frac{h}{mv}\right)$ needs correction.

If p be the momentum and m_0, the rest mass of the electron, then the relativistic expression for energy is, $E = \sqrt{p^2c^2 + m_0^2c^4}$ where, c is the velocity of light in free space.

The kinetic energy of the electron is,

$$E_k = E - m_0c^2 = \sqrt{p^2c^2 + m_0^2c^4} - m_0c^2$$

or
$$p^2c^2 + m_0^2c^4 = E_K^2 + m_0^2c^4 + 2m_0c^2E_K$$

or
$$p = \sqrt{\frac{E_K(E_K + 2m_0c^2)}{c}}$$

Then the de Broglie wavelength of electron is

$$\lambda = \frac{h}{p} = \frac{hc}{\sqrt{E_K(E_K + 2m_0c^2)}}$$

If V be the accelerating potential in volt, then

$$E_K = eV$$

$\therefore$
$$\lambda = \frac{hc}{\sqrt{eV(eV + 2m_0c^2)}}$$

or,
$$\lambda = \frac{hc}{e\sqrt{V\left(V + \frac{2m_0c^2}{e}\right)}}$$

3.4.2 Properties of de Broglie Waves (Matter Waves)

Matter waves possess the following properties:

1. Lighter is the particle, greater is the wavelength associated with it and vice-versa.
2. Smaller is the velocity of the particle, greater is the wavelength associated with it and vice-versa.
3. These waves are produced by the motion of the particles and are independent of the charge.
4. The velocity of matter wave depends on the velocity of the matter particle i.e., it is not a constant like the velocity of an electromagnetic wave.
5. The wave and particle aspects of moving bodies can never appear together in the experiment, i.e., waves have particle like properties and particles have wave like properties and are separately linked.
6. The wave nature of mater introduces an uncertainty in the position of the particle because a wave cannot be exactly at this point or at that point. However, where the wave is strong there is a better chance of finding the particle, while where the wave is weak there is feeble chance of finding the particle.

3.5 Experimental Evidence of Matter Wave : Proof of de Broglie's Hypothesis

The existence of matter wave or de Broglie's hypothesis can be demonstrated by a number of experiments. We shall now discuss some of them.

3.5.1 Davisson and Germer's experiment

The first proof of the existence of "matter waves" was obtained in 1927 by two American physicists Davisson and Germer. They succeeded in measuring the de Broglie wavelength for slow electrons, accelerated by a low potential difference by diffraction methods. The experimental arrangement is shown in the Fig. 3.1. The electron beam is produced from an electron gun consisting of tungsten filament F heated by low tension battery. The electrons exited by the filament are accelerated in an electric field of known potential difference from a high tension battery. The electrons are collimated to a fine beam and made to strike a Nickel target which is capable of rotation about an axis parallel to the axis of the incident beam. The electrons are scattered in all directions by the atoms of the crystal. The intensity of the electron beam scattered in a given direction is measured by allowing it to enter in a Faraday cylinder called collector C which can be moved along a graduated circular scale S, so that it is able to receive the reflected electrons at all angled between 20° and 90°.

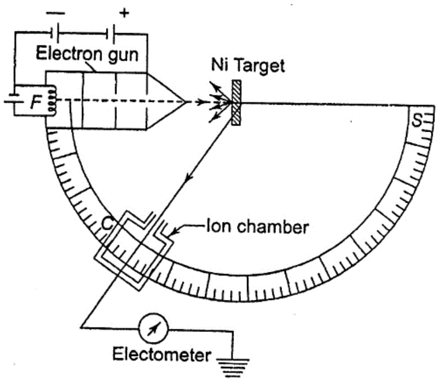


Fig. 3.1 : Davisson and Germer electron diffraction apparatus

Davisson and Germer noticed that the strongest of Davisson and Germer electron diffraction apparatus the scattered electron beams corresponded accurately to diffraction maxima that would be expected in the diffraction of X-rays by the same crystal. The angular distribution of scattered electrons was analogous to optical diffraction patterns from a plane diffraction grating whose lines consisted of the rows of nickel atoms in the surface of the target crystal. The wavelength associated with the diffraction pattern can be obtained using Bragg's law:

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

where$d$ is the distance between the rows of atoms.

It was observed by Davisson and Germer that when an electron beam accelerated by a potential of 54 volts was directed upon a Nickel target, a sharp diffraction maxima appeared in the electron currents. The incident and the scattered beams in this case make an angle of 65° with the family of Bragg's planes. The spacing of planes in this family which can be determined by x-ray diffraction is 0.91 Å. From above Bragg's equation, taking n = 1, we have,

$$2\times 0.91\times \sin 65^\circ = 1.\lambda \qquad \text{or} \lambda = 1.65 \text{ Å}$$

The wavelength of electrons accelerated through potential of 54 volts can be calculated as

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

Where*m* is the mass of the electron

$$m^2v^2 = 2meV$$

or

$$mv = \sqrt{2meV}$$

The de-Broglie wavelength of the electron will be given by

$$\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2meV}}$$

Putting $h = 6.6\times 10^{-34}$ J-s, $m = 9\times 10^{-31}$ kg and $e = 1.6\times 10^{-19}$ coulomb, we obtain

$$\lambda = \frac{12.27}{\sqrt{V}} \quad \text{with } V = 54 \text{ volts}$$

$$\lambda = 1.66 \text{ Å}.$$

There is an excellent agreement between the two results. Thus Davisson Germer experiment is a definite evidence that the electron beams do behave as waves and the wavelengths of these beams is thus given by the de-Broglie equation.

3.5.2 G.P. Thomson's Experiment

The wave nature of moving electron was confirmed through G.P. Thomson's electron diffraction experiment in 1928. A beam of electron of velocity *v* was passed through a thin foil of gold and the diffraction pattern obtained was found to be exactly similar to that obtained from X-rays, The experimental arrangement is shown in Fig 3.2.*T* is a closed tube in which the air pressure is made very low with the help of the pumps. At one end of T, there is a filament which is heated to produce electron beams. These electrons are then accelerated by a potential difference of 50,000V to the anode A. The electron beam passes through a narrow hole of the anode and falls normally on a gold foil G of thickness 10~8 m. The electrons suffer diffraction and are recorded on a photoplate P. The diffraction pattern was exactly similar to those obtained by diffraction of X-rays by powdered crystals in Debye-Scherrer method. The diffraction pattern was found to consist of a series of concentric rings about a central spot.

To be sure that the pattern was due to the electron beam and not due to the X-rays produced due to the impact of cathode rays on the film, the experiment was repeated by introducing a magnetic field between the film and the photographic plate. The diffraction pattern in presence of the magnetic field was found to be exactly similar except that the whole pattern is moved to one side due to the field. This proves that the diffraction pattern was due to the charged particles (electrons) all of them having the same velocity. On removing the film a central spot is recorded on the photoplate due to the direct electron beam. The experiment was repeated with beam of protons, neutrons and molecules, and all are found to show wave character under suitable conditions.

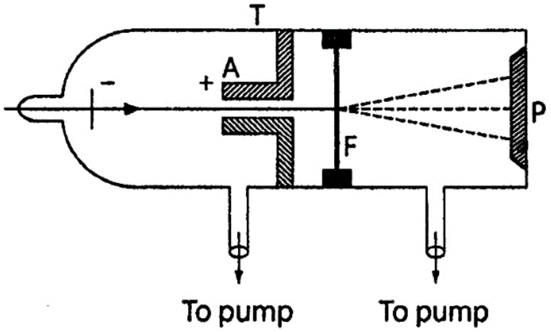


Fig 3.2: G.P. Thomson's experiment

Calculation of λ

The gold foil being polycrystalline, there are some atomic planes set at correct angle to give Bragg diffraction. If the number of crystals distributed at random be large, the Bragg reflection will form a series of concentric rings due to the intersection of the diffraction cone with the photographic plate.

In Fig 3.3, let PQ be the incident electron beam passing through the gold film at Q. The beam after suffering Bragg reflection at some crystal the reflected beam goes along QR meeting the photoplate at R. If O be the position of the central spot and OR = r, then,

$$r/l = \tan 2\theta ;\quad 2\theta$$

where, *l* is the distance QO and $\angle OQR = 2\theta$, the angle of scattering and θ is the glancing angle.

Again, if *d* be the distance between two parallel lattice planes and λ the wavelength of the de Broglie wave associated with the electron, then according Bragg's law, $2d \sin \theta = n\lambda$ [n is the order of diffraction.]

Again,

$$2d \sin \theta ;\quad 2d\theta = d \tan 2\theta \text{ [Q}\theta \text{ is small]}$$

or, $\quad d \tan 2\theta = 2d \sin \theta = n\lambda$

or,. $\quad d\dfrac{r}{l} = n\lambda,$

or, $\quad \lambda = \dfrac{rd}{nl}$

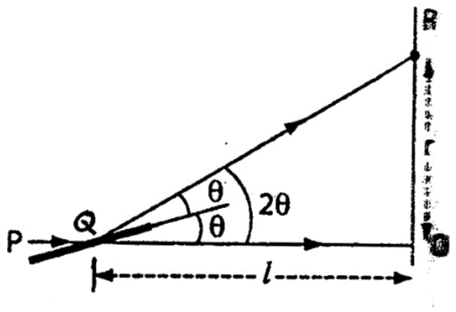


Fig. 3.3 Schematic diagram of G.P.Thomson's experiment

The value of λ calculated from the above relation agrees closely with the value calculated from $\lambda = \frac{12.27}{\sqrt{V}}$, V is the accelerating potential.

Thus we note that the experiment provides an excellent and direct confirmation wave nature of electrons proposed by de Broglie.

3.5.3 Electron Double Slit Experiment

The electron double slit experiment is another experiment that exhibits the existence of matter wave, for example waves associated with electrons.

The basic experimental arrangement is simple one thematically shown in the figure (Fig.3.4). A stream of focussed electrons from an electron gun impinges on a plate with two narrow slits separated a small distance apart. The electrons transmitted through the slits are observed to form a typical diffraction pattern, identical to that of Young's double slit experiment with visible light, on the fluorescent screen behind the slit plate. When the intensity of the electron source is very low, the locations of where electrons hit the screen and thereby causing a fluorescent spot, would appear to be completely arbitrary. However, if we either increase the intensity of the electron source or to allow the experiment to run for a very long time,a pattern on the screen will emerge. The pattern on the screen has a central bright band followed by a non-illuminated band and then a relatively less intense band on either sides of it. This intensity pattern cannot be predicted with electrons being treated in a classical manner, as a particle. This conceptual mystery can be resolved only with quantum mechanical concept assuming a wave associated with the moving electrons. The deflection of electrons has no classical explanation. The stripy interference pattern suggests that the electrons somehow interfere with each other so they don't arrive in the same places they would if they were alone. However, the interference pattern remains even when we fire the electrons one by one, so that they have no chance to interfere. But strongly, each individual electron contributes one dot to an overall pattern that looks like the interference pattern of a wave, but after lapse of some time only.

The result of his experiment suggests that what we call 'particle' such as electrons, somehow combine characteristics of waves the famous wave-particle duality.

3.6 Group and Wave Velocities

A particle while moving with velocity v can be explained as a group of waves which is moving along, a single direction. The group velocity is defined as the velocity with which a slowly varying envelope or packet due to group of waves travels in a medium

According to de Broglie hypothesis a material particle in motion is associated with a wave of wave - length $\lambda = h/mv$, where m is the mass and v the velocity of the particle. The group velocity can be shown equal to the velocity of the particle. If E is the energy of the particle and v the frequency of the wave then by quantum condition

$$E = h\nu \text{ or } \nu = E/h$$

But according to Einstein's mass-energy relation we have

$$E = mc^2, \quad \text{so that}$$

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

Thus the velocity of the propagation of the wave, called phase velocity, v_p is given by

$$v_p \quad = \quad \nu\lambda = \frac{mc^2}{h}.\frac{h}{mv}$$

or

$$v_p \ = \ \frac{c^2}{v} \tag{3.18}$$

which is also called de-Broglie wave velocity

According to special theory of relativity, the speed of light is the maximum speed that a particle in nature can attain i.e. the speed of material particle (v) is always less then the speed of light c. The above equation implies that the de-Broglie wave velocity must be greater than c. This is an unexpected result. Further, accordingly the de-Broglie wave associated with the particle would travel faster thanthe particle itself, thus leaving the particle far behind. So it is clear that a material particle cannot be equivalent to a single wave train.

This difficulty was resolved by Schrodinger by postulating that a material particle in motion is equivalent to a wave packet rather than a single wave.

3.7 Wave Packet and its formation

A wave packet is a type of wave motion comprising a group of waves, each with slightly differentvelocity and wavelength, with phases and amplitude so chosen that they interfere constructively only overa 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. Alternatively a wave packet is a localized disturbance that results from the sum of many different wave forms. In other words, the behaviour of then particle should be describable by a wave function $\psi(x, t)$ whose magnitude is large in regions wherethe probability of occurrence of the particle is large; in other regions where the particle is less likely tobe found, the magnitude of ψ is small.

The simplest type of wave is, a plane monochromatic wave expressed mathematically as

$$\psi(x,t) \;=\; A\exp[i(kx-\omega t)] \qquad (3.19)$$

which represents a disturbance of wavelength $\lambda = 2\pi / k$ travelling in the direction of its wave vector k with constant velocity ω/k. For the propagation of matter waves, the frequency ω is related to the be energy E of the particle as (given by eqn. 3.17)

$$E = h\nu \;=\; \frac{h\omega}{2\pi} = \hbar\omega$$

where

$$\hbar \;=\; \frac{h}{2\pi}$$

and from de-Broglie relation, the momentum, p and wave number k are connected by

$$p \;=\; \hbar k \qquad \left(\because\; p = \frac{h}{\lambda} = \frac{\hbar 2\pi}{\lambda} = \hbar k\right) \qquad (3.20)$$

A wave packet can be constructed by principle of superposition, which states that if a particle can be present in the states described by the wave function ψ_1 and ψ_2 it can also be in all states described by the wave function constructed from ψ_1 and ψ_2 by linear transformation

$$\psi = a_1\psi_1 + a_2\psi_2$$

Wherea_1 and a_2 are arbitrary complex numbers. Mathematically the wave packet in one dimension isdescribed as

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} A(k)\exp.[i(kx-\omega t)]dk \qquad (3.21)$$

where, $A(k)$ is the amplitude, a function of k and is called the Fourier transform of the function $\psi(x,t)$

Using eqns. (3.17) and (3.20) we may write eqn (3.21) in the following form

$$\psi(x,t) = \frac{1}{\sqrt{2\pi h}}\int_{-\infty}^{\infty} a(p)\exp.\left[\frac{i}{h}(px-Et)\right]dp \qquad (3.22)$$

A typical form for a wave packet is shown in fig 3.5 where $\psi(x,t)$ is plotted against x fora particular time t since $\psi(x,t)$ is in. general complex, what we have actually plotted is real part of$\psi(x,t)$ as a function of x for a particular time t. The average wavelength $\square_0$ and the approximate extension Δx of the wave packet are shown in the figure. :

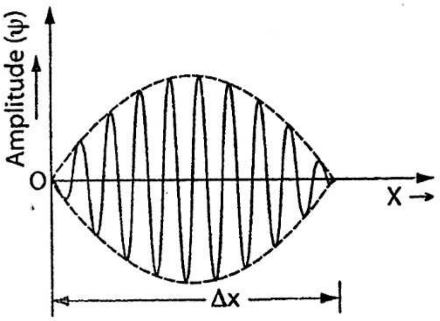


Fig 3.5:a wave packet

A wave packet consists of a group of waves each having slightly different velocity and wavelength. Such a packet moves with its own velocity v_g called the group velocity. The group velocity may be defined as "the velocity with which a slowly varying envelope or packet due to a group of waves travels in a medium". This is the velocity with which the energy in the wave group is transmitted.

One dimensional wave packet formed by superposition of plane waves is described by

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{i/(kx-\omega x)} dk$$

if the range of values of *k* for which the components have significant amplitude is limited, then it is possible to assign an average velocity to the wave packet. Assuming that,*A*(*k*) is negligible except when *k* lies in a small interval Δ*k* around k_0 the wave packet can be written as

$$\psi(x,t) \;=\; \int_{k_0-\frac{\Delta k}{2}}^{k_0+\frac{\Delta k}{2}} A(k) e^{i(kx-\omega t)} dk \qquad (3.23)$$

where the integration extends over the region *Δk*. Assuming that $\omega(k)$ varies slowly with *k*, it can be expanded in a Taylor series about $k = k_0$.

$$\omega(k) = \omega(k_0) + (k-k_0)\left(\frac{d\omega}{dk}\right)_{k=k_0} + \frac{1}{2}(k-k_0)^2 \left(\frac{d^2\omega}{dk^2}\right)_{k=k_0} + \ldots \qquad (3.24)$$

Assuming that the second and higher order terms can be neglected, we obtain

$$\psi(x,t) \approx \frac{1}{\sqrt{2\pi}} \int_{\Delta k} A(k) \exp.i \left\{ (k-k_0)x + k_0 x - \omega_0 t - \left(\frac{d\omega}{dk}\right)_{k=k_0} (k-k_0)t \right\} dk$$

$$\approx f(x,t) \exp[i(k_0 x - \omega_0 t)] \qquad (3.25)$$

where $\omega_0 = \omega(k_0)$ and $f(x,t)$, which determines the envelope of the wave packet, is given by

$$f(x,t)=\frac{1}{\sqrt{2\pi}}\int A(k)\exp\left[i\left(x-\frac{d\omega}{dk}t\right)_{k=k_0}(k-k_0)\right]dk \qquad (3.26)$$

Since the function $f(x,t)$ depends on *x* and *t* only through the combination $\left(x-\dfrac{d\omega}{dk}t\right)$ the wave packet propagates without distortion with velocity v_g where

$$v_g = \frac{d\omega}{dk} \qquad (3.27)$$

is known as the group velocity of the wave since it represents,the velocity of motion of a group of waves, which make up the wave packet. The wave packet remains undistorted as long as the neglect of second and higher order terms in equation (2.21) are justified.

Since $\omega = 2\pi v$

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

$$\therefore \qquad v_g = \frac{d\omega}{dk}=\frac{2\pi dv}{-(2\pi/\lambda^2)d\lambda}=-\lambda^2\frac{dv}{d\lambda} \qquad (3.28)$$

3.8 Relation Between Group Velocity and Particle Velocity

deBroglie's assumption that the equation $E = \hbar\,\omega$ is valid for matter as well as for radiation, may be made plausible by computing the group velocity of a wave packet that represents a non relativistic particle whose energy and momentum are connected by the relation. $E = \dfrac{p^2}{2m}$

and $\dfrac{dE}{dp} = \dfrac{p}{m} = v$

But from $E = \text{h}w$ and $p = \text{h}k$

$\therefore \quad dE = \text{h}dw$ and $dp = \text{h}dk$

or $$\frac{dE}{dp} = \frac{dw}{dk} = v_g \qquad \text{(by eqn. 3.27)}$$

Thus $$v_g = v \qquad (3.29)$$

i.e. group velocity of wave packet = velocity of the particle

For a relativistic particle

$$E^2 = p^2c^2 + m_0^2c^4$$

and $$\frac{dE}{dp} = \frac{pc^2}{E}$$

But $$E = \frac{m_0c^2}{\sqrt{1- v^2/c^2}} \text{ and } p = \frac{m_0v}{\sqrt{1- v^2/c^2}}$$

Therefore $$v_g = \frac{dE}{dp} = \frac{pc^2}{E}$$

putting for E and p we get, $$v_g = v \qquad (3.30)$$

Thus energy-frequency and momentum-wave vector relations introduced by de-Broglie, lead to the conclusion that the velocity of a particle is to be associated with the group velocity of the wave packet.

3.9 Relation Between Phase Velocity and Group Velocity

(i) Non-relativistic Particle: For particle which resemble a small wave packet rather than infinitely long wave, the phase velocity is given by

$$v_p = nl$$

According to de-Broglie hypothesis, the material particle associated with wave has wavelength

$$\square = \frac{h}{mv_g}$$

Total energy $$\mathrm{E} = \text{Kinetic Energy} = \frac{1}{2}mv_g^2$$

$$E = hv$$

so that $$v = \frac{E}{h} = \frac{\frac{1}{2}mv_g^2}{h}$$

or $$v_p = \frac{1}{2}v_g \qquad (3.31)$$

Thus for a non-relativistic free particle the phase velocity is half of the group velocity.

Further, as $$v_p = \frac{\omega}{k}$$

$$\omega = kv_p$$

Also from (3.29) $$v_p = \frac{d\omega}{dk} = \frac{d}{dk}(kv_p)$$

or $$v_g = v_p + k\frac{dv_p}{dk} \qquad (3.32)$$

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

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

Dividing, we get

$$\frac{k}{dk} = -\frac{\lambda}{d\lambda}$$

Putting in (3.32) we have

$$v_g = v_p - \lambda \frac{dv_p}{d\lambda} \tag{3.33}$$

(ii) For relativistic particle : The phase velocity v_p is defined by the relation

$$v_p = \frac{\omega}{k} \tag{3.34}$$

and represents the velocity of propagation of an infinitely long monochromatic plane wave. If □ is wavelength and ν the frequency of the wave then phase velocity given by eqn. (3.34) can also be written as

$$v_p = \nu\lambda \tag{3.35}$$

and as shown earlier in eqn. (3.18) the phase velocity of associated de-Broglie wave is given by

$$v_p = \frac{c^2}{v}$$

The group and phase velocities are equal only in the case where v_p is independent of k. A medium of which $\frac{d\omega}{dk}$ is independent of k (i.e. $\omega \propto k$) is known as dispersionless medium.

3.10 Summary

1. deBroglie suggested that like radiation, matter should also show dual character and hence material particles can also possess wave like character.
2. The wave associated with the particle has wavelength given by $\lambda = h/p = h/mv$, where p is momentum of the particle and h the Planck's constant.
3. A wave packet is a type of wave motion comprising a group of waves, each with slightly different velocity and wavelength, with phases and amplitude so chosen that they interfere constructively over only a small region of space where the particle can be located, outside of which they interfere destructively so that the amplitude reduces to zero rapidly.

4. The group velocity (v_p) is the velocity with which a slowly varying envelop or packet due to group of waves travel in a medium. The phase velocity (v_p) of a wave is the velocity with which the displacement of the crest or trough of the wave travels in a medium. In a dispersive medium v_p is different for different wavelength. The particle velocity is practically the group velocity.

   For no-relativistic particles the group and phase velocities are related as $v_p = ½v_g$

5. The wave character of particle can be observed through various experiments.

3.11 Glossary

- Wave-particle duality : Exhibiting both particle and wave like behaviour by light (radiation) and particle (matter) under suitable conditions.
- Matter waves : Waves associated with a particle in motion.
- deBroglie waves : Matter waves.
- deBroglie wavelength : The wavelength of the wave associated with a moving particle and given by the relation.

$$\lambda = h/mv$$

- Wave packet : A theoretical conception which are employed to explain the experimental findings.

  A wave packet is a short ' burst' or 'envelope' of localized wave action that travels as a unit.

- Group Velocity : The velocity with which a slowly varying envelope or packet due to group of waves travel in a medium.
- Phase velocity : The rate at which the phase of the wave propagates in space given.
- Particle velocity: The velocity of the particle which is equal to the group velocity of the waves.

3.12 References

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Self Assessment Questions (SAQ)

SAQ-1. What do you understand by wave-particle duality?

SAQ-2 What led deBroglie to suggest that the material particle should also show wave nature?

SAQ-3 What is the difference between light (electromagnetic) waves and matter waves?

SAQ-4 What do you understand by 'wave packet' and what is its importance?

SAQ-5 Why a monochromatic wave cannot represent a particle?

3.13 Solved Problems

Problem 1: What is the deBroglie wavelength of an electron moving with velocity $v = 3/5c$?

Solution: The deBroglie wavelength is

$$\lambda = h / mv$$

Here $v/c = 3/5$, so the electron mass undergoes relativistic variation by the relation

$$m = \frac{m_0}{\sqrt{(1 - v^2/c^2)}}, \qquad m_0 = \text{rest mass of electron}$$

$$\therefore \qquad \lambda = \frac{h}{m_0 v}\sqrt{1 - v^2/c^2} = \frac{6.63\times10^{-24}}{9.1\times10^{-31}\times\frac{3}{5}c}\times\sqrt{1-\frac{9}{25}}$$

$$= \frac{6.63\times10^{-34}\times4}{9.1\times10^{-31}\times3\times3\times10^{8}} = 0.323\times10^{-11}\,\text{m}$$

= 0.0323 Å.

Problem 2: What voltage must be applied to an electron microscope to produce electrons of wavelength 0.40 Å?

Solution: The deBroglie wavelength is given by

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

Here □ = 0.40 Å = 0.40×10^{-10} m

$h = 6.62 \times 10^{-34}$Js

$m = 9.1 \times 10^{-31}$ kg

$e = 1.6\times10^{-19}$ C

$$\therefore \qquad \lambda = \frac{6.62\times10^{-34}}{\sqrt{2\times9.1\times10^{-31}\times1.60\times10^{-19}}}\cdot\frac{1}{\sqrt{V}}$$

$$\text{or} \qquad \sqrt{V} = \frac{6.62\times10^{-34}}{0.4\times10^{-10}\times\sqrt{2\times9.1\times10^{-31}\times1.6\times10^{-19}}} = 30.6$$

$\therefore \qquad V = 936.36$ volts.

Problem 3: You have 10 *eV* photon and 10 *eV*electron, which one has shorter wavelength? Give reason.

Solution: Energy of a 10 eV photon

$$E = 10\times1.6\times10^{-19}\text{ J} \qquad (\because 1eV = 1.6\times10^{-19}\text{ J})$$

Again $$E = h\nu = \frac{hc}{\lambda}$$

$$\therefore \qquad \lambda = \frac{h}{p} = \frac{hc}{E} = \frac{6.62\times10^{34}\times3\times10^{8}}{10\times1.6\times10^{-19}} = 1240\times10^{-10}m = 1240\ \text{Å}$$

Now for an electron,

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

$mv = \sqrt{2mE}$ and the associated deBroglie wavelength is

$$\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2mE}} = \frac{6.62\times10^{-34}}{\sqrt{(2\times9.1\times10^{-31}\times10\times1.6\times10^{-19})}}$$

$$= 3.88\times10^{-10}\text{ m} = 3.88\text{ Å}$$

Hence electron will have shorter wavelength.

Problem 4: Find the deBroglie wavelength associated with a 50 eV electron.

Solution: We have,

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

Putting the values,

$$\lambda = \frac{6.62\times10^{-34}}{\sqrt{(2\times9.1\times10^{-31}\times50\times1.6\times10^{-19})}}$$

$$= 1.66\times10^{-10}\text{ m} = 1.66\text{ Å}.$$

3.14 Terminal Questions

3.14.1 Short Answer Type

1. What do you understand by wave-particle duality?
2. What are matter waves?
3. What led deBroglie to think that the material particles should also exhibit wave nature.
4. What is the difference between light (electromagnetic) waves and matter waves?
5. How matter waves are not electromagnetic?
6. Why we cannot observe matter or deBroglie waves associated with moving objects in our daily life?
7. What are wave-packets?
8. Why a monochromatic wave cannot represent a particle?
9. What is the significance of Davisson and Germer experimental result?
10. What are group velocity and phase velocity? Which one is greater?
11. Show that the deBroglie wavelength □of electron of energy $E = eV$ is given by $\lambda = \frac{h}{\sqrt{meV}}$.

3.14.2 Long Answer Type

1. Discuss the basic results that led to the formation of the wave concept of matter. What are deBroglie waves? Derive an expression for its wavelength.
2. State deBroglie theory of mater waves. Give experimental verification for this hypothesis.
3. Derive an expression for the deBroglie wavelength for a particle in terms of its kinetic energy.
4. What do you understand by wave packet? How does it represent a particle?

5. Distinguish between group velocity and phase velocity. Show that for a non-relativistic free particle the phase velocity is half of the group velocity.
6. What are group, phase and particle velocities? Show that phase velocity of associated waves is always greater thanthe velocity of light in vacuum.
7. On the basisof deBroglie's matter wave hypothesis establish the correspondence between particle concept and wave concept. Explain weave-particle dualism by Davisson-Germer's experiment.
8. Describe Davisson and Germer experiment on diffraction of electrons and explain how it explains the nature of an electron beam.
9. Show that group velocity $v_g = -\lambda^2 \frac{dv}{d\lambda}$, where the symbols have their usual meanings.
10. Prove that wave group associated with a moving particle travels with the same velocity as that of the particle.
11. Show that the deBroglie wavelength of an electron beam accelerated by a potential V volt, under relativistic condition, is given by

$$\lambda = \frac{h}{\sqrt{2m_0 eV}}\left[1 - \frac{eV}{m_0 c^2}\right]$$

12. Describe G.P. Thomson's experiment that demonstrates the wave-like behaviour of electrons. What are the practical applications of wave nature of electrons?

3.14.3 Numerical Answer Type

1. Calculate the de-Broglie wavelength of an electron which has kinetic energy equal to 15 eV (Ans. : 3.12 Å)
2. What voltage must be applied to an electron microscope to produce electrons of wavelength 0.5 Å? Given $e = 1.6 \times 0\ 10^{-19}$ C, $m = 9.1\times10^{-31}$ kg and $h = 6.62\times10^{-34}$ J-s

   [Ans : 602.4 V]

3. A bullet of mass 40 g travels at a speed of 1000 m/s What wavelength can be associated with it?

4. Find the energy of the neutron in eV whose deBroglie wavelength is 1 Å
(Ans : $8.13\times10^{-12} eV$)

5. A spectral line has wavelength 4000 Å. Calculate frequency and the energy ineV of the photon associated with it.[Ans. $\nu = 0.75\times10^{15}$ Hz, E = 3.1 eV]

6. Calculate the wavelength associated with an electron subjected to a potential difference of 1.25 kV [Ans. 11 Å]

Unit 4 : Heisenberg's Uncertainty Principle

Structure

4.1 Introduction

In the previous chapter we have discussed about the dual-character of light and particle in which light (e.m. waves) behaves as particles and particles like electrons protons, neutrons also behave as waves. Various explanations were given to explain this 'wave-particle duality' but the best known consequence of the wave-particle duality is the 'Uncertainty Principle'.

The uncertainty principle or principle of indeterminacy was proposed by Heisenberg in 1927.According to classical mechanics, a moving particle has a definite momentum and position in space and both the physical quantities i.e., position and momentum can be determined accurately. However, recently the classical view has been proved to be an approximation only and it is inadequate for describing the dynamical behaviour of microscopic objects like sub-atomic particles.

In quantum mechanics, a particle is described by a 'wave-packet' of linear extension (Δx) that surrounds the position of the classical particle and moves with group velocity. From Max Born'sprobability interpretation, the particle can be found everywhere within the wave packet. This means that the position of the particle is uncertain within the limit Δx. Again, a wavepacket is formed by the superposition of a large number of waves having different wavelengths. Hence, the wavelength of the wave packet cannot be said definitely.

In other way we can say that the wavelength of the wave packet lies within certain range $\lambda$to $\lambda + \Delta\lambda$.

As the momentum of a particle is related to the wavelength by deBroglie's relation-

$$\lambda = \frac{h}{p} \quad \text{or} \quad p = \frac{h}{\lambda} \tag{4.1}$$

or $$\Delta p = -\frac{h}{\lambda^2} d\lambda \tag{4.2}$$

and the particle momentum is also within range p to $p + \Delta p$. Therefore, now the momentum of the particle cannot have a definite value. Hence, because of the wave nature of particle there is uncertainty (Δx) in position and a corresponding uncertainty (Δp) in momentum of the particle.

Now if the number of superposed wave as well as their range of wavelength ($\Delta\lambda$) is increased, then the linear spread (Δx) of the wave packet decreases. But simultaneously the uncertainty (Δp) in momentum increases as $\Delta p \propto \Delta\lambda$, when $\Delta\lambda = \infty$, $\Delta p = \infty$ and $\Delta x = 0$, i.e. the wave packet reduces to a point. In this position, there is no uncertainty in the position of the particle.

Now for a definite λ, Δλ = 0, then Δp = 0 (as $\Delta p \propto \Delta\lambda$), and so there is no uncertainty in the momentum of the particle but in this case Δx = ∞, i.e., the position uncertainty is infinite since the associated wave with the particle may now extend upto∞.

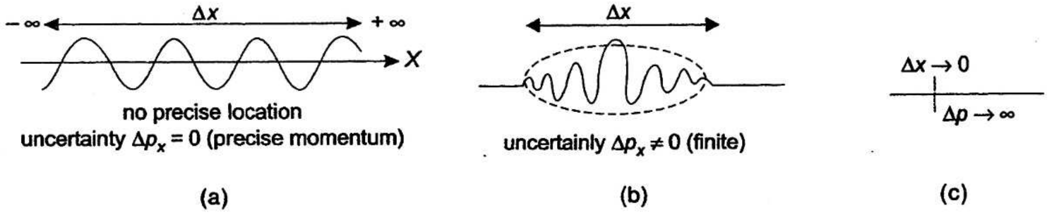

Fig. 4.1 :(a) a plane monochromatic wave ($k = a$ constant)

(b) a superposition of plane waves of slightly different k's, forming a wave group.

4.2 Objectives

After studying this chapter you should be able to understand the following points and answer same simple related questions.

1. Concept of uncertainty in measurement of physical quantities.
2. How fundamentally uncertainties are introduced in measurement of some dynamical conjugate variables associated with microscopic objects.
3. Statement and explanation of Heisenberg's uncertainty principle.
4. Uncertainty of position-momentum and energy-time.
5. Verification of uncertainty principle through various theoretical experiments.
6. Some applications of uncertainty principle and simple problems based on it.

4.3 Heisenberg's Uncertainty Principle

The uncertainty principle states that "It is fundamentally impossible to determine simultaneously the position and the momentum of a particle to an accuracy greater than one quantum of action *h*."

Mathematiclaly this principle can be expressed as

$$\Delta x \Delta p_x \geq h \tag{4.3}$$

where $h = h/2\pi$, h being the Planck's constant = 6.62×10^{-34} J-s. Here Δx is the error (uncertainty) in the determination of position of the particle and Δp_x is the error (uncertainty) in the determination of the *x*-component of momentum. If the position is determined accurately, then Δx becomes smaller and consequently larger is Δp_x and vice-versa. It must be kept in mind that the uncertainties do not lie in the apparatus used for the measurement but in the nature itself.

In three dimensions, the uncertainty relations are given as

$$\left.\begin{aligned} \Delta x \Delta p_x &\geq h \\ \Delta y \Delta p_y &\geq h \\ \Delta z \Delta p_z &\geq h \end{aligned}\right\} \tag{4.4}$$

4.3.1 Elementary Proof of Uncertainty Relation

For a particle moving along the *x*-direction, the deBroglie wavelength λ is given by

$$\lambda = h / p_x.$$

or,
$$p_x = \frac{h}{\lambda} = \frac{h}{2\pi}\cdot\frac{2\pi}{\lambda} = \hbar k \tag{4.5}$$

If the wave packet be considered as the superposition of two simple harmonic waves of propagation constants k and $k + \Delta k$, then linear extension of the wave packet is,

$$\Delta x = \frac{2\pi}{\Delta k} \tag{4.6}$$

As, the particle lies somewhere within the wave packet, Δx is the uncertainty in the position of the particle and Δk is the uncertainty in the corresponding propagation constant of the associated wave.

The uncertainty in the momentum $\Delta p_x$is obtained from eq. (4.5)

$$\Delta p_x = \hbar \Delta k \tag{4.7}$$

From eq. (4.6) and (4.7), we get the product of the uncertainty as

$$\Delta x.\Delta p_x = \frac{2\pi}{\Delta k} \times \hbar \Delta k = 2\pi\hbar = h$$

The above equality may be replaced by an inequality and then

$$\therefore \qquad \Delta x.\Delta p_x \geq h \qquad (4.8)$$

4.4 Conclusions from Uncertainty Relations

From the Heisenberg's uncertainty relation

$$\Delta x.\Delta p_x \geq \hbar$$

we may conclude that

(i) If $\Delta x = 0$, then $\Delta p_x = \frac{\hbar}{\Delta x} = \frac{\hbar}{0} = \infty$

Thus, if the uncertainty in the position measurement of a moving particle be zero, then at the same moment the uncertainty in the momentum measurement will be infinity.

(ii) If the momentum be measured accurately i.e., $\Delta p_x = 0$, then the uncertainty in the position mesurement will be infinite, that is

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

(iii) For a particle of mass *m*moving with velocity v_x along the *x*-direction, its momentum is $p_x = mv_x$, then from uncertainty relation

$$\Delta x.\Delta p_x = \hbar$$

or $$\Delta x.\Delta v_x = \frac{\hbar}{m}$$

For heavy particle,$m \to \infty$, then

$$\Delta x \cdot \Delta v_x = \frac{\hbar}{\infty} = 0\,.$$

For such a particle both the position and momentum can be determined accurately. This is true for macroscopic bodies whose motion can be discussed in classical mechanics.

Hence, the uncertainty relation bears no significance in classical mechanics rather only for microscopic objects like electron, proton, neutron, atom etc. where quantum mechanics is applicable.

4.5 Time-Energy Uncertainty Relation

The time-Energy Uncertainty Principle states that –

In any simultaneous determination of time and energy of a moving particle, the product of the uncertainty is of the order of Planck's constant, i.e.,

$$\Delta E.\Delta t \geq \hbar$$

Here, ΔE is the uncertainty in measurement of energy and Δt, the corresponding uncertainty in the measurement of time.

4.5.1 Elementary proof of Time-Energy Uncertainty Relation

Let a moving particle is represented by a wave packet whose group velocity is equal to the particle velocity. Now, if the wave packet extended in range Δx moved along the x-axis with group velocity v_g, then

$$v_g = \frac{\Delta x}{\Delta t}, \qquad \text{or} \qquad \Delta t = \frac{\Delta x}{v_g} \tag{4.9}$$

WhereΔt is the time in which the wave packet moves through Δx. Δx and Δt are the uncertainties in x-coordinate and time associated with the particle. If m be the mass, p_x the momentum and E the kinetic energy of the particle, then,

$$E = \frac{p_x^2}{2m},$$

or $$\Delta E = \frac{2p_x.\Delta p_x}{2m} = \frac{p_x}{m}\Delta p_x = \frac{mv}{m} \times \Delta p_x$$

or $$\Delta E = v_x \Delta p_x \tag{4.10}$$

From equations (4.9) and (4.10), we get

$$\Delta E.\Delta t = v_x \Delta p_x \cdot \frac{\Delta x}{v_g} = \Delta x \cdot \Delta p_x \qquad [\because v_x = v_g]$$

But, $\Delta x \cdot \Delta p_x \geq \hbar$.

Therefore, $\Delta E.\Delta t \geq \hbar$ (4.11)

Eq. (4.11) represents the time-energy uncertainty relation.

From eq. (4.11), we have

$$\Delta t = \frac{\hbar}{\Delta E} \tag{4.11a}$$

If ΔE be the maximum uncertainty in determining the energy for a system in a particular state, then from above equation Δt is the minimum i.e. the system remains in that state for a minimum time. Again

$$\Delta E = \frac{\hbar}{\Delta t} \tag{4.11b}$$

The above relation shows that if a system remains in a particular state for a maximum intervalof time then the uncertainty in the measurement of energy is the minimum.

4.6Angular Position-Angular Momentum Uncertainty Principle

The angular position angular momentum uncertainty principle is stated as below:

In any simultaneous determination of angular position and angular momentum of a particle, the product of the uncertainties in angular momentum ΔL and angular position$\Delta\phi$ is greater than or equal to the Planck's constant *h* i.e.

$$\Delta L.\Delta \phi \geq \hbar \tag{4.12}$$

In fact the Heisenberg's uncertainty principle is valid for any canonical conjugate variables.

4.7 Derivation of Uncertainty Principle from deBroglie's Wave Concept

It is possible to derive the Heisenberg's uncertainty principle using de-Broglie's wave concept which proposes that a particle in motion can be taken as a group of waves or a wave packet, the group velocity being equal to the particle velocity.

Let us consider a group of waves having only components of equal amplitude but having slightly different angular frequencies (0\ and o^. The wave displacements for two components are given as

$$\psi_1 = a\cos(\omega_1 t - k_1 x)$$

$$\psi_2 = a\cos(\omega_2 t - k_2 x)$$

where $\frac{\omega_1}{k_1}$ and $\frac{\omega_2}{k_2}$ represent their respective phase velocities.

The resultant displacement

$$\psi = \psi_1 + \psi_2 = 2a\cos\left[\frac{(\omega_1+\omega_2)}{2}t - \frac{(k_1+k_2)}{2}x\right] \times \cos\left[\frac{(\omega_1-\omega_2)}{2}t - \frac{(k_1-k_2)}{2}x\right]$$

$$= 2a\cos(\omega t - kx)\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right) \qquad (4.13)$$

$$\left.\begin{aligned} &\text{where} \quad \omega = \frac{(\omega_1+\omega_2)}{2};\ k = \frac{(k_1+k_2)}{2} \\ &\text{and} \quad \Delta\omega = \omega_1 - \omega_2; \quad \Delta k = k_1 - k_2 \end{aligned}\right] \qquad (4.14)$$

The resultant is plotted in Fig. (3.1), where the loop formed will travel with group velocity v_g. Now this group velocity is equal to the particle velocity and hence the loop is equivalent to the position of

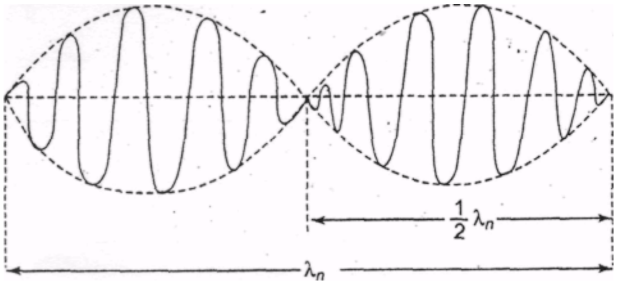

Fig. 4.2

the particle. Thus the position of the particle cannot be determined with certainty. It is expected to lie somewhere between the two consecutive nodes. In other words, the error in the measurement of the position of the particle is therefore equal to the distance between these two nodes.

Now a node is formed when

$$\cos\left(\frac{\Delta\omega}{2} - \frac{\Delta k}{2}x\right) = 0$$

or
$$\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right) = (2\pi + 1)\frac{\pi}{2} \text{ where n = 0, 1, 2, 3, ...}$$

Thus, if x_1 and x_2 represent the positions of two successive nodes, then at any instant *t*, we get

Thus, if x_1 and x_2 represent the positions of two successive nodes, then at any instant *t*, we get

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_1 = (2n+1)\frac{\pi}{2}$$

and
$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_2 = (2n+3)\frac{\pi}{2}$$

Subtracting, we get $\frac{\Delta k}{2}(x_1 - x_2) = (2n + 3 - 2n - 1)\frac{\pi}{2} = \pi$

Therefore, the error in the measurement of the position of the particle is

$$\Delta x = x_1 - x_2 = \frac{2\pi}{\Delta k} \tag{4.15}$$

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

$$\therefore \quad \Delta k = \frac{2\pi}{h}\Delta p \qquad (4.16)$$

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

$$\therefore \quad \Delta x \Delta p = h$$

or

$$\Delta x \cdot \Delta p \geq \hbar \qquad (4.17)$$

whereΔp represents the error in the measurement of momentum.

The treatment given above is very elementary. If we take a group of large number of waves having continuously varying frequencies, we get the product of the fundamental errors as $\Delta p \Delta x \approx \hbar/2$, which is exact form of uncertainty principle.

4.8 Illustration (Experimental Verification) of Heisenberg's Uncertainty Principle

The validation of Heisenberg's uncertainty principle may be illustrated by the following thought experiments: A thought experiment is an imaginary experiment which is not possible to be performed in practice however, it does not violate any fundamental law of nature.

4.8.1 Electron Diffraction through a Single Slit

Let a monoenergetic parallel beam of electrons moving along the x -direction be incident on a single slit of width Δy. As the electron in motion is associated with de Broglie wave, the electron beam after passing through the slit undergoes diffraction producing a Fraunhoferelectron diffraction pattern on the photoplate P, placed perpendicular to the x-axis [Fig 4.3].

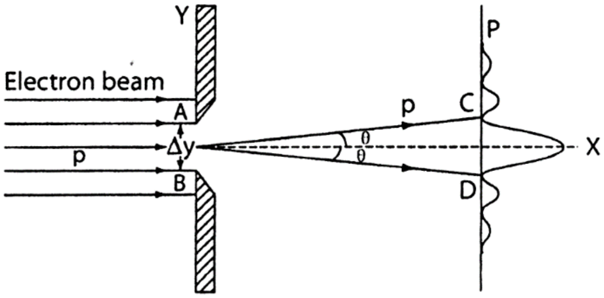

Fig.4.3 : Diffraction of electron wave through a single slit

The first minimum of the diffraction pattern satisfies the relation $\Delta y \sin\theta = \lambda$, where θ is the angle of diffraction for the first order and λ is the de Broglie wavelength. Nowthe uncertainty in the position of an electron in the slit is Δy as it is very difficult to exactly the position of the electron in the slit,

or, $$\Delta y = \frac{\lambda}{\sin\theta} \qquad (4.18)$$

Before incidence, let the momentum of the electron along the *x*-direction be *p*. After diffraction if the electron moves along *OC*, then the component of momentum *p* along the *y*-direction is *p*sinθ. If the electron moves along *OD* after diffraction, then the *y*component momentum is $-p\sin\theta$. Since the electron may be anywhere within –θ to +θ, the *y*-component of momentum must be anywhere between $-p\sin\theta$ to $p\sin\theta$.

Thus the uncertainty in the momentum measurement of the electron is,

$$\Delta p_y = p\sin\theta - (-p\sin\theta)$$

$$\Delta p_y = 2p\sin\theta$$

or $$\Delta p_y = 2h/\lambda p\sin\theta \qquad (\because \lambda = h/p) \qquad (4.19)$$

Multiplying equations (4.18) and (4.19) we get,

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

or $$\Delta y \Delta p_y = 2h$$

or $$\Delta y \Delta p_y \geq \hbar / 2 \tag{4.20}$$

To decrease the uncertainty in the determination position of the electron, Δy must be decreased. But equation (4.18) shows that a decrease in Δy leads to the increase in θ and the diffraction pattern will be wider. This will cause a larger uncertainty in Δp. Thus the electron diffraction experiment established the truth of uncertainty principle.

4.8.2 Gamma-Ray Microscope Experiment

This hypothetical experiment was suggested by Bohr and was developed by Heisenberg to establish the validity of uncertainty principle. The use of γ-ray in the experiment can be justified as follows:

The atomic radius is ~ 10^{-11} m. So to determine the position of an electron with an uncertainty of about 10% of the atomic radius, radiation of wavelength ~ 10^{-12} m = 0.01 Å is needed. The wavelength of γ-rays being ~ 0.01 Å, it is an efficient agent to conduct the experiment.

We suppose, O be the position of the electron and λ, the wavelength of the γ-ray. If α be the semi-vertical angle of the cone of the γ-rays entering into the microscope objective from the electron, then the resolving of the microscope is given by,

$$\Delta x = \frac{\lambda}{2 \sin \alpha} \tag{4.21}$$

Here, Δx is the distance between two points which can just be resolved by the microscope. This suggests that for greater resolving power Δx should be small which can be achieved if λ be small. We know that the γ-rays emitted from the atomic nuclei have smallest wavelength available in nature. That is why γ-rays are used to locate the position of the electron with minimum uncertainty. In this connection, it must be remembered that we cannot observe an object with the help of a microscope which uses γ-ray beam. The microscope using lens, etc. cannot refract γ-rays. This is why the experiment is known as athought experiment.

The incident γ-ray photon is scattered by the electron due to Compton effect and enters into the microscope. During bouncing off into the microscope the photon transfers momentum to the electron. The amount of transferred momentum is uncertain as the aperture of the microscope is definite.

The uncertainty in momentum of the recoil electron can be calculated as follows:

We suppose that a γ-ray photon of momentum $h\nu/c$strikes an electron of mass m at rest. After scattering the photon enters into microscope and making an angle ϕ with the direction of incidence and the electron moves with momentum mv along a direction making an angle θ with the x-axis as in Fig 4.4

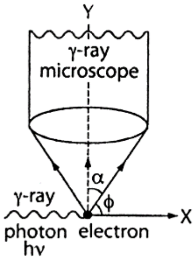

Fig 4.4 γ-ray microscope experiment

Now, from the momentum conservation principle along the x-direction [Fig 4.5],

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

or $$p_x = mv\cos\theta = \frac{h\nu}{c} - \frac{h\nu'}{c}\cos\phi$$

or $$p_x = \frac{h}{c}(\nu - \nu'\cos\phi) \qquad (4.22)$$

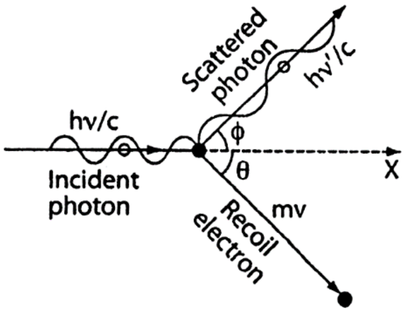

Fig 4.5 Scattering of photon by an electron

Here, p_x is the x-component of momentum of the electron. Since the limits of the angle ϕ through which the photon enters the microscope objective are from $(\pi/2 - \alpha)$ to $(\pi/2 + \alpha)$, the spread in the x-component of momentum is given by,

$$\frac{h}{c}\left[\nu - \nu'\cos\left(\frac{\pi}{2} - \alpha\right)\right] \le p_x \le \frac{h}{c}\left[\nu - \nu'\cos\left(\frac{\pi}{2} + \alpha\right)\right]$$

or $$\frac{h}{c}\left[\nu - \nu'\sin\alpha\right] \le p_x \le \frac{h}{c}\left[\nu - \nu'\sin\alpha\right]$$

The uncertainty in the momentum is given by,

$$\Delta p_x = \frac{h}{c}\left[\nu + \nu'\sin\alpha\right] - \frac{h}{c}\left[\nu - \nu'\sin\alpha\right]$$

$$= \frac{h\nu}{c} + \frac{h\nu'}{c}\sin\alpha - \frac{h\nu}{c} + \frac{h\nu'}{c}\sin\alpha$$

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

$$= \frac{2h}{\lambda}\sin\alpha \tag{4.23}$$

From equations (4.21) and (4.23),

$$\Delta x \Delta p_x = \frac{\lambda}{2\sin\alpha} \times \frac{2h}{\lambda}\sin\alpha = h \tag{4.24}$$

which is consistent with $\Delta x \Delta p_x \geq \hbar$.

Hence, the experiment established the validity of the uncertainty principle.

4.9 Applications of Uncertainty Principle

(i) Non-existence of free electronin the nucleus. The radius of the nucleus of any atom is of the order 10^{-14} m, so that if the electron is confined with nucleus, the uncertainty in its position must be greater than 10^{-14} m. According to uncertainty principle

$$\Delta x \Delta p_x = \hbar$$

whereΔx is the uncertainty in position and Δp is the uncertainty in momentum and $\hbar = h/2\pi$.

Thus $\Delta p = \frac{\hbar}{\Delta x} = \frac{6.63\times10^{-34}}{2\pi\times2\times10^{-14}} = \frac{6.63\times10^{-20}}{4\pi}$ $\quad [\because \Delta x = 2a = 2\times10^{-14} m]$

$\approx 5.275\times10^{-21}$ kg m/s.

If this is the uncertainty in momentum of the electron, the momentum of the electron must be at least comparable with its magnitude i.e.

$$p = 5.275 \times10^{-21} \text{ kgm/s.}$$

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

$$T = \frac{p^2}{2m} = \frac{(5.275\times10^{-21})^2}{2\times9\times10^{-31}} \qquad (m = 9.1\times10-31kg)$$

or, $$T = \frac{(5.275\times10^{-21})^2}{2\times9.1\times10^{-31}\times1.6\times10^{-19}}\text{eV} = 9.7\times10^7\text{eV} \approx 97\text{MeV}$$

This means that if the electrons exist inside the nucleus, their kinetic energy must be of the order of 97 MeV. But experimental observations show that an electron in the atom possesses energy in the range 4 MeV to 9 MeV. Clearly the inference is that the electrons do not exist in the nucleus,

ii) Determination of the size of atom. Consider the simplest atom, say, hydrogen atom which consists of an electron and a proton. Again assuming that electron is confined to a circular region of radius 'a' then the maximum uncertainty in the position of the electron w.r.t. nucleus is $\Delta a = a$.

From uncertainty principle the minimum uncertainty in the corresponding simultaneous momentum is

$$\Delta p \approx \frac{\hbar}{\Delta a} = \frac{\hbar}{a} \text{ where } \hbar = \frac{h}{2\pi}$$

(again the constants in uncertainty relation are chosen to get the exact result).

Since the momentum of electron cannot be less than Δp, then $p = \hbar / a$

Now, kinetic energy of electron = $\frac{p^2}{2m} \equiv \frac{\hbar^2}{2ma^2}$

as uncertainty principle relates Δx to $\Delta p_x, \Delta y$ to Δp_y and Δz to Δp_z

$$\therefore \qquad p^2 = p_x^2 + p_y^2 + p_z^2 \equiv (\Delta p_x)^2 + (\Delta p_y)^2 + (\Delta p_z)^2 = \frac{\hbar^2}{a^2}$$

The electrostatic potential energy is $-e^2/4\pi\in_0 a$. Therefore, the total energy is given by

$$E \equiv \frac{\hbar^2}{2ma^2} - \frac{e^2}{4\pi \in_0 a}$$

The ground state of the atom will correspond to a minimum value of E for which dE/da must be equal to zero. i.e., $dE / da = 0$

or $$\frac{dE}{da} = -\frac{\hbar^2}{2ma^3} + \frac{e^2}{4\pi \in_0 a^2} = 0$$

or $$\frac{e^2}{4\pi \in_0} = \frac{\hbar^2}{2ma}$$

or $$a = \frac{4\pi \in_0 \hbar^2}{me^2} = \frac{\in_0 h^2}{\pi me^2} \tag{4.25}$$

Putting the values of constants, we get $a = a_0 = 0.5 \times 10^{-10}\, m$, where a_0 represents the minimum value of *a*. Thus the finite size of the atom is due to the uncertainty principle. According to (4.25) the atomic dimensions are of the order of Angstrom which is indeed correct. The minimum energy is given by

$$E = \frac{\hbar^2}{2ma_0^2} - \frac{e^2}{4\pi \in_0 a_0}$$

Substituting values, we have

$$\mathrm{E} = -\,13.6\, eV \tag{4.26}$$

which in indeed the ground state energy of hydrogen atom.

(iii) Existence of neutrons, protons and α-particles in the nucleus. The rest mass of neutronsand protons is of the order ofm_0 = 1.67 × 10^{-27} kg. From the uncertainty principle

$$\Delta p_x \approx \frac{\hbar^2}{\Delta x}$$

As radius of the nucleus of atom is 10^{-14} m thus

$$\Delta x = 2a = 2 \times 10^{-14}$$

and $$\Delta p_x \approx p_x \approx 5.275 \times 10^{-21} \text{ kg m/s}$$

The corresponding value of kinetic energy,

$$E = \frac{p_x^2}{2m_0} = \frac{(5.275) \times 10^{-21})^2}{2 \times 1.67 \times 10^{-27}} = 8.4 \times 10^{-15} J = \frac{8.4 \times 10^{-15}}{1.6 \times 10^{-19}} = 52\, keV$$

The rest mass of α particle is approximately four times the proton mass, thus a-particle should have a minimum kinetic energy of 13*keV*. Since the minimum energy carried by protons or neutrons is of the order of $52 keV$ and for α-particles of the order of $13 keV$, thus these particles can exist in the nuclei.

(iv) The radiusof the Bohr's first orbit: Suppose ΔxandΔp represent the uncertainties in the position and momentum of the electron in the first orbit respectively. According to Heisenberg's uncertainty principle, we have

$$\Delta x\,\Delta p = h \text{ or } \Delta p = \frac{\hbar}{\Delta x}$$

The uncertainty in the kinetic energy of the electro0n may be put as follows:

$$\Delta T = \frac{1}{2} m (\Delta v)^2 \tag{4.27}$$

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

or
$$\Delta T = \frac{1}{2m}\left(\frac{\hbar}{\Delta x}\right)^2 = \frac{\hbar^2}{2m(\Delta x)^2} \tag{4.28}$$

The uncertainty in the potential energy of the same electron may be put as follows:

$$\Delta V = -\frac{Ze^2}{\Delta x} \tag{4.29}$$

The uncertainty in the total energy of the electron will therefore be

$$\Delta E = \Delta \mathrm{T} + \Delta V$$

or
$$\Delta E = \frac{\hbar^2}{2m(\Delta x)^2} - \frac{Ze^2}{\Delta x} \tag{4.30}$$

The uncertainty in the energy will be minimum provided

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

Equation (4.30) may be put as follows:

$$\frac{d(\Delta E)}{d(\Delta x)} = -\frac{\hbar^2}{m(\Delta x)^2} + \frac{Ze^2}{(\Delta x)^2} \tag{4.31}$$

If E is minimum, we must have

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

or

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

or

$$\Delta x \approx \frac{\hbar^2}{mZe^2} \tag{4.32}$$

On differentiating equation (4.31), we obtain

$$\frac{d^2(\Delta E)}{d(\Delta x)^2} \approx +\frac{3\hbar^2}{m(\Delta x)^2} - 2\frac{Ze^2}{(\Delta x)^3} \approx \frac{3\hbar^2}{m(\Delta x)^3\left(\frac{\hbar^2}{mZe^2}\right)} - \frac{2Ze^2}{(\Delta x)^3} \qquad \text{[by eqn. (4.32)]}$$

$$\approx \frac{3\text{Ze}^2}{(\Delta x)^3} - \frac{2Ze^2}{(\Delta x)^3} \approx \frac{2\text{Ze}^2}{(\Delta x)^3} = (+)\,\text{ve}$$

As equation (4.32) represents the condition of minimum in the first orbit, it means that the radius of the first orbit is given as follows:

$$r = \Delta x = \frac{\hbar^2}{mZe^2} = \frac{h^2}{4\pi^2 mZe^2} \tag{4.33}$$

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

(iv) Strength of nuclear force. If a nucleon is confined within the sphere of radius, r_0 (= 1.2×10^{-13} cm), the momentum must be of the order of $p = \hbar / r_0$. Thus, kinetic energy of the nucleon of mass M (proton or neutron) will be of the order

$$T \approx \frac{p^2}{2M} \approx \frac{1}{2M}\frac{\hbar^2}{r_0^2} \approx 10\ \text{MeV}$$

Now if the nucleon is bound in the nucleus, the binding energy must be more than kinetic energy and opposite in sign. The nuclear binding energy is of the order of 10 MeV.

(v) Stability of the atom. The ground state energy is the lowest possible energy with which the atom can have existence. This energy will be the sum of two terms (kinetic and potential) of opposite sign. If the electron is confined to a small region, the kinetic energy becomes large because the wave will be carrying large momentum. If the wave is spread in a large region, the potential energy will be small. Hence the ground state refers to the best possible compromise and this is the explanation for the stability of the atom against collapse.

(vi) Light quanta. Suppose an electromagnetic wave-packet is made by opening a shutter for a time interval Δt. Thus, a pulse of radiation is obtained which is passing any specific point in time Δt. Further the electric field will be large during time interval Δt.

Now suppose that the pulse of radiation has one quantum only and this pulse is incident on a target having many atoms. But only one of the atoms of the target will absorb the quantum. Therefore, the probability of the absorption will be proportional to $|E|^2$, where E refers to the strength of the electric field. It is, thus, evident that the momentum will be absorbed within time interval Δt because during this time there is maximum electric field in the region in the having the target. Hence Δt may be considered as uncertainty in the time during which the absorption of quantum takes place. But the pulse of radiation is having a range of angular frequencies given by

$$\Delta\omega \geq \frac{1}{\Delta t}$$

and, therefore, the range of energies will be

$$\Delta E = h\Delta\nu = \frac{h\Delta(2\pi\nu)}{2\pi} = \hbar\Delta\omega \geq \frac{\hbar}{\Delta t}$$

so that we obtain $\Delta E\,\Delta t \geq \hbar$

From above it is evident that in any process in which there occurs a transfer of quantum from radiation to the matter (or vice versa), the product of uncertainties in the time of transfer and in the quantity of energy transferred is never less than $\hbar$, i.e.,

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

Here, we knowingly avoided discussion on particle nature of light.

4.10 Discussion

We hardly find the uncertainty principle valid in our daily experience. We find that the calculation related to measurement of both position and momentum of terrestrial bodies remarkably accurate. This is due to the fact that for bodies having appreciable mass, the uncertainties in determining both position and momentum are so small that these are negligibly small compared to the normal experimental error. However, for very small particles such as electrons and photons, the uncertainties are large comparable to the quantities themselves. In such case the classical mechanics fails to explain the behaviour of such particles and hence wave or quantum mechanics becomes a necessity.

4.11 Summary

1. Heisenberg's uncertainty principle is the best known consequence of the wave-particle duality which states that "It is fundamentally in possible to determine simultaneously the position and the momentum of a particle to an accuracy greater than h the Planck's constant".
2. Mathematically, it can be expressed as

   $$\Delta x.\Delta p_x \geq \hbar$$

   where Δx is the error (uncertainty) in measurement of the position of the particle, Δp_x the error (uncertainty) in measuring the x-component of momentum of the particle and $\hbar = h/2\pi$, , h being the Planck's constant = 6.62×10^{-34} J-s.
3. The uncertainty relation is not only true for other components of position and momentum of the particle but also for other dynamical conjugate variables such as energy and time; angle and angular momentum etc. as well

   Thus, $\Delta y.\Delta p_y \geq \hbar$

   $\Delta z.\Delta p_z \geq \hbar$

   and $\Delta E.\Delta t \geq \hbar$

4. The uncertainty principle explains a number of facts which could not be explained by the classical concepts; such as non-existence of electrons in atomic nucleus, determination of size of the atom, the radius of Bohr's first orbit, existence of neutrons and protons in the nucleus etc.
5. The uncertainty principle can be validated by a number of theoretical experiments like gamma-ray microscope and electron diffraction by a slit.

4.12 Glossary

Uncertain: Something which is not sure or which is not known exactly.

*Uncertainty Principle:*A principle proposed by Heisenberg that states that "It is impossible to measure simultaneously the value of any two canonically conjugate variables with unlimited accuracy."

Angular momentum: The quantity of rotation of a body, which is the product of its moment of inertia and its angular velocity.

It is the rotational equivalent of linear momentum and denoted as

$$L = I\omega = r \times p, \quad \text{unit} = \text{kg m}^2\ \text{s}^{-1}.$$

*Wave packet:*A wave packet (or wave train) is a short 'burst' or 'envelope' of localized wave action that travels as a unit. It comprises a group of waves, each with slightly different velocity and wavelength, with phases and amplitude so chosen that they interfere constructively over only as a small region of space and destructively elsewhere. The particle can be located in the wave packet region.

*Gamma-ray microscope:*A hypothetical experiment proposed by Heisenberg to evaluate the order of limitations in the measurements of position and momentum of an electron or a photon. In other words, the experiment establishes the validity of uncertainty principle.

*α-particle:*Alpha particles, also called α-ray or α-radiation, consists of two protons and two neutrons bound together into a particle identical to helium-4 nucleus. They are generally produced in the process of α-decay but may be produced by other ways.

4.13 References

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Self Assessment Questions

SAQ1. If the number of superposed wave and the range of wavelength be increased, then what will happen to the linear spread of the wave packet?

SAQ2. How you can say that the uncertainty principle is the consequence of wave-particle duality?

SAQ3. In γ-ray thought experiment, why γ-rays is used?

SAQ4. The uncertainty principle has significance in the case of microscopic particles only. Why?

4.14 Solved Problems

Problem 1. An electron has a speed of 1 km/s with an accuracy of 0.05%. Calculate the uncertainty with which the position of the electron can be determined. Given mass of electron (m) = 9.1×10^{-31}kg,$h = 6.63\times10^{-34}$ J-s.

Solution: The uncertainty in momentum measurement is

$$\Delta p = \Delta(mv) = m\Delta v = 9.1\times10^{-31}\times1000\times\frac{0.05}{100} = 4.55\times10^{-31} \text{ kg m/s.}$$

From the uncertainty relation, the error in measurement of position is therefore,

$$\Delta x = \frac{h}{\Delta p} = \frac{6.63\times10^{-34}\,\text{Js}}{4.55\times10^{-31}\,\text{kg}\,\text{m/s}} = 1.45\times10^{-3}\ \text{m}$$

Problem 2. An electron is kept in a box of length 10^{-8} m. Find the minimum uncertainty in its velocity. Given m = 9.1×10^{-31} kg, and $\hbar$ = 1.05×10^{-34} J-s

Solution: From Heisenberg's relation

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

If Δx is maximum, Δp must be minimum.

i.e. $(\Delta x)_{\max}.(\Delta p)_{\min} \approx \hbar$

Given, $(\Delta x)_{\max}$ = maximum uncertainty in position = 10^{-8} m

Then, $(\Delta p)_{\min} = \dfrac{\hbar}{(\Delta x)_{\max}} = \dfrac{6.63\times10^{-34}}{2\times3.14\times10^{-8}} = 1.05\times10^{-26}\ \text{kg ms}^{-1}$

$$(\Delta p)_{\min} = m(\Delta v)_{\min} = 1.05\times10^{-26}\,\text{kgms}^{-1}.$$

$$\therefore \quad (\Delta v)_{\min} = \frac{1.05\times10^{-26}}{m} = \frac{1.05\times10^{-26}}{9.1\times10^{-31}} = 1.17\times10^{4}\,\text{ms}^{-1}$$

Problem 3. Life time of a nucleus in excited state is 10^{-12} s. Find the probability uncertainty in energy and frequency of a gamma-ray photon emitted by it.

Solution: According to Heisenberg's time-energy uncertainty relation

$$\Delta E.\Delta t = \hbar = h/2\pi$$

As the life time of a nucleus in the excited state is 10^{-12} s

$$\therefore \quad \Delta t = 10^{-12}\,\text{s}.$$

$$\therefore \qquad \Delta E = \frac{h}{2\pi\Delta t} = \frac{6.63\times10^{-34}\text{ J-s}}{2\times3.14\times10^{-12}\text{ s}} = 1.054\times10^{-22}\text{ J}$$

So the frequency of γ-ray photon is uncertain by an amount

$$\Delta\nu = \frac{\Delta E}{h} = \frac{1.054\times10^{-22}\text{ J}}{6.63\times10^{-34}\text{ Js}} = 1.59\times10^{11}\text{ Hz}$$

Problem 4. An electron has a speed of 1.05×10^4 m/s within the accuracy of 0.01%. Calculate the uncertainty in the position of the electron. Given $\hbar = 1.05\times10^{-34}$ Js, $m = 9.1\times10^{-31}$ kg.

Solution: The uncertainty in velocity, $\Delta\nu = 1.05\times10^{-4}\times\frac{0.01}{100}$ m/s

Uncertainty in momentum $\Delta p = m\Delta v = 9.1\times10^{-31}\times1.05\times10^{4}\times\frac{0.01}{100}$.

Using uncertainty relation

$\Delta p.\Delta x = \hbar$, we have

$$\Delta x = \hbar/\Delta p = \frac{1.05\times10^{-34}}{9.1\times10^{-31}\times1.05\times10^{4}\times\frac{0.01}{100}}\text{ m} = 1.1\times10^{-4}\text{ m.}$$

Problem 5. The position and momentum of a $1keV$ electron are simultaneously determined. If its position is located to within 1 Å, what is the percentage uncertainty in its momentum?

Solution: From uncertainty relation,

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

Here, Δx = 1 Å = 10^{-10} m, $h = 6.62\times10^{-34}$J-s

$$\therefore \qquad \Delta p = \frac{6.63\times10^{-34}}{2\times3.14\times10^{-10}} = 1.056\times10^{-24}\text{ kg m/s.}$$

Also, the momentum of electron = p = $\sqrt{2mE} = \sqrt{2meV}$,

$\therefore$ percentage uncertainty in momentum $\frac{\Delta p}{p}\times 100 = \frac{1.056\times 10^{-24}}{1.708\times 10^{-23}}\times 100 = 6.173\%$.

Problem 6. On the average, an excited state of a system remains in that state for 10^{-11} s. What is the minimum uncertainty in the energy of an excited state?

Solution: From the uncertainty relation,

$$\Delta E.\Delta t = \frac{\hbar}{2}$$

or $$\Delta E = \frac{\hbar}{2\Delta t} = \frac{1.054\times 10^{-34}}{2\times 10^{-11}} = 0.527\times 10^{-23} \text{ J.}$$

Problem 7. An electron has a speed of 300 m/s accurate to 0.01%. With what accuracy can the electron be located?

Solution: Momentum of the electron $p = mv = 9.1\times 10^{-31}\times 300 = 2.73\times 10^{-28}$ kg ms^{-1}.

$$\therefore \Delta p = 0.01\% \text{ of } p = 2.73\times 10^{-28}\times 10^{-4} = 2.73\times 10^{-32}\,\text{kgms}^{-1}.$$

$$\therefore \Delta x = \frac{\hbar}{\Delta p} = \frac{1.054\times 10^{-34}}{2.73\times 10^{-32}} = 3.86\times 10^{-3}\,\text{m.}$$

Problem 8. The maximum uncertainty in the position of an electron in a nucleus is 2×10^{-14}m. Find the minimum uncertainty in its momentum.

Solution: From Heisenberg's uncertainty relation

$$\Delta x.\Delta p_x \geq \frac{\hbar}{2}.$$

Here, max. uncertainty in position $\Delta x = 2\times 10^{-14}$ m.

The min. uncertainty in momentum is

$$\Delta p_x \geq \frac{\hbar}{2\Delta x} = \frac{6.63\times10^{-34}}{(2\times3.14)\times2\times(2\times10^{-14})} = 0.26\times10^{-20}\,\text{kgms}^{-1}.$$

4.15 Terminal Questions

4.15.1 Short Answer Type Questions

1) Is uncertainty principle the outcome of wave description of a particle? Justify your answer.

2) Why is uncertainty principle not applied for macroscopic objects in motion?

3) State and explain uncertainty principle is brief.

4) What is the significance and importance of uncertainty principle?

5) What is Heisenberg's uncertainty principle?

6) What is the use of γ-rays in thought experiment of gamma ray microscope?

7) What is the physical significance of uncertainty principle?

8) Using uncertainty relation show that electron cannot exist in a nucleus.

9) Do your expect to observe wave and particle aspect of a physical entity simultaneously in the same experiment? Justify your answer.

10) What is time-energy uncertainty relation?

11) Estimate the minimum uncertainty in the momentum of an electron confined in a box of length 1 μm.

12) Briefly explain one experiment to validate the uncertainty principle.

4.15.2 Long Answer Type Questions

1) Beginning from deBroglie wave concept, obtain Heisenberg's uncertainty principle. Give one illustration of this principle.

2) State and explain uncertainty principle. Discuss its significance and importance.

3) What is Heisenberg's uncertainty principle? Describe single slit electron diffraction experiment to prove the validity of this principle.

4) Give an elementary proof of the uncertainty relation between energy and time. What is its significance?

5) (a) Prove that proton, neutron and α-particle can exist within the nucleus.

   (b) Describe γ-ray microscope experiment to establish the truth of uncertainty principle.

6) Discuss various applications of uncertainty principle.

7) Explain the time-energy uncertainty relation. Why we cannot take measurement of physical property of a system without physically disturbing it?

8) Write uncertainty relation of position and momentum along all the three coordinates. Derive the position – momentum uncertainty relation along x-component.

4.15.3 Numerical Answer Questions

1. The uncertainty in velocity of an electron is 1 ms^{-1}. Calculate the uncertainty in the position of the electron. (Ans : 7.3×10^{-7} m).

2. An electron of energy 200 eV is passed through a circular hole of radius 10^{-4} cm. What is the uncertainty introduced in the angle of emergence? (Ans : 5.76×10^{-6} radians)

3. The average period that elapses between the excitation of an atom and the time it emits radiation is 10^{-8} s. Find the uncertainty in energy emitted and uncertainty in the frequency of light emitted. (Ans :$\Delta E = 1.054\times10^{-26}$ J, $\Delta\nu=1.59\times10^{7}$ Hz).

4. Calculate the minimum energy of a photon for its existence within the nucleus of diameter 10^{-14} m. (Ans : 4.9 MeV)

5. Wavelength can be determined with an accuracy of 1 part in 10^{6}. What is the uncertainty in the position of a 1 Å X-ray photon when its wavelength is simultaneously measured?

6. What is the uncertainty in momentum of the electron in H-atom of size 10^{-8}em and mass of electron = 9.1×10^{-31}kg. (Ans. : 1.054×10^{-24} kgms^{-1}

Unit 5: Schrodinger Wave Equation

5.1 Introduction

In previous chapters, we found that some experiments like Compton scattering showed that particles like proton, electron, neutron etc. exhibit wave like properties. In this chapter, we will obtain an equation, known as Schodinger's equation that describes the wave like behaviour of the particle and is consistent with Heisenberg's uncertainty principle. The trajectory of such particles is described by the wave function ψ, whereas $|\psi|^2 d\tau$ gives the probability of finding the particle in the volume element $d\tau$.

5.2 Objective

There has been a number of Formalisms available to deal with quantum mechanical problems. The two most famous formalisms are Heisenberg's formalism, also known as matrix mechanics, where he deals with the description of a quantum mechanical system through time evolution of matrix operators for different physical quantities required to describe the system like position, momentum etc. In this chapter we will learn about the second formalism given by Erwin Schrodinger. Schrodinger's formalism of quantum mechanical systems is based on the evolution of a wavefunction, describing the system as a function of time whereas the operators are considered as time independent. In this chapter we will also learn about quantum mechanical wavefunction for various physical systems and its various properties.

5.3 Schrodinger's Equation

The fundamental equation of quantum mechanics is the Schrodinger's equation. It was formulated by Erwin Schrodinger in 1926. We can say that Schrodinger's equation in Quantum

Mechanics is analogous to second law of motion in classical mechanics. In formulating his equation, Schrodinger used the concept of matter waves. In deriving the equation, Schrodinger used the assumptions that a) Material parties can't be created and destroyed b) and the velocity of material particles can be treated non-relativistically. Schrodinger's equation is a Second order homogeneous linear differential equation.

5.3.1 Time dependent Schrodinger equation

We know that the de-Broglie wavelength λ associated with a free particle having momentum *p* and mass *m* is

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

also the wave vector associatedwith wavelength λ is

$$k = \frac{2\pi}{\lambda} \qquad (2)$$

Combining equation (1) and (2) e get

$$p = \frac{h}{\lambda} = \frac{hk}{2\pi} = \hbar k \qquad (3)$$

Also the kinetic energy E and angular frequency 'ω' are related as

$$E = \hbar\omega \qquad (4)$$

Further $$E = \frac{p^2}{2m} \qquad (5)$$

Combining (4) and (5) we get

$$\omega = \frac{E}{k} = \frac{p^2}{2m}.\frac{1}{\hbar}$$

$$= \frac{h^2 k^2}{2m} \cdot \frac{1}{h} = \frac{\hbar k^2}{2m} \tag{6}$$

Now in quantum mechanics, the wavefunction 'ψ' plays the same role as the wave variable 'y' plays in wave motion. But unlike 'y', ψ. Can not be measured and therefore is complex. Also electrons and other subatomic particles exhibit wave like properties. Let such a wave be represented by a wave function $\psi(\vec{r},t)$ of free electron of Momentum $\vec{p}$ and energy E. Let us also assume that the wave associated with electrons to be free plane waves and hence $\psi(\vec{r},t)$ may be written as

$$\psi(\vec{r},t) = Ae^{i(\vec{k}.\vec{r}-\omega t)} \tag{7}$$

where k is given by equation (2)

In one dimension, eqn. (7) may be written as

$$\psi(x,t) = Ae^{i(kx-\omega t)} \tag{8}$$

Using eqn. (3) and (4) in eqn. (2) we get

$$\psi(x,t) = Ae^{\frac{i}{\hbar}(Px-Et)} \tag{9}$$

Eqns. (4), (5) and (9) reveals that the differential form of matter wave should have first derivative with respect to time 't' and second derivative with respect to position 'x'.

∴ Let the differential eqn. representing matter wave be of the form

$$\frac{\partial \psi}{\partial t} = \frac{\gamma \partial^2 \psi}{\partial x^2} \tag{10}$$

Differentia eqn. (8) with respect to time 't' and diff. eqn. (8) twice with respect to position 'x', we get

$$\frac{\partial \psi(x,t)}{\partial t} = -i\omega \psi(x,t) \tag{11}$$

and $$\frac{\partial^2 \psi(x,t)}{\partial x^2} = -k^2 \psi(x,t) \tag{12}$$

Using eqns. (11) and (12) in eqn. (10), we get

$$-i\omega \psi(x,t) = -k^2 \gamma \psi(x,t)$$

$$\Rightarrow \qquad \gamma = \frac{i\omega}{k^2} \tag{13}$$

Since $\omega = \frac{E}{\hbar}$

$$\Rightarrow \qquad \gamma = \frac{iE}{\hbar k^2} = \frac{iE}{\hbar \cdot P^2 / \hbar^2} = \frac{i\hbar E}{P^2} = \frac{i\hbar P^2}{2m.P^2} = \frac{i\hbar}{2m} \tag{14}$$

Using (14) in (10), we get the general form of differential equation for matter wave, which is

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

$$\Rightarrow \qquad i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \tag{15}$$

Eqn. (15) is the one-dimensional time dependent Schrodinger’s wave equation. The Schrodinger’s equation is linear in ψ and is second order homogeneous differential equation. In deriving eqn. (15), we have assumed that the particle is free. However if the particle is not free, (such as the electrons is an atom, where electrons more under the potential due to the nucleus of the atom) and speed of the particle is small then the total energy E can be written as the sum of kinetic energy and potential energy

i.e., $$E = \frac{P_x^2}{2m} + V(x,t) \tag{16}$$

Multiplying both sides of eqn. (16) by $\psi(x,t)$,

$$E\psi(x,t) = \frac{P_x^2}{2m} \psi(x,t) + V(x,t)\psi(x,t) \tag{17}$$

But $\psi = Ae^{i(P_x x - Et)}$

or $$\frac{\partial^2\psi}{\partial x^2} = -\frac{P_x^2\psi}{\hbar^2} \Rightarrow P_x^2\psi = -\hbar^2\frac{\partial^2\psi}{\partial x^2} \tag{18}$$

or ` $$\frac{\partial\psi}{\partial t} = -\frac{i}{\hbar}E\psi(x,t) \Rightarrow \; E\psi(x,t) = -\frac{\hbar}{i}\frac{\partial\psi(x,t)}{\partial t} \tag{19}$$

Using eqns. (18) and (19) in eqn. (17), we get

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

$\Rightarrow$ $$i\hbar\frac{\partial\psi(x,t)}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}(x,t) + V(x,t)\psi(x,t) \tag{20}$$

Above equation is the one-dimensional time dependent Schrodinger's equation for a particle under potential $V(x,t)$.Now if we know the potential due to the interaction of the particle with the surrounding, Schrodinger's equation can be solved.

5.3.2 Validity of Schrodinger's equation

Schrodinger's equation derived above used the wavefunction $\psi(x,t)$ of a free particles. But what we do not know is, if it is also valid for a bound particle is particle under same arbitrary potential. To verify Schrodinger's equation, we can solve it for any physical problem and compare the results with experimental results. If the two results agree, then we can say that the Schrodinger's equation is valid and if results do not match then Schrodinger's equation must be discarded. What we find is that Schrodinger's equation turns out to be accurate in predicting the experimental results. It is to be noted that Schrodinger's equation cannot be derived from other basic principles of physics, infect it is a basic principle in itself just like Newton's second law of motion in mechanics.

5.3.3 Time-dependent Schrodinger's equation in three dimensions

The one-dimensional Schrodinger's equation can be extended to three-dimension. The three dimensional wave eqn. can be written as

$$\psi(\vec{r},t) = Ae^{i(\vec{k}.\vec{r}-\omega t)}$$

or $$\psi(\vec{r},t) = Ae^{\frac{i}{\hbar}(\vec{P}.\vec{r}-Et)} \qquad (1)$$

$\Rightarrow$ $$\psi(\vec{r},t) = Ae^{\frac{i}{\hbar}(P_x x+P_y y+P_z z-Et)}$$

$\Rightarrow$ $$\frac{\partial\psi(\vec{r},t)}{\partial t} = \frac{-i}{\hbar}E\psi(\vec{r},t) \qquad (2)$$

$$\frac{\partial^2\psi(\vec{r},t)}{\partial x^2} = -\frac{P_x^2}{\hbar^2}\psi(\vec{r},t) \qquad (3)$$

$$\frac{\partial^2\psi(\vec{r},t)}{\partial y^2} = -\frac{P_y^2}{\hbar^2}\psi(\vec{r},t) \qquad (4)$$

$$\frac{\partial^2\psi(\vec{r},t)}{\partial z^2} = -\frac{P_z^2}{\hbar^2}\psi(\vec{r},t) \qquad (5)$$

Adding eqns. (3), (4) and (5) we get

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2 y}{\partial y^2}+\frac{\partial^2 z}{\partial z^2} = -\frac{(P_x^2+P_y^2+P_z^2)\psi}{h^2}$$

or $$\vec{\nabla}^2\psi(\vec{r},\, t) = -\frac{P^2}{\hbar^2}\psi(\vec{r},t)$$

$\Rightarrow$ $$\vec{\nabla}^2\psi(\vec{r},\, t) = -\frac{2Em}{\hbar^2}\psi(\vec{r},t)$$

$\Rightarrow$ $$\vec{\nabla}^2\psi(\vec{r},\, t) = -\frac{2m}{\hbar^2}\left(\frac{-\hbar}{i}\frac{\partial\psi(\vec{r},\, t)}{\partial t}\right)$$

$\Rightarrow$ $$i\hbar\frac{\partial\psi(\vec{r},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},\, t)$$

is three-dimensional have dependent Schrodinger's equation for a free particle.

5.4 Time independent Schrodinger's equation

5.4.1 One dimensional time independent Schrodinger's equation

The time dependent three-dimensional Schrodinger's equation is given by

$$\frac{-h^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}+V(\vec{r},t)\psi(\vec{r},t)=ih\frac{\partial\psi(\vec{r},t)}{\partial t} \tag{1}$$

above eqn. can be written in one-dimension as

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

When potential energy V does not dependexplicitly on time and is a function of position only, then the wavefunction $\psi(x,t)$ can be written as the product of two wave functions say $\psi(x)$ (function of position only) and $\phi(t)$ (function of time only).

therefore we can write

$$\psi(x,t)=\psi(x)\phi(t) \tag{3}$$

Using $\psi(x,t)$ from eqn. (3) in eqn. (1), we get

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

$$\Rightarrow \qquad -\frac{\hbar^2}{2m}\phi(t)\frac{\partial^2\psi(x)}{\partial x^2}+V\psi(x)\phi(t)=i\hbar\frac{\partial}{\partial t}\psi(x,t) \tag{4}$$

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

$$\Rightarrow \qquad \frac{\partial\psi(x,t)}{\partial t}=\frac{-i}{\hbar}AEe^{\frac{i}{\hbar}(P_x x-Et)}=\frac{-iE}{\hbar}\psi(x,t)$$

Eqn. (4) becomes

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

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

Dividing by $\phi(t)$, we get

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

or $$\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2m}{\hbar^2}(\mathrm{E}-V)\psi(x)=0 \qquad (5)$$

is one-dimensional time independent Schrodinger's equation.

5.4.2 Three-Dimensional time dependent Schrodinger's equation

Let $\psi(x,y,z,t)$ or simply $\psi(\vec{r},t)$ is the wave function representing the motion of a particle in three-dimension. In such a case, time independent Schrodinger's equation takes the form-

$$\frac{\partial^2}{\partial x^2}\psi(\vec{r},t)+\frac{\partial^2}{\partial y^2}\psi(\vec{r},t)+\frac{\partial^2}{\partial z^2}\psi(\vec{r},t)+\frac{2m}{\hbar^2}(E-V)\psi(\vec{r},t)=0$$

or $$\nabla^2\psi(x,y,z)+\frac{2m}{\hbar^2}(E-V)\psi(x,y,z)=0$$

5.5 Wave function

The quantity that describes the matter wave in space is known as a wavefunction. The wavefunction is a complex quantity having real and imaginary parts. It is a solution of Schrodinger equation. A wavefunction completely describes is system and contains every possible information about the system.

The wavefunction (ψ) being complex has no physical significance. This is because ψ, being an amplitude of a matter wave has both positive and negative amplitude. Since negative amplitude imply negative probability hencenegative amplitude is meaningless. Therefore ψ cannot represent a measurable quantity.

5.5.1 Physical Significance of wavefunction

The probability of funding the particle described by the wavefunction of a particle at a point (x, y, z) is proportional to $|\psi|^2$. $|\psi|^2$ always gives a real positive quantity.

because let $\psi = A + iB$

$$\psi^* = A - iB$$

$$\therefore \qquad |\psi|^2 = \psi^*\psi = |A|^2 + |B|^2 = \text{real.}$$

A greater value of $|\psi|^2$ implies large probability of funding the particle, whereas a sm

all value of $|\psi|^2$ means small probability of its presence. A non-zero value of $|\psi|^2$ at some (*x, y, z*) howsoever small always implies a definite, though small probability of finding the particle.

5.5.2 Conditions on a Wavefunctionψ

1. The wavefunctionψ must always be finite at (x, y, z).
2. ψmust be single valued.
3. ψmust be continuous in all regions except where potential energy is infinite.
4. Partial derivatives of ψ i.e. $\frac{\partial \psi}{\partial x}, \frac{\partial \psi}{\partial y}, \frac{\partial \psi}{\partial z}$ must also be continuous.

5.5.3 Probabilistic Interpretation of wavefunction

In the year 1926, Max Born postulated that "If a particle is described by a wavefunction $\psi(\vec{r},t)$, the probability offunding the particle within a volume element $d\tau = dxdydz$ about some point $\vec{r}$ at time t is.

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

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

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

where $\psi^*(\vec{r},t)$ is the complex conjugate of $\psi(\vec{r},t)$ and $P(\vec{r},t)$ denotes the probability density. Therefore if we know the wavefunction associated with a particle, we can always calculate the probability of an event and not the event itself. If the wavefunction is spread-out in space doesn't mean that the particle is also spread out. Spread of a wavefunction only implies probabilistic spread. It is for this reason that the wavefunction sometimes is also known as probability amplitude.

Above discussion shows that the quantum mechanical laws and the results of their measurement can be interpreted on the basis of probability interpretations.

5.5.4 Eigen values and Eigen vectors

When an operator $\hat{A}$ is such that when acts on a function $\psi(x)$ yields a constant times the same function back i.e,

$$\hat{A}\psi(x) = p\psi(x) \qquad (1)$$

Where p may be a complex constant then

(i) $\psi(x)$ is called the eigen function corresponding to the operator $\hat{A}$

(ii) The constant p is called the Eigen value of the operator $\hat{A}$, corresponding to Eigen function $f(x)$ and

(iii) the equation $\hat{A}\psi(x) = p\psi(x)$ is known as the Eigen value equation.

Each Eigen values of an operator is unique. If two or more eigen functions have same eigen values, then the eigen value is said to be degenerate. For example if,

$$\hat{A}\psi_1 = p\psi_1 and$$
$$\hat{A}\psi_2 = p\psi_2$$

Then the eigen value is said to be doubly degenerate. The eigen value is non degenerate, if there is only one eigen function corresponding to the eigen value.

5.5.5 Operator

An operator is a mathematical entity or a rule that transforms one function into another function.

e.g. differential operator $\frac{d}{dx}$ or D, differentiates with respect to *x*, when it operates on some function of *x*, say $\psi(x)$ and gives some other function $\phi(x)$.

i.e.let $\psi(x) = x^n$

$\therefore$ $\frac{d}{dx}(x^n) = nx^{n-1}$.

Linear operator →An operator D is said to be a linear operator if it satisfy following conditions:

(i) $D(p\psi) = pD(\psi) = p\phi$

(ii) $D(p_1\psi_1 + p_2\psi_2) = p_1D\psi_1 + p_2D\psi_2 = p_1\phi_1 + p_2\phi_2$

where p, p_1 and p_2 are complex constants.

Linearity is the fundamental aspect of wave theory and guarantees the addition of amplitudes before or after some operation is performed.

Differential operator $\frac{d}{dx}$ is a linear operator.

5.5.6 Normalized wavefunction

The probability of funding a particle in volume dτ is given by $|\psi|^2 \, d\tau$, where ψ is the wavefunction representing the particle. However, in real problems particles are bound by forces in some specified region. For e.g. particle in a box, electrons in an atom. In such constrained problems, the probability of finding the particle in the entire bound, region has to be unity.

i.e. $$\int \psi^* \psi d\tau = \int \ |\psi|^2 \, d\tau = 1 \qquad (1)$$

The wavefunctionψ which satisfy the eqn. (1) is known as normalized wave functions. If a wavefunction

If a wavefunction $\psi(\vec{r},t)$ is not normalized, it may be normalized by multiplying with a constant. For example if Schrodinger equations satisfied by a wavefunction $\psi(\vec{r},t)$ and the integration of probability density over the specified bound region is M, say

i.e. $$\int \psi^*(\vec{r},t)\psi(\vec{r},t)d\tau = M$$

then we can write

$$\int \frac{\psi^*(\vec{r},t)}{\sqrt{M}} \frac{\psi(\vec{r},t)}{\sqrt{M}} d\tau = 1$$

or $$\int \phi^*(\vec{r},t)\phi(\vec{r},t)d\tau = 1$$

{here $\phi(\vec{r},t)$ is also a Solution of Schrodinger's equation since Schrodinger's equation is a homogeneous linear differential equation}.

here M is known as the norm of the wavefunction $\psi(\vec{r},t)$ and $\frac{1}{\sqrt{M}}$ is known as normalization constant. Also $\phi(\vec{r},t)$ is the normalized wavefunction. A normalized wavefunction is one that has unit norm. Also a normalizable wavefunction has finite norm.For finite norm, $\psi(\vec{r},t)$ must satisfy the boundary condition

$$\psi(\vec{r},t) \to 0 \text{ as } r \to \pm\infty .$$

5.5.7 Orthogonal wavefunction

Another very important property of wavefunctionis that the set of wavefunctions $\psi_i(\vec{r},t),\ i=1,2,...,n$ is that they are orthogonalto each other.

For a pair of wavefunctions ψ_i and ψ_j to be orthogonal, they must satisfy the equation

$$\int_{-\infty}^{+\infty} \psi_i^* \psi_j d\tau = 0 \text{ if } i \neq j \tag{2}$$

If we combine eqns. (1) and (2), we can write

$$\int_{-\infty}^{+\infty} \psi_i^* \psi_j d\tau = \delta_{ij} \tag{3}$$

where δ_{ij} is kroncker delta and is defined as

$\delta_{ij} = 1$ if $i = j$ and

$= 0$ if $i \neq j$.

Any set of wavefunctions satisfying equation (3) are known as orthonormal wavefunctionsi.e, they are orthogonal as well as normalized.

5.5.8 Proof of orthogonality

Let ψ_i and ψ_j be two Eigen functions satisfying the Schrodinger's equation. Also let E_i and E_j be the corresponding Eigen values.

$\therefore$ time independent Schrodinger's equation for ψ_i and ψ_j can be writtenas

$$\frac{-\hbar^2}{2m}\frac{\partial^2 \psi_i}{\partial x^2} + V\psi_i = E_i\psi_i \tag{4}$$

and $$\frac{-\hbar^2}{2m}\frac{\partial^2 \psi_j}{\partial x^2} + V\psi_j = E_j\psi_j \tag{5}$$

Multiplying complex conjugate of eqn. (4) with ψ_j we get

$$\frac{-\hbar^2}{2m}(\psi_j)\frac{\partial^2\psi_i^*}{\partial x^2}+V\psi_i^*\psi_j=E_j\psi_i^*\psi_j \tag{6}$$

Multiplying eqn. (5) with ψ_i^*.

$$\frac{-\hbar^2}{2m}\psi_i^*\frac{\partial^2\psi_j}{\partial x^2}+V\psi_i^*\psi_j^*=E_j\psi_i^*\psi_j \tag{7}$$

Subtracting eqn. (7) from eqn. (6)

$$\frac{\hbar^2}{2m}\left[\psi_i^*\frac{\partial^2\psi_j}{\partial x^2}-\psi_j\frac{\partial^2\psi_i^*}{\partial x^2}\right]=(E_i-E_j)\psi_i^*\psi_j$$

$$=\frac{\hbar^2}{2m}\left[\psi_i^*\frac{\partial^2\psi_j}{\partial x^2}+\frac{\partial\psi_i^*}{\partial x}\frac{\partial\psi_j}{\partial x}-\psi_j\frac{\partial^2\psi_i^*}{\partial x^2}-\frac{\partial\psi_i^*}{\partial x}\frac{\partial\psi_j}{\partial x}\right]=(E_i-E_j)\psi_i^*\psi_j$$

$$=\frac{\partial}{\partial x}\left(\psi_i^*\frac{\partial\psi_j}{\partial x}\right)-\frac{\partial}{\partial x}\left(\psi_j\frac{\partial\psi_i^*}{\partial x}\right)=\frac{2m}{\hbar^2}(E_i-E_j)\psi_i^*\psi_j$$

Integrating both sides from –∞ to +∞

$$=\int_{-\infty}^{+\infty}\frac{\partial}{\partial x}\left(\psi_i^*\frac{\partial\psi_j}{\partial x}-\psi_j\frac{\partial\psi_i^*}{\partial x}\right)dx=\frac{2m}{\hbar^2}(E_i-E_j)\int_{-\infty}^{+\infty}\psi_i^*\psi_j \tag{8}$$

but $\psi,\ \psi^*,\ \frac{\partial\psi}{\partial x},\ \frac{\partial\psi^*}{\partial x}\to 0$ as $r\to\pm\infty$.

$\therefore$ L.H.S. of eqn. (8) is zero

$$\Rightarrow \quad \frac{2m}{\hbar^2}(E_i-E_j)\int_{-\infty}^{+\infty}\psi_i^*\psi_j dx=0 \tag{9}$$

but if $i\neq j$ then $E_i\neq E_j$

⇒ for eqn. (6) to be true

$$\int_{-\infty}^{+\infty} \psi_i^* \psi_j dx = 0$$

Hence Eigen functions corresponding to different Eigen values are orthogonal.

5.6 Solution of Schrodinger equation

The home time dependent Schrodinger's equation is given by

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t} \qquad (1)$$

here the wave function ψ is a function of three-position coordinates x, y and z and time t. Now if the potential V is independent of time and is a function of position only (x, y, z) then the solution of Schrodinger's equation is that of a standing wave. Therefore if potential V is independent of time, $\psi(x, y, z, t)$ can be written as –

$$\psi(x, y, z, t) = \phi(x, y, z)\xi(t) \qquad (2)$$

where $\phi(x, y, z)$ is a functions of position only and $\xi(t)$ is a function of time only.

Substituting eqn. (2) in eqn. (1), we get

$$\frac{-\hbar^2}{2m}\nabla^2(\phi(x, y, z)\xi(t)) + V(x, y, z)\phi(x, y, z)\xi(t) = i\hbar\frac{\partial}{\partial t}(\phi(x, y, z)\xi(t))$$

$$\Rightarrow \quad \xi(t)\left[-\frac{\hbar^2}{2m}\nabla^2(\phi(x, y, z)\right] + V(x, y, z)\phi(x, y, z)\xi(t) = \phi(x, y, z)i\hbar\frac{\partial}{\partial t}\xi(t)$$

Dividing throughout by $\phi(x, y, z)\xi(t)$ we get

$$\frac{1}{\phi(x, y, z)}\left[-\frac{\hbar^2}{2m}\nabla^2(\phi(x, y, z)\right] + V(x, y, z) = \frac{1}{\xi(t)}i\hbar\frac{\partial}{\partial t}\xi(t)$$

or
$$\frac{1}{\phi(x,y,z)}\left[-\frac{\hbar^2}{2m}\nabla^2+V(x,y,z)\right]\phi(x,y,z)=i\hbar\frac{1}{\xi(t)}\frac{\partial}{\partial t}\xi(t) \qquad (3)$$

In eqn. (3), right hand side is a function of time only while left hand side is a function of position only. Therefore equation (3) will be satisfied only if each side is equal to the same constant say E, therefore we have

$$i\hbar\frac{1}{\xi(t)}\frac{\partial}{\partial t}\xi(t)=E \qquad (4)$$

and
$$\frac{1}{\phi(x,y,z)}\left[-\frac{\hbar^2}{2m}\nabla^2+V(x,y,z)\right]\phi(x,y,z)=E$$

or
$$\nabla^2\phi(x,y,z)+\frac{2m}{\hbar^2}(E-V)\phi(x,y,z)=0 \qquad (5)$$

Equation (4) has a solution of the form

$$\xi(t)=e^{-iEt/\hbar} \qquad (6)$$

Here E, the constant is nothing but the energy of the particle can be found by solving the Schrodinger equation

Using eqn. (6), eqn. (2) becomes

$$\psi(x,y,z,t)=\phi(x,y,z)e^{-iEt/\hbar}$$

For bound states, like the particle in a box, E has only certain definite values and the allowed values of E are known as the Eigen values. Corresponding to every allowed value of Energy E, there is a function ψ, the solution of Schrodinger equation (5), known as Eigen function.

5.6.1 Stationary State Solution

We know that the wavefunctionψ is complex. But if in a particular state experimentally measurable quantity $\psi^*\psi$ i.e, the probability density is independent of time, then the state of the system is said to be stationary state.

Let the state of a system is given by the wavefunction

$$\psi(x,y,z,t) = c_1\phi_1(x,y,z)e^{-iE_1t/\hbar} + c_2\phi_2(x,y,z)e^{-iE_2t/\hbar} + \ldots$$

$$= \sum_n c_n\phi_n(x,y,z)e^{-iE_nt/\hbar}$$

It's complex conjugate will be

$$\psi^*(x,y,z,t) = \sum_n c_n^*\phi_n^*(x,y,z)e^{iE_nt/\hbar}$$

Now consider

$$\psi^*(x,y,z,t)\psi(x,y,z,t) = \left(\sum_n c_n^*\phi_n^*(x,y,z)e^{iE_nt/\hbar}\right)\left(\sum_n c_n\phi_n(x,y,z)e^{-iE_nt/\hbar}\right)$$

$$= \left(c_1^*\phi_1^*(x,y,z)e^{iE_1t/\hbar} + c_2^*\phi_2^*(x,y,z)e^{iE_2t/\hbar} + \ldots\right)\left(c_1\phi_1(x,y,z)e^{-iE_1t/\hbar} + c_2\phi_2(x,y,z)e^{-iE_2t/\hbar} + \ldots\right)$$

$$= c_1c_1^*\phi_1\phi_1^* + c_2c_2^*\phi_2\phi_2^* + \ldots + c_1\phi_1(x,y,z)e^{-iE_1t/\hbar}\Big[c_2^*\phi_2^*(x,y,z)e^{iE_2t/\hbar} +$$

$$c_3^*\phi_3^*(x,y,z)e^{iE_3t/\hbar} + \ldots\Big] + c_2\phi_2(x,y,z)e^{-iE_2t/\hbar}\Big[c_1^*\phi_1^*(x,y,z)e^{iE_1t/\hbar}$$

$$+c_3^*\phi_3^*(x,y,z)e^{iE_3t/\hbar} + \ldots\Big] + \ldots$$

$$= \sum_n c_nc_n^*\phi_n\phi_n^* + c_1\phi_1(x,y,z)e^{-iE_1t/\hbar}\sum_m c_m^*\phi_m^*\,e^{iE_mt/\hbar} +$$

$$c_2\phi_2(x,y,z)e^{-iE_2t/\hbar}\sum_m c_m^*\phi_m^*\,e^{iE_mt/\hbar} + \ldots$$

$$= \sum_n c_nc_n^*\phi_n\phi_n^* + \sum_n c_n\phi_n(x,y,z)e^{-iE_nt/\hbar}\sum_m{}' c_m^*\phi_m^*\,e^{iE_mt/\hbar}$$

$$= \sum_n c_n c_n^* \phi_n \phi_n^* + \sum_n \sum_m {}' c_m^* c_n \phi_m^* \phi_n e^{i(E_m - E_n)t/\hbar}$$

Where the summation $\sum_m {}'$ means excluding the terms where $m = n$.

Now in above equation first term is independent of time whereas the second term depends on time and hence the solutions not a stationary state.However $\psi^* \psi$ will be independent of time, only if $c_n\text{'}s = 0\text{'s}$ are zero for all values of n except for $m = n$.

Hence under the condition $c_n\text{'}s = 0$, wavefunction will consider only one term i.e,

$$\psi_n(x, y, z) = \phi_n(x, y, z) e^{-iE_n t/\hbar}$$

and hence the solution given by above equation is known as stationary state solution.

5.7 Expectation Value

We know that the wavefunction $\psi(x, y, z, t)$ contains every possible information regarding the variables of the particles. This information is probabilistic only (except for those variables, for which the solution of Schrodinger equation gives quantized values)and doesn't give definite values. Also we know that the quantity $\psi^*(x,t)\psi(x,t)dx$ gives the probability of finding the particles in a small distance dx. It makes us possible to find the expectation values or the average value of position denoted as $\langle x \rangle$ of the particle along the x-axis.

"The average or expectation value of a dynamical quantity is the Mathematical expression for the result of a single measurement. It may also be defined the average of the results of large number of measurements on independent identical systems".

As an example, Consider 'N' number of electrons, each being described by the same wave function $\psi(x,t)$.

Let at some time *t*, for each electron we makes an observation for position of electron and we find the number of electrons in the range, *x* and *x* + *dx*. Therefore the probability of an electron to be in the position anywhere between *x* and *x* + *dx* will be

$$= \frac{\text{No. of e}^{-}\text{'}s \text{ in the position between } x \text{ and } x + dx}{\text{No. of e}^{-}\text{'}s\,(N)} \tag{1}$$

But from wavefunction interpretation, this probability is given by

$$\psi^*(x,t)\psi(x,t)dx \tag{2}$$

where $\psi(x,t)$ is normalized wavefunction

From (1) and (2) we get

Number of electrons in the position between x and x + dx as $N\psi^*(x,t)\psi(x,t)dx$.

⇒ Summation of all measured values $x_1, x_2, ..., x_N$ of all the N electrons is given by

$$x_1 + x_2 + ... + x_N = \int_{-\infty}^{+\infty} xN\psi^*(x,t)\psi(x,t)dx$$

or

$$\frac{x_1 + x_2 + ... + x_N}{N} = \int_{-\infty}^{+\infty} \psi^*(x,t)x\psi(x,t)dx$$

but by definition $\frac{x_1 + x_2 + ... + x_N}{N}$ gives the average expectation values of *x*.

$$\langle x \rangle = \int_{-\infty}^{+\infty} \psi^*(x,t)x\psi(x,t)dx \tag{1}$$

Where $\psi(x,t)$ is normalized wavefunction

Eqn. (1) can be generalized for any function $f(x)$ as

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} \psi^*(x,t)f(x)\psi(x,t)dx \tag{2}$$

If the wavefunction $\psi(x)$ is not normalized, then the expectation value of some function $f(x)$ may be expressed as

$$\langle f(x)\rangle = \frac{\int_{-\infty}^{+\infty} \psi^*(x,t) f(x) \psi(x,t) dx}{\int_{-\infty}^{+\infty} \psi^*(x) \psi(x) dx}$$

Moreover, if the expectation values are defined using operators, the integrand consist of the operator operating on the wavefunction ψ, multiplied on left by ψ^*.

$$\therefore \qquad \langle \hat{f} \rangle = \frac{\int_{-\infty}^{+\infty} \psi^* \hat{f} \psi dx}{\int_{-\infty}^{+\infty} \psi^* \psi dx}$$

5.8 Summary

Schrodinger wave equations are the backbone of quantum mechanics, which are analogues to Newton's equation in classical mechanics but quantum mechanics is found different from classical physics. As we have learnt in the chapter that that the term evolution of state of a system is described by something, that we call wavefunction and the wavefunction is all we know about a system. Though wavefunction ψ does not have straightforward simple interpretation, its $|\psi|^2$ that represents the probability density of finding the system in a particular state. The probabilistic nature of quantum mechanics is in complete contrast with the deterministic nature of classical mechanics. From this probabilistic interpretation of wavefunction, we can also calculate the average values of the dynamical quantities of the system at any time.

5.9 Glossary

Validity - Credibility

Explicitely - Clear and Exact

Significance - Importance

Interpretation - Exposition

Unique - Distinctive

Fundamental - Elemental

Orthogonal - Independent

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5.11 Suggested Readings

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5.12 Solved Problems

Q.1 If ψ_1 and ψ_2 are two Eigenfunction corresponding to an operator with same Eigen values then show that their linear combinations will also be an eigen function.

Solution: Let $\psi = p_1\psi_1 + p_2\psi_2$ be the linear combination of ψ_1 and ψ_2

also $\hat{A}\psi_1 = a\psi_1$

$$\hat{A}\psi_2 = a\psi_2$$

Consider $A\psi = \hat{A}[p_1\psi_1 + p_2\psi_2]$

$$= p_1(\hat{A}\psi_1) + p_2(\hat{A}\psi_2)$$

$$= p_1(a\psi_1) + p_2(a\psi_2)$$

$$= a(p_1\psi_1 + p_2\psi_2)$$

$$= a\psi$$

hence the result.

Q.2 Explain if the wavefunction $\psi(x) = e^x$ is an acceptable quantum mechanical wavefunction or not?

Solution: Wavefunction $\psi(x)$ to be an acceptable wavefunction it should satisfy same general conditions i.e.

(a) $\psi(x)$ must be finite at all point in space

(b) $\psi(x)$ must be single valued at all points in space.

(c) $|\psi(x)|^2$ should be integrable.

(d) $\psi(x)$ and its partial derivatives must be continuous throughout.

But the given wave function $\psi(x) = e^x$ is such that

$$\psi(x) \to \pm\infty \text{ as } x \to \pm\infty$$

also $|\psi(x)|^2$ is not integrable, since

$$\int_{-\infty}^{+\infty} |\psi(x)|^2\, dx = \int_{-\infty}^{+\infty} e^{2x} dx = \infty$$

hence $\psi(x) = e^x$ does not represent an acceptable quantum mechanical wavefunction.

Q.3 The wavefunction of a particle is

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\frac{\pi x}{L} \qquad 0 < x < L$$

$$0 \qquad |x| > L$$

Find the probability of finding the particle in the region $0 < x < \frac{L}{2}$.

Solution: Probability of finding the particle inthe region $0 < x < \frac{L}{2}$ is given by

$$P = \int_0^{L/2} \psi^*(x)\psi(x)dx$$

$$= \int_0^{L/2} \left(\sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}\right)\left(\sqrt{\frac{2}{L}} \sin\frac{\pi x}{L}\right) dx$$

$$= \frac{2}{L}\int_0^{L/2} \sin^2\frac{\pi x}{L} dx$$

$$= \frac{1}{L}\int_0^{L/2} \left(1 - \cos\frac{2\pi x}{L}\right) dx$$

$$= \frac{1}{L}\int_0^{L/2} dx - \frac{1}{L}\int_0^{L/2} \cos\frac{2\pi x}{L} dx$$

$$= \frac{1}{L} x\Big|_0^{L/2} - \frac{1}{L}\frac{L}{2\pi}\sin\frac{2\pi x}{L}\Big|_0^{L/2}$$

$$=\frac{1}{L}\left(\frac{L}{2}-0\right)-\frac{1}{2\pi}\left(\sin\pi-\sin 0\right)$$

$$=\frac{1}{2}-\frac{1}{2\pi}(0-0)$$

$$=\frac{1}{2}.$$

Q4. Normalize the following wave function is one-dimension

$$\psi(x)=\begin{cases} Ae^{-\beta x} & \text{for } x>0 \\ Ae^{\beta x} & \text{for } x<0 \end{cases}$$

Whereβ is a real positive constant

Solution: Normalization condition is given by

$$\int_{-\infty}^{+\infty}\psi^*(x)\psi(x)dx=0$$

$$\therefore \qquad \int_{-\infty}^{0}A^*Ae^{+2\beta x}dx+\int_{0}^{+\infty}A^*Ae^{-2\beta x}dx=1]$$

$$\Rightarrow \qquad |A|^2\int_{-\infty}^{0}e^{2\beta x}dx+|A|^2\int_{0}^{+\infty}e^{-2\beta x}dx=0$$

$$=|A|^2\left[\frac{e^{2\beta x}}{2\beta}\bigg|_{-\infty}^{0}+\frac{e^{-2\beta x}}{-2\beta}\bigg|_{0}^{\infty}\right]$$

$$=|A|^2\left\{\left[\frac{1}{2\beta}-\frac{e^{-\infty}}{2\beta}\right]+\left[\frac{e^{-\infty}}{-2\beta}-\frac{e^{0}}{-2\beta}\right]\right\}=1$$

$$=|A|^2\left[\frac{1}{2\beta}-0+0+\frac{1}{2\beta}\right]=1$$

$$=|A|^2.\frac{1}{\beta}=1$$

$$|A|^2=\beta \text{ or } A=\sqrt{\beta}$$

Therefore the normalized wavefunction is

$$\psi(x)=\sqrt{\beta}e^{-\beta x} \text{ for} x>0$$

$$=\sqrt{\beta}e^{\beta x} \text{ for} x<0$$

Q.5 Normalize the one-dimensional wave function given by

$$\psi(x)=A\sin\left(\frac{\pi x}{a}\right) \qquad 0\le x\le a$$

Solution: The wavefunction $\psi(x)$ is said to be normalize if it satisfies the normalization condition

$$\int_{-\infty}^{+\infty}\psi^*\psi dx=1$$

we have $\psi(x)=A\sin\frac{\pi x}{a}$

$$\psi^*(x)=A^*\sin\frac{\pi x}{a}$$

Therefore $\int_0^a AA^*\sin^2\frac{\pi x}{a}dx$

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

or $$\frac{|A|^2}{2}\left[\int_0^a dx - \int_0^a \cos\frac{2\pi x}{a}dx\right]_0^a = 1$$

or $$\frac{|A|^2}{2}\left[x - \frac{a}{2\pi}\sin\frac{2\pi x}{a}\right]_0^a = 1$$

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

$$|A|^2 = \frac{2}{a}$$

if A is real, then we can write

$$A = \sqrt{\frac{2}{a}}$$

$\therefore$ Normalized wavefunctionis $\psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)$

Q.6. A particle described by a wavefunction

$$\psi(x) = \frac{x+ix}{1+ix^2}$$

Normalize the wavefunction and determine the region of the space wherethe particle is most likely to be found.

Solution: Let the normalized wavefunction is

$$\phi(x) = N\psi(x)$$

$$= N\left(\frac{x+ix}{1+ix^2}\right)$$

where N is the normalization constant

$$\therefore \qquad \phi^*(x) = N^*\left(\frac{x-ix}{1-ix^2}\right)$$

Now the normalization condition is

$$\int_{-\infty}^{+\infty} \phi^*(x)\phi(x)dx = 1$$

$$\Rightarrow \qquad N^*N\int_{-\infty}^{+\infty}\left(\frac{x-ix}{1-ix^2}\right)\left(\frac{x+ix}{1+ix^2}\right)dx = 1$$

$$\text{or} \qquad |N|^2\int_{-\infty}^{+\infty}\frac{x^2-i^2x^2}{1-(ix^2)^2}dx = 1$$

$$\text{or} \qquad |N|^2\int_{-\infty}^{+\infty}\frac{2x^2}{1+x^4}dx = 1$$

$$\text{or} \qquad |N|^2\int_{-\infty}^{\infty}\left(\frac{x^2+1}{1+x^4}+\frac{x^2-1}{1+x^4}\right)dx = 1$$

$$\text{or} \qquad |N|^2\left[\int_{-\infty}^{+\infty}\frac{1+\frac{1}{x^2}}{\left(x-\frac{1}{x}\right)^2+2}dx + \int_{-\infty}^{+\infty}\frac{1-\frac{1}{x^2}}{\left(x+\frac{1}{x}\right)^2-2}dx\right] = 1 \qquad (1)$$

Let $x-\frac{1}{x} = z$

$$\Rightarrow \qquad dx + \frac{1}{x^2}dx = dz$$

$$\text{or} \qquad \left(1+\frac{1}{x^2}\right)dx = dz$$

$\therefore$ 1st part of the integral on LHS of eqn. (1) becomes

$$\int_{-\infty}^{+\infty} \frac{dz}{z^2+2} = \int_{-\infty}^{+\infty} \frac{dz}{z^2+(\sqrt{2})^2}$$

$$= \frac{1}{\sqrt{2}} \tan^{-1} \frac{z}{\sqrt{2}} \Bigg|_{-\infty}^{+\infty}$$

$$= \frac{1}{\sqrt{2}} \left[\tan^{-1}(\infty) - \tan^{-1}(-\infty) \right]$$

$$= \frac{1}{\sqrt{2}} \left[2\tan^{-1}(\infty) \right] \qquad \{\because \tan^{-1}(-\theta) = -\tan^{-1}\theta\}$$

$$= \frac{1}{\sqrt{2}} .2\frac{\pi}{2} = \frac{\pi}{\sqrt{2}}$$

Similarly if we assume $x + \frac{1}{x} = t$

$$\Rightarrow \qquad \left(x - \frac{1}{x^2} \right) dx = dt$$

Then second integral on LHS of eqn. (1) becomes

$$\int_{-\infty}^{+\infty} \frac{dt}{t^2 - (\sqrt{2})^2} = \frac{1}{2\sqrt{2}} \log \left(\frac{t-\sqrt{2}}{t+\sqrt{2}} \right)_{-\infty}^{+\infty}$$

$$= \frac{1}{2\sqrt{2}} \left[\log \left\{ \frac{1 - \frac{\sqrt{2}}{t}}{1 + \frac{\sqrt{2}}{t}} \right\} \right]_{-\infty}^{+\infty}$$

$$= \frac{1}{2\sqrt{2}} \log(1) = 0$$

$\therefore$ eqn. (1) becomes

$$|N|^2\left[\frac{\pi}{\sqrt{2}}+0\right]=1$$

or $$|N|^2=\frac{\sqrt{2}}{\pi}$$

If N is real, then $N=\left(\frac{\sqrt{2}}{\pi}\right)^{1/2}$

Hence the normalized wave functions become

$$\left(\frac{\sqrt{2}}{\pi}\right)^{1/2}\left(\frac{x+ix}{1+ix^2}\right)$$

Now to find the most probable positionof the particle, we have to maximize $\psi^*\psi$

i.e. $$\frac{d}{dx}\left(\psi^*\psi\right)=0$$

$$x\frac{d}{dx}\left(\frac{x^2}{1+x^4}\right)=0$$

$$\frac{d}{dx}x^2(1+x^4)^{-1}=0$$

or $$x^2(-1(1+x^4)^{-2}\cdot 4x^3)+(1+x^4)^{-1}\cdot 2x=0$$

$\Rightarrow$ $$-4x^5(1+x^4)^{-2}+2x(1+x^4)^{-1}=0$$

or $$2x(1+x^4)^{-1}\left[1-\frac{2x^4}{1+x^4}\right]=0$$

or $$\frac{1+x^4-2x^4}{1+x^4}=0$$

or $$x^4=1 \quad \text{or} \quad x=1$$

Thus probability is maximum at $x = 1$.

Q.7 A normalized wave function is given by

$$\phi(x) = \frac{1}{a^{1/2}\pi^{1/4}} e^{\left(ik_0 x - \frac{x^2}{2a^2}\right)}$$

Find where the particle is most likely to be found.

Solution: The probability density of the particle is given by

$$|\phi(x)|^2 = \phi^2(x)\phi(x) = \frac{1}{a\,\pi^{1/2}} e^{-x^2/a^2}$$

Itis clear from above equation that

$|\phi(x)|^2$ is maximum at $x = 0$ and decreases exponentially for $|x| > 0$.

Therefore, the particle is most likely to be found in region of width 'a' on either side of the origin $x = 0$.

Q.8 A particle moving along the positive x-direction in region of potential energy $V(x)$ is given by the wave packet

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int A(p) e^{\frac{i}{\hbar}(P_x x - Et)} dp$$

Using non-relativistic energy expression, derive one-dimensional time-dependent Schrodinger equation.

Solution: Non-relativistic total energy in 1–D is given by

$$E = \frac{P_x^2}{2m} + V(x)$$

also we have

$$\psi(x,t)=\frac{1}{\sqrt{2\pi\hbar}}\int A(p)e^{\frac{i}{\hbar}(P_x x-Et)}dp \qquad (1)$$

Differentiating eqn. (1) w.r.t x.

$$\frac{\partial\psi(x,t)}{\partial x}=\frac{1}{\sqrt{2\pi\hbar}}\int A(p)\left(\frac{i}{\hbar}P_x\right)e^{\frac{i}{\hbar}(P_x x-Et)}dp$$

Again differentiating w.r.t. x

$$\frac{\partial^2\psi(x,t)}{\partial x^2}=\frac{1}{\sqrt{2\pi\hbar}}\int A(p)\left(\frac{i}{\hbar}P_x\right)^2 e^{\frac{i}{\hbar}(P_x x-Et)}dp$$

or $$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}=\frac{1}{\sqrt{2\pi\hbar}}\int \frac{P_x^2}{2m}A(p)e^{\frac{i}{\hbar}(P_x x-Et)}dp \qquad (2)$$

Differentiating eqn. (1) w.r.t to time

$$\frac{\partial\psi(x,t)}{\partial t}=\frac{1}{\sqrt{2\pi\hbar}}\int A(p)\left(\frac{-i}{\hbar}E\right)e^{\frac{i}{\hbar}(P_x x-Et)}dp$$

or $$i\hbar\frac{\partial\psi(x,t)}{\partial x}=\frac{1}{\sqrt{2\pi\hbar}}\int A(p)E\,e^{\frac{i}{\hbar}(P_x x-Et)}dp\,. \qquad (3)$$

Subtracting eqn. (3) from eqn. (2)

$\Rightarrow$ $$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}-i\hbar\frac{\partial\psi}{\partial t}=\frac{1}{\sqrt{2\pi\hbar}}\int\left(\frac{P_x^2}{2m}-E\right)A(p)E\,e^{\frac{i}{\hbar}(P_x x-Et)}dp$$

or $$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}-i\hbar\frac{\partial\psi}{\partial t}=\frac{1}{\sqrt{2\pi\hbar}}\int V(x)A(p)\,e^{\frac{i}{\hbar}(P_x x-Et)}dp$$

or $$\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}-i\hbar\frac{\partial\psi}{\partial t}=\frac{1}{\sqrt{2\pi\hbar}}V(x)\int A(p)\,e^{\frac{i}{\hbar}(P_x x-Et)}dp$$

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

or $$\boxed{\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+v(x)\psi=i\hbar\frac{\partial\psi}{\partial t}}$$

is the one–dimensional Schrodinger's time dependent wave equation.

Q9. Calculate the expectation value of x, P_x and P_x^2 for the wave function

$$\psi(x)=\begin{cases}\left(\frac{2}{L}\right)^{1/2}\sin\frac{\pi x}{L} & 0<x<L\\ 0 & |x|>L\end{cases}$$

Solution: The expectation value of x is

$$\langle x\rangle=\int \psi^*\hat{x}\psi\,dx$$

$$=\frac{2}{L}\int_0^L \sin\frac{\pi x}{L}(x)\left(\sin\frac{\pi x}{L}\right)dx$$

$$=\frac{2}{L}\int_0^L x\sin^2\frac{\pi x}{L}dx$$

$$=\frac{2}{L}\int_0^L \frac{x}{2}\left(1-\cos\frac{2\pi x}{L}\right)dx$$

$$=\frac{1}{L}\int_0^L xdx-\frac{1}{L}\int_0^L x\cos\frac{2\pi x}{L}dx$$

$$=\frac{1}{L}\frac{x^2}{2}\Bigg|_0^L-\frac{1}{L}\left(x.\sin\frac{\frac{2\pi x}{L}}{\frac{2\pi}{L}}\Bigg|_0^L-\int_0^L \sin\frac{\frac{2\pi x}{L}}{\frac{2\pi}{L}}dx\right)$$

$$=\frac{L}{2}-\frac{1}{L}.\frac{L}{2\pi}(L.\sin 2\pi-0)+\left(\frac{2\pi}{2}\right)^2\left(1-\cos\frac{2\pi x}{L}\right)^2$$

$$=\frac{L}{2}-0-\left(\frac{2\pi}{2}\right)^2(\cos 2\pi-\cos 0)$$

$$= \frac{L}{2} - 0 = \frac{L}{2}$$

$\therefore$ $$\langle x \rangle = \frac{L}{2}$$

(ii) $$\langle P_x \rangle = \int_{-\infty}^{+\infty} \psi^*(x,t)\hat{P}_x \psi(x,t)dx$$

$$= \frac{2}{L}\int_0^L \sin\frac{\pi x}{L}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\sin\frac{\pi x}{L}dx$$

$$= \frac{2}{L}.\frac{\hbar}{i}\frac{\pi}{L}\int_0^L \sin\frac{\pi x}{L}\cos\frac{\pi x}{L}dx$$

$$= \frac{\pi\hbar}{iL^2}\int_0^L \sin\frac{2\pi x}{L}dx$$

$$= \frac{-\pi\hbar}{iL^2}\times\frac{L}{2\pi}\cos\frac{2\pi x}{L}\bigg|_0^L$$

$$= \frac{-\hbar}{2iL}[\cos 2\pi - \cos 0]$$

$$= 0$$

$\therefore$ $$\langle P_x \rangle = 0$$

(iii) $$\langle P_x^2 \rangle = \int_{-\infty}^{+\infty} \psi^*(x,t)\hat{P}_x^2 \psi(x,t)dx$$

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

$$= \frac{-2\hbar^2}{L}\int_0^L \sin\frac{\pi x}{L}\frac{\partial^2}{\partial x^2}\left(\sin\frac{\pi x}{L}\right)dx$$

$$= \frac{-2\hbar^2}{L}\int_0^L \sin\frac{\pi x}{L}\left(-\sin\frac{\pi x}{L}\right)\left(\frac{\pi}{L}\right)^2 dx$$

$$= \frac{2\hbar^2}{L}.\frac{\pi^2}{L^2}\int_0^L \sin^2\frac{\pi x}{L}dx$$

$$= \frac{2\pi^2\hbar^2}{L^3}\int_0^L \frac{1}{2}\left(1-\cos\frac{2\pi x}{L}\right)dx$$

$$= \frac{2\hbar^2}{L}.\frac{\pi^2}{L^2}\int_0^L \sin^2\frac{\pi x}{L}dx$$

$$= \frac{2\pi^2\hbar^2}{L^3}\int_0^L \frac{1}{2}\left(1-\cos\frac{2\pi x}{L}\right)dx$$

$$= \frac{\pi^2\hbar^2}{L^3}\left\{x-\frac{\sin\frac{2\pi x}{L}}{\frac{2\pi}{L}}\right\}_0^L$$

$$= \frac{\pi^2\hbar^2}{L^3}\left\{L-\frac{L}{2\pi}(\sin 2\pi-\sin 0)\right\}$$

$$= \frac{\pi^2\hbar^2}{L^3}\{L-0\}$$

$$\langle P_x^2\rangle = \frac{\pi^2\hbar^2}{L^2}$$

5.13 Terminal Questions

5.13.1 Short Answer Questions

Q1 What is a wavefunction?

Q2 What do you understand by probabilistic interpretation in quantum mechanics?

Q3 What are the conditions that a wavefunction must satisfy and why?

Q4 What do you mean by normalization of a wavefunction?

Q5 Define the expectation value of an observable.

5.13.2 Long Answer Questions

Q1 Obtain the time dependent Schrodinger wave equation for bound and free particles.

Q2 State and prove the Ehrenfest theorem. Also explain its physical significance.

Q3 Why the wavefunction and its derivatives should be continuous everywhere?

Q4 Find the expression for expectation value of position, momentum and energy operator.

Q5 Derive time independent Schrodinger wave equation in one dimension**.**

5.13.3 Numerical Questions

Q1. An Eigen function of the operator ${d^3}/{dx^3}$ is $\psi(x) = e^{4x}$. Find the corresponding Eigenvalue.

Q2. Explain if the wavefunction $\psi(x) = A\tan x$ is an acceptable quantum mechanical wavefunction or not?

Q3. Explain if the wavefunction $\psi(x) = Ce^{-x^2}$ is an acceptable quantum mechanical wavefunction or not?

Q4. Why Schrodinger's wave equation is not valid for relativistic particles?

Q5. One dimensional wave function of a particle is given by $\psi(x) = \sqrt{a}e^{-ax}$. Find the probability of finding the particle between x=1/a and x = 3/a.

Q6. Determine the expectation value of position and momentum for a particle trapped in a box of length L.

Q7. Calculate the expectation values of momentum p and p^2 for the wavefunction $\psi(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{\pi x}{L}\right)$ in the region $0 < x < L$. Outside this region consider $\psi(x) = 0$.

Q8. Obtain the expectation value of the potential energy V(r) of the electron in a hydrogen atom in its ground state.

Unit 6 : Operators

6.1 Introduction

The quantity obtained by the process of measurement or observation on a physical system is called an observable. An observable is always a real entity, since it is a result of actual measurement. Classically we assume that an act of measurement does not disturb the system and various observables of the system can be measured with utmost accuracy. But quantum mechanically this is not the case. According to quantum mechanics, an act of measurement disturbs a physical system and therefore the value of an observable depends upon time. However if the value of an observable doesnot depend on time, it is known as constant of the system.

6.2 Objective

As we have learnt in unit 5, that the Schrodinger equation is fundamental equation of quantum mechanics, which provides us the wavefunction of the system. In physics we are mainly interested in finding the dynamical quantities of the system like position, momentum, angular momentum etc of the system at any time ‘t’. In this unit we will learn that the dynamical quantities in quantum mechanics are also represented by operators. We will also learn about the different relations satisfied by these operators. We will also learn that average values of these operators satisfies laws, analogues to the Newton’s second law.

6.3 Operators and Observables

An operator is a rule by means of which a given function is changes into another function. The measurable quantities like position, momentum energy etc. are called observable. Each observable has a definte operator associated with it.

6.3.1 Commuting and non-commuting operators

Let $\hat{A}$ and $\hat{B}$ be any two operators and ψ be any wavefunction

then $\hat{A}\hat{B}\psi$ means first $\hat{B}$ operators on ψs.t.

$\hat{B}\psi = \phi$ and then $\hat{A}$ operator on ϕs.t.

$\hat{A}\phi = \xi$

$\therefore \qquad \hat{A}(\hat{B}\psi) = \hat{A}\phi = \xi$

Now if $\hat{A}$ and $\hat{B}$ operators are such that

$\hat{A}\hat{B} - \hat{B}\hat{A} = 0$ then the two operators

$\hat{A}$ and $\hat{B}$ are said to be commuting, otherwise they are non-commuting.

6.3.2 Hermitian Operator:

An operator $\hat{A}$ is said to be Hermitian if it satisfy the equation

$$\int_{-\infty}^{+\infty} \psi^*(\hat{A}\phi)dx = \int_{-\infty}^{+\infty} (\psi\hat{A})^*\phi\, dx$$

when $\psi(x)$ and $\phi(x)$ are two well behaved wavefunction.

6.4 Dynamical Variables or Observables

The physical quantities that can be determined experimentally are known as observables or dynamical variables. For e.g. position of some particle with respect to some coordinates system, Momentum, Energy (kinetic and potential) are some observables or dynamical variables. In classical mechanics, observables have a continuous range of values whereas in quantum mechanics, observables have discrete or quantized values. In quantum mechanics, the observables are represented by operators. Below are some operators used in quantum mechanics.

6.4.1`Position Operator

In Cartesian Coordinates, position operators are represented as $\hat{x},\ \hat{y},\ \hat{z}$, when they act on any wavefunction ψ, they give the function times the corresponding coordinate

e.g. $\hat{x}\psi = x\psi,\qquad \hat{y}\psi = y\psi$ and $\hat{z}\psi = z\psi$

6.4.2 Linear Momentum Operator

We know that the wavefunction for a free particle is given by

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

$$\therefore \qquad \frac{\partial \psi}{\partial x} = A\left(\frac{i}{\hbar}P_x\right)e^{\frac{i}{\hbar}(P_x x - Et)}$$

$$= \frac{i}{\hbar}P_x\psi$$

or $$\frac{\hbar}{i}\frac{\partial \psi}{\partial x} = P_x\psi \quad or \quad \frac{\hbar}{i}\frac{\partial \psi}{\partial x} = P_x\psi \qquad (1)$$

Above equation is an Eigen value equation for x-component of momentum such that the operator $\frac{\hbar}{i}\frac{\partial}{\partial x}$ operators on a wavefunction ψ and gives x-component of momentum times the wavefunction.

the operator $\frac{\hbar}{i}\frac{\partial}{\partial x}$ is known the momentum operator and is denoted by $\hat{p}_x$

$$\therefore \qquad \hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x} \qquad (2)$$

Similarly $$\hat{p}_y = \frac{\hbar}{i}\frac{\partial}{\partial y}$$

$$\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial z}$$

The momentum operator $\hat{p} = i\hat{p}_x + \hat{j}\hat{p}_y + \hat{k}\hat{p}_z = \frac{\hbar}{i}\vec{\nabla}$ (3)

Such that $\hat{p}\psi = p\psi$.

∴ Momentum operator is defined as the operator which when operates on a wavefunction, reproduces the wavefunction multiplied by the Momentum.

6.4.3 Kinetic Energy Operator

We have the Momentum operator as

$$\frac{\hbar}{i}\frac{\partial}{\partial x}(\psi) = P_x\psi$$

Differentiating above eqn. w.r.t x,

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

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

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

or $$-\hbar^2\frac{\partial^2\psi}{\partial x^2} = p_x^2\psi \qquad \{i^2 = -1\}$$

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

but $\frac{p_x^2}{2m}$ = K.E. of the particle.

$\therefore$ The operator $-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ is known as kinetic energy operator $\hat{K}$.

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

6.4.4 Potential Energy Operator

Potential energy operator $\hat{V}(\vec{r})$ is such that when it operates on a wavefunction ψ, it gives potential energy multiplied by the wave function back.

i.e. $\hat{V}(\vec{r})\psi = V(\vec{r})\psi$

6.4.5 Hamiltonian operator or total Energy operator

Total energy of a particle moving along x-axis is given by

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

$$\Rightarrow \qquad \frac{p_x^2}{2m} = E - V(x)$$

Using value of $\frac{p_x^2}{2m}$ is eqn. (1)

$$\Rightarrow \qquad \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi = [E - V(x)]\psi$$

or $$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V\psi = E\psi$$

or $$\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right]\psi = E\psi$$

Above eqn. is the Eigen value equation of total energy and hence the operator $\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V$ is the total energy operator for the motion ofthe particle along x-direction and is denoted by $\hat{H}_x$

$$\therefore \qquad \hat{H}_x = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x) \tag{5}$$

In three dimensions, total energy operator is

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

or $\frac{-\hbar^2}{2m}\nabla^2+V$ and is denoted by $\hat{H}$ and is also known as Hamiltonian operator

$$\boxed{\hat{H} = \frac{-\hbar^2}{2m}\nabla^2+v} \tag{6}$$

Therefore total Energy operator or Hamiltonian operator is a differential operator, which operates on a wavefunction, reproduces the same wavefunction multiplied by the total energy.

6.4.6 Total Energy Operator as time derivative

We have the wavefunction of a free particle in one dimension as

$$\psi(x) = Ae^{i/h(P_x x-Et)}$$

Differentiating w.r.t. *t*, we get

$$\frac{\partial\psi}{\partial t} = A\left(\frac{-i}{\hbar}E\right)e^{i/h(P_x x-Et)}$$

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

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

From above equation we conclude that the total energy operator is

$$\therefore \qquad \hat{H} = i\hbar\frac{\partial}{\partial t} \tag{7}$$

6.5 Angular Momentum operator

6.5.1 Angular Momentum Operator in Cartesian Coordinates

The angular Momentum $\vec{L}$ is given by

$$\vec{L} = \vec{r}\times\vec{p} \tag{8}$$

where $\vec{r}$ is the position vector and $\vec{p}$ is the linear momentum operator.

In operator, form eqn. (8) can be written as

$$\hat{L} = \hat{r}\times\hat{p} \tag{9}$$

or

$$\hat{L} = \hat{r}\times -i\hbar$$

$$= -i\hbar\,\hat{r}\times\vec{\nabla} \tag{10}$$

But $\hat{r} = \hat{i}\,\hat{x} + \hat{j}\,\hat{y} + \hat{z}\,\hat{k}$ and $\vec{\nabla} = \hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}$

Therefore, $\hat{L} = -i\hbar(\hat{i}\,\hat{x} + \hat{j}\,\hat{y} + \hat{z}\,\hat{k})\times\left(\hat{i}\frac{\partial}{\partial x} + \hat{j}\frac{\partial}{\partial y} + \hat{k}\frac{\partial}{\partial z}\right)$

$$= -i\hbar\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{vmatrix}$$

$$= -i\hbar\left[\hat{i}\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right) + \hat{j}\left(\hat{z}\frac{\partial}{\partial x} - \hat{x}\frac{\partial}{\partial z}\right) + \hat{k}\left(\hat{x}\frac{\partial}{\partial y} - \hat{y}\frac{\partial}{\partial x}\right)\right]$$

If $\hat{L}_x, \hat{L}_y, \hat{L}_z$ be x, y, and z components of $\hat{L}$.

then
$$\hat{L}_x = -i\hbar\left(\hat{y}\frac{\partial}{\partial z} - \hat{z}\frac{\partial}{\partial y}\right), \tag{11}$$

$$\hat{L}_y = -i\hbar\left(\hat{z}\frac{\partial}{\partial x} - \hat{x}\frac{\partial}{\partial z}\right) \text{and} \tag{12}$$

$$\hat{L}_z = -i\hbar\left(\hat{x}\frac{\partial}{\partial y} + \hat{y}\frac{\partial}{\partial z}\right) \tag{13}$$

6.5.2 Angular Momentum Operator in Spherical Polar coordinates

The relation between Cartesian and Spherical polar coordinates is

$$\left.\begin{array}{l} x = r\sin\theta\cos\phi \\ y = r\sin\theta\sin\phi \\ z = r\cos\theta \end{array}\right\} \tag{14}$$

Where $\vec{r} = x\hat{i} + y\hat{i} + z\hat{k}$

also
$$\left.\begin{array}{l} r = (x^2+y^2+z^2)^{1/2} \\ \theta = \tan^{-1}\sqrt{\dfrac{x^2+y^2}{z}} \\ \phi = \tan^{-1} y/x \end{array}\right\} \tag{15}$$

$$\frac{\partial r}{\partial x} = \frac{1}{2}(x^2+y^2+z^2)^{-1/2}2x = \frac{x}{r} = \sin\theta\cos\theta \tag{16}$$

$$\frac{\partial r}{\partial y} = \frac{1}{2}(x^2+y^2+z^2)^{-1/2}2y = \frac{y}{r} = \sin\theta\sin\phi \tag{17}$$

$$\frac{\partial r}{\partial z} = \frac{1}{2}(x^2+y^2+z^2)^{-1/2}2z = \frac{z}{r} = \cos\theta \tag{18}$$

Again we have

$$z = r\cos\theta \qquad or \qquad \cos\theta = \frac{z}{r}$$

Differentiating w.r. to x.

$$-\sin\theta\frac{\partial\theta}{\partial x}=z\frac{\partial}{\partial x}\left(\frac{1}{r}\right)=\frac{-z}{r^2}\frac{\partial r}{\partial x}$$

Using eqns. (16) and (18), above eqn. becomes

$$-\sin\theta\frac{\partial\theta}{\partial x}=-\frac{1}{r}\sin\theta\cos\phi\cos\theta$$

or $$\frac{\partial\theta}{\partial x}=\frac{1}{r}\cos\theta\cos\phi \qquad (19)$$

Similarly $$-\sin\theta\frac{\partial\theta}{\partial y}=\frac{-z}{r^2}\frac{\partial r}{\partial y}$$

or $$\frac{\partial\theta}{\partial y}=\frac{1}{r}\cos\theta\sin\phi \qquad (20)$$

and $$\frac{\partial\theta}{\partial z}=\frac{-1}{r}\sin\theta \qquad (21)$$

also we have

$$\tan\phi=\frac{y}{x}$$

Differentiating w.r. t. x, we get

$$\sec^2\phi\frac{\partial\phi}{\partial x}=\frac{-y}{x^2}$$

or $$\sec^2\phi\frac{\partial\phi}{\partial x}=\frac{-y}{x}.\frac{1}{x}=-\tan\phi.\frac{1}{r\sin\theta\cos\phi}$$

⇒ $$\sec^2\phi\frac{\partial\phi}{\partial x}=-\frac{\sin\phi}{\cos\phi}.\frac{1}{r\sin\theta\cos\phi}$$

⇒ $$\frac{\partial\phi}{\partial x}=-\frac{\sin\phi}{r\sin\theta} \qquad (22)$$

Similarly $$\frac{\partial\phi}{\partial y}=\frac{\cos\phi}{r\sin\phi} \tag{23}$$

and $$\frac{\partial\phi}{\partial z}=0 \tag{24}$$

Now consider

$$\frac{\partial}{\partial x}=\frac{\partial r}{\partial x}.\frac{\partial}{\partial r}+\frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta}+\frac{\partial\phi}{\partial x}\frac{\partial}{\partial\phi}$$

$$\frac{\partial}{\partial x}=\sin\theta\cos\phi\frac{\partial}{\partial r}+\frac{1}{r}\cos\theta\cos\phi\frac{\partial}{\partial\theta}-\frac{\sin\phi}{r\sin\theta}\frac{\partial}{\partial\phi} \tag{25}$$

$$\frac{\partial}{\partial y}=\frac{\partial r}{\partial y}.\frac{\partial}{\partial r}+\frac{\partial\theta}{\partial y}\frac{\partial}{\partial\theta}+\frac{\partial\phi}{\partial y}\frac{\partial}{\partial\phi}$$

$$\sin\theta\sin\phi\frac{\partial}{\partial r}+\frac{1}{r}\sin\phi\cos\theta\frac{\partial}{\partial\theta}+\frac{\cos\phi}{r\sin\theta}\frac{\partial}{\partial\phi} \tag{26}$$

and $$\frac{\partial}{\partial z}=\frac{\partial r}{\partial z}\frac{\partial}{\partial r}+\frac{\partial\theta}{\partial z}\frac{\partial}{\partial\theta}+\frac{\partial\phi}{\partial z}\frac{\partial}{\partial\phi}$$

$$=\cos\theta\frac{\partial}{\partial r}-\frac{\sin\theta}{r}\frac{\partial}{\partial\theta} \tag{27}$$

Now $\hat{L}_x=-i\hbar\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right)$

Using above relations,

$$\hat{L}_x=-i\hbar\left[r\sin\theta\sin\phi\cos\theta\frac{\partial}{\partial r}-\sin^2\theta\sin\phi\frac{\partial}{\partial\theta}-r\cos\theta\sin\theta\sin\phi\frac{\partial}{\partial r}\right.$$
$$\left.-\cos^2\theta\sin\phi\frac{\partial}{\partial r}-\frac{\cos\theta}{\sin\theta}\cos\phi\frac{\partial}{\partial\phi}\right]$$

$$\hat{L}_x = i\hbar\left[\sin\phi\frac{\partial}{\partial r} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right] \tag{28}$$

Similarly $\hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) = -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$ (29)

and $\hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial\phi}$ (30)

6.5.3 Operator for Square of total angular Momentum ($\hat{L}^2$)

Operator for total angular momentum in Cartesian Coordinates is –

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$$= \hat{L}_x\cdot\hat{L}_x + \hat{L}_y\cdot\hat{L}_y + \hat{L}_z\cdot\hat{L}_z \tag{31}$$

Consider

$$\hat{L}_x\cdot\hat{L}_x = -\hbar^2\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$= -\hbar^2\left[\sin^2\phi\frac{\partial^2}{\partial\theta^2} + \sin\phi\cos\phi\frac{\partial}{\partial\theta}\left(\cot\theta\frac{\partial}{\partial\theta}\right) + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\left(\sin\phi\frac{\partial}{\partial\theta}\right)\right.$$

$$\left. + \cot^2\theta\cos\phi\frac{\partial}{\partial\phi}\left(\cos\phi\frac{\partial}{\partial\phi}\right)\right]$$

$$= -\hbar^2\left[\sin^2\phi\frac{\partial^2}{\partial\theta^2} + \sin\phi\cos\phi\cot\theta\frac{\partial^2}{\partial\theta\partial\phi} - \sin\phi\cos\phi\,\mathrm{cosec}^2\theta\frac{\partial}{\partial\phi}\right.$$

$$+ \cot\theta\cos\phi\sin\phi\frac{\partial^2}{\partial\phi\partial\theta} + \cot\theta\cos^2\phi\frac{\partial}{\partial\theta} + \cot^2\theta\cos^2\phi\frac{\partial^2}{\partial\phi^2}$$

$$\left. - \cot^2\theta\cos\phi\sin\phi\frac{\partial}{\partial\phi}\right] \tag{32}$$

Similarly, $\hat{L}_y \cdot \hat{L}_y = -\hbar^2 \left[\cos^2\phi \frac{\partial^2}{\partial\theta^2} + \cos\phi \sin\phi \operatorname{cosec}^2\theta \frac{\partial}{\partial\phi} - \cos\phi \sin\phi \cot\theta \frac{\partial^2}{\partial\theta\partial\phi} \right.$

$$-\cot\theta \sin\phi \cos\phi \frac{\partial^2}{\partial\phi\partial\theta} + \cot\theta \sin^2\phi \frac{\partial}{\partial\theta} + \cot^2\theta \sin\phi \cos\phi \frac{\partial}{\partial\phi}$$

$$\left. +\cot^2\theta \sin^2\phi \frac{\partial^2}{\partial\phi^2} \right] \tag{33}$$

and $\hat{L}_z.\hat{L}_z = \left[-i\hbar \frac{\partial}{\partial\phi} \right] \left[-i\hbar \frac{\partial}{\partial\phi} \right] = -\hbar^2 \frac{\partial^2}{\partial\phi^2}$ (34)

Using eqns. (32), (33) and (34) in eqn. (31)

$$\hat{L}^2 = -\hbar^2 \left[(\sin^2\phi + \cos^2\phi) \frac{\partial^2}{\partial\theta^2} + \cot\theta (\sin^2\phi + \cos^2\phi) \frac{\partial}{\partial\theta} \right.$$

$$\left. +\cot^2\theta (\sin^2\phi + \cos^2\phi) \frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial\phi} \right]$$

$$= -\hbar^2 \left[\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \cot^2\theta \frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial\phi^2} \right]$$

$$= -\hbar^2 \left[\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + (\cot^2\theta + 1) \frac{\partial^2}{\partial\phi^2} \right]$$

$$= -\hbar^2 \left[\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \operatorname{cosec}^2\theta \frac{\partial^2}{\partial\phi^2} \right]$$

$$= -\hbar^2 \left[\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]$$

$$= -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]$$

Therefore operator for square of total angular momentum $\hat{L}^2$ is given by

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \right] \tag{35}$$

6.6 Commutation relation

The commutator $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ plays a vital role in quantum mechanics, we will now consider commutation of position and momentum. The position and momentum in quantum mechanics are represented by the operators $\hat{r}$ and $\frac{\hbar}{i}\vec{\nabla}$.

If we consider the z component of position and momentum operator for z and p_z such that $\hat{z} = z$ and $\hat{p}_z = \frac{\hbar}{i}\frac{\partial}{\partial z}$

Then consider the commutator $[z,\ p_z]\psi$

$$= \left[z, \frac{\hbar}{i}\frac{\partial}{\partial z} \right]\psi$$

$$= \frac{\hbar}{i}\left[z, \frac{\partial}{\partial z} \right]\psi = \frac{\hbar}{i}\left(z\frac{\partial}{\partial z}\psi - \frac{\partial}{\partial z}(z\psi) \right) \left\{ \left(\hat{A}\hat{B} - \hat{A}\hat{B}\right)\psi = \hat{A}\hat{B}\psi - \hat{A}\hat{B}\psi \right\}$$

$$= \frac{\hbar}{i}\left(z\frac{\partial\psi}{\partial z} - \psi - z\frac{\partial\psi}{\partial z} \right)$$

$$= -\frac{\hbar}{i}\psi$$

or $\quad [z,\ p_z]\psi = i\hbar\psi$

$\Rightarrow \quad [z,\ p_z] = i\hbar$

Similarly, $\quad [x,\ p_x] = [y,\ p_y] = i\hbar$

Consider $$[y,\ p_x]\psi = \frac{\hbar}{i}\left[y,\ \frac{\partial}{\partial x}\right]\psi$$

$$= \frac{\hbar}{i}\left(y\frac{\partial\psi}{\partial x} - \frac{\partial}{\partial x}(y\psi)\right)$$

$$= \frac{\hbar}{i}\left(y\frac{\partial\psi}{\partial x} - y\frac{\partial\psi}{\partial x}\right) = 0$$

Similarly $[z,\ p_x] = [x,\ p_y] = [x,\ p_z] = [y,\ p_x],\ [y,\ p_z] = 0$

Above relations can be expressed as

$$[x_i,\ p_j] = i\hbar\,\delta_{ij}$$

When δ_{ij} is Kronecker delta function and is defined as

$\delta_{ij} = 0$, if $i \neq j$

$= 1$, if $i = j$

also $x_1 = x,\ x_2 = y,\ x_3 = z$ and $p_1 = p_x,\ p_2 = p_y,\ p_z = p_z$

6.6.1 Commutation relation between angular momentum operators:

(i) $[\hat{L}_x,\ \hat{L}_y]$

Consider $[\hat{L}_x,\ \hat{L}_y]\psi = \hat{L}_x\hat{L}_y\psi - \hat{L}_y\hat{L}_x\psi$

Where psi is any arbitrary wavefunction, therefore we have

$$= (-i\hbar)^2\left[\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\psi - \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\right]\psi$$

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

$$= -\hbar^2\left[y\frac{\partial}{\partial z}\left(y\frac{\partial\psi}{\partial x}\right) - z\frac{\partial}{\partial y}\left(z\frac{\partial\psi}{\partial x}\right) - y\frac{\partial}{\partial z}\left(x\frac{\partial\psi}{\partial z}\right) + z\frac{\partial}{\partial y}\left(x\frac{\partial\psi}{\partial z}\right)\right]$$

$$+\hbar^2\left[z\frac{\partial}{\partial x}\left(y\frac{\partial\psi}{\partial z}\right)-z\frac{\partial}{\partial x}\left(z\frac{\partial\psi}{\partial y}\right)-x\frac{\partial}{\partial z}\left(y\frac{\partial\psi}{\partial z}\right)+x\frac{\partial}{\partial z}\left(z\frac{\partial\psi}{\partial y}\right)\right]$$

$$=-\hbar^2\left[y\frac{\partial\psi}{\partial x}+yz\left(\frac{\partial^2\psi}{\partial z\partial x}\right)-z^2\frac{\partial^2\psi}{\partial y\partial x}-yx\frac{\partial^2\psi}{\partial z^2}+zx\frac{\partial^2 y}{\partial y\partial z}\right]$$

$$+\hbar^2\left[zy\frac{\partial^2\psi}{\partial x\partial z}-\frac{z^2\partial^2\psi}{\partial x\partial y}-xy\frac{\partial^2\psi}{\partial z^2}+x\frac{\partial\psi}{\partial y}+xz\frac{\partial^2\psi}{\partial z\partial y}\right]$$

$$=-\hbar^2 y\frac{\partial\psi}{\partial x}+\hbar^2 x\frac{\partial\psi}{\partial y}=\hbar^2\left[x\frac{\partial\psi}{\partial y}-y\frac{\partial\psi}{\partial x}\right]$$

$$\therefore [\hat{L}_x,\,\hat{L}_y]\psi=(i\hbar)(-i\hbar)\left[x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right]\psi$$

$$\text{but}\,-i\hbar\left[x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right]=\hat{L}_z$$

Therefore $\quad [\hat{L}_x,\,\hat{L}_y]\psi=i\hbar\hat{L}_z\psi$

or $\quad [\hat{L}_x,\,\hat{L}_y]=i\hbar\,\hat{L}_z \qquad (1)$

Similarly we can prove

$$[\hat{L}_y,\,\hat{L}_z]=i\hbar\,\hat{L}_x \qquad (2)$$

and $\quad [\hat{L}_z,\,\hat{L}_x]=i\hbar\,\hat{L}_y \qquad (3)$

The commutation relations (1), (2) and (3) can be combined as

$$[\hat{L}_i,\,\hat{L}_j]=i\hbar\,\hat{L}_k$$

where $i,\ j,\ k$ being *x, y* and *z* resp. taken in cyclic order.

6.6.2 Commutation relations between Square Angular Momentum Operator ($\hat{L}^2$) and $\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$

(i) $[\hat{L}^2, \hat{L}_x]$

$$\vec{L}^2 = \vec{L} \cdot \vec{L} = L_x^2 + L_y^2 + L_z^2$$

the operator corresponding to the observable L^2 is L^2 and can be expressed as

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$$[\hat{L}^2, \hat{L}_x] = [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_x]$$

$$= [\hat{L}_x^2, \hat{L}_x] + [\hat{L}_y^2, \hat{L}_x] + [\hat{L}_z^2, \hat{L}_x]$$

$$= \hat{L}_x[\hat{L}_x, \hat{L}_x] + [\hat{L}_x, \hat{L}_x]\hat{L}_x + \hat{L}_y[\hat{L}_y, \hat{L}_x] + [\hat{L}_y, \hat{L}_x]\hat{L}_y + \hat{L}_z[\hat{L}_z, \hat{L}_x] + [\hat{L}_z, \hat{L}_x]\hat{L}_z$$

$$\left\{\because \left[\hat{A}\hat{B}, \hat{C}\right] = \hat{A}\left[\hat{B}, \hat{C}\right] + \left[\hat{A}, \hat{C}\right]\hat{B}\right\}$$

$$= 0 + 0 - \hat{i}\,\hbar\,\hat{L}_y\hat{L}_z - i\,\hbar\,\hat{L}_z\hat{L}_y + i\hbar\,\hat{L}_z\hat{L}_y + i\hbar\,\hat{L}_y\hat{L}_z = 0$$

$\therefore$ $[\hat{L}^2, \hat{L}_x] = 0$

Similarly $[\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z] = 0$

6.7 Ehrenest Theorem

P. Ehrenfest established the correspondence between the Motion of a wave packet representing a particle and the motion of a classical particle and stated that

"The expectation values or averages of the quantum mechanical variable satisfy the same equation of motion as the corresponding classical variables in the corresponding classical picture.

i.e. We can write

$$\frac{d}{dt}\langle x \rangle = \frac{1}{m}\langle P_x \rangle$$

and $$\frac{d}{dt}\langle P_x\rangle = \left\langle -\frac{dV(x)}{dx}\right\rangle$$

under the constraint that the wavefunction. $\psi(x,t)$ w.r.t which the averages are computed satisfy the time dependent Schrodinger's equation

$$i\hbar\frac{\partial\psi}{\partial t}(x,t) = \hat{H}\psi(x,t)$$

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

6.7.1 Proof of Ehrenfest Theorem

Let x be the position coordinate of a particle of mass m at time 't'. Also let the particle is under the action of a potential $V(x)$. If $\psi(x,t)$ be the wavefunction of the particle at position x and time t, then we have

$$\langle x\rangle = \int_{-\infty}^{+\infty} \psi^*(x,t)x\psi(x,t)dx \tag{1}$$

Differentiating w.r. t. time

$$\frac{d\langle x\rangle}{dt} = \frac{\partial}{\partial t}\int_{-\infty}^{+\infty} \psi^*(x,t)x\psi(x,t)dx \tag{2}$$

Also time dependent Schrodinger equation is

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

or $$\frac{\partial\psi(x,t)}{\partial t} = \frac{-i}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x,t) \tag{3}$$

Complex conjugate of eqn. (3) is

$$\frac{\partial \psi^*(x,t)}{\partial t} = \frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi^*(x,t) \qquad (4)$$

eqn. (2) can also be written as

$$\frac{d\langle x\rangle}{dt} = \int_{-\infty}^{+\infty} \frac{\partial \psi^*}{\partial t}(x,t)x\psi(x,t)dx + \int_{-\infty}^{+\infty} \psi^*(x,t)x\frac{\partial \psi(x,t)}{\partial t} \qquad (5)$$

Substituting eqns. (3) and (4) in eqn (5)

$$\frac{d\langle x\rangle}{dt} = \int_{-\infty}^{+\infty} \frac{i}{\hbar}\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi^*(x,t)x\psi(x,t)dx$$

$$+\int_{-\infty}^{+\infty} \psi^*(x,t)x\left(-\frac{i}{\hbar}\right)\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x,t)dx$$

$$\Rightarrow \quad \frac{d\langle x\rangle}{dt} = \frac{i\hbar}{2m}\int_{-\infty}^{+\infty} \left[-\frac{\partial^2\psi^*(x,t)}{\partial x^2}x\psi(x,t) + \frac{2m}{\hbar^2}V(x)\psi^*(x,t)x\psi(x,t)\right.$$

$$\left. +\psi^*(x,t)x\frac{\partial^2\psi(x,t)}{\partial x^2} - \frac{2m}{\hbar^2}\psi^*(x,t)x\psi(x,t)V(x)\right]dx$$

$$\Rightarrow \quad \frac{d\langle x\rangle}{dt} = \frac{i\hbar}{2m}\int_{-\infty}^{+\infty} \left[x\psi^*(x,t)\frac{\partial^2\psi(x,t)}{\partial x^2} - x\psi(x,t)\frac{\partial^2\psi^*(x,t)}{\partial x^2}\right]dx \qquad (6)$$

Let $I_1 = \int_{-\infty}^{+\infty} x\psi(x,t)\frac{\partial^2\psi^*(x,t)}{\partial x^2}dx$

$$= x\psi(x,t)\frac{\partial \psi^*(x,t)}{\partial x}\Bigg|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \frac{\partial}{\partial x}(x\psi(x,t))\frac{\partial \psi^*(x,t)}{\partial t}dx$$

But $\psi(x,t) \to 0$ as $x \to \pm\infty$

$$\therefore I_1 = -\int_{-\infty}^{+\infty} \frac{\partial}{\partial x}(x\psi(x,t))\frac{\partial \psi^*}{\partial t}(x,t)dx$$

or $$I_1 = \frac{-\partial}{\partial x}(x\psi(x,t))\psi^*(x,t)\Big|_{-\infty}^{+\infty} + \int_{-\infty}^{+\infty} \frac{\partial^2}{\partial x^2}(x\psi(x,t))\frac{\partial}{\partial t}\psi^*(x,t)\,dx$$

Again using the boundary conditions, we get

$$I_1 = \int_{-\infty}^{+\infty} \psi^*(x,t)\frac{\partial^2}{\partial x^2}(x\psi(x,t))dx$$

$$= \int_{-\infty}^{+\infty} \psi^*(x,t)\frac{\partial}{\partial x}\left(\psi(x,t) + x\frac{\partial\psi(x,t)}{\partial x}\right)dx$$

$$= \int_{-\infty}^{+\infty} \psi^*(x,t)\left(\frac{\partial}{\partial x}\psi(x,t) + x\frac{\partial^2\psi(x,t)}{\partial x^2} + \frac{\partial\psi(x,t)}{\partial x}\right)dx$$

$$= \int_{-\infty}^{+\infty} \psi^*(x,t)\left(x\frac{\partial^2\psi(x,t)}{\partial x^2} + \frac{2\partial\psi(x,t)}{\partial x}\right)dx \qquad (7)$$

Using I$_1$ in eqn. (6), we get

$$\frac{d\langle x\rangle}{dt} = \frac{i\hbar}{2m}\int_{-\infty}^{+\infty}\left[x\psi^*(x,t)\frac{\partial^2\psi(x,t)}{\partial x^2} - \psi^*(x,t)x\frac{\partial^2\psi}{\partial x^2}(x,t) - 2\psi^*(x,t)\frac{\partial\psi}{\partial x}(x,t)\right]dx$$

$$= \frac{i\hbar}{2m}\int_{-\infty}^{+\infty} -2\psi^*(x,t)\frac{\partial\psi}{\partial x}(x,t)dx$$

or $$\frac{d\langle x\rangle}{dt} = \frac{1}{m}\int_{-\infty}^{+\infty}\psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x,t)dx$$

But by definition

$$\langle P_x\rangle = \int_{-\infty}^{+\infty}\psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x,t)dx$$

Therefore eqn. (9) gives

$$\boxed{\frac{d\langle x\rangle}{dt}=\frac{\langle P_x\rangle}{m}} \tag{9}$$

(ii) By definition

$$\langle P_x\rangle=\int_{-\infty}^{+\infty}\psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x,t)dx$$

Differentiating w.r.t time

$$\frac{\partial}{\partial x}\langle P_x\rangle=\frac{\partial}{\partial t}\int_{-\infty}^{+\infty}\psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x,t)dx$$

$$=-i\hbar\int_{-\infty}^{+\infty}\frac{\partial\psi^*}{\partial t}(x,t)\frac{\partial\psi}{\partial x}(x,t)dx-i\hbar\int_{-\infty}^{+\infty}\psi^*(x,t)\frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial t}(x,t)\right)dx \tag{10}$$

Substituting $\frac{\partial\psi^*(x,t)}{\partial t}$ and $\frac{\partial\psi(x,t)}{\partial t}$ from eqn. (3) and (4) in eqn. (10) we get

$$\frac{d\langle P_x\rangle}{dt}=-i\hbar\int_{-\infty}^{+\infty}\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}dx$$

$$-i\hbar\int_{-\infty}^{+\infty}\psi^*(x,t)\left(\frac{-i}{\hbar}\right)\frac{\partial}{\partial x}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right)\psi(x,t)dx$$

$$=-\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\frac{\partial^2\psi^*(x,t)}{\partial x^2}\frac{\partial\psi(x,t)}{\partial x}dx+\int_{-\infty}^{+\infty}V(x)\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}dx$$

$$+\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\psi^*(x,t)\frac{\partial}{\partial x}\left(\frac{\partial^2\psi}{\partial x^2}(x,t)\right)dx-\int_{-\infty}^{+\infty}\psi^*(x,t)\frac{\partial}{\partial x}\big(V(x)(x,t)\big)dx$$

$$=\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\left[\psi^*(x,t)\frac{\partial}{\partial x}\left(\frac{\partial^2}{\partial x^2}\psi(x,t)\right)-\frac{\partial^2\psi^*(x,t)}{\partial x^2}\frac{\partial\psi(x,t)}{\partial x}\right]dx$$

$$+\int_{-\infty}^{+\infty}\left[V(x)\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x}-\psi^*(x,t)\frac{\partial}{\partial x}\big(V(x)\psi(x,t)\big)\right]dx$$

$$=\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\left[\frac{\partial}{\partial x}\left(\psi^*(x,t)\frac{\partial^2\psi}{dx^2}(x,t)\right)-\frac{\partial\psi^*(x,t)}{\partial x}\frac{\partial^2\psi(x,t)}{\partial x^2}-\frac{\partial^2\psi^*(x,t)}{\partial x^2}\frac{\partial^2\psi(x,t)}{\partial x^2}\right]dx$$

$$+\int_{-\infty}^{+\infty}\psi^*(x,t)\left(-\frac{\partial V(x)}{\partial x}\right)\psi(x,t)dx$$

$$=\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\left[\frac{\partial}{\partial x}\left(\psi^*(x,t)\frac{\partial^2\psi}{dx^2}(x,t)\right)-\frac{\partial}{\partial x}\left(\frac{\partial\psi^*(x,t)}{\partial x}\frac{\partial\psi(x,t)}{\partial x}\right)\right]dx+\left\langle-\frac{\partial V(x)}{\partial x}\right\rangle$$

$$=\frac{\hbar^2}{2m}\left[\psi^*(x,t)\frac{\partial^2\psi}{dx^2}(x,t)\Big|_{-\infty}^{+\infty}-\frac{\partial\psi^*}{\partial x}(x,t)\frac{\partial\psi}{dx}(x,t)\Big|_{-\infty}^{+\infty}\right]+\left\langle-\frac{\partial V(x)}{\partial x}\right\rangle$$

Again due to boundary conditions first two terms are zero

∴ We are left with

$$\frac{d\langle P_x\rangle}{dt}=\left\langle-\frac{\partial V(x)}{\partial x}\right\rangle \tag{11}$$

But force corresponding to potential energy V_x is

$$F_x=-\frac{\partial V(x)}{\partial x} \tag{12}$$

∴ eqn. (11) becomes

$$\frac{d\langle P_x\rangle}{dt}=\langle F_x\rangle \tag{13}$$

In the limiting case of the wave packet reducing to a point i.e, particle is localized then

$\langle x\rangle = x$ $\quad\langle P_x\rangle = P_x$ $\quad$ and $\quad\langle F_x\rangle = F_x$

Hence eqn. (9) becomes

$$\frac{dx}{dt} = \frac{P_x}{x} \qquad \text{or} \qquad P_x = m\frac{dx}{dt}, \text{ classical definition of momentum}$$

and eqn. (11) becomes

$$F_x = \frac{dP_x}{dt}; \text{ Newton's Second law of Motion.}$$

6.8 Summary

In this chapter, we learnt that the dynamical quantities in quantum mechanics are represented by operators. Also we learnt that the Heisenberg's uncertainty relation, mathematically in a concise form, can be presented in terms of commutation relations satisfied by these operators. We have also learned about Ehrenfest theorem, which in quantum mechanics, is analogues of Newton's second law.

6.9 Glossary

Utmost – Greatest

Observable - Noticeable

Correspondence - Correlation

Analogues - Similar

Concise - Compact

Uncertainty - Unpredictability

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1) Concept of Modern Physics, Arthur Beiser, 2002, McGraw-Hill.
2) Introduction to quantum Mechanics, David J. Griffith, 005, Pearson Education

3) Quantum Mechanics, Theory and Application, Ajoy Ghatak and S Loknathan, MacMillan India Ltd.

4) Theory and Problems of Modern Physics, Schaum's outline, R. Gautreau and W. Savin, 2nd edition, Tata MacGraw Hill Publishing.

6.11 Suggested Readings

1) Concept of Modern Physics, Arthur Beiser, 2002, McGraw-Hill.

2) Quantum Physics, Berkeley Physics, Vol. 4, E. H. Wichman, 2008, 2008, Tata McGraw-Hill Co.

3) Modern Physics, R. A. Serway, C. J. Moses and C.A. Moyer, 2005, Cengage Learning.

6.12 Solved Problems

Q1. Show that the operator $\hat{A} = \frac{\partial}{\partial x}$ and $\hat{B} = x^2$ do not commute when they operate on a function y^2.

Solution: Consider $\hat{A}\,\hat{B}(y^2) = \hat{A}(x^2y^2) = \frac{\partial}{\partial x}(x^2y^2) = 2xy^2$

$$\hat{B}\,\hat{A}(y^2) = \hat{B}\frac{\partial}{\partial x}(y^2) = x^2.0 = 0$$

$\therefore$ $(\hat{A}\,\hat{B} - \hat{B}\hat{A})y^2 = 2xy^2 - 0 = 2xy^2 \neq 0$

$\therefore$ $\hat{A}$ and $\hat{B}$ do not commute.

Q2. Show that the operator $\hat{A} = \frac{\partial}{\partial x}$ and $\hat{B} = p$; where p is a constant commute when operate on a function y^2.

Solution: $\hat{A}\hat{B}\,y^2 = \hat{A}(py^2) = \frac{\partial}{\partial x}(by^2) = 0$

$$\hat{B}\,\hat{A}(y^2) = \hat{B}\left(\frac{\partial}{\partial x}y^2\right) = p \cdot 0 = 0$$

Since $(\hat{A}\hat{B} - \hat{B}\hat{A})\,y^2 = 0.$ $\therefore\ \hat{A}$ commute with $\hat{B}$.

Q3. Show that $\frac{d^n}{dx^n}$ is a linear operator when n is a positive integer

Solution: Consider $\frac{d^n}{dx^n}c_1\psi_1 = c_1\frac{d^n\psi_1}{dx^n}$

and $\frac{d^n}{dx^n}c_2\psi_2 = c_2\frac{d^n\psi}{dx^n}$

$\therefore$ $\frac{d^n}{dx^n}(c_1\psi_1 + c_2\psi_2) = c_1\frac{d^n\psi_1}{dx^n} + c_2\frac{d^n\psi_2}{dx^n}$

Therefore $\frac{d^n}{dx^n}$ is a linear operator.

Q4. If $\hat{A}\psi = e^{-\psi}\psi$, then shows that $\hat{A}$ is not a linear operator. Consider

Solution: $\hat{A}(c_1\psi_1) = e^{-c_1\psi_1} \cdot c_1\psi_1$

$\hat{A}(c_2\psi_2) = e^{-c_2\psi_2} \cdot c_2\psi_2$

i.e. $\hat{A}(c_1\psi_1 + c_2\psi_2) = e^{-(c_1\psi_1 + c_2\psi_2)} \cdot (c_1\psi_1 + c_2\psi_2)$

$$= c_1\psi_1 e^{-(c_1\psi_1 + c_2\psi_2)} + c_2\psi_2 e^{-(c_1\psi_1 + c_2\psi_2)} \neq c_1\psi_1 e^{-c_1\psi_1} + c_2\psi_2 e^{-c_2\psi_2}$$

$\therefore$ $\hat{A}$ is not a linear operator.

Q5. Show that the operator $\hat{A} = \frac{d^2}{dx^2}$ is Hermitian

Solution: For an operator to be Hermitian, we have

$$\int_{-\infty}^{+\infty} \psi^* \left(\hat{A}\phi\right) dx = \int_{-\infty}^{+\infty} (\psi \hat{A})^* \phi dx$$ When ψ and ϕ are same function of x.

Let $\hat{A} = \frac{d^2}{dx^2}$.

$$\Rightarrow \quad \int_{-\infty}^{+\infty} \psi(x) \frac{d^2}{dx^2} \phi(x)\, dx = \int_{-\infty}^{+\infty} \left(\psi(x) \frac{d^2}{dx^2}\right)^* \phi(x)\, dx$$

Consider LHS $\int_{-\infty}^{+\infty} \psi^* \frac{d^2}{dx^2} \phi(x)\, dx = \psi^* \frac{d\phi}{dx}\Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} \frac{d\psi^*}{dx} \frac{d\phi}{dx} dx$

$$= \psi^* \frac{d\phi}{dx}\Big|_{-\infty}^{+\infty} - \phi \frac{d\psi^2}{dx}\Big|_{-\infty}^{+\infty} + \int_{-\infty}^{+\infty} \frac{d^2\psi^*}{dx^2} \phi\, dx$$

But wavefunctions ψ and ϕ must vanish as x →±∞.

$$\therefore \quad \int_{-\infty}^{+\infty} \psi^* \frac{d^2\phi(x)}{dx^2} dx = \int_{-\infty}^{+\infty} \left(\frac{d^2\psi^*}{dx^2}\right) \phi\, dx$$

Hence the operator $\hat{A} = \frac{d^2}{dx^2}$ is Hermitian.

Q6. Find the commutator $[x_i, x_j] and [p_i, p_j]$

Solution: Consider $[x_i, x_j]\psi$

$$= [x_i x_j - x_j x_i]\psi$$

If $i = j$

$$[x_i, x_j] = [x_i \ x_i - x_i x_i]\psi = 0$$

if $i \neq j$; let i = 1, j = 2 $\therefore x_1 = x, \ \ x_2 = y$

$$[xy - yx]\psi = 0$$

$\therefore \qquad [x_i,\, x_j] = 0$

Consider $[x_i,\, p_j]\psi = [x_i p_j - p_j x_i]\psi$

case 1 if $i = j = 1$

$$[x_1 p_1 - p_1 x_1]\psi$$

but $\qquad p_1 = p_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$ and $\qquad x_1 = x$

$\Rightarrow \qquad [xp_x - p_x x]\psi$

$$= \frac{\hbar}{i}\left[x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x\right]\psi$$

$$= \frac{\hbar}{i}\left(x\frac{\partial \psi}{\partial x} - \frac{\partial}{\partial x}(x\psi)\right)$$

$$= \frac{\hbar}{i}\left(x\frac{\partial \psi}{\partial x} - x\frac{\partial \psi}{\partial x} - \psi\right)$$

$$= -\frac{\hbar}{i}\psi$$

$\therefore \qquad [x,\, p_x]\psi = i\hbar\psi$

or $\qquad [x,\, p_x] = i\hbar$

Case 2 if $i \neq j$, let $i = 1, j = 2$

$\Rightarrow \qquad x_1 = x; \quad p_2 = p_y$

$$[x, p_y]\psi = [xp_y - p_y x]\psi$$

$$\frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - \frac{\partial}{\partial y}x\right)\psi$$

$$\frac{\hbar}{i}\left(x\frac{\partial\psi}{\partial y}-\frac{\partial}{\partial y}(x\psi)\right)$$

$$\frac{\hbar}{i}\left(x\frac{\partial\psi}{\partial y}-x\frac{\partial\psi}{\partial y}-0\right)$$

$$\frac{\hbar}{i}(0)=0$$

$\therefore \quad [x,\ p_y]=0$

Similarly $[z,\ p_y]=[x,p_z]=[y,p_x]=[y,\ p_z]=0$

$\therefore$ is general we can write $[x_i,\ p_j]=i\hbar\,\delta_{ij}$

(iii) Consider $[p_i,\ p_j]\psi$

Case 1 if $i=j=1$

$$[p_1,\ p_1]\psi=[p_x,\ p_x]\psi=[p_xp_x-p_xp_x]\psi=0$$

Case 2 $i\neq j;$ let $i=1,\ j=2$

$\therefore \quad p_1=p_x$ and $p_2=p_y$

Hence the commutation relation becomes

$$[p_x,\ p_y]\psi=[p_xp_y-p_yp_x]\psi$$

$$=\left(\frac{\hbar}{i}\right)^2\left[\frac{\partial}{\partial x}\left(\frac{\partial}{\partial y}\right)-\frac{\partial}{\partial y}\left(\frac{\partial}{\partial x}\right)\right]\psi$$

$$=-\hbar^2\left[\frac{\partial}{\partial x}\left(\frac{\partial\psi}{\partial y}\right)-\frac{\partial}{\partial y}\left(\frac{\partial\psi}{\partial x}\right)\right]$$

$$= -\hbar^2 \left[\frac{\partial^2 \psi}{\partial x \partial y} - \frac{\partial^2 \psi}{\partial y \partial x} \right] = -\hbar^2 \times 0 = 0$$

$\therefore$ in general we can write

$$[p_i, \, p_j] = 0$$

Q.7 Evaluate the commutation relations

$$[\hat{P}_x, \, \hat{L}_x], [\hat{P}_x, \, \hat{L}_y], [\hat{P}_x, \, \hat{L}_z]$$

Sol. Consider $[\hat{P}_x, \, \hat{L}_x]\psi = \hat{P}_x \hat{L}_x \psi - \hat{L}_x \hat{P}_x \psi$

$$= -i\hbar \frac{\partial}{\partial x}(-i\hbar)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right) - (-i\hbar)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right)(-i\hbar)\frac{\partial}{\partial x}\psi$$

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

$$= -\hbar^2 \left[y\frac{\partial^2 \psi}{\partial x \partial z} - z\frac{\partial^2 \psi}{\partial x \partial y} \right] + \hbar^2 \left[y\frac{\partial^2 \psi}{\partial z \partial x} - z\frac{\partial^2 \psi}{\partial x^2} \right]$$

$$= 0$$

Thus $[\hat{P}_x, \, \hat{L}_x] = 0$

(ii) Consider $[\hat{P}_x, \, \hat{L}_y]\psi = [\hat{P}_x \hat{L}_y - \hat{L}_y \hat{P}_x]\psi$

$$= -i\hbar \frac{\partial}{\partial x}\left[-i\,\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right)\psi - (-i\hbar)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right) \times -i\hbar\frac{\partial \psi}{\partial x} \right]$$

$$= -\hbar^2 \frac{\partial}{\partial x}\left(z\frac{\partial \psi}{\partial x} - x\frac{\partial \psi}{\partial z} \right) + \hbar^2 \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right)\frac{\partial \psi}{\partial x}$$

$$= -\hbar^2 \left(z\frac{\partial^2 \psi}{\partial x^2} - x\frac{\partial^2 \psi}{\partial x \partial z} - \frac{\partial \psi}{\partial z} \right) + \hbar^2 \left(z\frac{\partial^2 \psi}{\partial x^2} - x\frac{\partial \psi}{\partial z \partial x} \right)$$

$$= \hbar^2 \frac{\partial \psi}{\partial z}$$

$$= i\hbar\left(-i\hbar\frac{\partial}{\partial z}\right)\psi$$

$$= i\hbar\,\hat{P}_z\psi$$

$$[\hat{P}_x,\,\hat{L}_y] = i\hbar\,\hat{P}_z$$

(iii) Consider $[\hat{P}_x,\,\hat{L}_z]\psi = \hat{P}_x\hat{L}_z\psi - \hat{L}_z\hat{P}_x\psi$

$$= -i\hbar\frac{\partial}{\partial x}(-i\hbar)\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi - (-i\hbar)\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\times -i\hbar\frac{\partial}{\partial x}\psi$$

$$= -\hbar^2\frac{\partial}{\partial x}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi + \hbar^2\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\frac{\partial\psi}{\partial x}$$

$$= -\hbar^2\left(\frac{\partial\psi}{\partial y} + x\frac{\partial^2\psi}{\partial x\partial y} - y\frac{\partial^2\psi}{\partial x^2}\right) + \hbar^2\left(x\frac{\partial^2\psi}{\partial y\partial x} - y\frac{\partial^2\psi}{\partial x^2}\right)$$

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

$$= (-i\,\hbar)\left((-i\,\hbar)\frac{\partial}{\partial y}\right)\psi$$

$$= -i\,\hbar\,\hat{P}_y\psi$$

$$= [\hat{P}_x,\,\hat{L}_z] = -i\hbar\hat{P}_y$$

Q.8 Find the commutators

(i) $[\hat{x},\,\hat{L}_x]$ (ii) $[\hat{x},\,\hat{L}_y]$ (iii) $[\hat{x},\,\hat{L}_z]$

Sol. (i) Consider $[\hat{x},\,\hat{L}_x]\psi = \hat{x}\,\hat{L}_x\psi - \hat{L}_x\hat{x}\psi$

$$= x(-i\hbar)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\psi - (-i\hbar)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)x\psi$$

$$= -i\hbar\, xy\frac{\partial \psi}{\partial z} + i\hbar\, xz\frac{\partial}{\partial y}\psi + i\hbar\, xy\frac{\partial \psi}{\partial z} - i\hbar\, xz\frac{\partial \psi}{\partial y} = 0$$

$\therefore \quad [\hat{x},\ \hat{L}_x] = 0$

(ii) Consider $[\hat{x},\ \hat{L}_y]\psi = [\hat{x}\hat{L}_y - \hat{L}_y\hat{x}]\psi$

$$= x(-i\hbar)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\psi - (-i\hbar)\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)x\psi$$

$$= -i\hbar\, xz\frac{\partial \psi}{\partial x} + i\hbar x^2\frac{\partial \psi}{\partial z} + i\hbar z\psi + i\hbar zx\frac{\partial \psi}{\partial z} - i\hbar x^2\frac{\partial \psi}{\partial z}$$

$$= i\hbar\, z\,\psi$$

Thus $[\hat{x},\ \hat{P}_y] = i\hbar\hat{z}$

(iii) Consider $[\hat{x},\ \hat{L}_z]\psi = \hat{x}\hat{L}_z\psi - \hat{L}_z\hat{x}\psi$

$$= x(-i\hbar)\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi - (-i\hbar)\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)x\psi$$

$$= -i\hbar x^2\frac{\partial \psi}{\partial y} + i\hbar x\, y\frac{\partial \psi}{\partial x} + i\hbar x^2\frac{\partial \psi}{\partial y} - i\hbar yx\frac{\partial y}{\partial x} - i\hbar y\psi$$

$$= -i\hbar\, y\psi$$

then $\quad [\hat{x},\ \hat{L}_z] = -i\hbar\,\hat{y}$

Q.9 Show the commutation $[\hat{L}_z,\ \cos\phi] = i\hbar\sin\phi$ where ϕ is the azimuthal angle.

Solution: We know that us polar coordinates $(r, \theta,\ \phi)$,

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial \phi}$$

Consider $[\hat{L}_z,\ \cos\phi]\psi = (\hat{L}_z\cos\phi - \cos\phi\hat{L}_z)\psi$

whereψ is a function of (r, θ, ϕ)

therefore $$[\hat{L}_z, \cos\phi]\psi = -i\hbar\frac{\partial}{\partial\phi}(\cos\phi\psi) - \cos\phi\left(-i\hbar\frac{\partial}{\partial\phi}\psi\right)$$

$$= -i\hbar\ (-\sin\phi)\psi - i\hbar\cos\phi\frac{\partial\psi}{\partial\phi} + i\hbar\cos\phi\frac{\partial\psi}{\partial\phi}$$

$$= i\hbar\ \sin\phi\psi$$

Thus $\boxed{[\hat{L}_z, \cos\phi] = i\hbar\sin\phi}$

6.13 Terminal Questions

6.13.1 Short Answer Questions

Q1 Show that the sum of two linear operators is also a linear operator.

Q2 Show that the product of two linear operators is also a linear operator.

Q3 Show that the momentum operator is Hermitian.

Q4 Show that xe^{-x^2} is an eigenfunction of the linear operator $\frac{d^2}{dx^2} - 4x^2$. Also find the corresponding eigen value.

Q5 Find $\left[xyz, p_x^2\right]$.

6.13.2 Long Answer Questions

Q1 Find the values of angular momentum operator in

i) Spherical polar coordinates

ii) Cartesian coordinates

Q2 Calculate the value of the operator for square of total angular momentum in spherical polar coordinate.

Q3 i) Define eigen value and eigen function

ii) The operator for z-component of angular momentum is $\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$, find if $\sin(m\phi)$ is its eigenfunction or not.

6.13.3 Numerical problems

Q1. Evaluate the commutator $[\hat{L}_z, \sin 2\phi]$.

Q2. Evaluate the commutators $\left[\hat{p}_i, \hat{L}_j\right]$ where $i \neq j$

Q3 An Eigen function of the operator ${d^2}/{dx^2}$ is $\sin(mx)$, where m = 1,2,3...Find the corresponding eigenvalues.

Q4. State and Prove Ehrenfest Theorem.

Unit-7: One Dimensional Potential Well and Barrier Potential

CONTENTS

7.1 Introduction:

Insight into how quantum particles can be bound or scattered by potential energy fields can be obtained by considering models based on square wells and square barriers. In these models, the Schrödinger equation may be solved easily using elementary mathematics, the possible energies of a particle may be found and the properties of the wave functions are self-evident. We begin by considering the quantum states of a particle in a one-dimensional square-well potential. We shall show that there are unbound states with a continuous range of energies and that there are, when the well is deep enough, bound states with discrete energies. We shall then consider a particle incident on a square potential barrier.

In this unit, Schrödinger's equation is used to solve one-dimensional problems in which the potential is discontinuous and is such that between two points of discontinuity it is a constant. These problems are interesting since there exist many physical phenomena whose motion is one dimensional. The application of the Schrödinger's equation to one-dimensional problems enables us to compare the predictions of classical and quantum mechanics in a simple setting. Besides being simple to solve, one-dimensional problems will be used to illustrate some non-classical effects.

7.2 Objective

- To know about the Schrödinger equation and its application in one dimensional problem
- To define the bound and unbound state in one dimensional potential
- Derive an expression for one dimensional potential wells
- To determine the energy eigen value of one dimensional square well potential
- Define the meaning of potential barrier
- To calculate the transmission coefficient for single step potential barrier

7.3 Properties of one-dimensional motion

The Schrödinger's equation describing the dynamics of a microscopic particle of mass m in a one-dimensional time-independent potential is given by

$$\frac{d^2\psi(x)}{dx^2}+\frac{2m}{\hbar^2}\left(E-V(x)\right)\psi(x)=0 \tag{7.1}$$

where E is the total energy of the particle. The solution of this equation yield the allowed energy eigenvalues E_n and the corresponding wave function $\psi_n(x)$. To solve this partial differential equation, we need to specify the potential *V(x)* as well as the boundary conditions; the boundary conditions can be obtained from the physical requirements of the system. The solutions of the Schrödinger equation for time-independent potentials are stationary,

$$\psi(x,t) = \psi(x)e^{-iEt/\hbar} \tag{7.2}$$

for the probability density does not depend on time. We begin by examining some general properties of one dimensional motion and discussing the symmetry character of the solutions. Then, we apply the Schrödinger equation to various one-dimensional potentials: the potential well, finite potential wells etc.

To study the dynamic properties of a single particle moving in a one-dimensional potential, let us consider a potential *V(x)* that is general enough to allow for the illustration of all the required features.

One such potential is displayed in Fig.7.1; it is finite at $x \to \pm\infty, V(-\infty) = V_1$ and $V(+\infty) = V_2$ with V_1 smaller than V_2, and it has a minimum, V_{min}. In particular, we want to study the conditions under which discrete and continuous spectra occur. As the character of the states is completely determined by the size of the system's energy, we will be considering separately the cases where the energy is smaller and larger than the potential.

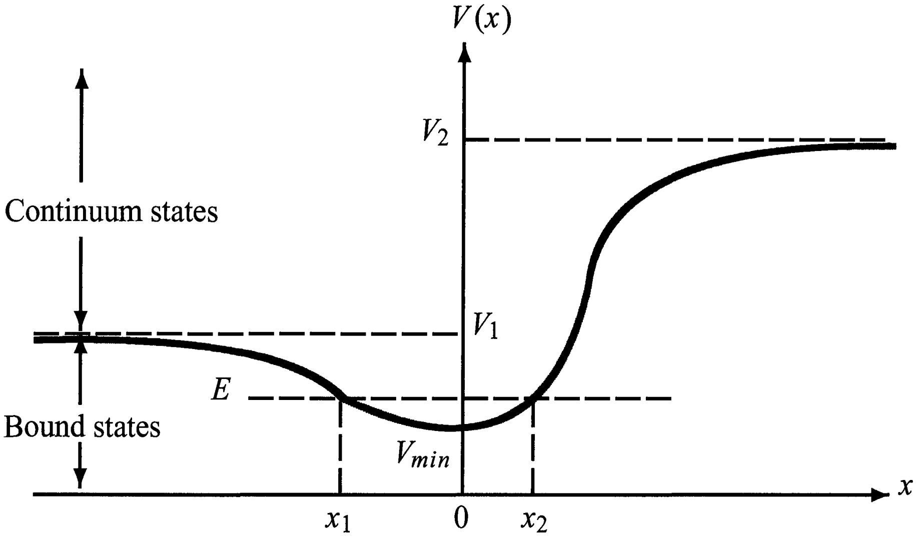

Fig.7.1: General Potential Shape

7.4 Bound States (Discrete Spectrum)

At first, we want to know about the bound states in one dimensional potential. Bound states occur whenever the particle cannot move to infinity. That is, the particle is confined or bound at all energies to move within a finite and limited region of space which is delimited by two classical turning points. The Schrödinger equation in this region admits only solutions that are discrete. The infinite square well potential and the harmonic oscillator are typical examples that display bound states.

In the potential of Fig.7.1, the motion of the particle is bounded between the classical turning points x_1 and x_2 when the particle's energy lies between V_{min} and V_1:

$$V_{min} < E < V_1. \tag{7.3}$$

The states corresponding to this energy range are called bound states. They are defined as states whose wave functions are finite (or zero) at $x \to \pm\infty$, usually the bound states have energies smaller than the potential *E<V*. For the bound states to exist, the potential *V(x)* must have at least one minimum which is lower than$V_1 (V_{min} < V_1)$. The energy spectra of bound states are discrete.

7.5 Unbound States (Continuous Spectrum)

On the other hand, the unbound states occur in those cases where the motion of the system is not confined; a typical example is the free particle. For the potential displayed in Fig.7.1 there are two energy ranges where the particle's motion is finite: $V_1 < E < V_2$and $E > V_2$.

- **Case-I: $(\boldsymbol{V_1} < E < \boldsymbol{V_2})$**
  In this case the particle's motion is infinite only towards $x = -\infty$, that is, the particle can move between $x = x_2$ and $x \to -\infty, x_2$ is a classical turning point. The energy spectrum is continuous and none of the energy eigenvalues is degenerate. The non-degeneracy can be shown to result as follows. Since the Schrödinger equation is a second order differential equation, it has, for this case, two linearly independent solutions, but only one is physically acceptable.

- **Case-II: $(\boldsymbol{E} > \boldsymbol{V_2})$**
  The energy spectrum is continuous and the particle's motion is infinite in both directions od *x* (i.e., towards $x \to \pm\infty$,). All the energy levels of this spectrum are doubly degenerate. To see this, note that the general solution to equation (7.1) is a linear combination of two independent oscillatory solutions, one moving to the left and the other to the right. In the previous nondegenerate case only one solution is retained, since the other one diverge as $x \to +\infty$ and it has to be rejected.

7.6 One dimensional potential well

Suppose a particle is moving from left to right in a region in which potential is zero. However, after a certain time it reaches in a region in which potential becomes infinite as shown in Fig.7.2.

Now the problem arises how to find the boundary condition at the surface of infinite potential. We know that the Schrödinger's equation is as follows:

$$\frac{d^2\psi_2}{dx^2}+\frac{2m}{\hbar^2}(E-V)\psi=0 \qquad (7.4)$$

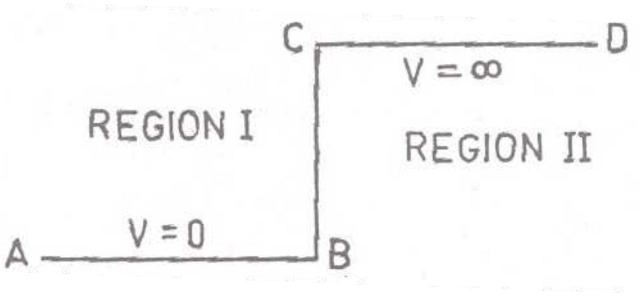

Fig. 7.2: Boundary conditions at the surface of infinite potential

For region I, the Schrödinger equation may be put as follows:

$$\frac{d^2\psi}{dx^2}+\frac{2m}{\hbar^2}E\psi_1=0\left(\because \mathrm{V}=0\right)$$

or $$\frac{d^2\psi}{dx^2}+\alpha^2\psi_1=0,\ \text{where}\ \alpha^2=\frac{2\mathrm{mE}}{\hbar^2} \qquad (7.5)$$

The general solution of equation (7.4) [for x<0] is as follows

$$\psi_1 = \mathrm{A}\cos\alpha x + \mathrm{B}\sin\alpha x, \qquad (7.6)$$

The Schrödinger equation for the region II is as follows

$$\frac{d^2\psi_2}{dx^2}+\frac{2m}{\hbar^2}(E-V)\psi_2=0, \qquad \text{(Because V>E)}$$

$$\frac{d^2\psi_2}{dx^2}-\beta^2\psi_2=0 \qquad (7.7)$$

where $\beta^2=\frac{2m(V-E)}{\hbar^2}$

The general solution of equation (7.5) [for x > 0] is as follows

$$\psi_2 = \mathrm{C}e^{\beta x} + \mathrm{D}e^{-\beta x} \qquad (7.8)$$

As the first term in Eq. (7.8) is representing an exponentially growing function for x=0, this means that it does not remain finite as x→∞. Thus, only well-behaved part in ψ_2 is second term which is the solution in the region II (x>0).

$$\psi_2 = De^{-\beta x} \tag{7.10}$$

The solutions (7.6) and (7.10) have to be continuous at x = 0, i.e. ψ_1 at x = 0 should be the same as ψ_2 at x = 0,

or $$(\psi_1)_{\alpha=0} = (\psi_2)_{\alpha=0}$$

From equation (7.6), we have $(\psi_1)_{\alpha=0} = A$.

From equation (7.8), we have $(\psi_2)_{\alpha=0} = D$.

$$\therefore \quad A = D \tag{7.11}$$

$\left(\frac{d\psi}{dx}\right)$ has also to be continuous i.e., $\left(\frac{d\psi_1}{dx}\right)_{\alpha=0} = \left(\frac{d\psi_2}{dx}\right)_{\alpha=0}$

$$\left(\frac{d\psi_1}{dx}\right)_{\alpha=0} = \beta x$$

$$\left(\frac{d\psi_2}{dx}\right)_{\alpha=0} = \beta D$$

$$\therefore B\alpha = -\beta D$$

or $$\frac{B}{D} = -\frac{\beta}{\alpha} \tag{7.12}$$

From equation (7.12) it follows that if V →∞, β also tends to infinity, and as B cannot be infinite, it implies that D should be zero

$$\therefore A = D = 0$$

or $$\psi_2 = 0$$

Hence at the surface of infinite potential wave function will be zero.

7.7 Energy levels for one-dimensional square well potential of finite depth (*OR* finite potential well)

Let us now consider a simple one-dimensional well potential of finite depth which gives rise to discrete energy levels. Suppose the potential is equal to zero within a distance on either side of the origin and is equal to +V elsewhere, as depicted in Fig. 7.3).

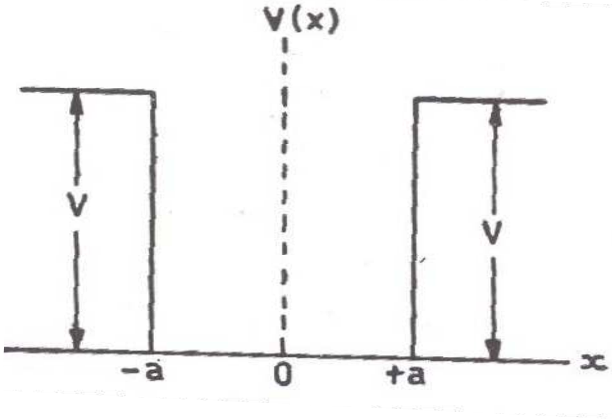

Fig. 7.3: Finite potential well.

$$V = \begin{cases} 0 & \text{for } -a < x < a \\ V & \text{for } -a > x > a \end{cases}$$

Such a potential energy function is termed as a square well potential.

In the region | x | <a, the wave equation may be put as follows:

$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}E\psi_1 = 0, \ \text{(V=0)}$$

$$\frac{d^2\psi_1}{dx^2} + \alpha^2\psi_1 = 0, \qquad \text{where } \alpha^2 = \frac{2mE}{\hbar_2} \tag{7.13}$$

The general solution of this equation is as follows:

$$\psi_1 = A\cos\alpha x + B\sin\alpha x \tag{7.14}$$

The wave equation outside this region may be put as follows:

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(V - E)\psi_2 = 0$$

or $$\frac{d^2\psi_2}{dx_2} - \beta^2\psi_2 = 0, \quad \text{where}\beta^2 = \frac{2m}{\hbar^2}\left(V - E\right) \quad (7.15)$$

The general solution of this equation for E<V (bound states) may be put as follows :

$$\psi_2 = Ce^{Bn} + De^{-Bn} \qquad (7.16)$$

On applying the boundary conditions at x = ±∞ we need that in the region

x> a, C = 0

x<-a, D=0.

Hence we get

$$\psi_1 = A \cos \alpha x + B \sin \alpha x. \qquad -a<x<a, \qquad (7.17)$$

$$\psi_2 = Ce^{Bn} \qquad x< - a \qquad (7.18)$$

$$\psi_3 = De^{-Bn}, \qquad x > a. \qquad (7.19)$$

Let us now put restrictions that ψ and $(d\psi/dx)$ should be continuous at x = ±a.

If equations (7.17) and (7.19) are considered at x = +a, and then we apply $(\psi_1)_{x=a}=(\psi_3)_{x=a}$. We obtain

$$A \cos \alpha a + B \sin \alpha a = De^{-B\alpha} \qquad (7.20)$$

and if we apply $\left(\frac{d\psi_1}{dx}\right)_{x=a}$, we obtain

$$- A^{\alpha} \sin \alpha a + B\alpha \cos \alpha a = - \beta De^{-\beta\alpha}. \qquad (7.21)$$

If Eqs. (7.17) and (7.18) are considered at x = -a and then we apply $(\psi_1)_{z=-a}=(\psi_2)_{z=-a}$ we obtain

$$A \cos \alpha a - B \sin \alpha a = Ce^{-\beta\alpha} \qquad (7.22)$$

and $\left(\frac{d\psi_1}{dx}\right)_{x=-a} = \left(\frac{d\psi_2}{dx}\right)_{x=-a}$, we get

$$- A\, \alpha \sin \alpha a + B\alpha \cos \alpha a = C\beta e^{-B\alpha} \qquad (7.23)$$

On adding and subtracting equations (7.20) and (7.22), we get

$$2A \cos \alpha a = (C+D)\, e^{-\beta\alpha} \qquad (7.24)$$

$$2B\sin\alpha a = (D-C)\, e^{-\beta\alpha} \qquad (7.25)$$

Similarly, on adding and subtracting Eqs. (7.21) and (7.23), we get

$$2B\alpha \cos \alpha a = (C - D)\, \beta e^{\beta\alpha}, \tag{7.26}$$

$$2A\alpha \sin\alpha a = (C + D)\, \beta e^{\beta\alpha}, \tag{7.27}$$

From Eqs. (7.24) and (7.27), we get

$$\alpha \tan \alpha a = \beta \tag{7.28}$$

and from Eqs. (7.25) and (7.26), we get

$$\alpha \cot\alpha a = -\beta \tag{7.29}$$

It is possible to get a solution of the equations (7.28) and (7.29) graphically.

Now the equation (7.28) is considered and put $\xi = \alpha a$ and $\beta a = \eta$ then

$$\xi \tan \xi = \eta \qquad ...(7.30)$$

and $$\xi^2 + \eta^2 = \alpha^2 a^2 + \beta^2 a^2 = a^1[\alpha^2 + \beta^2] = \frac{2mVa^2}{\hbar^2} \qquad ...(7.31)$$

= constant for a given system

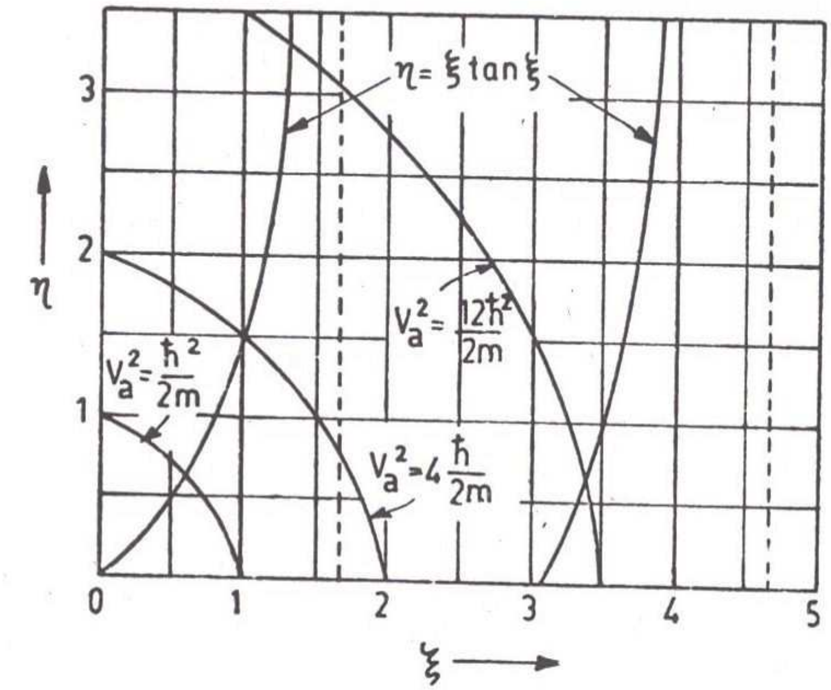

Fig. 7.4: Graphical solution of equation

As ξ and η have been restricted to positive values, it becomes possible to find out the energy levels front he intersection in the first quadrant of the curve ξ tan α plotted against ξ with the circle of known radius.

$$\left\{\frac{2mVa^2}{\hbar^2}\right\}^{\frac{1}{2}}$$

In Fig. 7.4, there are curves for three values of Va^2. For each of the two smaller of those values there occurs one solution of equation and for the largest there are two solutions.

$$\xi \tan \xi = \eta$$

Now we will consider the equation

$$\alpha \cot a = -\beta$$

$$\Rightarrow \xi \cot \xi = - \eta$$

In Fig. 7.5, there have been shown the intersections of the same circles with the curves of $-\xi \cot \xi$ versus ξ. The smallest value Va^2 does not furnish any solution while the two larger values furnish one each. Hence the three increasing values of Va^2 yield altogether one, two and three energy levels respectively.

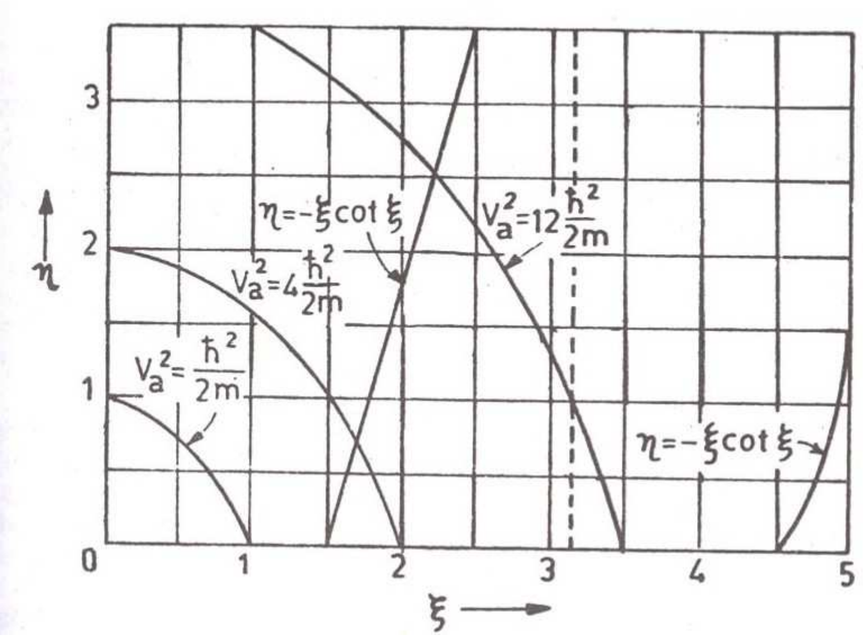

Fig. 7.5: Graphical solution of equation

$$\xi \cos \xi = - \eta$$

Let us now undertake a special case in which V approaches infinity, i.e., when the potential barrier is infinitely high. For the first group of solutions, we obtain

$$\tan \alpha a = \beta/\alpha = \infty$$

or $$\alpha a = (2n + 1)\, \pi/2 \qquad \text{...(7.32)}$$

The characteristic energy values may be put as follows:

$$E_\eta = \frac{(2n+1)^2 \pi^2 \hbar^2}{8ma^2} \qquad \text{...(7.33)}$$

For the second group of solutions, we have

$$\tan \alpha a = \frac{-\alpha}{\beta} \rightarrow 0$$

$$\therefore \qquad \alpha a = n\pi \qquad \text{...(7.34)}$$

The characteristic energy values may be put as follows:

$$E_n = \frac{(2n)^2 \pi^2 \hbar^2}{8ma^2} \qquad \text{...(7.35)}$$

One gets interesting results by finding the value of ψ at $x = \pm a$ as V is changed and also that of ψ_x = a as V approaches unity. It follows that ψ_x = a approaches zero as V approaches infinity. This result is also obtained from Eqs. (7.18) and (7.19). The general shape of ψ within the well has been found to be same as in the well of infinite depth. However, exponential tails are present on the wave functions in region on two sides of the well. These tails possess larger amplitude and fall off less rapidly with increasing distance away from the well.

An interesting new result is obtained that ψ and therefore ψ^2 is not zero in outer regions. This result is not expected when we apply the classical theory to this problem. In the outer regions kinetic energy is negative (V > E). By the negative kinetic energy, it means that classically the particle should get turned around at the edge to the well and should never appear in negative kinetic energy regions. However, the quantum mechanics predicts a probability that a particle is able to penetrate some distance into a classically forbidden region of negative kinetic energy. But it follows from the form of the wave function that ψ_n remains appreciable in size beyond the barrier provided (V – E) is small. Therefore, the degree of penetration will be a rapidly varying function of the negative kinetic energy.

The ψ does not get reduced to zero at the edges of the well. Therefore, the wave length of the oscillation within the well becomes somewhat longer, i.e., the energy levels are somewhat lower than in the preceding case. It is possible to put this conclusion in another form, i.e., walls are separated by a distance greater than 2a. It is not necessary that the wave function may not complete $\frac{1}{2}, 1, \frac{3}{2}$ etc. oscillation within the well but will have ‘little left’ over for joining smoothly with exponential tails.

Self Assessment Question (SAQ) 1:A particle with mass m is in an infinite square well potential with walls at $x = -l/2$ and $x = l/2$. Write the wave functions for the states $n = 1, n = 2, n = 3$.

Self Assessment Question (SAQ) 2:A particle is in the nth energy state $\psi_n(x)$of an infinite square well potential with width$L$. Determine the probability $P_n(\frac{1}{a})$that the particle is confined to the first$\frac{1}{a}$of the width of the well.

7.8 Potential step or a single step barrier

When the force field acting on a particle is zero or nearly zero everywhere except in a limited region, it is known as a potential step or a single step barrier. A potential step is shown in Fig. 7.6.

The potential function of a potential step may be put as follows :

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

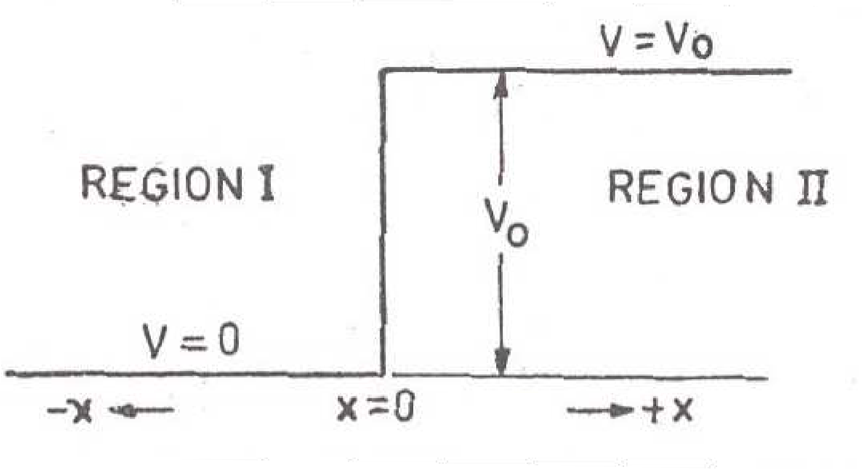

Fig. 7.6: Potential step or a single step barrier.

Suppose the electrons of energy E move from left to right, i.e., along the positive direction of x-axis. Suppose we apply quantum mechanics to this problem according to which the electrons behave like a wave when moving from left to right and face a potential hill of height $V_{(x)} = V_0$ at x = 0.

The analogy for this problem is that if light strikes a sheet of glass, the wave is partly reflected and partly transmitted. Hence in this problem the electrons at the discontinuity will be partly reflected and partly transmitted.

As V(x) = 0 for region I, the Schrödinger wave equation for this region will be

$$\frac{\partial^2\psi}{\partial x^2}+\frac{2m}{\hbar^2}E\psi=0, \qquad ...(7.36)$$

The Schrödinger wave equation for the region II will be

$$\frac{\partial^2\psi}{\partial x^2}+\frac{2m}{\hbar^2}(E-V_0)\psi=0 \qquad ...(7.37)$$

The general solutions of Eqs. (7.36) and (7.37) may be expressed as

$$\psi_1 = A\,e^{ip_1x/\hbar}+B\,e^{-ip_1x/\hbar} \qquad ...(7.38)$$

and

$$\psi_2 = C\,e^{ip_2x/\hbar}+D\,e^{-ip_2x/\hbar} \qquad ...(7.39)$$

where ψ_1 and ψ_2 are the wave functions for the regions I and II respectively; A, B, C and D are constants of integration and can be evaluated by the boundary conditions; ρ_1 and ρ_2 are the momenta in the regions I and II respectively and are given by

$$\left.\begin{aligned}\rho_1 &= \sqrt{}(2mE)\\ \rho_2 &= \sqrt{}[2m(E-V_0)]\end{aligned}\right\} \qquad ...(7.40)$$

In Eq. (7.38), the first term represents a wave advancing in the positive direction of x-axis in the first region, i.e., incident wave and the second term represents a wave moving in the negative direction of x, i.e., reflected wave.

Similarly, in Eq. (7.39), the first term represents a wave advancing in the positive direction of x-axis in the region II, i.e., transmitted wave and the second term represents a wave moving in the negative direction of x-axis in the region II, i.e., reflected wave. As there occurs discontinuity only at x=0 in the region II and after which there occurs no discontinuity in this region, it means that the reflection will not take place in this region, i.e., D=0.

Hence Eq. (7.39) becomes as follows:

$$\psi_2 = Ce^{ip_2x/\hbar} \qquad ...(7.41)$$

7.8.1 Boundary conditions

In order for ψ to be finite, E and V must be finite because infinite energies do not occur in nature. Then, from Schrödinger equation, it follows that $\frac{\partial^2\psi}{\partial x^2}$ is not necessarily continuous but is everywhere finite. In order for $\frac{\partial^2\psi}{\partial x^2}$ to be finite, $\frac{\partial\psi}{\partial x}$ should be continuous everywhere. By the continuity of $\frac{\partial\psi}{\partial x}$, it means that

$$\frac{\partial\psi_1}{\partial x} = \frac{\partial\psi_2}{\partial x} \text{ at } x = 0, i.e.,$$

i.e., $$\left(\frac{\partial\psi_1}{\partial x}\right)_{x=0} = \left(\frac{\partial\psi_2}{\partial x}\right)_{\mathrm{x=0}} \qquad ...(7.42a)$$

This is the first boundary condition.

In order for $\frac{\partial\psi}{\partial x}$, ψ must be continuous. By the continuity of ψ it implies that $\psi_1=\psi_2$ and x=0, i.e.,

$$(\psi_1)_{x=0} = (\psi_2)_{x=0} \qquad ...(7.42b)$$

This is the second boundary condition.

On applying the boundary condition Eq. (7.42b) to Eqs. (7.38) and (7.39), we get

$$A + B = C \qquad ...(7.43)$$

On differentiating Eqs. (7.38) and (7.42), we obtain

$$\frac{\partial\psi_1}{\partial x} = \frac{ip_1}{\hbar}\left[Ae^{ip_1x/\hbar} - Be^{-ip_1x/\hbar}\right] \qquad ...(7.44)$$

$$\frac{\partial\psi_1}{\partial x} = \frac{ip_2}{\hbar}Ce^{ip_2x/\hbar} \qquad ...(7.45)$$

On applying the boundary condition (7.42a) to Eqs. (7.44) and (7.45), we obtain

$$p_xC=p_1[A + B] \qquad ...(7.46)$$

On solving Eqs. (7.43) and (7.46) for B and C, we obtain

$$C = \frac{2p_1A}{p_1 + p_2} \qquad ...(7.47)$$

$$B = \frac{p_1 - p_2}{p_1 + p_2}A, \qquad ...(7.48)$$

In the above equations, B and C are denoting the amplitudes of reflected and transmitted beam in terms of the amplitude of incident wave.

In order to understand further steps, we should define reflectance and transmittance at the potential discontinuity.

At the potential discontinuity, the reflectance, reflectivity or reflection coefficients may be defined as the ratio of magnitude of reflected current to the magnitude of incident current, i.e.

$$\text{Reflectance, } \mathrm{R} = \frac{\text{magnitude of reflected current}}{\text{magnitude of incident current}} \qquad ...(7.49)$$

At the potential discontinuity, the transmittance may be defined as the ratio of magnitude of transmitted current to the magnitude of incident current

$$\text{Transmittance, } \mathrm{T} = \frac{\text{magnitude of transmitted current}}{\text{magnitude of incident current}} \qquad ...(7.50)$$

Two cases may arise :

(a) $E > V_0$

(b) $E < V_0$

Let us discuss these one by one.

- ***Case-I:*** **$E > V_0$**

When $E > V_0$, ρ_2 is real. In this case we will now derive the current density in the I and II regions.

In region I, we have

$$\psi_1 = Ae^{i\rho_1 x/\hbar} + Be^{-i\rho_1 x/\hbar} \qquad ...(7.51)$$

Its complex conjugate ψ_1^* would become as follows :

$$\psi_1^* = A^* e^{-i\rho_1 x/\hbar} + B^* e^{i\rho_1 x/\hbar} \qquad ...(7.52)$$

On differentiating Eqs. (7.51) and (7.52) with respect to x, we get

$$\frac{\partial \psi_1}{\partial x} = \frac{i\rho_1}{\hbar}\left[Ae^{i\rho_1 x/\hbar} - Be^{-i\rho_1 x/\hbar}\right] \qquad ...(7.53)$$

$$\frac{\partial \psi_1}{\partial x} = -\frac{i\rho_1}{\hbar}\left[A^{*}{}_{e}{}^{-i\rho_1 x/\hbar} - B^{*}{}_{e}{}^{i\rho_1 x/\hbar}\right] \qquad ...(7.54)$$

We know that the probability current may be defined as follows :

$$J = \frac{\hbar}{2im}\left[\psi^* \nabla \psi - \psi \nabla \psi^*\right]$$

When this relation is applied to region I, it becomes as follows :

$$\left(J_x\right)_1 = \frac{\hbar}{2im}\left[\psi_1^* \frac{\partial \psi_1}{\partial x} - \psi_1 \frac{\partial \psi_1^*}{\partial x}\right] \qquad \text{...(7.55)}$$

On substituting Eqs. (7.51), (7.52), (7.53) and (7.54), we obtain

$$\left(J_x\right)_1 = \frac{\hbar}{2im}\left[\left\{\left(Ae^{ip_1x/\hbar} + B^* e^{ip_1x/\hbar}\right)\right.\right.$$

$$X\left(\frac{-ip_1}{\hbar}\right)\left(A^{*-}e^{ip_1x/\hbar}\right)\Big\} - \Big\{\left(Ae^{ip_1x/\hbar} + Be^{-ip_1x/\hbar}\right)$$

$$X\left(\frac{-ip_1}{\hbar}\right)\left(A^{*-}e^{ip_1x/\hbar} - B^* e^{ip_1x/\hbar}\right)\Big\}\Big],$$

$$= \frac{p_1\left(AA^* - B^*B\right)}{m} = \frac{p_1}{m}\left[|A|^2 - |B|^2\right] \qquad \text{...(7.56)}$$

From the above relation it is evident that the current in the region I is equal to the difference between two terms, of which the first one which is proportional to$p_1|A|^2$ represents the incident beam travelling from the left to right, whereas the second one which is proportional to $p_1 |B|^2$ represents the reflected beam travelling from right to left. Hence,

The probability current of the incident beam = $|A|^2 \frac{p_1}{m}$ ...(7.57)

and the probability current of the reflected beam = $|B|^2 \frac{p_1}{m}$ ...(7.58)

Let us now consider the region II. In this region, we have

$$\psi_2 = Ce^{ip_2x/\hbar} \qquad \text{...(7.59a)}$$

Its complex conjugate would be given as follows :

$$\psi_2^* = C^* e^{-ip_2x/\hbar} \qquad \text{...(7.59b)}$$

On differentiating Eqs. (7.59a) and (7.59b) with respect to x, we get

$$\frac{\partial \psi_2}{\partial x} = \frac{ip_2}{\hbar} C e^{ip_2 x/\hbar} \qquad \text{...(7.59c)}$$

$$\frac{\partial \psi_2^*}{\partial x} = -\frac{ip_2}{\hbar} C * e^{-ip_2 x/\hbar} \qquad \text{...(7.59d)}$$

The expression for probability current in region II becomes as follows :

$$(J_x)II = \frac{\hbar}{2im}\left[\psi_2 * \frac{\partial \psi_2}{\partial x} + \psi_2 \frac{\partial \psi_2 *}{\partial x}\right] \qquad \text{...(7.59e)}$$

On substituting Eqs. (7.59a), (7.59b), (7.59c), and (7.59d) in Eq. (7.59e), we get

$$(J_x)II = \frac{\hbar}{2im}\left[\left\{C^* e^{ip_2 x/\hbar}\left(\frac{ip_2}{\hbar}\right)C e^{ip_2 x/\hbar}\right\} - \left\{C e^{ip_2 x/\hbar}\left(-\frac{ip_2}{\hbar}\right)C^* e^{-ip_2 x/\hbar}\right\}\right]$$

$$= \frac{p_2}{2m}\left[CC^* + CC^*\right]$$

$$= \frac{p^2}{m}(CC*) = \frac{|C|^2 \, p_2}{m} \qquad \text{...(7.60)}$$

From Eqs. (7.60), it is evident that there is only transmitted wave in region II, Thus, Eq. (7.60) represents the transmitted current.

Let us now find the expressions for reflectance and transmittance for the case when E>V_0 or p_1 is real.

Thus, we have

$$\text{Reflectance } \mathrm{R} = \frac{\text{magnitude of reflected current}}{\text{magnitude of incident current}}$$

On substituting Eqs. (7.57) and (7.58) in the above relation, we get

$$R = \frac{|B|^2 \, p_1 / m}{|A|^2 \, p_1 / m} \qquad \text{...(7.60a)}$$

where we have

$$B = \frac{p_1 - p_2}{p_1 + p_2}.A$$

or

$$\frac{B}{A} = \frac{p_1 - p_2}{p_1 + p_2}$$

On substituting the above relation in Eq. (7.60a), we get

or $$R = \frac{(p_1 - p_2)^2}{(p_1 + p_2)^2} \qquad ...(7.61)$$

Thus we have

$$\text{Transmittance } T = \frac{\text{Magnitude of transmitted current}}{\text{magnitude of incident current}}$$

From the above relations we get

$$T = \frac{|C|^2 \; p_2/m}{|A|^2 \; p_1/m}$$

$$T = \left(\frac{2p_1}{p_1 + p_2}\right)^2 . \frac{p_2}{p_1}$$

$$T = \frac{4p_1p_2}{(p_1 + p_2)} \qquad ...(7.62)$$

From the definitions of reflectance and transmittance, it follows that the sum of reflectance and transmittance must be equal to unity. This can be verified by using Eqs. (7.61) and (7.62).

$$R + T = \frac{(p_1 - p_2)^2}{(p_1 + p_2)^2} + \frac{4p_1p_2}{(p_1 + p_2)^2}$$

$$= \frac{(p_1 - p_2)^2 + 4p_1p_2}{(p_1 + p_2)^2} = \frac{(p_1 + p_2)^2}{(p_1 + p_2)^2} = 1 \qquad ...(7.63)$$

From Eq. (7.61) it follows that

(i) the reflectance approaches zero as p_2 approaches p_1 and

(ii) the reflectance approaches unity as p_2 approaches zero

We also know

$$p_2 = \sqrt{2m(E - V_0)}$$

$$p_1 = \sqrt{2mE}$$

From the above expressions it follows that p_2 would approach zero when V_0 is zero, i.e., the reflectance would be zero when V_0 becomes equal to zero. It means that some reflection must take place even if $E>V_0$. The reflectance would be large only when V_0 is almost comparable in size with E. It is to be kept in mind that it is the wave nature of matter that gives rise to the property of reflection from a sudden change in potential. However, the classical theory does not give rise to this property when $E>V_0$. Thus, it may be concluded that the property of reflection from a sudden change in potential is purely a quantum mechanical effect.

- ***Case-II:* $E<V_0$**

When $E<V_0$,p_2 is imaginary. We know,

$$p_2 = i\sqrt{2m}\{(V_0 - E)\} \qquad ...(7.64)$$

Its complex conjugate would be

$$p_2^* = \sqrt{[2m(V - E)]} = -p_2 \qquad ...(7.65)$$

As p_2 is imaginary, it is possible to calculate the probability current associated with wave function ψ_2 in the following way.

$$\psi_2 = Ce^{ip_2 x/h} \qquad ...(7.66)$$

$$\psi_2^* = C^* e^{-ip_2^* x/h} (\because\ p_2 \text{ is imaginary}) . \qquad ...(7.67)$$

On differentiating Eqs. (7.56) and (7.67), we get

$$\frac{\partial \psi_2}{\partial x} = \frac{ip_2}{\hbar} Ce^{ip_2 x/\hbar} \qquad ...(7.68)$$

$$\frac{\partial {\psi_2}^*}{\partial x} = -\frac{i{p_2}^*}{\partial x} C^* p^{-i{p_2}^* x/\hbar} \qquad ...(7.69)$$

The probability current in this case would be given by

$$J_x = \frac{\hbar}{2im}\left[{\psi_2}^* \frac{\partial \psi_2}{\partial x} \psi_2 \frac{\partial {\psi_2}^*}{\partial x} \right] \qquad ...(7.70)$$

or

$$J_x = \frac{\hbar}{2im}\left[C^* e^{ip^* x/\hbar} \left(\frac{ip_2}{\hbar} \right) Ce^{+ip_2 x/\hbar} \right.$$

$$\left. - Ce^{ip_2 x/\hbar} \left(\frac{i{p_2}^*}{\hbar} \right) C^* e^{-i{p_2}^* x/\hbar} \right] \qquad ...(7.71)$$

But $p_2^{\,*} = p_2$

$$\therefore J_x = \frac{\hbar}{2im}\left[C^* e^{ip_2x/\hbar}\left(\frac{ip_2}{\hbar}\right)Ce^{+ip_2x/\hbar} - CC^*\left(\frac{ip_2}{\hbar}\right)e^{ip_2x/\hbar}e^{ip_2x/\hbar}\right]$$

$$=0 \qquad \text{...(7.72)}$$

It means that the transmittance current is zero. Also we know

$$\text{The transmittance} = \frac{\text{magnitude of transmitted current}}{\text{magnitude of reflected current}}$$

$$= \frac{0}{\text{magnitude of reflected current}}$$

i.e., $T = 0$ ...(7.73)

We also know,

$$\text{The reflectance } R = \frac{\text{magnitude of reflected current}}{\text{magnitude of incident current}}$$

$$R = \frac{(BB^*)\frac{p_1}{m}}{(AA^*)\frac{p_1}{M}}$$

$$R = \frac{\left(\frac{p_1 - p_2}{p_1 + p_2}\right)A\left(\frac{p_1 - p_2}{p_1 + \hbar_2}\right)^* A^*}{AA^*} = \frac{(p_1 - p_2)(p_1 - p_2)}{(p_1 + p_2)(p_1 + p_2)}$$

[By using Eq. (7.48) and its complex conjugate]

$$R = \frac{(p_1 - p_2)(p_1 - p_2^{\,*})}{(p_1 + p_2)(p_1 + p_2^{\,*})} = \frac{(p_1 - p_2)(p_1 + p_2)}{(p_1 + p_2)(p_1 + p_2)} \qquad \left(\text{since } p_2^* = -p_2\right)$$

or $R=1$ ...(7.74)

From Eqs. (7.73) and (7.74), it is evident that the entire wave gets reflected when $E<V_0$, i.e., no electrons are transmitted but all are reflected.

Self Assessment Question (SAQ) 3: Write the difference between reflectance and transmittance coefficient.

Example7.1:*Suppose a beam of electrons gets impinged on an energy barrier of height 0.035 eV and of infinite width. Calculate the fraction of electrons reflected and transmitted at the barrier when the energy of the impinging electrons is*

(i) *0.035 eV*
(ii) *0.045 eV*
(iii) *0.020 eV.*

Sol. *(i)* Here E = V_0

$$p_1 = \sqrt{2mE}$$

$$= \sqrt{2 \times 9 \times 10^{-28} \times 0.035 \times 1.6 \times 10^{-12}} \text{ g cm/sec}$$

$$= 1.0039 \times 10^{-20} \text{ g cm/sec}$$

$$p_2 = \sqrt{2m(E - V_0)}$$

$$= 0 \qquad (\because E = V_0)$$

Fraction of electrons reflected

$$= \frac{(p_1 - p_2)^2}{(p_1 + p_2)^2}$$

$$= \frac{(1.0039 \times 10^{-20} - 0)^2}{(1.0039 \times 10^{-20} + 0)^2} = 1$$

Fraction of electrons transmitted

$$= \frac{4 p_1 p_2}{(p_1 + p_2)^2}$$

$$= \frac{4 \times 1.0039 \times 10^{-20} \times 0}{(1.0039 + 0)^2}$$

=0. Ans.

(ii) Here E= 0.045 eV

$=0.045 \times 1.6 \times 10^{-12}$ erg. $= 7.2 \times 10^{-14}$ erg.

$V_0 = 0.035$ eV

$= 0.035 \times 1.6 \times 10^{-12}$ erg $= 5.6 \times 10^{-14}$eg.

$$p_1 = \sqrt{2mE} \qquad (\because m = 9\times10^{-25} \text{ g.})$$

$$= \sqrt{2\times9\times10^{-28}\times7.2\times10^{-44}\text{ erg}}$$

$=1.1384 \times 10^{-20}$ g cm/sec.

$$p_2 = \sqrt{2m(E-V_0)}$$

$$= \sqrt{2\times9\times10^{-28}(7.2\times10^{-14}-5.6\times10^{-14}}$$

$$= \sqrt{2\times9\times10^{28}\times1.6\times10^{-14}}$$

$=5.3665 \times 10^{-21}$ g cm/sec.

But $E > V_0$,

$$\text{Reflectance} \quad = \frac{(p_1 - p_2)^2}{(p_1 + p_2)^2}$$

$$= \frac{(1.1384\times10^{-20} - 5.3665\times10^{21})^2}{(1.1384\times10^{-20} + 5.3665\times10^{21})^2}$$

$$= \frac{3.6210\times10^{-41}}{2.8057\times10^{-40}}$$

$=0.1290.$

Fraction of electrons reflected ≈ 0.13.

Fraction of electrons transmitted

$$= \frac{4p_1p_2}{(p_1+p_2)^2}$$

$$= \frac{4\times1.1384\times10^{-20}\times5.3665\times10^{-21}}{(1.1384\times10^{-20}+5.3665\times10^{21})^2}$$

$$= \frac{2.4436\times10^{40}}{2.8057\times10^{-40}}$$

=0.87094.

Fraction of electrons transmitted ≈ 0.87.

(iii) In this case, $E < V_0$. It means that

Transmission coefficient = 0

Thus, the fraction of electrons transmitted = 0.

and, the fraction of electrons reflected = 1.

Example 7.2:*A particle of mass m moves in a potential $V(r)=-V_0$ when $r<a$, and $V(r)=0$ when $r>a$. Find the least value of V_0 such that there is a bound state of zero energy and zero angular momentum.*

Sol.: Since there is no angular momentum, the Schrödinger equation reduced to

$$-\frac{\hbar^2}{2m}\left\{\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right\}\psi = E\psi \quad \text{(outside the well)}$$

and

$$-\frac{\hbar^2}{2m}\left\{\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}\right\}\psi = (V_0+E)\psi \quad \text{(inside the well)}$$

With the introduction of $U=r\psi$, the wave equation is

$$U'' - \alpha^2 U = 0 \qquad (r > a),$$

and

$$U'' + \beta^2 U = 0 \qquad (0 \le r \le a),$$

where

$$\alpha = \left[-\frac{2mE}{h^2}\right]^{1/2}$$

$$\text{and} \quad \beta = \left[\frac{2m(V_0+E)}{h^2}\right]^{1/2}$$

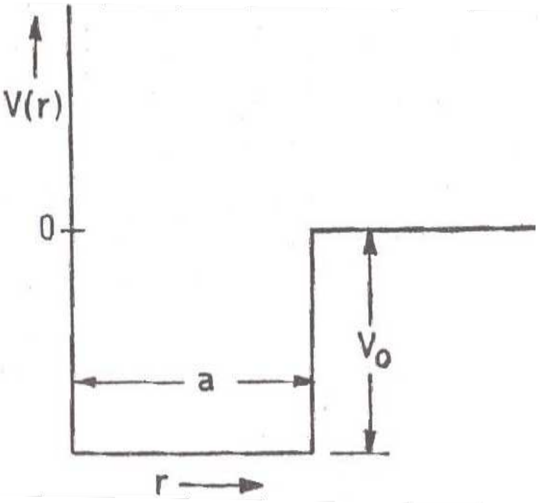

Fig. 7.7

We are interested in the limit E→0. Solutions are

$$\psi = A\frac{\rho e^{-\alpha r}}{r}(r > a),$$
$$\psi = B\frac{\sin\beta r}{r}(r < a),$$

where we have eliminated the solution singular at the origin. Continuity of ψ and its derivative at $r=a$ (equivalently, and easier, continuity of U and its derivate) requires that $\beta\cot\beta a = -\alpha$. As $E\to 0, \alpha\to 0$; hence cot $(\beta a)\to 0$. This happens when $\beta a=\pi/2$, or $V_0=\pi^2 h^2/8ma^2$.

Example 7.3:*Calculate the value of* E_0 *for an electron moving back and forth between potential barriers* 10^{-7} *cm apart* ($m=9.1 \times 10^{-28}$ *g).*

Sol. We know $$E_0 = \frac{h^2}{8ma^2}$$

$$= \frac{\left(6.63\times10^{-27}\right)^2}{8\times9.1\times10^{-28}\times\left(10^{-7}\right)^2}$$

$=6.04\times10^{-13}$ erg.Ans.

Example 7.4:*Calculate the value of the difference between the energy of a molecule of the moving back and forth on a path 1 cm long when n=2 and n=3 at T=298°K.*

Sol. We know $$E_n = n^2 \frac{h^2}{8m^2}$$

$$E_2 = \frac{2^2 \times \left(6.63\times10^{-27}\right)^2}{8\times\frac{4}{6.02\times10^{28}}\times1^2}$$

$$E_3 = \frac{3^2 \times \left(6.63\times10^{-27}\right)^2}{8\times\frac{4}{6.02\times10^{23}}\times1^2}$$

$$E_3 - E_2 = (-4)(8.27\times10^{-31})$$

$=4.13\times10^{-30}$ ergAns.

Example 7.5: *If the electron having de Broglie's wave length as 1.21×10^{-8} cm is confined in a one-dimensional box, how far apart must the walls of the box be when five loops of the de Broglie wave span the distance from one wall to the other?*

Sol. A loop is just half as long as the wave length, i.e., $(1.21\times10^{-8})/2$ or 0.605×10^{-8} cm. If there are five loops between the walls of the box, the distance between the walls must be five times the length of the loop i.e., $5\times0.605\times10^{-8}$ cm or 3.03×10^{-8} cm.

7.9 Summary:

This unit has considered a particle in the potential energy field given in Fig. 7.2. We have chosen this simple potential because it permits the solution of the Schrodinger equation using elementary methods and because it leads to wave functions which are easy to visualize. Clearly, the detail of the results is only relevant to this particular potential, but the following general features are relevant in atomic, nuclear and particle physics:

- Wave functions undulate in classically allowed regions and fall off exponentially in classically forbidden regions.
- Potentials give rise to bound states with discrete energies when they are sufficiently attractive.

7.10References:

1. Beiser A., *Concepts of Modern Physics*, 6th Edition, Mcgraw Hill (2003) Isbn 0-07-244848-2.
2. Zettili Nouredine,*Quantum Mechanics: Concepts and Applications*, John Wiley and Son's Publishers,United Kingdom(2009) Isbn 978-0-470-02678-6.

3. Shankar, R., *Principles Of Quantum Mechanics*, Kluwer Academic / Plenum Publishers New York (1994) Isbn 0-306-44790-8.
4. Chatwal, G. R.; Anand, S. K.; Arora, M., *Quantum Mechanics,* Himalaya Publishing House (2007) Isbn 978-9-350-24732-7.

7.11 SuggestedReading:

1. Quantum Mechanics by E Merzbacher
2. A Text book of Quantum Mechanics by P M Mathews and K Venkatesan
3. Introduction to Quantum Mechanics by J Griffiths David
4. Quantum Mechanics: A Textbook for Undergraduates by Jain Mahesh

7.12TERMINAL QUESTIONS:

Objective type questions:

a) According to Schrödinger a particle is equivalent to a-
- (i) Single wave
- (ii) Wave packet
- (iii) Light wave
- (iv) Cannot behave as wave

b) Of the following having the same kinetic energy, which has the longest wavelength?
- (i) An electron
- (ii) A proton
- (iii) A neutron
- (iv) An alpha particle

c) In case of a potential step of height V_0. If a classical particle of energy $E<V_0$ the transmittance is-
- (i) Zero
- (ii) Finite non-zero
- (iii) Infinite
- (iv) 1

d) The wave $\Psi = A \exp{(ikx)}$ represents-
- (i) The wave travelling along x-axis
- (ii) The wave travelling along negative x-axis
- (iii) The wave travelling along any direction
- (iv) None of these

Short Answer type questions:

Q.7.1 Define bound and unbound states for one dimensional potential.

Q.7.2 Write the Schrodinger equations for one dimensional potential walls.

Q.7.3 What are the impotency of boundary conditions?

Q.7.4 Discuss the one dimensional potential step.

Q.7.5 Define the probability current for any complex wave function.

Long Answer type questions:

Q.7.6 Derive an expression for one dimensional finite potential wall potential and deduce the eigen value equations.

Q. 7.7 The potential function for a certain particle moving along positive direction of X-axis is represented as

$$\begin{aligned} V(x) &= 0 \; for \; x < 0 \\ &= V_0 \; for \; x \geq 0 \, . \end{aligned}$$

Calculate the transmittance and reflectance at the potential $R + T = 1$, where R is reflectance and T is the transmittance.

Q. 7.8A particle is moving in a one-dimensional potential, given by

$$\begin{aligned} V(x) &= 0 \; for \; x < 0 \\ &= V_0 \; for \; x \geq 0 \, . \end{aligned}$$

(a) Write down the Schrödinger wave equation for the particle and solve it.
(b) Find the reflection and transmission coefficients for the case of (i) $E>V_0$ and (ii) $0<E<V_0$, where *E* is the total energy of the particle.

Q. 7.9 An electron having kinetic energy 10eV at $x = \infty$ is moving from left to right along X-axis. The potential energy is V= 0 for x<0 and V= 20eV for x>0. Treating to electron as a one dimensional plane wave:

(a) Write Schrödinger equation for x<0 and x>0.

(b) Sketch to solution of Schrödinger equation in the two regions x<0 and x>0.

(c) What is the wavelength of electron in x<0.

(d) What are the boundary conditions at x= 0.

(e) What is the probability of finding the electron at some positive value of x.

Q. 7.10 Calculate the discrete energy levels of a particle in one-dimensional square well potential with (i) perfectly rigid walls (ii) finite potential step.

Q. 7.11 Given that V= 0 for x<0 and x>0 and that a potential barrier of arbitrary shape V(x) exists in 0<x<a. Shaw that the coefficient of reflection of particle incident on the barrier is same whether they approach from the right or from the left.

Q. 7.12 An alpha particle is trapped in a nucleus whose radius is r₀ = $1.4 \times 10^{-15} m$. What is the probability that an alpha particle will escape from the nucleus if its energy is 2MeV? The potential barrier at the surface of the nucleus is 4 MeV.

7.14 (a) Answers of Self Assessment Question (SAQ):

Ans.1: $\psi_1(x) = \sqrt{2/L}\cos\left(\frac{\pi x}{L}\right)$

$$\psi_2(x) = -\sqrt{2/L}\sin\left(\frac{2\pi x}{L}\right)$$

$$\psi_3(x) = -\sqrt{2/L}\cos\left(\frac{3\pi x}{L}\right)$$

Ans.2: $P_n\left(\frac{1}{a}\right) = \int_0^{L/a} \psi^2{}_n(x)\, dx = \frac{1}{a} - \frac{sin 2n\pi/a}{2n\pi}$

Ans.3: Refer section 7.8 to ans.

(b) Answers of Terminal Questions:

Answer of objective questions: a) (ii) **b)** (i) **c)**(i) **d)**(i)

Ans.7.6: Refer section 7.7 to solve.

Ans.7.7 to 7.11: Refer section 7.8 to solve.

Ans. 7.12: P = 0.124.

Unit-8: Reflection and Transmission Coefficients for a Rectangular Barrier in One Dimension

CONTENTS

8.1 Introduction

In the present unit we describe that how a particle interacts with the rectangular barrier in case of one dimension. The ability to penetrate and tunnel through a classically forbidden region is one of the most important properties of a quantum particle. In the previousunit, we discovered that the wave function of a bound particle extends beyond the region of confinement of a bound classical particle. Now, we shall show how particles can tunnel through potential barriers. Here we checked thatif a classical particle approaches the barrier from the left, it would be reflected if its energy is below of the barrier and it would be transmitted if its energy is above the barrier. We shall see that when a quantum particle encounters the barrier, the outcome is uncertain; it may be reflected or it may be transmitted. Most importantly, we shall show that the particle may be transmitted even when its energy is below ofthe barrier, and we shall calculate the probability for this to happen.

8.2 Objective

- To define the rectangular potential barrierin one dimensional
- Derive and write the transmission and reflected coefficients
- To discuss the classical and quantum approach of the tunneling effect
- Explain the various examples of the tunneling phenomena
- To study the attractive square well potential

8.3 Rectangular potential barrier

In this unit we shall study some applications of Schrödinger equation which beyond the potential step. Suppose there is one-dimensional problem (Fig. 8.1) where the potential function may be defined as follow :

$$\left.\begin{aligned} V(x) &= 0 \text{ for } x < 0 \\ &= V_0 \text{ for } 0 < x < a \\ &= 0 \text{ for } x > a \end{aligned}\right\} \qquad \ldots(8.1)$$

Here there is a potential barrier between *x=0* and *x=a*.If a particle having energy less than V_0, i.e., $E<V_0$ approaches this barrier from the left, i.e., from region I, classically the particle will always get reflected and will not penetrate the barrier. However, wave mechanics predicts that the particle will not necessarily be reflected by the barrier but there is always a probability that it may cross the barrier and continue its forward motion to the region III. This probability of crossing the barrier is termed as the tunnel effect.

Further, if $E>V_0$, classical mechanics predicts that the particle will always get transmitted whereas wave mechanics predicts that the particle is having finite probability of transmission and therefore it is not certain that the particle will penetrate the barrier.

In order to solve this problem, the Schrödinger's wave equation will be written for three regions one by one.

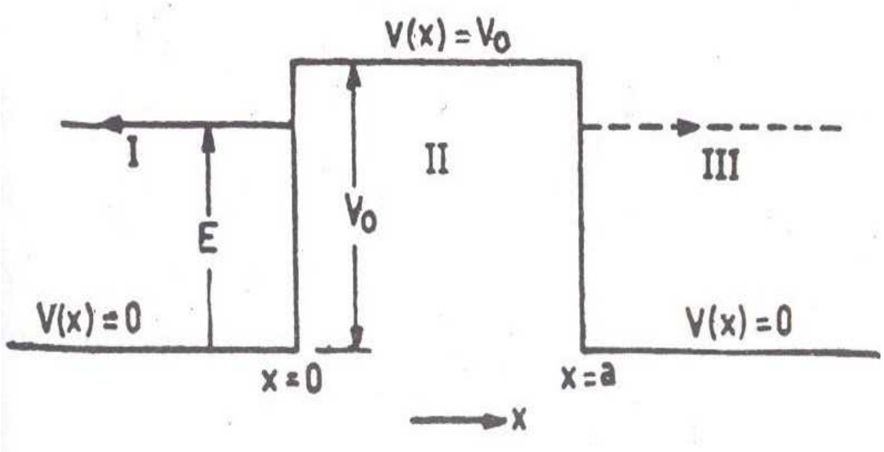

Fig. 8.1 Rectangular potential barrier

The Schrödinger equation for regions I may be put as follows :

$$\frac{\partial^2\psi_1}{\partial x^2} + \frac{2m}{\hbar^2}E\psi_1 = 0, \quad (\text{Since } V = 0) \qquad \ldots(8.2)$$

The Schrödinger equation for region II may be put as follows:

$$\frac{\partial^2\psi_z}{\partial x^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_2 = 0 \qquad \ldots(8.3)$$

Similarly, the Schrödinger equation for region III may be put as follows :

$$\frac{\partial^2\psi_z}{\partial x^2}+\frac{2m}{\hbar^2}E\psi_3=0 \qquad ...(8.4)$$

In Eqs. (8.2), (8.3) and (8.4) ψ_1, ψ_2 and ψ_3 represent wave-function for region I, II and III respectively.

The general solutions of equations (8.2), (8.3) and (8.4) may be put as follows :

$$\psi_1=A_1e^{ip_1x/\hbar}+B_1e^{-ip_1x/\hbar} \qquad ...(8.5)$$

$$\psi_z=A_2e^{ip_2x/\hbar}+B_2e^{-ip_2x/\hbar} \qquad ...(8.6)$$

$$\psi_2=A_3e^{ip_3x/\hbar}+B_3e^{-ip_3x/\hbar} \qquad ...(8.7)$$

where p_1, p_2 and p_3 represent the momenta of particle in the corresponding regions and are given as follows :

$$\left.\begin{aligned} p_1 &= \sqrt{(2mE)}=p_3 \\ p_2 &= \sqrt{\ }[2m(E-V_0)] \end{aligned}\right\} \qquad ...(8.8)$$

In Eqs. (8.5), (8.6) and (8.7) A_1, A_2, A_3, B_1, B_2, B_3 are constants whose values can be determined by boundary conditions.

Also, in Eq. (8.5), the first term is representing the wave which is travelling along +ve X-axis in the region I, i.e., the incident wave, while the second term is representing the wave reflected at x=0.

In Eq. (8.6), the first term is representing the wave travelling along +ve X-axis in the region II, i.e., the wave transmitted at x=0 whereas the second term is representing the wage travelling along –ve X-axis in the region II, i.e., the wave reflected at x=a.

Similarly, in Eq. (8.7), the first term is representing the wave travelling along +ve X-axis in the region III i.e., the wave transmitted at X-a, while the second term is representing the wave travelling along –ve X-axis in the region III. However, no wave is travelling back from infinity in region III. Hence, B_3=0. Therefore, it means that Eq. (8.7), which is the solution of Eq. (8.4), may be put as follows :

$$\psi_3=A_3e^{ip_1x/\hbar} \qquad ...(8.9)$$

In order to evaluate the constant A_1, B_1, A_2, B_2 and A_3, the conditions are to be applied at the boundaries x=0 and x=a. These conditions are as follows:

(a) Condition–*i)*: Theψ must be continuous at the boundaries, i.e.,

$$\psi_1=\psi_2 \text{ at } x=0 \qquad ...(8.10a)$$

$$\psi_2=\psi_3 \text{ at } x=0 \qquad ...(8.10b)$$

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

$$\frac{\partial\psi_1}{\partial x} = \frac{\partial\psi_2}{\partial x} \text{ at } x = 0 \qquad \text{...(8.11a)}$$

and

$$\frac{\partial\psi_2}{\partial x} = \frac{\partial\psi_3}{\partial x} \text{ at } x = a \qquad \text{...(8.11b)}$$

If we apply boundary condition (8.10a) to equations (8.5) and (8.6), we get

$$A_1 + B_1 = A_2 + B_2 \qquad \text{...(8.12)}$$

If we apply boundary condition (8.10b) to equations (8.6) and (8.9), we get

$$A_2 e^{ip_2 a/\hbar} + B_2 e^{-ip_2 a/\hbar} = A_3 e^{ip_1 a/\hbar} \qquad \text{...(8.13)}$$

Now we differentiate equations (8.5) and (8.9), we obtain

$$\frac{\partial\psi_1}{\partial x} = \frac{ip_1}{\hbar}\left[A_1 e^{ip_1 x/\hbar} - B_1 e^{-ip_1 x/\hbar}\right] \qquad \text{...(8.14)}$$

$$\frac{\partial\psi_2}{\partial x} = \frac{ip_2}{\hbar}\left[A_2 e^{ip_2 x/\hbar} - B_2 e^{-ip_2 x/\hbar}\right] \qquad \text{...(8.15)}$$

$$\frac{\partial\psi_2}{\partial x} = \frac{ip_1}{\hbar} A_3 e^{ip_1 x/\hbar} \qquad \text{...(8.16)}$$

If we apply boundary conditions (8.11a) and (8.11b) to these equations, we obtain

$$p_1[A_1 - B_1] = p_2[A_2 - B_2]$$

and

$$p_2\left[A_2 e^{ip_2 a/\hbar} - B_2 e^{-ip_2 a/\hbar}\right] = p_1\left[A_3 e^{ip_1 a/\hbar}\right]$$

or

$$A_1 - B_1 = \frac{p_2}{p_1}(A_2 - B_2) \qquad \text{...(8.17)}$$

$$A_2 e^{ip_2 a/\hbar} - B_2 e^{ip_2 a/\hbar} = \frac{p_1}{p_2} A_3 e^{ip_1 a/\hbar} \qquad \text{...(8.18)}$$

If we solve Eqs. (8.12) and (8.17) for A_2 and B_2, we obtain

$$A_1 = \frac{A_2}{2}\left(1 + \frac{p_2}{p_1}\right) + \frac{B_2}{2}\left(1 - \frac{p_2}{p_1}\right) \qquad \text{...(8.19)}$$

$$B_1 = \frac{A_1}{2}\left(1 - \frac{p_2}{p_1}\right) + \frac{B_2}{2}\left(1 + \frac{p_2}{p_1}\right) \qquad ...(8.20)$$

If we solve Eqs. (8.13) and (8.18) for A_2 and B_2, we obtain

$$A_2 = \frac{A_3}{2}\left(1 + \frac{p_1}{p_2}\right)e^{i(p_1 - p_2)a/\hbar} \qquad ...(8.21)$$

$$B_2 = \frac{A_3}{2}\left(1 + \frac{p_1}{p_2}\right)e^{i(p_1 + p_2)a/\hbar} \qquad ...(8.22)$$

$$B_2 = \frac{A_3}{4}e^{ip_1a/\hbar}\left[\left(1 - \frac{p_2}{p_1}\right)\left(1 + \frac{p_1}{p_2}\right)e^{-ip_2a/\hbar}\right.$$

$$\left. + \left(1 + \frac{p_2}{p_1}\right)\left(1 - \frac{p_1}{p_2}\right)e^{ip_2a/\hbar}\right] \qquad ...(8.23)$$

It is possible to rewrite Eq. (8.23) in the form:

$$\frac{A_3}{A_1} = \frac{4e^{-ip_1a/\hbar}}{\left\{\left(1 + \frac{p_2}{p_1}\right)\left(1 + \frac{p_1}{p_2}\right) - e^{ip_2a/\hbar} + \left(1 - \frac{p_2}{p_1}\right)\left(1 - \frac{p_1}{p_2}\right)e^{ip_2a/\hbar}\right\}}$$

$$= \frac{4p_1p_2e^{ip_1a/\hbar}}{(p_1 + p_2)^2 e^{ip_2a/\hbar} - (p_1 - p_2)^2 e^{i_2pa/\hbar}}$$

$$= \frac{4p_1p_2e^{-ip_1a/\hbar}}{\left(p_1{}^2 + p_2{}^2\right)\left(e^{-ip_2a/\hbar}\right) + 2p_1p_2\left(e^{-ip_2a/\hbar} + e^{ip_2a/\hbar}\right)}$$

$$= \frac{2p_1p_2e^{-ip_1a/\hbar}}{\left(p_1{}^2 + p_2{}^2\right)\frac{\left(e^{-ip_2a/\hbar} - e^{ip_2a/\hbar}\right)}{2} + 2p_1p_2\frac{\left(e^{-ip_2a/\hbar} + e^{ip_2p/\hbar}\right)}{2}}$$

As $E < V_0$, $p_a = \sqrt{[2m(E - V_0)]}$ is imaginary and therefore ip_2 is real, so that we may obtain

$$\frac{A_3}{A_1} = \frac{2p_1p_2e^{-ip_1a/\hbar}}{\left(p_1{}^2 + p_2{}^2\right)\sinh\left(ip_2a/\hbar\right) + 2p_1p_2\cosh\left(ip_2a/\hbar\right)}$$

$$=\frac{2p_1p_2e^{-ip_1a/\hbar}}{\cosh(ip_2a/\hbar)\left[\left(p_1^{\,2}+p_2^{\,2}\right)\tanh(ip_2a/\hbar)+2p_1p_2\right]}$$

$$=\frac{2p_1p_2\operatorname{sech}(ip_1a/\hbar)e^{-ip_1a/\hbar}}{\left(p_1^{\,2}+p_2^{\,2}\right)\tanh(ip_2a/\hbar)+2p_1p_2} \qquad ...(8.25)$$

The complex conjugate of above equation may be put as follows :

$$\frac{A_3^{\,*}}{A_1^{\,*}}=\frac{2p_1p_2^{\,*}\operatorname{sech}\left(-ip_2^{\,*}a/\hbar\right)e^{ip_1a/\hbar}}{\left(p_1^{\,2}+p_2^{\,*2}\right)\tanh\left(-ip_2^{\,*}a/\hbar\right)+2p_1p_2^{\,*}} \qquad ...(8.26)$$

But we get

$$p_2^{\,*}=-i\sqrt{[2m(V_0-E)]}=-p_2$$

$$\left[\because \qquad p_2=\sqrt{\{2m(E-V_0)\}}=i\sqrt{\{2m(V_0-E)\}}\text{ as }V_0>E\right]$$

$$\therefore p_2^{\,*2}=p_2^{\,2}.$$

Then, Eq. (8.26) becomes as follows :

$$\frac{A_2^{\,*}}{A_1^{\,*}}=\frac{-2p_1p_2\operatorname{sech}(ip_2a/\hbar)e^{ip_1a/\hbar}}{\left(p_1^{\,2}+p_2^{\,2}\right)\tanh(ip_2a/\hbar)-2p_1p_2} \qquad ...(8.27)$$

The transmittance or the transmission coefficient may be defined as follows :

$$T=\frac{\text{magnitude of transmitted current}}{\text{magnitude of incident current}}$$

$$=\frac{\left(A_3A_3^{\,*}\right)p_1/m}{\left(A_1A_1^{\,*}\right)p_1.m}=\frac{A_3A_3^{\,*}}{A_1A_1^{\,*}}$$

$$=\frac{\left\{2p_1p_2\operatorname{sech}(ip_2a/\hbar)e^{-ip_1a/\hbar}\right\}\left\{-2p_1p_2\operatorname{sech}\left(ip_2a/\hbar\, e^{ip_2a/\hbar}\right)\right\}}{\left\{\left(p_1^{\,2}+p_2^{\,2}\right)\tanh(ip_2a/\hbar)+2p_1p_2\right\}\left\{\left(p_1^{\,2}+p_2^{\,2}\right)\tanh(ip_2a/\hbar)-2p_1p_2\right\}}$$

[Using Eqs. (8.25) and (8.27)]

or

$$T=\frac{-4p_1^{\,2}p_2^{\,2}\operatorname{sech}^2(ip_2a/\hbar)}{\left(p_1^{\,2}+p_2^{\,2}\right)\tanh^2(ip_2a/\hbar)-4p_1^{\,2}p_2^{\,2}} \qquad ...(8.28)$$

As p_2 is imaginary, it means that ip_2 is real and so p_2^2 is real. Hence T is real.

The reflectance of the barrier or the reflection coefficient may be defined as follows :

$$R = \frac{\text{magnitudeof reflectedcurrent}}{\text{magnitudeof incident current}}$$

$$= \frac{B_1 B_1^*}{A_1 A_1^*} \qquad ...(8.29)$$

If we use equations (8.23) and (8.24), their conjugates and remembering that $p_2^* = -p_2$, equation (8.29) on simplification becomes as follows :

$$R = \frac{\left(p_1^2 - p_2^2\right)^2 \tanh^2(ip_2 a/\hbar)}{\left(p_1^2 + p_2\right)^2 \tanh^2(ip_2 a/\hbar) - 4p_1^2 p_2^2} \qquad ...(8.30)$$

It is possible to obtain the reflection coefficient on the basis of the fact

$$R + T = 1 \qquad ...(8.31)$$

i.e., $R=1-T$

The property of barrier penetration has been entirely ascribed to the wave nature of the matter and has been found to be much similar to the total internal reflection of light waves. If there are two glass plates having a layer of air as a medium between them, then there occurs transmission of light from one plate to another, even though the angle of incidence is greater than the critical angle. However, the intensity of transmitted wave will decrease exponentially with thickness of the layer of air. In this case, there occurs decrease in the intensity of transmitted wave exponentially with the thickness of the barrier. The wave function will be of the form as depicted in Fig. 8.2.

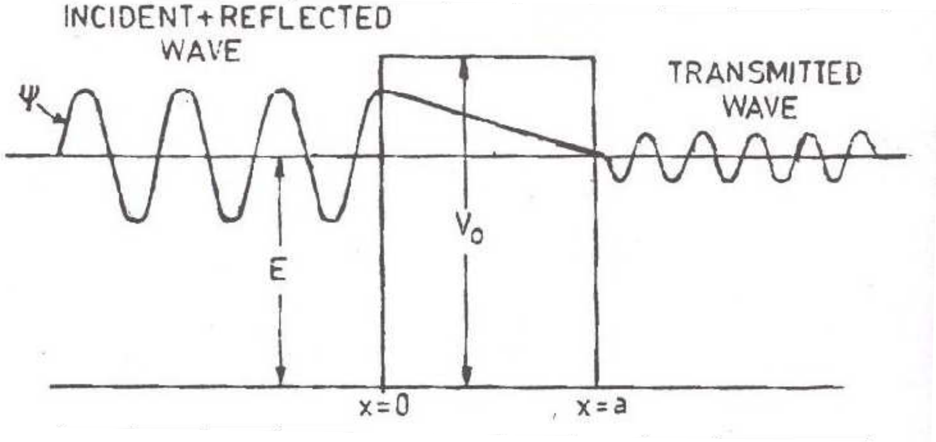

Fig. 8.2 Transmission wave functionand its amplitude

Now we will undertake a special case when the barrier is thick. It means that

$$ip_2a > \hbar, \qquad \text{because a is very large.}$$

In this case $\tanh\{(ip_2)a/\hbar\} = 1$

$$\sec h\left(\frac{(ip_2)a}{\hbar}\right) = 2e^{ip_2a/\hbar}$$

As p_2 is imaginary, it means that ip_2 and p_2^2 are real and negative. Then, equations (8.28) and (8.30) become as follows :

$$T = \frac{-16p_1^2p_2^2e^{2ip_2a/\hbar}}{(p_1^2+p_2^2)^2 - 4p_1^2p_2^2}$$

or

$$T = \frac{-16p_1^2p_2^2e^{2ip_2a/\hbar}}{(p_1^2-p_2^2)^2} \qquad \text{...(8.32)}$$

$$R = \frac{(p_1^2-p_2^2)}{(p_1^2+p_2^2)^2 - 4p_1^2p_2^2}$$

$$= \frac{(p_1^2-p_2^2)^2}{(p_1^2-p_2^2)^2} = 1. \qquad \text{...(8.33)}$$

If the values of p_1 and p_2 from equation (8.8) are substituted in equation (8.32), we get

$$T = \frac{-16(2mE)2m(E-V_0)e^{[2i\sqrt{\{2m(E-V_0)\}}\,a/\hbar}}{\{2mE - 2m(E-V_0)\}^2}$$

$$= \frac{16E(V_0-E)}{V_0^2}e^{[-2\sqrt{\{m(V_0-E)\}a/\hbar}]} \qquad \text{...(8.34)}$$

Eq. (8.34) represents the expression for transmission coefficient for a very large barrier. The phenomenon of penetrating the potential barrier by the particles such as electrons is known as tunnel effect. This effect finds valid applications in thermionic and field emission.

Self Assessment Question (SAQ) 1: What are the difference between one dimensional square well and rectangular potential barrier?

Self Assessment Question (SAQ) 2: Write an expression for transmission coefficient for a very large barrier.

8.4Tunnelling Phenomena

Although the walls of the potential well were of finite height, they were assumed to be infinitely thick. As a result, the particle was trapped forever even though it could penetrate the walls. We next look at the situation of a particle that strikes a potential barrier of height *U,* again with *E<U,* but here the barrier has a finite width (Fig.8.3). In this figure, ψ_{I+} is incident de-Broglie wave, ψ_{I-} is reflected wave while ψ_{III+} is the quantum phenomena of transmission waves.

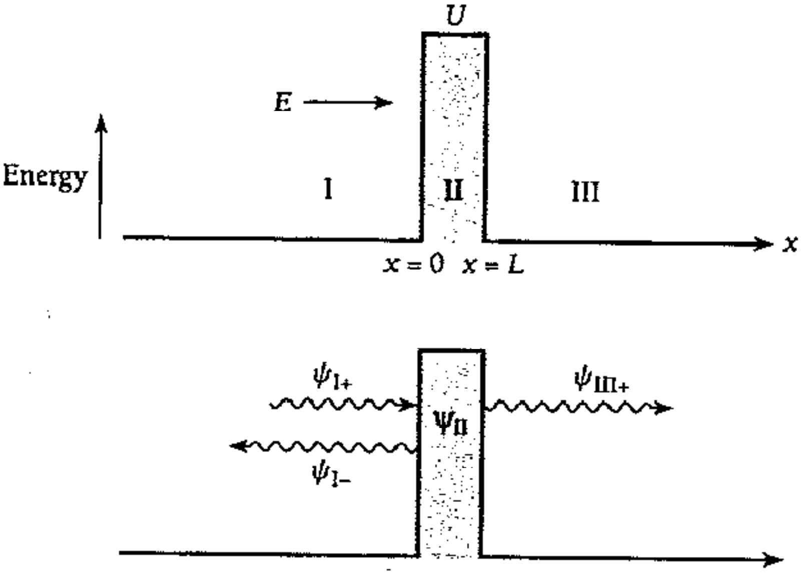

Fig: 8.3Classical and quantum approaches when a particle *E<V.*

The tunnel effect actually occurs, notably in the case of the alpha particles emitted by certain radioactive nuclei. An alpha particle whose potential wall is perhaps 25MeV high. The probability of escape is so small that the alpha particle might have to strike the wall 10^{38}or mora times before it emerges, but sooner or later it does get out. Tunnelling also occurs in the operation of certain semiconductor diodes in which electrons pass through potential barriers even though their kinetic energies are smaller than the barrier heights.

Examples of Tunnel effect: There are many examples in mature of quantum mechanical tunneling. We consider a few of them.

- **Alpha Decay:** The tunnel effect occurs in the emission of alpha particles from radioactive nuclei. The average energy of an alpha particle formed within a nucleus is only a few MeV whereas the potential barrier around the nucleus (formed by the nuclear binding forces) is about 25MeV high.

Classically, the alpha particle cannot escape from the nucleus but quantum mechanically it "tunnels" through the barrier. This tunnelling constitutes radioactive alpha decay.

- **Field Emission:** The tunnel effect has also been found responsible for the "field emission" of electrons from metals. This is the emission by cold metals in vacuum subjected to strong electric fields. Classically, the field must be much stronger than the actual fields at which the emission occurs. The actual field however, reduces the width of the barrier for the electrons at the metal-vacuum interface, so that electrons of energy less than the barrier height can "tunnel" through the barrier.
- **Field Ionisation:** The tunnel effect also explains "field ionisation" of electrons inside solid insulators. In this phenomena the electrons break away from their parent atoms under the influence of electric fields applied to insulators which thus undergo dielectric break down. Here too, the actual field is weaker than classical physics requires it to be. But it makes the electrons to "tunnel" through the potential barriers around the atoms.
- **Tunnel Diode:** Crystal diodes are modified by an extremely thin layer of insulation between the two faces in contact. These are called "tunnel diodes" in which current flows by electrons tunnelling from one side to the other through potential barriers higher than the kinetic energy of the regulated merely by changing the height of the barrier, which can be done with an applied voltage. This can be done rapidly, so that frequencies higher than 10^9Hz can be obtained. (ordinary diodes depend on the diffusion of electrons across a junction and therefore operate at much lower frequencies.)

8.5 Application of barrier penetration, i.e.Radioactive emission of α-particles (α-decay)

There are certain nuclei which emit α-particles and get converted into new nuclei with atomic number less by two and mass number less by four. This process is known as α-decay and is depicted as follows :

$$\mathbf{{}^{A}_{Z}K} \rightarrow \mathbf{{}^{A-4}_{Z-2}M + {}^{4}_{2}He} \qquad \text{...(8.35)}$$

When an α-particle is present inside the nucleus, the energy of α-particle cannot be greater than the height of the potential barrier which is existing around the nucleus. It implies that it is never possible to detect or observe the α-activity or it means that α-particle should never come out of the nucleus. When classical mechanics was applied to explain α-decay, many difficulties were realised which are as follows :

(i) The first difficulty involves the energy of the α-particle in the field of the nucleus. It was concluded from Rutherford's scattering experiments that the force experienced by α-particles is a coulomb force which acts at a very small distance ($\approx 10^{-12}$ cm) from the centre of the nucleus. After this distance, coulomb's law breaks down and the boundary of the nucleus starts. Thus, there is only coulomb potential outside the nucleus which is depicted in Fig. 8.4. As soon as the α-particle enters the nucleus (0<r<a), it will be under the influence of very strong attractive nuclear forces from the nuclear constituents. These forces are represented by a potential well as depicted in Fig. 8.4.

(ii) If the radius of radium nucleus is 9.1×10^{-13} cm, then the coulomb potential outside the nucleus is 27.8 MeV. However, the energy of the α-particle emitted by a radium nucleus is 4.88 MeV only. Now the simple question arises : How can an α-particle of 4.88 MeV energy go through a potential barrier of 27.8 MeV?

(iii) The second difficulty is concerned with the law of causality. According to the radioactive decay law, the amount of radium left after 1620 years should be half. After several periods of 1620 years, a small fraction of radium should be left. Now the simply question arises: Why are some radium atoms decaying in the first few years and why are some others surviving for thousands of years?

When quantum mechanics was applied to the problem of α-decay, the difficulties of classical mechanics as described above disappear. According to quantum mechanics, every particle is assigned a wave aspect. If this fact is taken into consideration, difficulty disappears completely because an electrostatic potential barrier, although very high, cannot completely rule out the passage of wave through it.

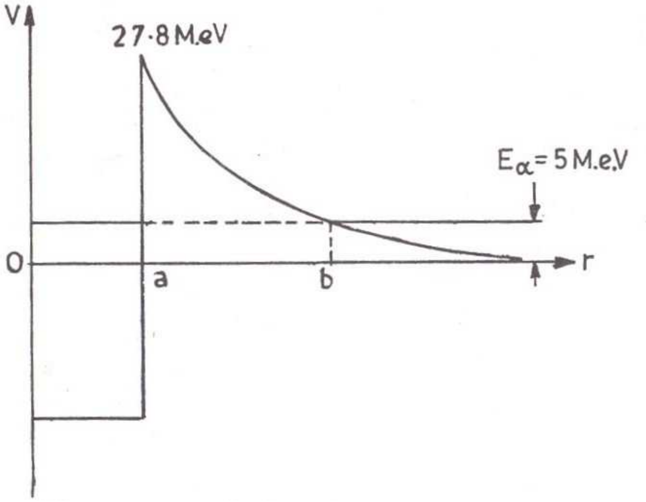

Fig. 8.4: Potential for the α-particle in the nucleus.

There always exists certain probability of the particle to penetrate through the barrier, however the small the energy might be. It is possible to obtain some quantitative features of the theory from the expression of the transmission:

$$T = \frac{16E(V_0 - E)}{V_0^{\,2}} e^{\left[-2\sqrt{\{2m(V_0-E)\}}a/\hbar\right]} \qquad ...(8.36)$$

In quantum mechanics, we are only concerned with the probability of doing something; the probability may become reality in a few years or after many thousand years. Thus, no question of causality exists.

Now an attempt is being made to calculate the mean rate of emission in case of uranium nucleus which is having radius of about 10^{-12} cm. There is an evidence that the α-particle moves back and forth freely with an average speed of 10^{9} cm/sec. Thus, the α-particle will strike the barrier $10^{9}/10^{-12}=10^{21}$ times/sec. The α-particle strikes the barrier each time. The probability that it penetrates the barrier is equal to the transmittance or transmission coefficient T which is given by Eq. (8.36).

Hence the probability that α-particle leaks out in one second

$$P = 10^{21}\ T \text{ per sec.}$$

$$= 10^{21}\,\frac{16E\left(V_0 - E\right)}{{V_0}^2}\,e^{\left[-2\sqrt{\{m(V_0-E)\}}a/\hbar\right]}$$

For uranium, E=4.2 MeV and V_0 = 30 MeV,

Mass of α-particle = 4×mass of proton

$$= 4\times1.6\times10^{-24}\ \text{g}$$

$$\hbar = 1.05\times10^{-27}\ \text{erg-sec.}$$

$$a = 2\times 10^{-12}\ \text{cm}$$

Thus,
$$P = 10^{21}\times16\times\frac{(4.2\text{MeV})\times\{(30-4.2)\text{MeV}\}}{(30\text{MeV})^2}$$

$$\times\, e^{\left[-2\sqrt{\{2m(V_0-E)\}}a/\hbar\right]}$$

$$= 10^{21}\times\frac{16\times4.2\times25.8}{30\times30}$$

$$\exp\left[\frac{\left[-2\sqrt{\left(2\times4\times1.6\times10^{-24}\times25.8\times10^{6}\times1.6\times10^{-12}\right)}\right]\times2\times10^{-12}}{1.05\times10^{-27}}\right]$$

$$= 1.9\times10^{22}\,e^{(\cong-90)}$$

$$\approx 10^{-18} \text{ per sec.}$$

$$\cong 10^{-11} \text{ per year.}$$

∵ The average life time of the nucleus is equal the reciprocal of P, i.e.,

$$\tau = \frac{1}{10^{-11}} \text{ years} = 10^{11} \text{ years.}$$

But experimentally, τ had been found to be 10^{19} years. Thus the theory is not valid. The discrepancy has been ascribed to the fact that the barrier is not rectangular and hence the present treatment is not very good for this case. A better treatment due to W.K.B. approximation is used.

It may also be understood that the life times of different elements have been found to vary widely because $V_0 - E$ and a are different for different elements and the exponential is very sensitive to these quantities.

Self Assessment Question (SAQ) 3: What is alpha particle? Define.

8.6 Attractive square well potential

Suppose there is an attractive square well potential as shown in Fig. 8.5. Suppose the potential between $x=a$ and $x=-a$ be $-V_0$and zero elsewhere.

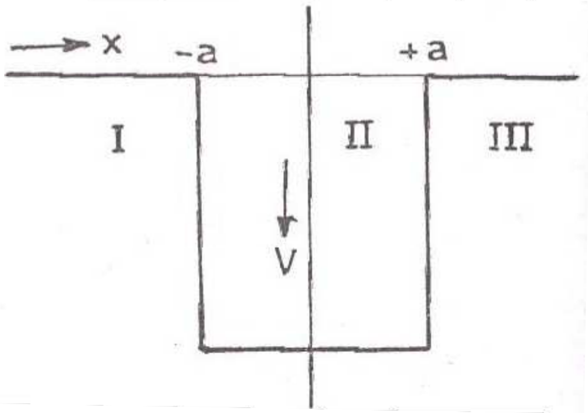

Fig. 8.5 Attractive square well potential

Suppose a stream of electrons is directed from the left side. According to the classical physics, there occurs no reflection of electrons from the potential barrier but due to wave reflection of electrons from the potential barrier but due to wave nature there occurs reflection of some electrons from the sharp edges at $x = a$ and $x = -a$. As a result, there will be reflected and transmitted wave.

The Schrödinger wave equation for the first region may be put as follows :

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

(because the potential V = 0)

Suppose we take $p_1 = \sqrt{(2mE)}$ where p_1 represents the momentum in this region. Then,

$$\frac{d^2\psi_1}{dx^2} + \frac{p_1^{\,2}}{\hbar^2}\psi_1 = 0$$

The solution of this equation is as follows :

$$\psi_1 = Ae^{ip_1x/\hbar} + Be^{-ip_1x/\hbar} \qquad ...(8.37)$$

where A and B are constants.

Schrödinger wave equation for the second region may be put as follows:

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

or $$\frac{d^2\psi_2}{dx^2} + \frac{p_2^{\,2}}{\hbar^2}\psi_2 = 0 \text{ where } p_2\sqrt{\;}[2m(E + V_0)],$$

The solution of this equation may be put as follows :

$$\psi_2 = Ce^{ip_2x/\hbar} + De^{-ip_2x/\hbar} \qquad ...(8.38)$$

Schrödinger's wave equation for the third region is as follows :

$$\frac{d^2\psi_3}{dx^2} + \frac{2mE}{\hbar^2}\psi_3 = 0$$

or $$\frac{d^2\psi_3}{dx^2} + \frac{p_1^{\,2}}{\hbar^2}\psi_3 = 0. \qquad \text{where } p_1 = \sqrt{(2mE)}$$

The solution of this equation may be put as follows :

$$\psi_3 = Fe^{ip_1x/\hbar} + Ge^{-ip_1x/\hbar}$$

As there occurs no reflected wave in the third region, the factor $Ge^{-ip_1x/\hbar}$ gets discarded. Hence

$$\psi_3 = Fe^{ip_1x/\hbar} \qquad ...(8.39)$$

It is possible to obtain the values of those constants by applying the following boundary conditions as:

$$(\psi_1)_{x=-a} = (\psi_2)_{x=-a,}$$

$$\left(\frac{d\psi_1}{dx}\right)_{x=-a} = \left(\frac{d\psi_2}{dx}\right)_{x=-a}$$

Similarly $(\psi_2)_{x=+a}=(\psi_3)_{x=+a}$

$$\left(\frac{d\psi_2}{dx}\right)_{x=a}=\left(\frac{d\psi_3}{dx}\right)_{x=a}$$

It we apply those boundary conditions, we obtain

$$Ae^{-(ip_1a)/\hbar}+Be^{+(ip_1a)/\hbar}=Ce^{-(ip_2a)/\hbar}+De^{(ip_2a)/\hbar} \quad ...(8.40)$$

or $$\left(\frac{ip_1}{\hbar}\right)Ae^{-(ip_1a)/\hbar}-\left(\frac{ip_1}{\hbar}\right)Be^{(ip_1a)/\hbar}$$

$$=\left(\frac{ip_2}{\hbar}\right)Ce^{-(ip_1a)/\hbar}-\left(\frac{ip_1}{\hbar}\right)Be^{(ip_1a)/\hbar} \quad ...(8.41)$$

$$Ce^{(ip_2a)/\hbar}+De^{-(ip_2a)\hbar}=Fe^{(ip_1a)\hbar} \quad ...(8.42)$$

$$\left(\frac{ip_2}{\hbar}\right)Ce^{(ip_2a)/\hbar}-\left(\frac{ip_2}{\hbar}\right)De^{-(ip_2a)/\hbar}$$

$$=\left(\frac{ip_1}{\hbar}\right)Fe^{(ip_1a)/\hbar} \quad ...(8.43)$$

Equations (8.41) and (8.41) on simplification become as follows :

$$Ae^{-(ip_1a)/\hbar}+Be^{(ip_1a)/\hbar}=Ce^{-(ip_2/a)/\hbar}+De^{(ip_2a)/\hbar} \quad ...(8.44)$$

and $$Ae^{-(ip_1a)/\hbar}-Be^{(ip_1a)/\hbar}$$

$$=\left(\frac{p_2}{p_1}\right)Ce^{-(ip_2a)/\hbar}-\left(\frac{p_2}{p_1}\right)De^{+(ip_2a)/\hbar} \quad ...(8.45)$$

On adding Eqs. (8.44) and (8.45), we have

$$2Ae^{-[ip_1a]/\hbar}=\left(1-\frac{p_2}{p_1}\right)Ce^{-(ip_2a)/\hbar}+\left(1-\frac{p_2}{p_1}\right)De^{+(ip_1a)/\hbar}$$

or $$A=\frac{1}{2}\left[\left(1+\frac{p_2}{p_1}\right)Ce^{-(ip_2a)/\hbar}+\left(1-\frac{p_2}{p_1}\right)De^{+(ip_2a)/\hbar}\right]\times e^{(ip_1a)/\hbar}$$

$$\frac{1}{2}\left[\left(1+\frac{p_2}{p_1}\right)Ce^{i(p_1-p_2)a/\hbar}+\left(1-\frac{p_2}{p_1}\right)De^{i(p_1-p_2)a/\hbar}\right] \quad ...(8.46)$$

On simplifying Eqs. (8.42) and (8.43), we get

$$\mathrm{C}e^{(\mathrm{i}p_2\mathrm{a})/\hbar}+\mathrm{D}e^{-(\mathrm{i}p_2\mathrm{a})\hbar}=\mathrm{F}e^{(\mathrm{i}p_1\mathrm{a})\hbar} \qquad ...(8.47)$$

$$\mathrm{C}e^{(\mathrm{i}p_2\mathrm{a})/\hbar}+\mathrm{D}e^{-(\mathrm{i}p_2\mathrm{a})/\hbar}=\left(\frac{\mathrm{p}_1}{\mathrm{p}_2}\right)\mathrm{F}e^{(\mathrm{i}p_1\mathrm{a})/\hbar} \qquad ...(8.48)$$

If Eqs. (8.47) and (8.48) are added and subtracted, we obtain

$$2Ce^{(ip_2a)/\hbar}=\left(1+\frac{p_1}{p_2}\right)Fe^{(ip_1a)/\hbar}$$

or

$$C=\frac{1}{2}\left(1+\frac{p_1}{p_2}\right)Fe^{i(p_1-p_2)a/\hbar} \qquad ...(8.49)$$

and similarly

$$D=\frac{1}{2}\left(1-\frac{p_1}{p_2}\right)Fe^{i(p_1+p_2)a/\hbar} \qquad ...(8.50)$$

If the values of C and D from Eqs. (8.49) and (8.50) are substituted in Eq. (8.46), we get

$$A=\frac{1}{4}\left(1+\frac{p_2}{p_1}\right)\left(1+\frac{p_1}{p_2}\right)Fe^{2i(p_1-p_2)a/\hbar}$$

$$+\frac{1}{4}\left(1-\frac{p_2}{p_1}\right)\left(1-\frac{p_1}{p_2}\right)Fe^{2i(p_1+p_2)a/\hbar}$$

$$=\frac{F}{4}e^{(2ip_1a)/\hbar}\left[\left(1+\frac{p_2}{p_1}\right)\left(1-\frac{p_2}{p_1}\right)e^{0(2ip_2a)/\hbar}\right.$$

$$\left.+\left(1-\frac{p_2}{p_1}\right)\left(1-\frac{p_1}{p_2}\right)e^{(2ip_2a)/\hbar}\right]$$

$$=\frac{F}{4}e^{(2ip_1a)/\hbar}\left[\left(1+\frac{p_2}{p_1}+\frac{p_1}{p_2}+1\right)e^{-(2ip_2a)/\hbar}\right.$$

$$\left.+\left(1-\frac{p_2}{p_1}-\frac{p_1}{p_2}+1\right)e^{-(2ip_2a)/\hbar}\right]$$

$$=\frac{F}{4}e^{(2ip_1a)\hbar}\left[2e^{-(2ip_2a)/\hbar}+\left(\frac{p_2}{p_1}+\frac{p_1}{p_2}\right)e^{-(2ip_2a)/\hbar}\right.$$

$$\left.=2e^{(2ip_2a)/\hbar}-\left(\frac{p_2}{p_1}+\frac{p_1}{p_2}\right)e^{(2ip_2a)/\hbar}\right]$$

$$=\frac{F}{4}e^{(2ip_1a)/\hbar}\left[2\cos\left(\frac{2p_2}{\hbar}\right)-i2\sin\left(\frac{p_2a}{\hbar}\right)+\left(\frac{p_2}{p_1}+\frac{p_1}{p_2}\right)\right.$$

$$\cos\left(\frac{2p_2a}{\hbar}\right)-i\left(\frac{p_2}{p_1}+\frac{p_1}{p_2}\right)\sin\left(\frac{2p_2a}{\hbar}\right)+2\cos\left(\frac{2p_2a}{\hbar}\right)$$

$$+2i\sin\left(\frac{2p_2a}{\hbar}\right)-\left(\frac{p_2}{p_1}+\frac{p_1}{p_2}\right)\cos\left(\frac{2p_2a}{\hbar}\right)$$

$$\left.-i\left(\frac{p_2}{p_1}+\frac{p_1}{p_2}\right)\sin\left(\frac{2p_2a}{\hbar}\right)\right]$$

$$=\frac{F}{4}e^{(2ip_1a)/\hbar}\left[4\cos\left(\frac{2p_2a}{\hbar}\right)-2i\left(\frac{p_2}{p_1}+\frac{p_1}{p_2}\right)\sin\left(\frac{2p_2a}{\hbar}\right)\right]$$

$$=Fe^{(2ip_1a)/\hbar}\left[\cos\left(\frac{2p_2a}{\hbar}\right)-\frac{i}{2}\left(\frac{p_2}{p_1}+\frac{p_1}{p_2}\right)\sin\left(\frac{2p_2a}{\hbar}\right)\right] \qquad \text{...(8.51)}$$

Now the transmissivity may be obtained as follows :

$$T=\frac{|F|^2\ v}{|A|^2\ v}=\frac{|F|^2}{|A|^2}$$

$$=\frac{|F|^2}{\left[Fe^{(2ip_1a)/\hbar}\left\{\left(\cos\frac{2p_2a}{\hbar}-\frac{i}{2}-\frac{p_2}{p_1}+\frac{p_1}{p_2}\right)\sin\frac{2p_2a}{\hbar}\right\}\right]^2}$$

$$=\frac{1}{\left[\cos^2\left(\frac{2p_2a}{\hbar}\right)+\frac{1}{4}\left(\frac{p_1}{p_2}+\frac{p_2}{p_1}\right)\sin^2\left(\frac{2p_2a}{\hbar}\right)\right]}$$

$$= \frac{1}{\left[1 - \sin^2\left(\frac{2p_2 a}{\hbar}\right) + \frac{1}{4}\left(\frac{p_1}{p_2} + \frac{p_2}{p_1}\right)^2 \sin^2\left(\frac{2p_2 a}{\hbar}\right)\right]}$$

$$= \frac{1}{\left[1 + \left\{\frac{1}{4}\left(\frac{p_1}{p_2} + \frac{p_2}{p_1}\right)^2 - 1\right\}^2 \sin^2\left[\frac{2p_2 a}{\hbar}\right]\right]}$$

$$T = \frac{1}{1 + \frac{1}{4}\left\{\frac{p_1}{p_2} + \frac{p_2}{p_1}\right\}^2 \sin^2\left\{\frac{2p_2 a}{\hbar}\right\}} \qquad \text{...(8.52)}$$

From Eq. (8.52), it is evident that if $p_1 = p_2$, then T is unity, i.e., T=1. It is expected because there exists no potential well at all. If $p_1 \neq p_2$, transmissivity will be less than unity. It implies that there will occur some reflection. However, this reflection is taking place from an attractive potential due to wave nature and further this reflection has resemblance with the reflection of round wave from the open end of an organ pipe.

For $p_1=p_2$, transmissivity is unity, i.e., when

$$\sin^2\left\{\frac{2p_2 a}{\hbar}\right\} = 0 \qquad \text{or} \qquad p_2 = \frac{N\pi\hbar}{2a}$$

where N represents an integer. This problem has been somewhat similar to the Febry-Perot interferometer in optics.

The result could be understood as follows :

The wave which gets reflected from the surface x=a, arrives back at x=0 with a phase shift of $n\pi$, then it interferes constructively with the next wave coming in and consequently the transmitted wave gets reinforced.

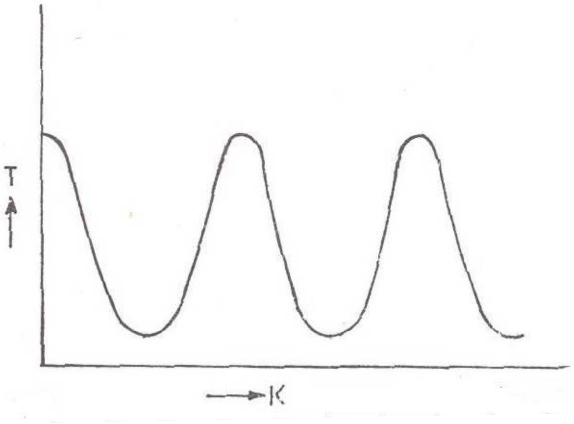

Fig. 8.6A wavenumber the transmittance

Hence, for certain wavelengths the transmittance or transmission coefficient becomes unity. As a wavenumber the transmittance has been shown in Fig. 8.6.

Example 8.1: *Electrons with energies of 10.0eV and 2.0eV are incident on a barrier 10.0eV high and 0.50 nm wide. (a) Find their respective transmission probabilities. (b) How are these affected if the barrier is doubled in width?*

Sol:

(a) For the 1.0eV electrons

$$k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

$$= \frac{\sqrt{2(9.1 \times 10^{-31})[10 - 1](1.6 \times 10^{-19})}}{1.054 \times 10^{-34}}$$

$$= 1.6 \times 10^{10} m^{-1}$$

Since $L = 0.50nm = 5.0 \times 10^{-10} m$, and $2k_2L = 2 \times 1.6 \times 10^{10} \times 5.0 \times 10^{-10} = 16,$

The approximate transmission probability is

$$T_1 = e^{-2k_2L}$$

$$= e^{-16}$$

$$= 1.1 \times 10^{-7}$$

One 1.0eV electron out of 8.9 million can tunnel through the 10eV barrier on the average. For the 2.0eV electrons a similar calculation gives $T_2 = 2.4 \times 10^{-7}$. These electrons are over twice as likely to tunnel through the barrier.

(b) If the barrier is doubled in width to 1.0nm, the transmission probabilities become

$$T'_1 = 1.3 \times 10^{-14},$$

$$T'_2 = 5.1 \times 10^{-14}.$$

Evidently T is more sensitive to the width of the barrier than to the particle energy here.

Example 8.2: *A spherical square well has depth V_0 and radius a. A particle of positive energy E and mass m is caught in a state of angular momentum $L \neq 0$. Estimate the lifetime τ of the particle, ignoring the angular momentum inside the well.*

Sol.: The spherical square well may be treated as a one-dimensional square well, provided the potential is replaced by the effective potential:

$V(r) = -V_0 + (h^2/2mr^2)\, L(L+1)$ (inside the well)

And $= V(r) + (h^2/2mr^2)\, L(L+1)$ (outside)

The transmission factor, the ratio of the flux outside and inside the well, is given, in WKB-approximation, as

$$T = \left(\frac{E}{E+V_0}\right)^{1/2} e^{-2\int k(x)dx}$$

where $$\frac{h^2k^2}{2m} = V - E;$$

thus $$T = \left(\frac{E}{E+V_0}\right)^{1/2} \exp.\left\{-2\int_a^b dr\left[\frac{L(L+1)}{r^2} - \frac{2mE}{h^2}\right]^{1/2}\right\}$$

Here, b is the point at which the radicand vanishes. Each time the particle, which may be pictured as bouncing back and forth inside the well, strikes the wall, the probability of escaping is T. The particle hits the wall $(v/2a = [(2/m)(E+V_0)]^{1/2}/2a)$ times/sec. So

$$\frac{1}{\tau} = \left[\frac{(E+V_0)}{2ma^2}\right]^{1/2} T.$$

Upon change of variables the integral in the expression for T becomes

$$\sqrt{L(L+1)}\int_\gamma^1 dx\left(\frac{1}{x^2} - 1\right)^{1/2}$$

where $$\gamma = \left[\frac{2mEa^2}{h^2 L(L+1)}\right]^{1/2}$$

The exact integration is somewhat involved; however, in the case $\gamma < 1,$ one has

$$\int_{\gamma}^{1} \frac{dx}{x}\left(1-x^2\right)^{1/2} \sim \log\left(\frac{1}{\gamma}\right)$$

and the expression for τ becomes

$$\tau = \left(\frac{2ma^2}{E}\right)^{1/2} \left\{\frac{h^2 L(L+1)}{2ma^2 E}\right\}^{\sqrt{L(L+1)}}$$

Example 8.3: *A particle of mass m is confined to a one-dimensional box with the origin at the centre of the box. The box extends from* $-a/2 \text{ to} + a/2.$ *The potential energy is*

$$V(x) = \begin{cases} 0, & -\dfrac{a}{2} < x < \dfrac{a}{2} \\ \infty, \ |x| > \dfrac{a}{2} \end{cases}$$

(a) Write the Schrödinger equation for this problem showing separate equations for the inside and the outside of the box.

(b) Assume a solution (inside the box) of the form

$$\psi(x) = A\sin(cx) + B\cos(cx)$$

Give a rule that determines all the possible values of c, and for each possible c give the conditions on A and B that make ψ(a) satisfactory solution.

(c) Express the energy in terms of c.

Sol. (a) Inside :

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

Outside : $$-\frac{h^2}{8\pi^2 m}\frac{d\psi}{dx^2} + \infty\psi = E\psi$$

Then $\psi = 0$ outside.

(b) $\psi = A\sin(cx) + B\cos(cx)$

For continuity of inside and outside functions,

$$\psi\left(-\frac{a}{2}\right) = -A\sin\frac{ca}{2} + B\cos\frac{ca}{2} = 0$$

$$\psi\frac{a}{2} = A\sin\frac{ca}{2} + B\cos\frac{ca}{2} = 0$$

$$2A\sin\frac{ca}{2} = 0$$

Either A=0 or sin (ca/2)=0

$$\frac{ca}{2 = n\pi,} \quad n = 1 \pm 1, \quad \pm 2, ...$$

$$c = \frac{2n\pi}{a}$$

$$\psi = A\sin\frac{2n\pi x}{a}$$

$$2B\cos\frac{ca}{2} = 0$$

Either B=0, or cos $ca/2 = 0$

$$\frac{ca}{2} = \left(n - \frac{1}{2}\right)\pi, n = 0, \pm 1, \pm 2, ...$$

$$c = \frac{(2n-1)\pi}{a}$$

$$\psi = B\cos\left[\frac{(2n-1)\pi x}{a}\right]$$

(c) $$\frac{d^2\psi}{dx^2} = -c^2\psi$$

$$\frac{-h^2}{8\pi^2 m}\left(-c^2\psi\right) = E\psi$$

$$E = \frac{h^2}{8\pi^2 m} = \frac{h^2 j^2}{8ma^2}, \qquad j = 2n \text{ or } 2n-1$$

=±1, ±2, ...

Example 8.4: *Calculate the reflection and transmission coefficients for a particle incident on the potential*

$$V(x) = -\alpha\delta(x).$$

Sol. The solution to the Schrödinger equation in position space is

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}, \quad x < 0$$

$$\psi_2(x) = Ce^{ikx} \quad x > 0$$

where the infinite potential well is at $x = 0$. Continuity of the wave function means

$$Ae^{ik(0)} + Be^{-ik(0)} = Ce^{ik(0)}$$

$$\Rightarrow A + B = C$$

The first derivatives in regions $\psi_1(x)$and $\psi_2(x)$ are

$$\psi'_1(x) = ikAe^{ikx} - ikBe^{-ikx},$$

$$and \ \ \psi'_2(x) = ikCe^{ikx}$$

Thus we obtain,

$$\psi'_1(0) - \psi'_2(0) = -\frac{2m}{\hbar^2}\alpha\,\psi(0)$$

$$\Rightarrow \ ikAe^{ik(0)} - ikBe^{-ik(0)} - ikCe^{ik(0)} = -\frac{2m}{\hbar^2}\alpha\,\psi(0)$$

Using $\psi_2(0) = C$,

$$ikA - ikB - ikC = -\frac{2m}{\hbar^2}\alpha\, C$$

$$ik(A - B) = -C\left(ik - \frac{2m}{\hbar^2}\alpha\right)$$

and we use the continuity condition, $A + B = C$, to eliminate C, so

$$ik(A - B) = -(A + B)\left(ik - \frac{2m}{\hbar^2}\alpha\right)$$

$$k(A - B) = -A\left(ik - \frac{2m}{\hbar^2}\alpha\right) + B\left(ik - \frac{2m}{\hbar^2}\alpha\right)$$

$$\Rightarrow \quad B = A\left[\frac{\left(\frac{2m}{\hbar^2}\alpha\right)}{\left(2ik - \frac{2m}{\hbar^2}\alpha\right)}\right] = \frac{m\alpha A}{ik\hbar^2 - m\alpha}.$$

The reflection coefficient is

$$R = \frac{|B|^2}{|A|^2}$$

$$= \frac{m^2\alpha^2}{k^2\hbar^4 + m^2\alpha^2}$$

$$= \frac{1}{1 + \frac{k^2\hbar^4}{m^2\alpha^2}}.$$

The transmission coefficient is

$$T = 1 - R = 1 - \frac{m^2\alpha^2}{k^2\hbar^4 + m^2\alpha^2}$$

$$= \frac{k^2\hbar^4}{k^2\hbar^4 + m^2\alpha^2}$$

$$= \frac{1}{1 + \frac{m^2\alpha^2}{k^2\hbar^4}}.$$

Example 8.5:*Prove that all the wave functions belonging to the maximum eigen value of the square of the total spin operator of a system of N electrons are symmetric in the spin coordinates of the individual electrons.*

Sol. All $(2S_{\max} + 1)$ of the wave functions belong to $S_{\max}$ have the same symmetry, since the raising and lowering operators, $S_x \pm iS_y$ of S_z are symmetric functions of the individual particle operators (e.g., $S_z = S_{1\alpha} + \ldots + S_{N\alpha}$, which is symmetric under particle exchange).

Now S_z attain its maximum value N/2 only when each S_{ix} is oriented along the z-direction; i.e., if

$$\psi = \psi_1\left(\frac{1}{2},\frac{1}{2}\right) \ldots\ldots \psi_N\left(\frac{1}{2},\frac{1}{2}\right),$$

where the argument of the single-electron wave function gives the spin and its projection on the z-axis. Now $\psi$is completely symmetric under interchange of spinors; therefore by the argument of the first paragraph, all wave functions in question are symmetric.

8.7 Summary:

In this unit, we have expressed the reflection and transmission coefficients if a particle passing through the potential barrier. We know from the photoelectric effect that the minimum energy needed to eject an electron from the surface of a metal is of the order of a few electron volts. This energy is needed because electrons in a metal reside in an attractive potential energy field which increases at the surface of the metal to give a potential step which is a few electron volts above the energy of the most energetic electrons in the metal. When two metal surfaces are placed in close proximity, there are two regions of low potential energy separated by a potential barrier which is similar to that shown in Fig. 8.1. But this barrier does not prevent electrons from moving across the gap between the surfaces. Electrons are quantum particles that can tunnel through the barrier with a finite probability. We have discussed the various examples of the tunnelling effect. Moreover, we have explained the tunnel effect occurs in the emission of alpha particles from radioactive nuclei.

8.8 Glossary:

Boundary conditions-a condition that is required to be satisfied at all or part of the boundary of a region in which a set of differential conditions is to be solved.

Thermionic emission- the emission of free electrons from a heated source.

Radioactive-emitting or relating to the emission of ionizing radiation or particles.

Ionization-*it* is the process by which an atom or a molecule acquires a negative or positive charge by gaining or losing electrons to form ions.

Reinforced-to make something stronger.

8.9 References:

1. Beiser A., *Concepts of Modern Physics*, 6th Edition, McGraw Hill (2003) ISBN 0-07-244848-2.
2. Shankar, R., *Principles of Quantum Mechanics*, Kluwer Academic / Plenum Publishers New York (1994) ISBN 0-306-44790-8.
3. Chatwal, G. R.; Anand, S. K.; Arora, M., *Quantum Mechanics,* Himalaya Publishing House (2007) ISBN 978-9-350-24732-7.
4. Zettili Nouredine, *Quantum Mechanics: Concepts and Applications*, John Wiley and Son's Publishers, United Kingdom(2009) ISBN 978-0-470-02678-6.

8.10 Suggested Reading:

1. Quantum Mechanics by E Merzbacher

2. A Text book of Quantum Mechanics by P M Mathews and K Venkatesan

3. Introduction to Quantum Mechanics by J Griffiths David

4. Quantum Mechanics: A Textbook for Undergraduates by Jain Mahesh

8.11 Terminal Questions:

Objective Type Questions:

a) Which of the following wave functions can be solutions of Schrodinger's equation for all valves of *x?*

(i) $\Psi = A \sec x$

(ii) $\Psi = A \tan x$

(iii) $\Psi = A \exp x^2$

(iv) $\Psi = A \exp(-x^2)$

b) A particle of energy E is incident on a potential step of infinite width and height V_0. According to quantum mechanics, if $E>V_0$, then-

(i) The particle will definitely get transmitted

(ii) The reflectivity of the particle will be zero

(iii) The reflectivity and transmittance of particle will be finite

(iv) The particle will definitely get reflected

c) A particle of energy E is incident on a potential step of infinite width and height V_0. If $E<V_0$, then-

(i) R = 0, T = 1

(ii) R = 1, T = 0

(iii) R = 0.5, T = 0.5

(iv) R = 0.16, T = 0.48

(d) The probabilities of transmission through a potential barrier of height V_0 and width *a* for

a particle of energy E ($E<V_0$)-

(i) Is inversely proportional to the width *a* of the barrier

(ii) Is directly proportional to the width *a* of the barrier

(iii) Does not depend on the width *a* of the barrier

(iv) Decreases exponentially with the width *a* of the barrier

Short Answer Type Questions:

Q.8.1 What is the potential barrier? Explain.

Q.8.2 Write Schrodinger wave equations for one dimensional rectangular potential barrier.

Q.8.3 Why Tunnelling phenomena is called quantum phenomena?

Q.8.4 Explain the examples of quantum mechanical tunneling.

Q.8.5 What would be the difficulties when classical mechanics was applied to explain alpha-decay? Explain briefly.

Long Answer Type Questions:

Q.8.6 Calculate the transmission coefficient of electrons of energy E through one-dimensional rectangular barrier. Discuss the phenomenon associated with this problem.

Q. 8.7(a) What do you mean by tunnelling through a barrier? A particle travelling with energy E along X-axis has a potential barrier defined as

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

Derive the expression for the reflection and transmission coefficients of the particle.

(b) Show that coefficient of reflection of particles inside on barrier is same whether they approach from right of from left.

Q. 8.8A beam of particles with energy E is incident on a potential barrier with potential function:

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

Show that there is a finite probability of transmission even if $E < V_0$.

Q. 8.9 Determine the transmission coefficient for a particle of energy $E < V_0$ for a rectangular one-dimensional potential barrier given by

$$\begin{aligned} V &= 0 \text{ for } x < -a \text{ and } x > a \\ &= V_0 \text{for} - a < x < a \end{aligned}$$

Discuss briefly its application to the observed phenomenon of alpha-decay.

Q. 8.10 Explain the problem of the leakage of a particle through a rectangular potential barrier of finite width and explain the quantum theory of α −particle decay.

Q. 8.11 A particle travelling with energy E along X-axis has in its path a rectangular potential barrier of height V<E and width *a*. Calculate the transmission coefficient of the particle and discuss briefly its application to the observed phenomenon of alpha decay in nuclei.

Q. 8.12 A beam of electrons of energy 100eV fall on one-dimensional rectangular potential barrier of height 110eV and width 1mm. Calculate the percentage of electrons transmitted.

8.12 Answers of Self Assessment Question (SAQ):

Answer of the objective questions: a) (iv) **b)** (ii) **c)** (ii) **d)** (iv)

Ans.1&2: Refer section 8.3.

Ans.3: Alpha particles consist of two protons and two neutrons bound together into a particle identical to a helium-4 nucleus.

Answers of Terminal Questions:

Ans.8.7& 8.8: Refer section 8.3
Ans.8.12: follow example 8.1

Unit-9: Free Particle in One Dimensional Box and Eigen Functions

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CONTENTS

9.1 Introduction

In this unit we study a quantum view of a particle in one dimensional particle in a box. The quantum mechanics is the theoretical structure whose results are closest to experimental reality, we must explore its methods and applications to understand modern physics. In present unit, we shall see, even a modest mathematical background is enough for us to follow the trains of thought that have led quantum mechanics to its greatest achievements.

9.2 Objective

- Define the meaning of free particle
- To study a quantum mechanical problem of a particle that trapped in a box
- To calculate the expectation value of position and momentum
- Describe the infinite symmetrical square potential wall problem
- To study the behaviour of the three-dimensional box system

9.3 Particle in a box

The simplest quantum mechanical problem is that of a particle trapped in a box with infinitely hard walls.This is called afree particle since it has no forces acting on it. A particle does not lose energy when it collides with such walls, so that its total energy stays constant. Let us consider a particle restricted to move along the x-axis between $x = 0$ ad $x = L$ by ideally reflecting infinitely high walls of a box (Fig: 9.1). Suppose that the potential energy V of the particle is zero inside the box, but rises to infinity on the outside, that is,

$$V = 0 \text{ for } \quad 0 \leq x \leq L$$

$$= \infty \text{ for } \quad x < 0 \text{ and } x > L\,.$$

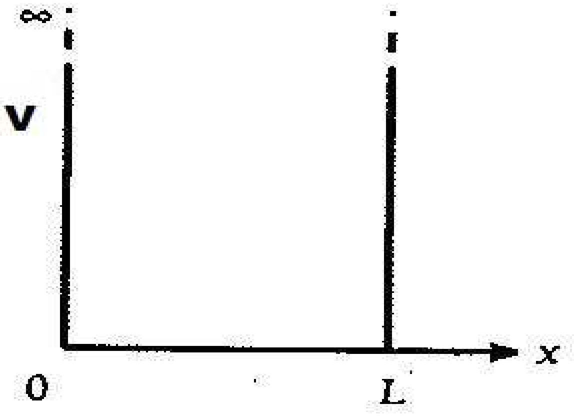

Fig. 9.1 Particle in a box.

Because the particle cannot have an infinite amount of energy, it cannot exist outside the box, and so its wave function ψ is 0 for $x \leq 0$ and $x \geq L$. Thus our task is to find what ψ is with in the box, namely between $x = 0$ and $x = L$.

The Schrödinger equation for the particle within the box (V = 0) or free particle is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0$$

or $$\frac{d^2\psi}{dx^2} + k^2\psi = 0, \qquad \text{where } k^2 = \frac{2mE}{\hbar^2} \tag{9.1}$$

The general solution of this differential equation is of the form of

$$\psi(x) = A \sin kx + B \cos kx \tag{9.2}$$

$$\text{or } \psi(x) = A \sin \frac{\sqrt{2mE}}{\hbar} x + B \cos \frac{\sqrt{2mE}}{\hbar} x$$

where the constant A and B are to be determined by the boundary conditions. The boundary condition $\psi(x) = 0$ at $x = 0$ applied to Eq. (9.2) requires

$$B = 0,$$

and the condition $\psi(x) = 0$ at $x = L$ requires

$$A \sin kL = 0$$

$$\text{or} \quad kL = n\pi$$

$$\Rightarrow k = \frac{n\pi}{L} \tag{9.2a}$$

Where the quantum number $n = 1,2,3, \dots \dots \dots$ (n= 0 is not admissible because it yields $\psi(x)$ zero everywhere which means that the particle is nowhere). Substitution of this value of k in Eq. (9.1) shows that the energy E can have only the values

$$\frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{L}, \qquad n = 1,2,3,, \dots \dots \tag{9.3}$$

From Eq.(9.3) it is clear that the energy of the particle can have only certain values, which are called the eigenvalues. These eigenvalues constituting the energy levels of the system, are found by solving Eq. (9.3) for E_n which gives

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \text{ Joules} \tag{9.4}$$

The wave function of a particle in a box whose energies are E_n are, from Eq. (9.2) with $B = 0$,

$$\psi_n(x) = A\, sin\, \frac{\sqrt{2mE_n}}{\hbar}\, x \tag{9.5}$$

Substituting Eq. (9.4) for E_n gives

$$\psi_n(x) = A\, sin\, \frac{n\pi}{L}\, x \tag{9.6}$$

for the eigen functions corresponding to the energy eigenvalues E_n .

It is easy to verify that these eigenfunctions meet all the requirements, i.e. for each quantum number n, $\psi_n(x)$ will be finite, single-valued function of x, and $\psi_n(x)$ and $\partial \psi_n(x)/\partial x$ become continuous (except at the ends of the box). Furthermore, the integral of $|\psi_n(x)|^2$ over all space will be finite.

As we can see by integrating $|\psi_n(x)|^2 dx$ from $x = 0$ to $x = L$ (since the particle is confined within these limits). With the help of the trigonometric identity $sin^2\theta = \frac{1}{2}(1 - cos2\theta)$, we find that

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 dx = \int_0^L |\psi_n(x)|^2 dx$$

$$= A^2 \int_0^L sin^2\left(\frac{n\pi x}{L}\right) dx$$

Solving the above integral as,

$$\int_0^L \left|\psi_n(x)\right|^2 dx = \frac{A^2}{2}\left[\int_0^L dx - \int_0^L cos\left(\frac{2n\pi x}{L}\right) dx\right]$$
$$= \frac{A^2}{2}\left[x - \left(\frac{L}{2n\pi}\right) sin\frac{2n\pi x}{L}\right]_0^L$$
$$= A^2\left(\frac{L}{2}\right).$$

(9.7a)

The normalize $\psi_n(x)$ we must assign a value to *A* such that $|\psi_n(x)|^2 dx$ is equal to the probability $P\ dx$ of finding the particle between *x* and *x*+*dx*, rather than merely proportional to $P\ dx$. If $|\psi_n(x)|^2 dx$ is to equal $P\ dx$, then it must be true that

$$\int_{-\infty}^{\infty} \left|\psi_n(x)\right|^2 dx = 1$$

(9.7b)

Comparing Eqs. (9.7a) and (9.7b), we see that the wave functions of a particle in a box are normalized if

$$A = \sqrt{\frac{2}{L}}$$

Thus the normalized wave functions of the particle are therefore

$$\psi_n(x) = \sqrt{\frac{2}{L}}\, sin\,\frac{n\pi}{L}\,x, \qquad n = 1,2,3, \dots \dots \dots$$

(9.8)

The normalized wave functions ψ_1, ψ_2, and $\psi_3$together with the probability densities, $|\psi_1|^2$, $|\psi_2|^2$and $|\psi_3|^2$ are plotted in Fig.9.2. Although ψ_n may be negative as well as positive, $|\psi_n|^2$ is negative and, since ψ_n is normalized, its value at a given *x* is equal to the probability density of finding the particle there. In every case $|\psi_n|^2 = 0$ at *x = 0,* and *x = L,* the boundaries of the box.

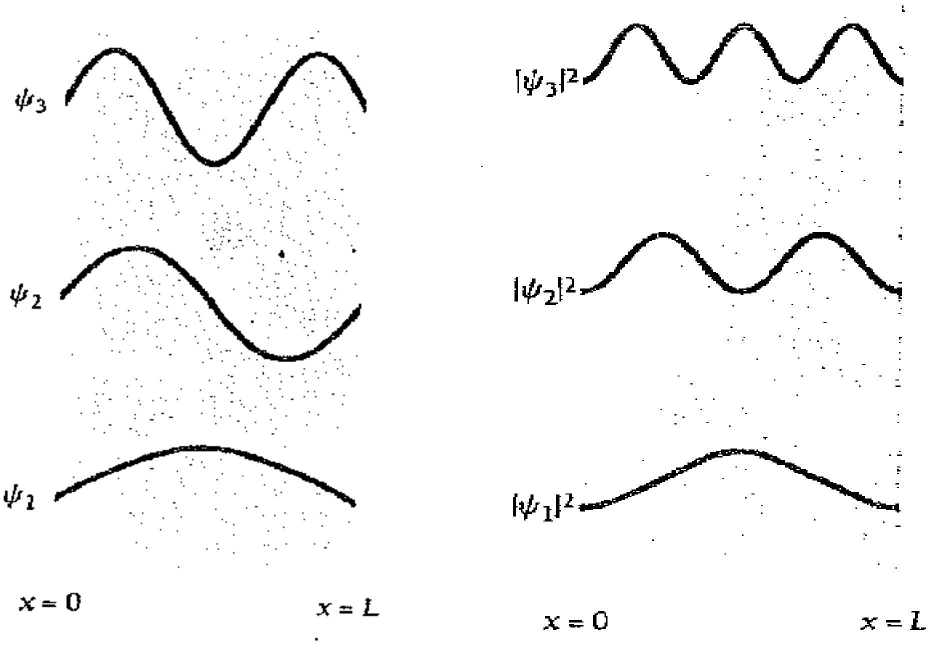

Fig. 9.2 Wave functions and probabilities of a particle in a box

At a particular place in the box the probability of the particle being present may be very different for different quantum numbers given by fig. 9.2. For instance, $|\psi_1|^2$ has its maximum value of *2/L*in the middle of the box, while $|\psi_2|^2 = 0$ there.

A particle in the 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, suggest the same probability for the particle being anywhere in the box.

The significant feature of the particle-in-a-box quantum states is the occurrence of nodes. These are points, other than the two end points (which are fixed by the boundary conditions), at which the wavefunction vanishes.At a node there is exactly zero probability of finding the particle.

The*n*th quantum state has, in fact,$n - 1$ nodes. It is generally true that thenumber of nodes increases with the energy of a quantum state, which can be rationalized by the following qualitative argument. As the number ofnodes increases, so does the number and steepness of the `wiggles' in the wavefunction. It's like skiing down a slalom course. Accordingly, the average curvature, given by the second derivative, must increase. But the second derivative is proportional to the kinetic energy operator. Therefore, the more nodes, the higher the energy. This will prove to be an invaluable guide in more complex quantum systems.

Self Assessment Question (SAQ) 1: Find the value of *A* in the following wave state

$$\psi = A\, exp.\left(\frac{-\omega m x^2}{2\hbar} - \frac{i\omega t}{2}\right)$$

Self Assessment Question (SAQ) 2: Write the first and second energy eigen value for one dimensional particle in a box.

Self Assessment Question (SAQ) 3: What are the physical significant of the particle in a box?

9.4 The expectation value <*x*>(*OR* Average position of a particle in a box)

In quantum mechanics, the expectation value is the probabilistic expected value of the result (measurement) of an experiment. It is not the *most* probable value of a measurement; indeed, the expectation value may have zero probability of occurring. It is a fundamental concept in all areas of quantum physics.We know that the formula of the expectation value of *x* is

$$< x >= \int_{-\infty}^{\infty} x\Psi(x,t)^* \Psi(x,t)dx$$

where $\Psi(x,t)$ has to benormalized

we need normalized wave functions, from the above relation (9.8) we have

$$\psi_n = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L}, \qquad n = 1,2,3,...$$

The modulus & square of this equations, simply called probability of finding the particle, i.e.

$$\psi_n^{\ 2} = \frac{2}{L}\sin^2\frac{n\pi x}{L}, \qquad n = 1,2,3,...$$

so the integral becomes

$$< x > = \int_{-\infty}^{\infty} x\,\psi(x)^*\psi(x)dx$$

$$= \frac{2}{L}\int_0^L x(\sin\frac{n\pi x}{L})(\sin\frac{n\pi x}{L})dx$$

or

$$< x > = \frac{2}{L}\int_0^L x \cdot \sin^2 \frac{n\pi x}{L}\, dx$$

$$= \frac{2}{L}\left[\frac{x^2}{4} - \frac{x\sin(\frac{2n\pi x}{L})}{\frac{4n\pi}{L}} - \frac{\cos(\frac{2n\pi x}{L})}{8(\frac{n\pi}{L})^2}\right]_0^L$$

since sin (nπ) = 0, cos (2nπ) = 1 and cos 0 = 1, for all values of n, thus the expectation value of x is

$$< x >= \frac{2}{L}(\frac{L^2}{4}) = \frac{L}{2}$$

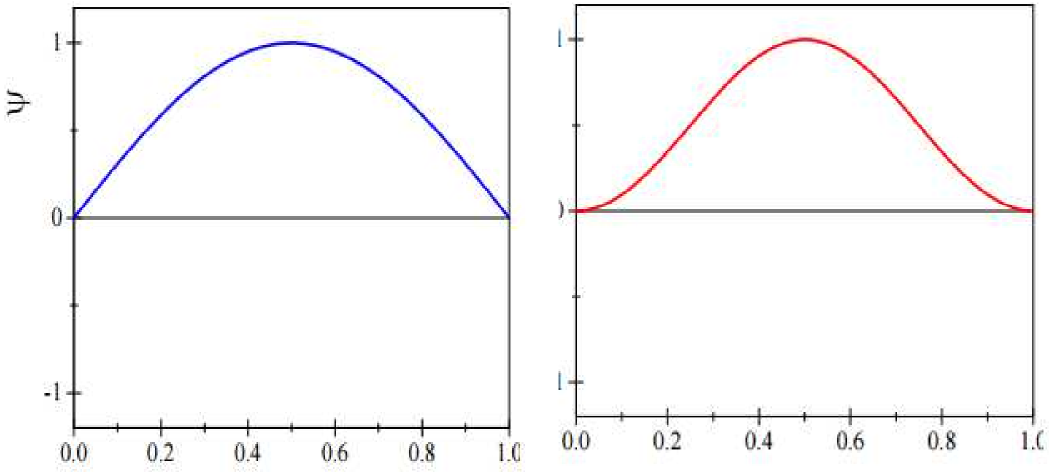

Fig. 9.2a*(left)* *The ground-state (n=1) wave function for a particle in a box.*

(right) *The ground-state (n=1) probability for a particle in a box.*

Therefore, in all quantum states, the arithmetic mean position of the particle is in the middle of the box. In Fig.9.2a, we show the nature of a wavefunction and probability for moving a particle in a box.

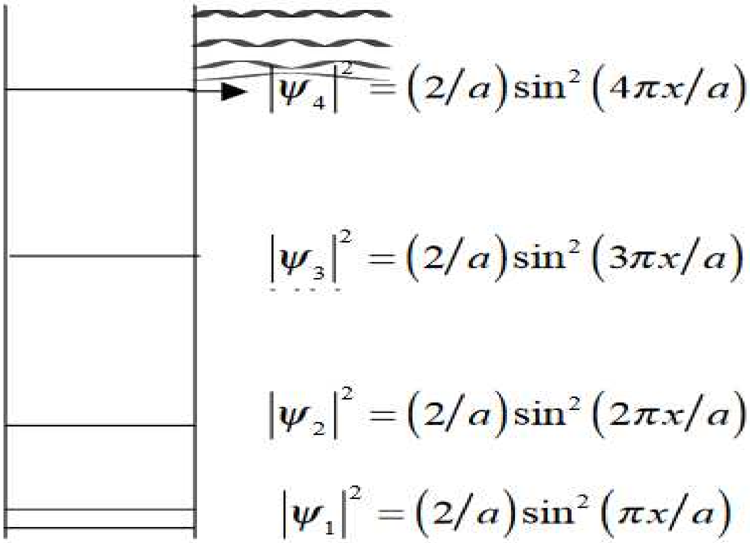

Fig 9.2b: Probability distribution in particle in a box.

Now, the interpretation of $|\psi_n|^2$ based on measurements (Fig. 9.2b). Each measurement of the position gives one result. Many measurements give a probability distribution of outcomes. Moreover, we know that Max Born interpreted that $|\psi_n(x)|^2 = \psi_n{}^*(x)\,\psi_n(x)$ is a probability distribution or probability density for the particle in the interval *x* and *x*+*dx*.

9.5 Expectation value of $<p_x>$(*OR* Average momentum of a particle)

What is the average momentum of a particle in the box? We start with the momentum operator as

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

We note that the particle-in-a-box wavefunctions are **not** eigen functions of the momentum operator, but we can calculate the expectation value for the momentum.
First write the expectation value integral with the momentum operator. Then insert the expression for the wavefunction and evaluate the integral as shown here.

$$< p_x > = \int_0^L \Psi(x,t)*\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi(x,t)dx$$

Substituting the wavefunction of particle in a box, we get

$$< p_x > = \int_0^L \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}\left(-i\hbar\frac{\partial}{\partial x}\right)\sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} dx$$

$$= -i\hbar\left(\frac{2}{L}\right)\int_0^L \sin\left(\frac{n\pi x}{L}\right)\left(\frac{\partial}{\partial x}\right)\sin\left(\frac{n\pi x}{L}\right)dx$$

$$= -i\hbar\left(\frac{2}{L}\right)\left(\frac{n\pi}{L}\right)\int_0^L \sin\left(\frac{n\pi x}{L}\right)\cos\left(\frac{n\pi x}{L}\right)dx$$

$$= 0$$

Note that this makes sense since the particles spends an equal amount of time traveling in the $+x$ and $-x$axisdirection.

Why are we not aware of quantization in daily experience: In our daily life we come across particles of large mass and systems of large dimensions. In such case the allowed energy states do not appear to be quantized and for all practical purposes, form a continuum. To show this, let us find the spacing between two adjacent energy levels for different values of the mass of a particle moving in boxes of different sizes.

The difference in energies of two adjacent levels is

$$\begin{aligned}\Delta E_n &= E_{n+1} - E_n\\ &= \frac{(n+1)^2h^2}{8ml^2} - \frac{n^2h^2}{8ml^2}\\ &= \frac{h^2}{8ml^2}(2n+1).\end{aligned}$$

Let us take $m$to be the mass of the molecule ($\approx 10^{-26} kg$) and L to be 10cm. That is, for the molecule of a gas in a vessel, we have

$$\begin{aligned}\Delta E_n &= \frac{(6.62\times10^{-34})^2(2n+1)}{8\times10^{-26}\times(0.1)^2}\\ &= 5.5\times10^{-40}(2n+1)\text{joule}\end{aligned}$$

$$\begin{aligned}&= \frac{5.5\times10^{-40}(2n+1)}{1.6\times10^{-19}}\\ &= 3.4\times10^{-21}(2n+1)\text{eV}.\end{aligned}$$

The permissible energy levels are so very close together that they may be regarded as being practically continuous. Although energy quantization occurs in principle, it will not affect the motion of the molecules. Hence in the domain of everyday experience quantum effects are imperceptible. This accounts for the success of Newtonian mechanics in everyday life.

A similar result is obtained if we take *m*to be the mass of an electron ($\approx 9 \times 10^{-31}$kg) but *L* same as above. In this case of free electrons in a metal, we have

$$\Delta E_n = 3.8 \times 10^{-17}(2n + 1)\mathrm{eV}\,.$$

Thus in a trap of macroscopic size the energy of an electron behaves in classical manner, it can take continuous values.

An absolutely different result is, however, obtained for an electron moving ina region of atomic dimensions ($m = 9 \times 10^{-31}\mathrm{kg}, L = 1\text{Å}$). In this case,

$$\Delta E_n = \frac{(6.62 \times 10^{-34})^2(2n + 1)}{8 \times (9 \times 10^{-31}) \times (10^{-10})^2}$$

$$= 6.0 \times 10^{-18}(2n + 1)\mathrm{joule}$$

$$= \frac{6.0 \times 10^{-18}(2n + 1)}{1.6 \times 10^{-19}}$$

$$= 38(2n + 1)\mathrm{eV}\,.$$

The spacing between the lowest (n = 1) and the next level is 114 eV, and increases in higher adjacent levels. Thus these energy level are sufficiently far apart to make the quantization of energy conspicuous.

Thus, in passing from atomic to much larger dimensions the results of wave mechanics approach those of the classical physics.

Self Assessment Question (SAQ) 4: Express the quantum operators for classical position, momentum and energy.

9.6 Infinite symmetrical potential wall or one-dimensional symmetrical box

In order to calculate discrete energy levels of particle in quantum mechanics, let us consider the one-dimensional motion of a particle which is restrained by reflecting walls. Here we shall assume a square well potential with infinitely high sides as shown in Fig. 9.3. This is corresponding to a particle which is bounded by impenetrable walls of width 2a. In Fig. 9.3, it can be seen that

$V(x) = 0$ *for* $-a < x < a$

and $V(x) = +\infty$, *for* $|x| > a$ and walls at points $x = \pm a$.

The proper boundary condition which is to be imposed is that the wave functions gets vanished at the walls, i.e. $(x)_{x=a} = 0$ and $(\psi)_{x=-a} = 0$.

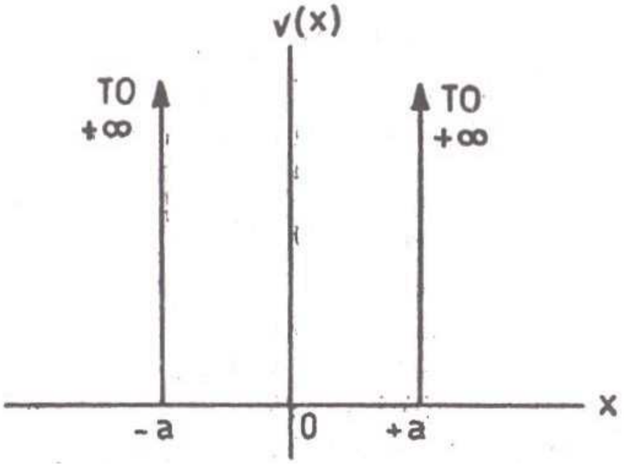

Fig. 9.3: One dimensional square well potential with perfectly rigid walls.

The wave equation for | x | > a is as follows :

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0 \qquad \text{[because V = 0]}$$

or $$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0, \qquad \text{where } \alpha^2 = \frac{2mE}{\hbar^2} \qquad (9.9)$$

The general solution of this equation is

$$\psi = A \cos x + B \sin x \qquad (9.10)$$

On applying the boundary conditions at x = ±a, we get

i.e., $\psi = 0$ at $x = a$

and $\psi = 0$ at $x = - a$

$$A \cos \alpha a + B \sin \alpha a = 0, \qquad (9.11)$$

$$A \cos \alpha a - B \sin \alpha a = 0, \qquad (9.12)$$

On adding Eqs. (9.11) and (9.12), we get

$$2A \cos \alpha a = 0$$

either $a = 0$ or $\cos \alpha a = 0$

On subtracting Eq. (9.12) from (9.11), we get

$$2B \sin \alpha a = 0$$

either $B = 0$ or $\sin \alpha a = 0.$

Both A and B cannot be zero because we would get the physically uninteresting solution $\psi = 0$. Further, both $\sin \alpha a$ and $\cos \alpha a$ cannot be made zero for a given value of α and E. However, two possible classes of solutions are as follows:

(i) $A = 0,$ $\sin \alpha a = 0$

(ii) $B = 0,$ $\cos \alpha a = 0$

For the class (i) ($\sin \alpha a = 0$), we have

$$\alpha a = \pi, 2\pi, \frac{5\pi}{2}\ldots\ldots\ldots\ldots\ldots$$

$$= \frac{n\pi}{2} \qquad (9.13)$$

where n is an even integer.

Similarly, for the class (ii) (cos αa = 0), we have

$$\alpha a = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}\ldots\ldots\ldots\ldots$$

$$= \frac{n\pi}{2} \qquad (9.14)$$

where n is an odd integer.

If we apply Eqs. (9.13) and (9.14) to Eq. (9.9), we obtain

$$\psi = A\cos\frac{n\pi\pi}{2}, \text{ when n is odd.}$$

$$\psi = B\cos\frac{n\pi\pi}{2}, \text{ when n is even}$$

and

$$\alpha^2 = \frac{2mE}{\hbar^2} \text{ or } E = \frac{\alpha^2\hbar^2}{2m}$$

$$E_n = \frac{n^2\pi^2\hbar^2}{8ma^2} \text{ Joules} \qquad (9.15)$$

Thus, corresponding to all integral values of n, there is an infinite sequence of discrete energy levels. In the above discussion, the n numbers are called quantum numbers while the E values are called energy levels.

If a particle is described by a wave function with a certain n value, it is said to be the quantum state, n. On the other hand, the quantum state with higher values of n (=2, 3, ...etc) are termed as excited states.

According to quantum mechanics (but not in accordance to classical mechanics), the kinetic energy is not equal to zero in ground state. The result is applicable to all problems. Further, if a particle is bound to a small region of space, the quantum mechanics only predicts the discrete energy levels and quantum numbers. On the other hand, classical mechanics does not need any such requirement of discrete energy levels for bound systems. It does not imply that quantum mechanics does not agree with classical mechanics in the region of laboratory-scale sizes where classical theory is known to be applicable. In the laboratory sizes, the energy levels are so closely spaced that they could not be distinguished experimentally from a continuous set.

Let us now give few interesting facts about the foregoing problem.

(a) It is possible to deduce the quantum condition of discreteness of energy levels by taking into consideration of the interference of de Broglie wave reflected back and forth between the walls. Any value of E not given by Eq. (9.15) will give rise to destructive interference while any value of E given by Eq. (9.15) will give rise to constructive interference.

(b) It is possible to compare this problem mathematically with that of the vibrations of the violin string. The value of ψ represents the displacement of point on the string. As the string is fixed at each end, y = 0 at x = ±a. The solution of this problem is same what we get in the violin case (sinusoidal oscillations); the string is having a fundamental mode of vibration (n=1) and set of overtones (n=2, 3, ...) each with a characteristic frequency.

(c) It is also possible to compare this problem with a section of transmission line or wave guide which is shorted at both ends and here the voltage *V* is used in place of ψ. Further *V* become equal to zero at each end as termination becomes short (impedance z=0) at each end.

9.6.1 Wave function

It is possible to put the general form of wave equation in the following form :

$$\psi_n = A\cos\frac{n\pi x}{2a}\left(n = 1, 2, ...5\right) \tag{9.16}$$

$$\psi_n = B\sin\frac{n\pi x}{2a}\left(n = 2, 4, ...6\right) \tag{9.17}$$

Let us now normalise ψ_n in Eq. (9.16)

$$\int_{-a}^{a} A^2 \cos^2\frac{n\pi x}{2a}\,dx = 1$$

$$\int_{-a}^{a} \frac{A^2}{2}\left(1+\cos\frac{2n\pi x}{2a}\right)dx = 1$$

$$A^2 = \frac{1}{a}$$

$$A = \sqrt{\frac{1}{a}} \tag{9.18}$$

Similarly, normalise ψ_n in Eq. (9.17) to yield

$$\Rightarrow \qquad B = \sqrt{\frac{1}{b}} \tag{9.19}$$

Hence normalised wave functions of Eqs. (9.16) and (9.17) are as follows :

$$\psi_n = \frac{1}{\sqrt{a}}\cos\frac{\text{n}\pi\text{x}}{2\text{a}}(n = 1, 2, 5...) \tag{9.20}$$

$$\psi_n = \frac{1}{\sqrt{b}}\sin\frac{\text{n}\pi\text{x}}{2\text{a}}(n = 2, 4, 6...) \tag{9.21}$$

In Fig. 9.4, the energy levels and wave functions have been depicted. From Fig.9.4, it can be seen that there is only one-half wave length for the lowest energy state called zero-point energy E_0 while the successive energy states are differing in having an additional half wave-length more.

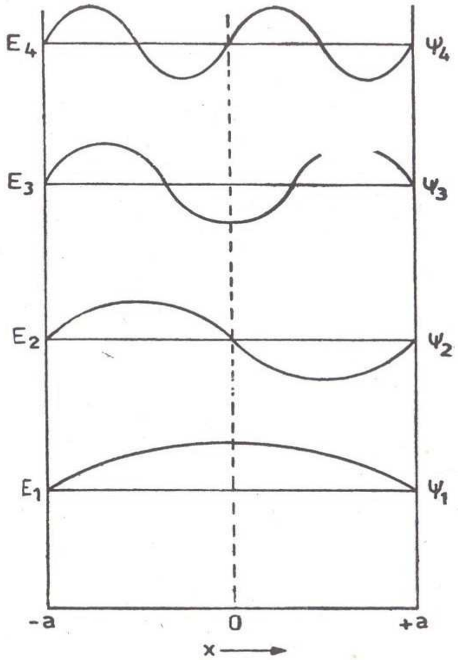

Fig. 9.4: First few energy levels and wave functions of a particle in a box.

There are certain points between a≤x≤-a at which the wave function gets vanished. These points are known as nodes. It can be seen that the number of nodes, excluding those at the extremities, go on increasing as we go up the energy scale. For a particular energy state which is characterised by the quantum number n, there will be (n-1) intermediate nodes.

As wave-functions represented by Eq. (9.20) are symmetrical about the origin x=0, it means that $\psi_n(x)$ for odd n are even for function of x. Such functions are considered to be having an even parity. Similarly, $\psi_n(x)$ of Eq. (9.21) are odd function of x (anti-symmetric about x=0) and are considered to be having an odd parity.

9.7 The three dimensional box: (Application of Schrödinger equation)

Let us consider a particle which is enclosed inside a rectangular box having edges a, b and c in length (Fig. 5.5).

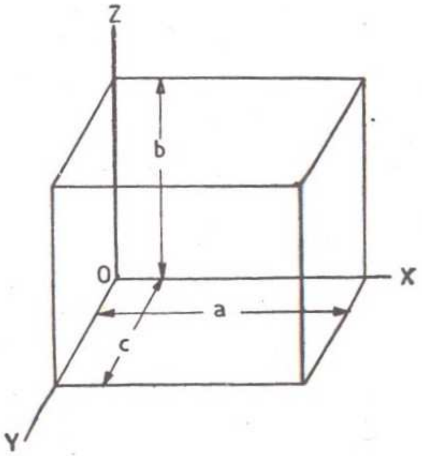

Fig. 5.5 Three dimensional box

The potential function V(x, y, z) is having a constant value of zero in the regions given as follows :

V(x, y, z), = 0, 0<x<a,

V(x, y, z) = 0, 0 <y< b,

and V(x, y, z) = 0, 0<z<c.

The potential outside the box is infinite. The Schrödinger time independent wave equation inside the box may be put as follows :

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{2m}{\hbar^2}E\psi=0 \tag{9.22}$$

It is possible to separate Eq. (9.22) by making the following substitutions:

$$\psi(x,y,z)=X(x)Y(y)Z(z)=XYZ \tag{9.23}$$

Differentiating Eq. (9.23) with respect to x, y and z separately by keeping the remaining two factors as constant, we obtain

$$\frac{\partial^2\psi}{\partial x^2}=X"YZ,\frac{\partial^2\psi}{\partial y^2}=XY"Z,\text{ and }\frac{\partial^2\psi}{\partial z^2}=XYZ" \tag{9.23a}$$

On substituting Eq. (9.23a) in Eq. (9.22), we obtain

$$X"YZ+XY"Z+XYZ"=-\frac{2mE}{\hbar^2}XYZ$$

On dividing the above equation by XYZ, we obtain

$$\frac{X"}{X}+\frac{Y"}{Y}+\frac{Z"}{Z}=-\frac{2mE}{\hbar^2} \tag{9.24}$$

For the given energy of the particle, the term $\left(-8\pi^2 mE/h^2\right)$ is constant and each term on the left side is a function of one variable only. If we allow only one of these (x or y or z) to vary at a time and keep the other two constants (say we vary x keeping y and z constant), the sum of the three terms is still equal to the constant on the right-hand side. This means that each of the three terms on the left is itself a constant and is independent of the other variables, present in it. Let us represent the constants for the three terms as $-\alpha_1{}^2, -\alpha_2{}^2$ and $-\alpha_3{}^2$. These have a minus sign because the term on the right side of equation has minus sign. This gives three differential equations. Now

$$\frac{X"}{X}=\frac{2mE}{\hbar^2}-\frac{Y"}{Y}-\frac{Z"}{Z}=-\alpha_1{}^2 \tag{9.25}$$

or

$$\frac{X"}{X}=-\alpha_1{}^2$$

or

$$\frac{d^2X}{dx^2}+\alpha_1{}^2X=0 \tag{9.26}$$

and from Eq. (9.25), we have

$$\frac{Y"}{Y}=-\frac{2mE}{\hbar^2}-\frac{Z"}{Z}+\alpha_2{}^2 \tag{9.27}$$

or $$\frac{Y''}{Y} = -\alpha_2{}^2$$

or $$\frac{d^2Y}{dy^2} + \alpha_2{}^2 Y = 0 \qquad (9.28)$$

Again from Eq. (9.27), we have

$$\frac{Z''}{Z} = -\frac{2mE}{\hbar^2} + \alpha_1{}^2 + \alpha_2{}^2 = -\alpha_3{}^2 \qquad (9.29)$$

or $$\frac{d^2Z}{dz^2} + \alpha_3{}^2 Z = 0 \qquad (9.30)$$

On substitutingEqs. (9.26), (9.28) and (9.30) in Eq. (9.24), we obtain

$$\alpha_1{}^2 + \alpha_2{}^2 + \alpha_3{}^2 = \frac{2mE}{\hbar^2} \qquad (9.31)$$

The solutions of Eqs. (9.26), (9.28) and (9.30) are as follows :

$$X = A_1 \cos \alpha_1 x + B_1 \sin \alpha_1 x \qquad (9.32)$$

$$Y = A_2 \cos \alpha_1 y + B_2 \sin \alpha_2 y \qquad (9.33)$$

$$Z = A_3 \cos \alpha_3 x + B_3 \sin \alpha_3 x \qquad (9.34)$$

In the above equations, A_1, A_2 and A_3 are constants; B_1, B_2 and B_3 are also constants. It is possible to obtain the values of these constants by applying the boundary conditions. As ψ vanishes at the surface of infinite potential, it means that

$$\psi = 0 \text{ when} \left.\begin{matrix} x=0 \\ \text{x=a} \end{matrix}\right\} \left.\begin{matrix} y=0 \\ y=b \end{matrix}\right\} \left.\begin{matrix} z=0 \\ z=b \end{matrix}\right\}.$$

If these boundary conditions are applied, then we have

$$A_1 = A_2 = A_3 = 0$$

Also $$B_1 \neq 0 \quad \therefore \quad \sin \alpha_1 a = 0, \quad \text{i.e.,} \quad \alpha_1 a = n_\alpha \pi \text{ or } \alpha_1 = \frac{n_\alpha \pi}{a}$$

$$B_2 \neq 0 \quad \therefore \quad \sin \alpha_2 b = 0, \quad \text{i.e.,} \quad \alpha_2 b = n_\alpha \pi \text{ or } \alpha_2 = \frac{n_y \pi}{b}$$

$$B_3 \neq 0 \quad \therefore \quad \sin \alpha_3 c = 0, \quad \text{i.e.,} \quad \alpha_3 c = n_\alpha \pi \text{ or } \alpha_3 = \frac{n_\alpha \pi}{c}$$

Hence $$X = B_1 \sin \frac{n_z \pi x}{a} \tag{9.35}$$

where n_z represents any integer ($n_\alpha = 1, 2, 3 ...$).

Also, $$Y = B_2 \sin \frac{n_y \pi y}{b} \tag{9.36}$$

$n_y = 1, 2, 3$

and $$Z = B_3 \sin \frac{n_z \pi z}{c} \tag{9.37}$$

$n_z = 1, 2, 3$

$$\therefore \quad \psi_{n_x n_y n_z}(x, y, z) = B_1 B_2 B_3 \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{b} \sin \frac{n_z \pi z}{c}$$

or $$\psi_{n_x n_y n_z}(x, y, z) = k \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{b} \sin \frac{n_z \pi z}{c} \tag{9.38}$$

In the above equation, k is termed as normalisation constant. It is possible to obtain the value of k by using the normalised condition, i.e.,

$$\int_0^a \int_0^b \int_0^c \psi \psi^* \, dx \, dy \, dz = 1 \tag{9.39}$$

or $$k^2 \int_0^a \int_0^b \int_0^c \sin^2 \frac{n_\alpha \pi x}{a} \sin^2 \frac{n_y \pi x}{b} \sin^2 \frac{n_z \pi x}{c} \, dx \, dy \, dz = 1 \tag{9.40}$$

But, $$\int_0^a \sin^2 \frac{n_\alpha \pi x}{a} dx = \int_0^a \left[\frac{1}{2} - \frac{1}{2} \cos \frac{2\pi n_\infty}{a} \right] dx = \frac{a}{2}$$

Similarly $$\int_0^b \sin^2 \frac{n_y \pi y}{b} dy = \frac{b}{2}$$

and $$\int_0^a \sin^2 \frac{n_z \pi y}{c} dz = \frac{c}{2}$$

$$\therefore \quad k^2 \frac{a}{2} . \frac{b}{2} . \frac{c}{2} = 1 \tag{9.41}$$

or $$k = \frac{2\sqrt{2}}{\sqrt{(abc)}} \tag{9.42}$$

$$\psi_{n_x n_y n_z}(x,y,z) = \frac{2\sqrt{2}}{\sqrt{(abc)}} \sin\frac{n_\alpha \pi x}{a} \sin\frac{n_y \pi y}{b} \sin\frac{n_z \pi z}{c} \tag{9.43}$$

From Eq. (9.31), we have

$$\alpha_1{}^2 + \alpha_2{}^2 + \alpha_3{}^2 = \frac{2mE}{\hbar^2} \tag{9.44a}$$

$$\frac{n_\alpha{}^2 \pi^2}{a^2} + \frac{n_y{}^2 \pi^2}{b^2} + \frac{n_z{}^2 \pi^2}{c^2} = \frac{2mE}{\hbar^2} \tag{9.44b}$$

or

$$E_{n_\alpha n_y n_z} = \frac{\hbar^2}{2m}\left[\frac{n_\alpha{}^2}{a^2} + \frac{n_y{}^2}{b^2} + \frac{n_z{}^2}{c^2}\right]\pi^2 \tag{9.44c}$$

or

$$E_{n_z n_y n_z} = \frac{\hbar^2}{8m}\left[\frac{n_z{}^2}{a^2} + \frac{n_y{}^2}{b^2} + \frac{n_z{}^2}{c^2}\right] \tag{9.44d}$$

But if we consider a box that is cubical in shape such that $a=b=c$, energy can be expressed by

$$E = \frac{h^2}{8ma^2}\left(n_\alpha{}^2 + n_y{}^2 + n_z{}^2\right)$$

For the lowest quantum state (111), in which n_α, n_y and n_z, respectively, are equal to unity, it is seen that $E = 3h^2/8ma^2$. There is only one set of quantum numbers that gives this energy state, and this level is said to be non-degenerate.

If we now consider the second energy state as shown in Fig. 9.6, it is seen that there are three sets (112), (121) and (211) of the quantum numbers n_α, n_y and n_z, that will give the same energy level, $E = 3h^2/4ma^2$. Such level is said to degenerate, and in this particular case the level of triply degenerate. For a cubical box, it can be concluded from the Fig. 9.6, that virtually all the energy levels are degenerate to some degree.

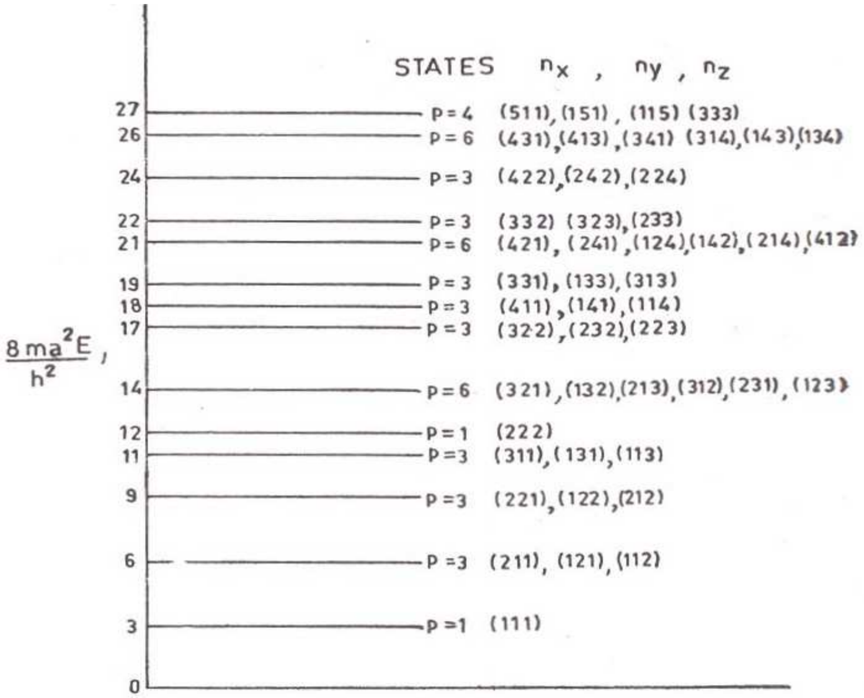

Fig. 9.6: Energy levels, degree of degeneracy and quantum numbers of a particle in a cubical box.

The next problem is to know about the number of allowed energy values which are lying between a given energy *E* and *E+dE*. The exact solution of this problem is quite a difficult task. However, the task becomes much easier for such cases in which the integers n_z, n_y and n_z are very large. In order to solve this problem, a three-dimensional lattice is set up in which $\frac{1}{a}, \frac{1}{b}$ and $\frac{1}{c}$ are the sides of a unit cell respectively (Fig. 9.6). The energy is given as follows:

$$\frac{8mE}{h^2} = \left(\frac{n_\alpha{}^2}{a^2} + \frac{n_y{}^2}{b^2} + \frac{n_z{}^2}{c^2} \right) \tag{9.45}$$

From the above equation it is evident that each brick yields one energy state and now only the problem is to know the number of bricks in the energy between *E* and *E+dE*.

If a sphere of radius $\sqrt{8mE/h^2}$ is considered, then all energy states would be situated in this sphere. It means that the number of eigen values lying in this energy interval *E* and*E+dE*would be equal to the number of bricks which are lying between the octant of the sphere of radius *r* corresponding to energy and octant of the sphere of radius r+*dr* corresponding to energy *E+dE*. This can be obtained by knowing the total volume of the bricks within energy *E* and*E+dE*and then dividing it by the volume of one brick. Now the number of bricks up to energy *E* would be given as follows:

$$= \frac{1}{8}\frac{4\pi}{3}\left(\frac{8mE}{h^2}\right)^{3/2} . \frac{1}{\frac{1}{a}.\frac{1}{b}.\frac{1}{c}}$$

$$=\frac{1}{8}.\frac{4\pi}{3}abc\left(\frac{8mE}{h^2}\right)^{3/2}$$

$$=\frac{abc.\pi}{6h^2}.8.(2mE)^{3/2}$$

$$=\frac{4\pi}{3}\frac{V}{h^3}(2mE)^{3/2} \qquad (9.46)$$

And therefore energy states between E and $E+dE$would be given as follows :

$$=\frac{d}{dE}\left[\left(\frac{\pi}{3}\right)\left(\frac{V}{h^2}\right)(2mE)^{3/2}\right]$$

$$=\frac{4\pi V}{3h^3}(2m)^{3/2}.\frac{3}{2}E^{1/3}$$

$$=2\pi V\left(\frac{2m}{h^2}\right)^{3/2}E^{1/2} \qquad (9.47)$$

Thus, from above Eq. (9.47), we can easily calculate the energy state density for the case of three dimensional box.

Self Assessment Question (SAQ) 5: What do you mean by the degeneracy for energy levels.

Example 9.1:*Prove that the value of energy obtained for a particle of mass m moving in a one-dimensional box can also be obtained with the help of relation used to obtain expectation value.*

Sol. The normalised wave function for a particle of mass m in one dimensional box may be put as follows :

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

The Hamiltonian operator may be put as follows:

$$\hat{H}=\frac{1}{2}m{v_\infty}^2=\frac{{p_x}^2}{dx^2}$$

$$=-\frac{h^2}{8\pi^2 m}\frac{d^2}{dx^2}$$

$$\overline{E} =< E >= \int_0^a \psi_n{}^*(x)\hat{H}\psi_n(x)dx$$

$$= -\frac{h^2}{8\pi^2 m}\int_0^a \sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x$$

$$\times\frac{d^2}{dx^2}\left(\sqrt{\frac{2}{a}}\sin\frac{n\pi}{a}x\right)dx$$

$$= \frac{2h^2}{8\pi^2 am}\int_0^a \sin\frac{n\pi}{a}x\left(-\frac{n^2\pi^2}{a^2}\sin\frac{n\pi}{a}x\right)dx$$

$$= \frac{2h^3}{8\pi^2 am}\times\frac{n^2\pi^2}{a^2}\int_0^a \sin^2\frac{n\pi}{a}x\,dx$$

$$= \frac{\pi^2h^2}{4ma^3}\left[\frac{1}{2}\int_0^a\left(1-\cos\frac{2n\pi}{a}x\right)dx\right]$$

or $$\overline{E} =< E >= \frac{n^2h^2}{8ma^3}\left\{[x]_0^a - \frac{a}{2n\pi}\left[\sin\frac{2n}{a}x\right]_0^a\right\}$$

$$= \frac{n^2h^2}{8ma^3}(a-0) = \frac{n^2h^2}{8ma^2}$$

This value is the same obtained by solving Schrödinger's equation.

Example 9.2: *What is the lowest energy that a neutron (mass* $1.67 \times 10^{-27}\,\mathrm{kg}$*) can have if confined to move along the edge of an impenetrable box of length* 10^{-14}*meter? (*$h = 6.63 \times 10^{-34}\,\mathrm{joule-sec}$*).*

Sol. The quantised energies of a particle of mass *m* in a one-dimensional box of length *L* are given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}\text{ joules}$$

$$= \frac{n^2h^2}{8mL^2}\text{ joules,} \qquad (\mathrm{n} = 1,2,3,......)$$

The lowest energy corresponds to n = 1, and is thus

$$E_1 = \frac{h^2}{8mL^2}\text{ joules}$$

Substituting the given values, we have

$$E_1 = \frac{(6.63 \times 10^{-34}\text{joule} - \text{sec})^2}{8 \times (1.67 \times 10^{-27}\text{kg}) \times (10^{-14}\text{meter})^2}$$

$$= 3.29 \times 10^{-13}\text{joule}$$

$$= \frac{3.29 \times 10^{-13}}{1.6 \times 10^{-13}}\text{MeV}$$

Here $1\text{MeV} = 1.6 \times 10^{-13}\text{joule}$

$$\boldsymbol{E_1 = 2.06\ \text{MeV}}.$$

Example 9.3: *An electron is confined to move between two rigid walls separated by* 10^{-9}*meter. Find the de Broglie wavelengths representing the first three allowed energy states of the electron and the corresponding energies. (electron mass* $9.1 \times 10^{-31}\text{kg}$ *and* $h = 6.63 \times 10^{-34}\text{joule} - \text{sec}$*).*

Sol: The electron moving back and between rigid walls will form a stationary wave-pattern with nodes at the walls. For this, the distance *L* between the walls must be a whole multiple of the de- Broglie half-wave-lengths. Thus

$$L = n\frac{\lambda}{2}, \qquad n = 1,2,3, \dots\dots$$

Or

$$\lambda = \frac{2L}{n}.$$

Here, $L = 10^{-9}meter = 10\text{Å}$

So that,

$$\lambda = \frac{2 \times 10\text{Å}}{n} \qquad n = 1,2,3, \dots\dots$$
$$= 20\text{Å}, 10\text{Å}, 6.7\text{Å}, \dots\dots$$

The corresponding energies are given by

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

Here *m*= 9.1×10^{-31}kgand *L*= $10^{-9}meter$.

Therefore,

$$E_n = \frac{(6.63 \times 10^{-34})^2 n^2}{8 \times (9.1 \times 10^{-31}) \times (10^{-9})^2}$$

$$= 6.04 \times 10^{-20} n^2, \quad \text{joule}$$

$$= \frac{6.04 \times 10^{-20} n^2}{1.6 \times 10^{-19}} \text{eV}$$

$$= 0.38\, n^2 \text{eV}\,.$$

For $n = 1,2,3,$ we have

$$\boldsymbol{E_1 = 0.38\ eV}$$

$$\boldsymbol{E_2 = 1.52\ eV}$$

$$\boldsymbol{E_3 = 3.42\ eV}\,.$$

Example 9.4: Calculate the energy difference between the ground state and the first excited state for an electron in a one-dimensional rigid box of length 10^{-8} cm. *(electron-mass* 9.1×10^{-31}kg,and$h = 6.626 \times 10^{-34}\text{joule} - \text{sec}$*).*

Sol: The energy of a particle of mass *m* in a one –dimensional rigid box of side *L* is given by

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

or

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

$$= 0.60 \times 10^{-27} n^2, \quad \text{joule}$$

$$= \frac{0.60 \times 10^{-27} n^2}{1.6 \times 10^{-19}} \text{eV}$$

$$= 38\, n^2 \text{eV}\,.$$

For the ground state (n = 1); E_1 = 38 eV and for the first excited state (n = 2); E_2 = 152 eV. The energy difference is 152-38 = **114 eV.**

Example 9.5: *Can you observe the energy states for a ball of mass 10 gm moving in a box of length 10 cm.* ($h = 6.626 \times 10^{-34} joule - sec$).

Sol.: No. On calculating as above, we shall have

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

or

$$E_n = 3.4 \times 10^{-45} n^2 \ eV.$$

The first few energies (n = 1, 2, 3, ….) will be:

$$\mathbf{3.4 \times 10^{-45}} \, \boldsymbol{eV},$$

$$\mathbf{13.6 \times 10^{-45}} \, \boldsymbol{eV},$$

$$\mathbf{30.6 \times 10^{-45}} \, \boldsymbol{eV},$$

$$\dots \dots \dots$$

$$\dots \dots \dots$$

These are so near to each other that a continuum will be observed.

Example 9.6: *Find the probabilities of finding a particle trapped in a box of length L in the region from 0.45L to 0.55L for the ground state and the first excited state.*

Sol:

The eigenfunctions of a particle trapped in a box of length *L* are:

$$\psi_n(x) = \sqrt{\left(\frac{2}{L}\right)} \, sin \, \frac{n\pi}{L} \, x, \qquad n = 1,2,3, \dots \dots \dots$$

The probability of finding the particle between x_1 and x_2 when it is in the nth state, is

$$P = \int_{x_1}^{x_2} \left|\psi_n(x)\right|^2 dx$$

$$= \frac{2}{L} \int_{x_1}^{x_2} sin^2 \frac{n\pi x}{L} dx$$

$$= \frac{2}{L} \left[\int_{x_1}^{x_2} \frac{1}{2} \left(1 - \cos\left(\frac{2n\pi x}{L}\right)\right) dx \right]$$

$$= \frac{1}{L} \left[x - \left(\frac{L}{2n\pi}\right) \sin \frac{2n\pi x}{L} \right]_{x_1}^{x_2}$$

Here $x_1 = 0.45L$, $x_2 = 0.55L$ and for the ground state, n = 1,

$$P = \frac{1}{L} \left[x - \left(\frac{L}{2\pi}\right) \sin \frac{2\pi x}{L} \right]_{0.45L}^{0.55L}$$

$$= \frac{1}{L} \left[\left(0.55L - \left(\frac{L}{2\pi}\right) \sin 1.10\pi\right) - \left(0.45L - \left(\frac{L}{2\pi}\right) \sin \ 0.90\pi\right) \right]$$

$$= \left(0.55 - \left(\frac{1}{2\pi}\right)\sin 198°\right) - \left(0.45 - \left(\frac{1}{2\pi}\right)\sin 162°\right)$$
$$= (0.55 - 0.45) - \left(\frac{1}{2\pi}\right)[\sin 198° - \sin 162]°$$
$$= 0.10 - \frac{1}{\pi}(\cos 180° \sin 18°)$$
$$= 0.10 + \frac{0.3090}{3.14}$$
$$= 0.198 = \mathbf{19.8}\%$$

Similarly, for the first excited state (n= 2), we shall have $\boldsymbol{P} = \mathbf{0.65}\%$.

9.8 Summary:

In this unit we have discussed the behaviour of a particle in a one dimensional box. We also have discussed the quantum structure of it. We have derived the eigen values and eigen functions for one dimensional box system and also calculate the expectation value of position & momentum. It seems that this means the particle in a box does not have any momentum, which is incorrect because we know the energy is never zero. In fact, the energy that we obtained for the particle-in-a-box is entirely kinetic energy because we set the potential energy at 0. Since the kinetic energy is the momentum squared divided by twice the mass, it is easy to understand how the average momentum can be zero and the kinetic energy finite. Further, we have calculated discrete energy levels of particle in quantum mechanics for the case of one-dimensional motion of a particle which is restrained by reflecting symmetrical walls. For this case, the wave-functions also represented symmetrical nature about the origin $x = 0$, it means that $\psi_n(x)$ for odd n are even for function of x and vice-versa. Similarly, we have extended one dimensional concept in three dimensional form and calculate the eigen value and the eigen function for a particle.

9.9 Glossary:

Trapped- confined, imprisoned

Free particle-a free particle is a particle that, in some sense, is not bound by an external force, or equivalently not in a region where its potential energy varies.

Eigenvalue-each of a set of values of a parameter for which a differential equation has a non-zero solution (an eigen-function) under given conditions.

Eigenfunction- wavefunction or each of a set of independent functions which are the solutions to a given differential equation.

Distinguished-differentiate or discriminate.

Degenerate-an energy level corresponding to more than one quantum state.

9.10 References:

5. Beiser A., *Concepts of Modern Physics*, 6th Edition, McGraw Hill (2003) ISBN 0-07-244848-2.
6. Shankar, R., *Principles of Quantum Mechanics*, Kluwer Academic / Plenum Publishers New York (1994) ISBN 0-306-44790-8.
7. Chatwal, G. R.; Anand, S. K.; Arora, M., *Quantum Mechanics,* Himalaya Publishing House (2007) ISBN 978-9-350-24732-7.

9.11 Suggested Reading:

1. Quantum Mechanics by E Merzbacher

2. Introduction to Quantum Mechanics by J Griffiths David

3. Quantum Mechanics: A Textbook for Undergraduates by Jain Mahesh

9.12 Terminal Questions:

Objective Type Questions:

a) The quantum state energy of an atom probably depends on-
   - (i) Principal quantum number
   - (ii) Orbital quantum number
   - (iii) Magnetic quantum number
   - (iv) Spin quantum number

b) If the width L between two sides of one dimensional potential well is decreased to a smaller width *l*then-
   - (i) Energy of each level decreases
   - (ii) Number of energy levels decreases
   - (iii) The energy of each energy level remains unchanged
   - (iv) The energy difference between consecutive energy levels increases

c) The lowest energy possible for a particle in a potential box is 2eV. The next highest energy the particle can have is-
   - (i) 4eV
   - (ii) 8eV
   - (iii) 16eV
   - (iv) 32eV

d) The energy of a particle constrained to move in a cube of side *a* is given by

$$E = \frac{h^2}{8ma^2}\left(n_\alpha{}^2 + n_y{}^2 + n_z{}^2\right)$$

If n_x, n_y and n_z may have either values out of 1,2,3, the degree of degeneracy of this energy level is-

(i) 2
(ii) 3
(iii) 6
(iv) 8

Short Type Answer Questions:

Q.9.1 Write the Schrodinger wave equations for free particles in 1D and 3D box.

Q.9.2 What are the difference between unsymmetrical and symmetrical one dimensional potential wall in view of eigen function and eigen values?

Q.9.3 What is the reason that the value of $n \neq 0$ for a particle in a box with infinite walls.

Q.9.4 Show that any two wave functions corresponding to different energy levels are orthogonal in case of particle in a box problem.

Q.9.5 Show thatthe function $\psi = A \exp\,[i(kx - \omega t)]$ satisfies the Schrödinger's equation.

Q.9.6 Sketch the energy levels diagram along with their wave functions for one dimensional particle in a box.

Long Type Answer Questions:

Q.9.7A box was considered that extends from $x = 0$ to $x = L$. Suppose the box instead extends form $x = x_0$ to $x = x_0 + L$, where $x_0 \neq 0$. Would the expression for the wave functions of a particle in this box be any different from those in the box that extends from $x = 0$ to $x = L$? Would the energy levels be different?

Q.9.8 Show that the expectation valve $\langle x \rangle$ of a particle trapped in a box *L* wide is *L/2,* which means that its average position is the middle of the box. Find the expectation value of $\langle x^2 \rangle$.

Q.9.9 Find the normalization constant *B* for the linear combination of two wave functions for the same system, i.e.,

$$\psi = B\left(\sin\frac{\pi x}{L} + \sin\frac{2\pi x}{L}\right)$$

for the $n = 1$ and $n = 2$ states of a particle in a box *L* wide.

Q.9.10 Find the probability that a particle in a box *L* wide can be found between $x = 0$ and $x = (L/n)$ when it is in the *n*th state.

Q.9.11 The particle in a box is in its ground state of $n_x = n_y = n_z = 1$.

(a) Find the probability that the particle will be found in the volume defined by $0 \leq x \leq \frac{L}{4},\ 0 \leq y \leq \frac{L}{4},\ 0 \leq z \leq \frac{L}{4}$.

(b) Do the same for $\frac{L}{2}$ instead of $\frac{L}{4}$.

Q.9.12 An important property of the eigenfunctions of a system is that they are orthogonal to one another, which means that

$$\int_{-\infty}^{+\infty} \psi_n \psi_m dV = 0, \qquad n \neq m$$

Verify this relationship for the eigenfunctions of a particle in a one-dimensional box.

Q.9.13A particle is in a cube box with infinitely hard walls whose edges are L long. The wave functions of the particle are given by

$$\psi_{n_x n_y n_z} = A \sin\frac{n_x \pi x}{L} \sin\frac{n_y \pi y}{L} \sin\frac{n_z \pi z}{L}$$

where n_x, n_y, n_z are the quantum numbers of values 1, 2, 3,….. . Find the value of the normalization constant *A*.

9.13(a) Answers of Self Assessment Question (SAQ)

Ans.1: Using Eq.(9.7b), $A = \left(\frac{m\omega}{\hbar\pi}\right)^{1/4}$

Ans.2: $E_1 = E$, and $E_2 = 4E$, where $E = \frac{h^2}{8mL^2}$

Ans.3: Refer section-9.3

Ans.4:$x \longrightarrow \hat{x},\ \ p \longrightarrow \hat{p} = -i\hbar\frac{\partial}{\partial x}\ ,\ \ E \longrightarrow \hat{E} = i\hbar\frac{\partial}{\partial t}$

Ans.5: Refer section-9.7

(c) Answers of Terminal Questions:

Answer of objective questions: a) (i) **b)** (iv) **c)** (ii) **d)** (iii)

Ans.9.8:$\langle x^2\rangle = \frac{L^3}{3} - \frac{L^2}{2n^2\pi^2}$

Ans.9.9: $B = \left(\frac{1}{L}\right)^{1/2}$

Ans.9.10: $1/n$

Ans.9.13: $A = \left(\frac{2}{L}\right)^{3/2}$

Unit-10: Linear Harmonic Oscillator and Hydrogen atom

CONTENTS

10.1 Introduction:

In this unit, we study about the quantum phenomena of linear harmonic oscillator and hydrogen atom. Let us consider two masses which are joined together by some type of interaction force between them. Suppose these are vibrating with respect to each other. This system will execute harmonic oscillations if the restoring force exerted by one vibrating mass upon the other is proportional to its respective displacement. In such a situation, the system will constitute a harmonic oscillator. If the vibrations are confined to one dimension, the system will form a linear harmonic oscillator.

10.2 Objective:

- Explain and define the meaning oflinear harmonic oscillator
- To derive the eigen value and eigen function of linear harmonic oscillator
- Illustrate thephysical interpretation of harmonic oscillator wave function
- Describe the spherical symmetric systems and potentials
- To study the hydrogen atom and its eigen value and eigen state

10.3 Linear harmonic oscillator:

When the potential energy of two atoms is plotted as a function of their separation, a curve of the type shown in Fig. 10.1 is obtained. At $x=a$, the potential will be minimum. This point is corresponding to a stable equilibrium position. Ear this point it becomes possible to expand the potential as a series of powers of (x-a) and but $\frac{\partial V}{\partial x} = 0$ at this point. Therefore, we have

$$V = \frac{K}{2}(x-a)^2 \qquad ...(10.1)$$

In the above expansion, the higher order terms have been neglected.Eq. (10.1) represents the harmonic oscillator potential. In general, it is possible to represent any system in stable equilibrium near the equilibrium position by means of a harmonic oscillator (Fig.10.1).

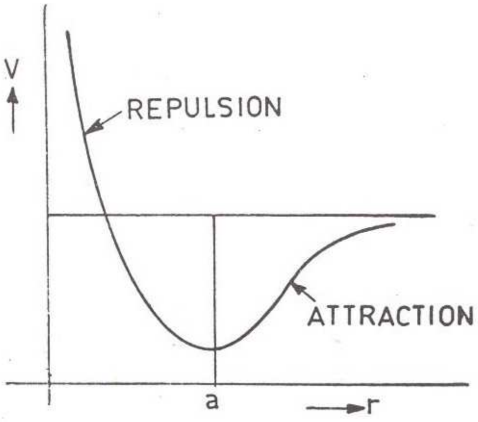

Fig. 10.1 Harmonic potential

10.3.1 Asymptotic behaviour:

In the case of a linear harmonic oscillator, it is possible to represent the force *F=Kx* by the potential energy

$$V(x) = \frac{1}{2}Kx^2 \qquad ...(10.2)$$

It is possible to derive the above equation in the following manner. Suppose the particle of mass m in undergoing simple harmonic motion with amplitude *a*. The displacement from the origin at time t is given as follows :

$$x = a \sin wt$$

or $$\frac{dx}{dt} = aw \cos wt$$

$$\therefore \text{Kinetic energy} = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2$$

$$= \frac{1}{2}m\, a^2 w^2 \cos^2 wt$$

Maximum value of K.E. will be obtained, when $\cos wt = 1$

$$\therefore \text{(Kinetic Energy)}_{\max} = \frac{1}{2}ma^2w^2$$

Further, $(\text{K.E.})_{\max} = \text{K.E.} + \text{Potential Energy (V)}$

or $$\frac{1}{2}ma^2w^2 = \frac{1}{2}ma^2w^2\cos^2 wt + V$$

$$V = \frac{1}{2} m a^2 w^2 \left(1 - \cos^2 wt\right)$$

$$= \frac{1}{2} m a^2 w^2 \sin^2 wt$$

$$= \frac{1}{2} m w^2 x^2 \qquad [\because \quad x = a \sin\, wt]$$

$$= \frac{1}{2} K x^2$$

where K=mw^2. It is to be proved. If we substitute Eq. (10.2) in the Schrödinger's equation in one dimension, we obtain

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}Kx^2\right)\psi = 0 \qquad ...(10.3)$$

Now it is possible to convert Eq. (10.3) in dimensionless form by introducing $\xi = \alpha x$.

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

and
$$\frac{d^2\psi}{dx^2} = \frac{d}{dx}\left(\frac{d\psi}{d\xi}\alpha\right) = \frac{d}{d\xi}\frac{d\xi}{dx}\left(\frac{d\psi}{d\xi}\alpha\right) = \alpha^2\frac{d^2\psi}{d\xi} \qquad ...(10.4)$$

If the above equations are introduced in Eq. (10.3), we obtain

$$\alpha^2\frac{d^2\psi}{d\xi^2} + \left[\frac{2mE}{\hbar^2} - \frac{mK}{\hbar^2}\frac{\xi^2}{\alpha^2}\right]\psi = 0$$

$$\frac{d^2\psi}{d\xi^2} + \left[\frac{2mE}{\hbar^2\alpha^2} - \frac{mK\xi^2}{\alpha^4{}_0\hbar^4}\right]\psi = 0 \qquad ...(10.5)$$

Suppose α is so chooses that

$$\frac{mK}{\hbar^2\alpha^4} = 1 \text{ or } \alpha^4 = \frac{mK}{\hbar^2}, \text{ i.e., } \alpha = \left[\frac{mK}{\hbar^2}\right]^{1/2}$$

and suppose
$$\lambda = \frac{2mE}{\hbar^2\alpha^2}$$

$$\lambda = \frac{2mE\hbar}{\hbar^2\sqrt{(mK)}} = \frac{2E}{\hbar}\left(\frac{m}{K}\right)^{1/2} \qquad ...(10.6)$$

If Eq. (10.6) substituted in Eq. (10.5), we obtain

$$\frac{d^2\psi}{d\xi^2} + \left(\lambda - \xi^2\right)\psi = 0 \qquad ...(10.7)$$

Now such functions are needed which are able to satisfy this equation throughout the region of value -∞ to +∞ for ξ and are acceptable wave functions. It means that we desire such functions which are continuous, single valued and finite throughout the region.

Now an attempt is being made to get the solution of Eq. (10.7) throughout configuration space ($-\infty<\xi<+\infty$). This is based upon the asymptotic behaviour. Suppose the solution is of the following form :

$$\psi(\xi) = H(\xi)e^{-\xi^2/2} \qquad ...(10.8)$$

where H(ξ) represents a polynomial of finite order in ξ. If positive sign is taken in the exponent, ψ get diverged as $\psi\rightarrow\infty$.

From Eq. (10.5), $\frac{d\psi}{d\xi} = H'(\xi)\ \text{exp.}\left[\frac{-\xi^2}{2}\right] - \xi H(\xi)\exp\left[\frac{-\xi^2}{2}\right]$

and $$\frac{d^2\psi}{d\xi^2} = H'(\xi)\ \text{exp.}\left[\frac{-\xi^2}{2}\right] = H'(\xi)\xi\exp\left[\frac{-\xi^2}{2}\right]$$

$$-H(\xi)\ \text{exp.}\left[\frac{-\xi^2}{2}\right] - \xi H'(\xi)\ \text{exp.}\left[\frac{-\xi^2}{2}\right] - \xi H(\xi)\ \text{exp.}\left[\frac{-\xi^2}{2}\right]$$

$$= H''(\xi)\ \text{exp.}\left[\frac{-\xi^2}{2}\right] - 2\xi H'(\xi)\ \text{exp.}\left[\frac{-\xi^2}{2}\right] + (\xi^2-1)\,H(\xi)\ \text{exp.}\left[\frac{-\xi^2}{2}\right]$$

If the values of $\frac{d\psi}{d\xi}$ and $\left[\frac{d^2\psi}{d\xi^2}\right]$ are substituted in Eq. (10.7), we obtain

$$\text{exp.}\left[\frac{-\xi^2}{2}\right]\left[H''(\xi) - 2\xi H'(\xi) + \xi^2 H(\xi) - H(\xi) + (\lambda - \xi^2)H(\xi)\right] = 0$$

or $$H''(\xi) - 2\xi H'(\xi) + (\lambda - 1)H(\xi) = 0$$

or $$H''-2\xi H'+(\lambda-1)H=0, \qquad ...(10.9)$$

In Eq. (10.9) primes represent differentiation with respect to ξ.

10.3.2 Energy levels:

It is possible to solve Eq. (10.6) by the series method by putting.

$$H(\xi)=\xi^s\left(a_0+a_1\xi+a_2\xi^2+...\right) \qquad a_0\neq 0, s\geq 0$$

$$=\xi^s\sum_{v=0}^{\infty}a_v\xi^v=\sum_{v=0}^{\infty}a_v\xi^{s+v}$$

$$\frac{dH}{d\xi}=\sum_v a_y(s+v)\xi^{s+v-1}$$

and $$\frac{a^2H}{d\xi^2}=\sum_v a_v(s+v)(s+v-1)\xi^{s+v-2}$$

If these values are substituted in equation (10.9), we get

$$\sum_v a_v(s+v)(s+v-1)\xi_s^{+v-2}-2\xi\sum_v a_v(s+v)\xi^{s+v-1}+(\lambda-1)\sum_v a_v\xi^{s+v}=0$$

$$\sum_v a_v(s+v)(s+v-1)\xi^{s+v-2}-2\sum_v a_v(s+v)\xi^{s+v-1}+(\lambda-1)\sum a_v\xi^{s+v}=0 \qquad ...(10.11)$$

If this series is to vanish for all values of ξ i.e., $H(\xi)$ is to be a solution of Eq. (10.9), it means that the coefficient of individual powers of ξ must vanish separately. If the coefficients of various powers of ξ are equated to zero, we obtain

$$s(s-1)a_0=0 \qquad ...(10.12a)$$

$$(s+1)(s)a_1=0 \qquad ...(10.12b)$$

$$(s+2)(s+1)a_2-(2s+1+\lambda)a_0=0 \qquad ...(10.12c)$$

$$(s+3)(s+2)a_2-(2s-3-\lambda)a_1=0 \qquad ...(10.12d)$$

... ...

... ...

$$(s+v+2)(s+v+1)a_{v+2}-(2s+2v+1-\lambda)a_0=0 \qquad ...(10.12e)$$

$$a_{v+2} = \frac{2s+2v+1-\lambda}{(s+v+1)(s+v+2)} a_v \qquad ...(10.13)$$

where *v* represents an integer.

Eq. (10.13) is termed as a recursion formula. As a_0 cannot be zero, it follows from Eq. (10.12a) that s=0 or s=1. If a_0 is put equal to zero, only odd powers will appear; with a, zero, the series will be having even powers only.

If arbitrary values are given to the energy parameters λ, the series given in Eq. (10.13) will give rise to an infinite number of terms but they do not correspond to satisfactory wave function. If the convergence of the power solution defined by Eq. (10.13) is examined very carefully, it is found that as $v \to \infty, (a_{v+2})/a_v \to 2/v$ so that the series gets converged for all finite values of ξ. Now we will consider the series gets converged for all finite values of ξ. Now we will consider the series expansion of $e^{+\xi 2}$, i.e.,

$$e^{\xi 2} = 1 + \xi^2 + \frac{\xi^4}{2!} + \frac{\xi^6}{3!} + ... + \frac{\xi^v}{(v/2)!} + \frac{\xi^{v+2}}{(v/2+1)!} + ...$$

$$b_0 + b_2\xi^2 + b_4\xi^4 + ... + b_v\xi^v + b_v\xi^v + b_{v+2}\xi^{v+2} + ...$$

and $$\frac{b_{v+2}}{b_v} = \frac{\frac{1}{(v/1+1)!}}{\frac{1}{(v/2)!}} = \frac{2}{2+v}$$

or $$\underset{v\to\infty}{Lim} \frac{b_{v+2}}{b_v} = \frac{2}{v}$$

From the above it follows that $H(\xi)$ gets diverged approximately as $e^{\xi 2}$ and the product $H(\xi)\, e^{-\xi^2/2}$ will behave in a similar manner as $H(\xi)\, e^{+\xi^2/2}$ in this region. It implies that it is unacceptable as wave function.

In order to avoid this situation, the value of λ is chooses in such a way that the power series of $H(\xi)$ gets cut off at some terms, thereby making $H(\xi)$ a polynomial. From Eq. (10.13), it follows that the value of λ which makes the series to cut off at nth terms, should be

$$\lambda = 2s + 2v + 1$$

The value of index, *s*, may be either 0 or 1. Corresponding to these values of *s* the values of λ will be equal to *2v+1* or *2v+3* where *2v* is an even integer. It is possible to express both these cases in terms of a quantum number *n*, i.e., Then $$\frac{2E_n}{\hbar}\frac{\lambda=(2n+1)}{\sqrt{\frac{m}{k}}=(2n+1)}$$

or $$E_n=\left(n+\frac{1}{2}\right)\hbar\omega, \qquad n=0,\ 1,\ 2,\ 3, \qquad \text{...(10.14)}$$

where $\omega_c=\sqrt{\frac{K}{m}}$ is the classical angular frequency of the oscillator.

10.3.3 Zero-point energy:

The energy levels obtained by using Eq. (10.14) are discrete and possess equal spacing. If n=0 put in Eq. (10.14), then the finite value of grand state energy will be $\frac{1}{2}\hbar\omega_c$, called the zero point energy, i.e.,

$$E_0=\frac{1}{2}\hbar\,\omega_c \qquad \text{...(10.15)}$$

From the above equation it is evident that all the energy levels get shifted by an amount which is equal to half the separation of energy levels.

In Fig. 10.2, five lowest energy of a harmonic oscillator have been depicted. In this figure, it can be seen that the system in its lowest state is having an energy greater than that which it would be having when it was at rest in its equilibrium position. Zero-point energy has been found to be characteristic of quantum mechanics. Further it is related to the uncertainty principle given by Heisenberg.

Fig. 10.2: Energy level diagram for a liner harmonic oscillator.

10.3.4 Hermite polynomials:

When $\lambda = (2n+1)$, Eq. (10.9) becomes as follows :

$$H_n''-2\xi H_n'+2nH_n = 0 \qquad ...(10.16)$$

The polynomials $H_n(\xi)$, are known as the Hermite polynomials. The first few Hermite Polynomials are as follows :

$$H_0(\xi) = 1,$$
$$H_1(\xi) = 2\xi,$$
$$H_2(\xi) = 4\xi^2 - 2,$$
$$H_3(\xi) = 8\xi^3 - 12\xi,$$
$$H_4(\xi) = 16\xi^4 - 48\xi - 12.$$

10.3.5 Harmonic oscillator wave function:

The solution of the equation $H_n''-2\xi H_n'+2nH_n = 0$ will be $\psi_n(\xi) = H_n(\xi)e^{-\xi^2/2}$. The general solution may be put as follows :

$$\psi_n(\xi) = N_n H_n(\xi)e^{-\xi^2/2}. \qquad (10.17)$$

where N_n is a constant. In order to evaluate this constant now proceed as follows:

From the Hermite Polynomials, we have

$$e^{-S^2+2S\xi} = \sum_{n=0}^{\infty}\frac{H_n(\xi)}{n!}s^n. \qquad (10.18)$$

Similarly, it can be put as follows:

$$\text{exp.}\left(-t^2+2t\xi\right) = \sum_{m=0}^{\infty}\frac{H_n(\xi)}{m!}t^m. \qquad (10.19)$$

By power series, we also obtain

$$\int_{-\infty}^{+\infty} H_n{}^2(\xi)e^{-\xi^2}d\xi = \pi^{1/2}2^n(n)!, \text{ when } n = m \qquad (10.20)$$

$$\int_{-\infty}^{-\infty} H_n(\xi)H_m(\xi)e^{-\xi 2}d\xi = 0. \text{ If } n \neq m. \qquad (10.21)$$

By normalised condition, we have

$$\int_{-\infty}^{+\infty} |\psi_n(x)|^2 \, dx = \frac{|N_n|^2}{\alpha} \int_{-\infty}^{+\infty} H_n{}^2(\xi) e^{-\xi 2} d\xi = 1 \qquad (10.22)$$

i.e., $$\frac{|N_n|^2}{\alpha} \pi^{1,2} 2^n (n) A = 1$$

or $$N_n = \left\{ \frac{\alpha}{\pi^{1/2} 2^n (n)!} \right\}^{1/2} \qquad ...(10.23)$$

Therefore, the wave function of harmonic oscillator is

$$\psi_n(\xi) = \left\{ \frac{\alpha}{\pi^{1/2} 2n(n)!} \right\}^{1/2} H_n(\xi) e^{-\xi 2/2} \qquad ...(10.24)$$

Self Assessment Question (SAQ) 1: Define linear harmonic oscillator. How potential energy varies for that.

Self Assessment Question (SAQ) 2: Calculate the energy eigen value of linear harmonic oscillator for third energy state.

Self Assessment Question (SAQ) 3: What isthe frequency of emitted radiation if electron jumps from third exited level to second exited level.

10.4 Physical interpretation of harmonic oscillator wave functions:

We should know about the physical significant of the harmonic oscillator wave functions. For the lowest energy state (n=0), the wave function $\psi_0(\xi)$ and the quantity $[\psi_0(\xi)]^2$ when plotted as a function of ξ are depicted in Fig. 10.3(a) and (b).

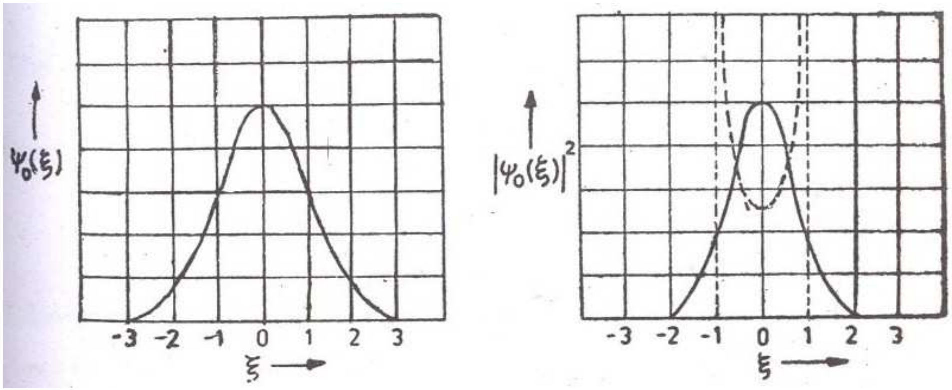

Fig. 10.3(a) The wave function $\psi_0(\xi)$ for the normal state of the harmonic oscillator wave function

(b) Probability distribution function $|\psi_0(\xi)|^2$ classically distribution curve is shown by dashed curve

From Fig. 10.3(b), it can be seen that the result for quantum mechanics for this case is not having any agreement with the probability function which is found out classically for a harmonic oscillator with the same energy.

From the classical theory, it is evident that a limit exists beyond which oscillator cannot go and the classical probability density tends to approach infinity at this limit. From the quantum mechanics, it is evident that there occurs a small probability outside of it.

The kinetic energy of the classical oscillator reduces to zero and the potential energy equals the total energy at the two end point of the classically permitted region. Outside this region, the potential energy would become higher than the total energy and the particle would be having a negative kinetic energy which is not possible at all in classical mechanics. This unexpected result is closely related to the Heisenberg's uncertainty relation. This forms the characteristic feature of quantum mechanics. It is of interest to note that the agreement between classical and quantum probability densities tends to increase rapidly with increasing value of *n*. This can be seen from Fig. 10.4, having a plot of $|\psi_n(\xi)|^2$ for n=10 (solid curve) and of the density of a classical oscillator of total energy $\frac{21}{2}\hbar\omega_0$ (shown by dotted curve). It will be seen that the agreement is fairly good on the average.

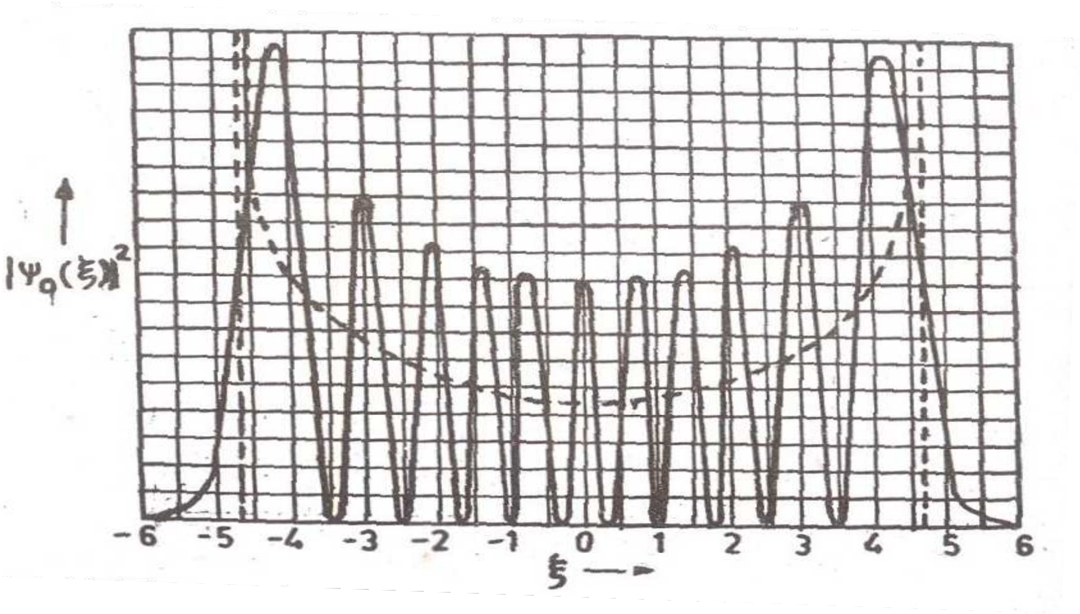

Fig. 10.4: The probability distribution function $|\psi_{10}(\xi)|^2$ for state n=10 of the harmonic oscillator. Dashed curve represents the probability function for the classical harmonic oscillator with the energy.

In fig 10.5, we represent the nature of wave functions if the values of n are going to 0 to 5. Each of these wave functions, the peak shows the probability of finding of particle.

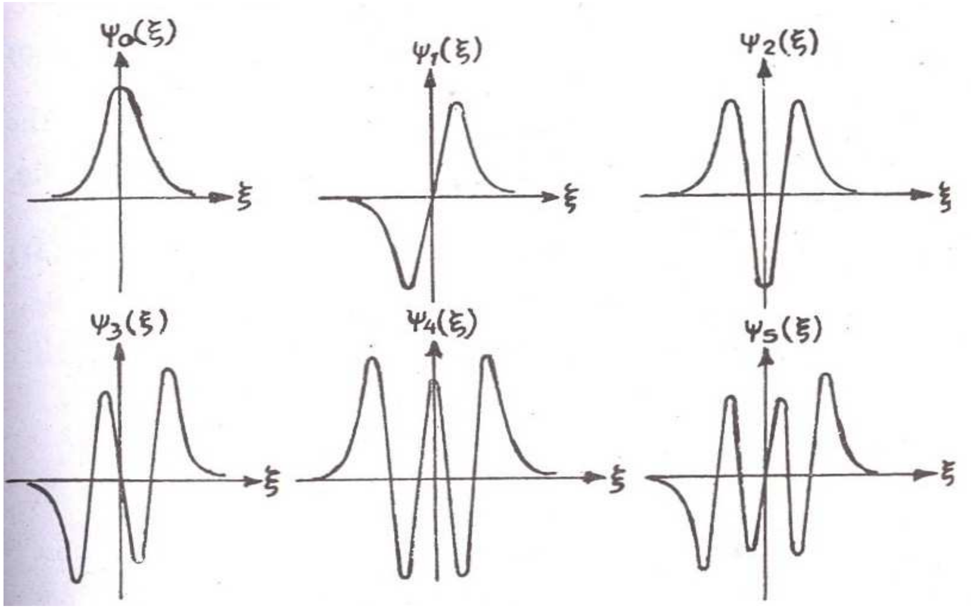

Fig. 10.5: Representation of the wave-function of harmonic oscillatorfor n = 0 to 5

But H_n is representing a polynomial of degree n. Therefore, ψ_n will be having n zeros or points where ψ_n will cut the zero line. The probability of finding the particle at these points will be zero.

10.4.1 Probability inside or outside the classical region :

The wave functions for a linear harmonic oscillator may be put as follows :

$$\psi_n(\xi) = \left\{ \frac{\alpha}{\pi^{1/2} 2^n (n)!} \right\}^{1/2} H_n(\xi) e^{-\xi 2/2}$$

In the ground state, i.e., n=0, the above equation becomes as follows :

$$\psi_0(\xi) = \left[\frac{\alpha}{\pi^{1/2}} \right]^{1/2} .1.e^{-\xi^2}/2 \qquad ...(10.25)$$

The classical probability becomes as follows :

$$= \int_{-a}^{+a} |\psi|^2 \, dx = 2\int_0^a \frac{\alpha}{\pi^{1/2}} e^{\xi 2} dx$$

$$= 2\int_{-a}^{a} \frac{\alpha}{\pi^{1/2}} e^{-\alpha^2 x^2} dx \qquad ...(10.26)$$

(The amplitude varies from –a to +a)

According to quantum mechanics, we have

$$E = \frac{1}{2}\hbar\omega_0 = \frac{1}{2}\hbar\sqrt{\left(\frac{K}{m}\right)} = \frac{1}{2}Kx^2 \text{ or } x^2 = \frac{\hbar}{\sqrt{(mK)}} = \frac{1}{\alpha^2}$$

$$\therefore \qquad x = \pm\frac{1}{\alpha}, \qquad ...(10.27)$$

i.e., quantum mechanically x tends to vary from $-\frac{1}{\alpha}$ to $+\frac{1}{\alpha}$. The classical and quantum mechanical limits have been depicted in Fig. 10.6. Hence quantum mechanical probability is given by

$$P = 2\int_0^{+1/\alpha} \frac{\alpha}{\pi^{1/2}} e^{-\alpha^2 x^2} dx \qquad ...(10.28)$$

If we put $\alpha x = t$, we get

$$P = \frac{2}{\sqrt{\pi}} \int_0^1 e^{-t^2} dt \ldots (10.29)$$

Or

$$P = \frac{2}{\sqrt{\pi}} \int_0^1 \left[1 - \frac{t^2}{1!} + \frac{t^4}{2!} - \frac{t^6}{3!} + \frac{t^8}{4!} + \ldots \right] dt$$

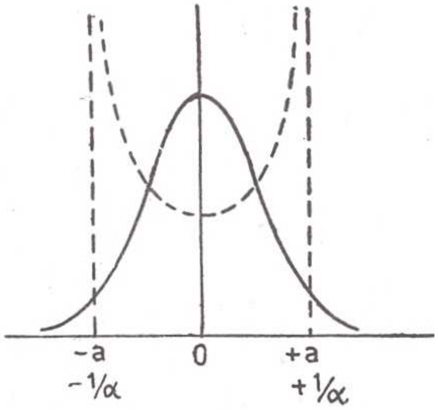

Fig. 10.6: Showing the classical and quantum mechanical limits.

$$= \frac{2}{\sqrt{\pi}} \left[t - \frac{t^3}{3(1)!} + \frac{t^5}{5(2)!} - \frac{t^7}{7(3)!} - \frac{t^9}{9(4)!} + \ldots \right]_0^1$$

$$= \frac{2}{\sqrt{\pi}} \left[1 - \frac{1}{3(1)!} + \frac{1}{5(2)!} - \frac{1}{7(3)!} - \frac{1}{9(4)!} + \ldots \right]$$

$$P = 0.83$$

or $$P = 83\%$$

Therefore, it can be concluded that the probability of finding the oscillator inside the classical limit will be 83% while outside the classical limit will be only 17%.

Self Assessment Question (SAQ) 4: Write the physical significant of wave vector (Ψ).

10.5 Spherical symmetric systems and potentials:

There are certain systems in which the potential energy of the particle is not dependent upon θ and ϕ but is only the function of radius vector *r*. Such systems are termed as spherical symmetric systems.

A **hydrogen atom** consists of one electron which is moving around the positively charged nucleus. Our interest lies in the motion of two particles namely nucleus and electron. These two are attracted by a force which depends upon only on the distance between them. Whenever this problem is to be solved, the important assumptions made are that the nucleus is at rest while the mass of the electron is replaced by μ. The potential energy V(r) of such a system is given by $-e^2/r(Z=1)$. Actually, is equal to the attractive coulomb interaction between an atomic nucleus of charge +e and an electron of charge –e. Thus,

$$V(r) = -\frac{e^2}{r}$$

Such potentials are termed as spherically symmetrical potentials.

10.5.1 The hydrogen atom: (Application of the Schrödinger's equation)

In the field of atomic and molecular structure, the problem of structure of hydrogen atom is regarded as very important because it forms the basis for the discussion of more complex atomic systems. The wave-mechanical treatment, which is applied to hydrogen atom, is also used for hydrogen-like or closely related atoms.

In the hydrogen atom there are two interacting particles, namely, nucleus and electron. The interaction between these two particles gives rise to the Coulombic attraction. If the charge on the nucleus is Ze and the charge on the electron –e, then the potential energy of the system in the absence of electric field is $-Ze^2/r$ where r represents the distance between the electron and the nucleus.

The Schrödinger's wave equation for the system consisting of two particles of mass m_1 and m_2 and having Cartesian coordinates x_1, y_1, z_1 and x_2, y_2, z_2 may be put as follows :

$$\frac{1}{m_1}\left(\frac{\partial^2\psi_T}{\partial x_1^2}+\frac{\partial^2\psi_T}{\partial y_1^2}+\frac{\partial^2\psi_T}{\partial z_1^2}\right)+\frac{1}{m_2}\left(\frac{\partial^2\psi_T}{\partial x_2^2}+\frac{\partial^2\psi_T}{\partial y_2^2}+\frac{\partial^2\psi_T}{\partial z_2^2}\right)$$

$$+\frac{2}{\hbar^2}(E_T - V)\psi_T = 0 \quad ...(10.30)$$

In Eq. (10.30), the subscript $_T$ refers to total and is put along E and ψ to indicate that these quantities are referring to the complete system. Eq. (10.30) also defines the complete behaviour of the system.

As the potential energy of the system depends upon the relative coordinates of the two particles $\{V = V(x_1 - x_2, y_1 - y_2, z_1 - z_2)\}$ and the effect of external interaction is well shown by centre of mass, it becomes essential to transform the above equation in terms of coordinates x, y, z and coordinates of the centre of mass X, Y, Z which are represented as follows :

$x=x_1-x_2$ $\qquad$ $y=y_1-y_2$ $\qquad$ $z=z_1-z_2$

$$\begin{aligned} MX &= m_1x_1 + m_2x_2, \\ MY &= m_1y_1 + m_2y_2, \\ MZ &= m_1z_1 + m_2z_2. \end{aligned} \qquad ...(10.31)$$

In the above equation, $M(=m_1+m_2)$ denotes the total mass of the system. If Eqs. (10.31) are substituted in Eq. (10.30), we obtain the equation in terms of new coordinates.

$$\frac{1}{m}\left(\frac{\partial^2\psi}{\partial X^2}+\frac{\partial^2\psi}{\partial Y^2}+\frac{\partial^2\psi}{\partial Z^2}\right)+\frac{1}{\mu}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)$$

$$+\frac{8\pi^2}{h^2}\left[(E_t+E)-V(x,y,z)\right]\psi = 0 \qquad ...(10.32)$$

where $\mu = \frac{m_1m_2}{m_1+m_2}$ is termed as the reduced mass of the system; $E_T = E_t + E,$ with E_t represents the energy of translation and E the total energy excluding that of translation.

It is possible to separate Eq. (10.32) into two equations given below:

$$\frac{1}{M}\left(\frac{\partial^2\psi}{\partial X^2}+\frac{\partial^2\psi}{\partial Y^2}+\frac{\partial^2\psi}{\partial Z^2}\right)+\frac{8\pi^2}{h^2}E_t\psi = 0 \qquad ...(10.33)$$

and

$$\frac{1}{\mu}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)+\frac{8\pi^2}{h^2}\left[E-V(x,y,z,)\right]\psi = 0 \qquad ...(10.34)$$

Eq. (10.33) is applicable to the translation of the center of mass of the system while Eq. (10.34) is concerned with the internal motion and is having the potential energy term.

As Eq. (10.33) yields the solution of a free particle only, it will not be discussed further. However, Eq. (10.34) is our interest only.As the force is central and is acting along the line connecting the particles, it becomes essential to express the potential energy as a function of single variable called *r*, the distance between the particles, in terms of spherical polar coordinates. The Schrödinger's wave equation may be put as follows:

$$\nabla^2\psi + \frac{2m}{\hbar^2}[E-V]\psi = 0 \qquad \text{...(10.35)}$$

Here *r*, the distance of the point from the origin, θ is the angle from the Z-axis, ϕ is the angle included between the XZ plane and the vector r.

From Fig. 10.7, it is seen that the spherical coordinates define

$x = r \sin\theta \cos\phi$

$y = r \sin\theta \sin\phi$

$z = r \cos\theta$

In terms of spherical polar coordinates, the value ∇^2 may be put as follows:

$$\nabla^2 = \frac{1}{r}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial}{\partial\phi^2} \qquad \text{...(10.36)}$$

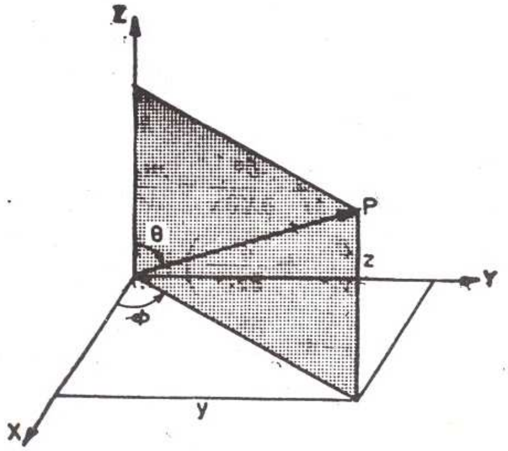

Fig. 10.7: Spherical coordinates.

If the above equation is substituted in Eq. (10.36), we obtain the Schrödinger's wave equation with a spherically symmetric potential in spherical coordinates

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{dr}\right) + \frac{1}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)$$

$$+\frac{1}{\sin^2\theta}.\frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2}+\frac{2\mu}{\hbar^2}\left[E-V(r)\right]\psi=0 \qquad ...(10.37)$$

Equation (10.37) is a second order partial differential equation. This contains three variables. In order to separate the variables it becomes necessary to assume that ψ may be represented by the product of three wave functions, each having only one of the three variables, r, θ and ϕ. If we let

$$\psi(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi)$$

Now it is possible to separate Eq. (10.37) in different variables by using the above equation.

$$\frac{1}{r^2R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{1}{r^2\sin^2\theta}\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}$$

$$+\frac{1}{r^2\sin\theta}\frac{1}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\frac{2\mu}{\hbar^2}\{E-V(r)\}=0 \qquad ...(10.38)$$

If the above equation is multiplied by $r^2\sin^2\theta$, we get

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{1}{\Theta}\frac{d^2\Phi}{d\phi^2}+\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\frac{2\mu r^2\sin^2\theta}{\hbar^2}\{E-V(r)\}=0$$

$$...(10.39)$$

As the second term of Eq. (10.39) depends on ϕ and rest part of this equation is independent of Φ, it means that the second term should be equal to a constant, i.e.

$$\frac{d^2\Phi}{d\phi^2}=-m^2\Phi$$

or

$$\frac{d^2\Phi}{d\phi^2}+m^2\Phi=0. \qquad ...(10.40)$$

With this value of second term equation (10.39) becomes as follows:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{1}{\sin\theta}\frac{1}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)-\frac{m^2}{\sin^2\theta}+\frac{2\mu r^2}{\hbar^2}\{E-V(r)\}=0.$$

$$...(10.41)$$

In Eq. (10.41), the I and IV terms depend only on r and II and III terms only on θ. Therefore each part has to be put equal to a constant:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2\mu r^2}{\hbar^2}(E-V)-\frac{m^2}{\sin^2\theta}-\frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)=\lambda,$$

so that we may write as follows :

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)+\left(\lambda-\frac{m^2}{\sin^2\theta}\right)\Theta=0. \qquad ...(10.42)$$

and

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{d\theta}\right)+\left[\frac{2\mu}{\hbar^2}\{E-V(r)\}-\frac{\lambda}{r^2}\right]R=0. \qquad ...(10.43)$$

The equations (10.41), (10.42) and (10.43) are termed as ϕ, θ and r equations respectively. The complete solution of equation (10.37) will be depending upon the solution of (10.41), (10.42) and (10.43). Now the solutions of these equations will be given as follows :

10.5.2 Solution of Φ equations:

The Φ equation may be put as follows :

$$\frac{d^2\Phi}{d\phi^2}+m^2\Phi=0.$$

The above equation is a second order differential equation having solution as given below :

$$\Phi=Ae^{\pm im\phi}, \qquad ...(10.44)$$

where A is known as an arbitrary constant. It is possible to evaluate the constant A by normalizing Φ, i.e.,

$$\int_0^{2\pi}\Phi^*\Phi\,d\phi=1$$

or

$$\int_0^{2\pi}A^2d\phi=1. \qquad ...(10.45)$$

or

$$A=\frac{1}{\sqrt{(2\pi)}}.$$

Hence the solution becomes as follows :

$$\Phi=\frac{1}{\sqrt{(2\pi)}}e^{\mp im\phi}. \qquad ...(10.46)$$

As the function Φ is single valued, it means that it should have same value at $\phi=0$ and $\phi=2\pi$, i.e.,

$$\Phi=A=Ae^{\mp 2\pi m}$$

or $$e^{\mp 2\pi i m} = \cos 2\pi m \mp i \sin 2\pi m. \quad \text{...(10.47)}$$

The equation (10.47) will be valid only if m is zero or an integer (positive or negative). Thus it may be written as follows :

$$\Phi = \frac{1}{\sqrt{(2\pi)}} e^{im\phi}, \quad \text{...(10.48)}$$

where m=0, ±1, ±2, ±3...

It implies that positive and negative values of m are corresponding to the distinct solution while for m=0, there is only one solution.

The quantity m is termed as the magnetic quantum number which is having obviously the integral nature: (the postulatory concept is now natural consequence of mathematical formulation).

However, it is possible to get real solutions of ϕ equation by taking linear combinations of complex solutions for Φ and they are as follows

$$\Phi = \frac{1}{\sqrt{\pi}} \sin m\phi, \quad \text{or} \quad \frac{1}{\sqrt{\pi}} \cos m\phi, \quad \text{for } m = \pm 1, \pm 2...$$

and $$\Phi = \frac{1}{\sqrt{(2\pi)}} \text{ for } m = 0. \quad \text{...(10.49)}$$

Thus, the wave functions of hydrogen atom are given by

$$\psi_{n,l,m_l}(r,\theta,\phi) = R_{n,l}(r)\, \Theta_{l,m_l}(\theta)\, \Phi_{m_l}(\phi)$$

The real form of the wave functions of hydrogen atom for ground state is given below:

$$R_{1,0}(r)\, \Theta_{0,0}(\theta) \qquad \Phi_0(\phi) \qquad \Rightarrow \psi_{1,0,0}(r,\theta,\phi)$$

$$\frac{2}{a_0^{3/2}} e^{-r/a_0} \qquad \frac{1}{\sqrt{2}} \qquad \frac{1}{\sqrt{2\pi}} \qquad \Rightarrow \frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0}$$

10.5.3 Energy of atomic levels and degeneracy:

If$E_n$is the eigen value, then we get

$$E_n = -|E_n| = -\frac{\mu Z^2 e^4}{2\hbar^2 n^2} \qquad ...(10.50)$$

Eq. (10.50) represents the equation for energy of an atomic state which is defined by the principal quantum number, n. We know that associated Laugerre polynomial L_q^p is accepted solution of associated Laugerre equation in which both p and q must be zero or integer.

It implies that for accepted solution of r equation the equivalent values of p and q have to follow the same rule, i.e., it means that $(2l+1)$ and $(n+l)$ must be zero or integral. As l takes integral values (including zero), it means that n must be either zero or integral.

When $n=0$ is substituted in Eq. (10.50), it becomes infinite. However, it becomes impossible as a normal electron will not be having infinite value of energy. Thus, the minimum value of n will be unity and takes the values as 1, 2, 3, ..., ∞. Hence energy values of different atomic energy levels are discrete.

For given value of n, the following equation will get satisfied for various combinations of n_r and l.

$$n=n_r+l+1 \qquad ...(10.51)$$

It implies that several wave functions are possible for given energy value (n is fixed) when it takes place, the state is termed as to be degenerate. This will be true for every value of n except unity. It is possible to calculate the degeneracy in the following manner.

In Fig. 10.8 the different eigen states in case of hydrogen like atom have been depicted.From Eq. (10.50) it is evident that the energy eigen values depend upon n. Therefore, they are degenerate with respect to both l and m.

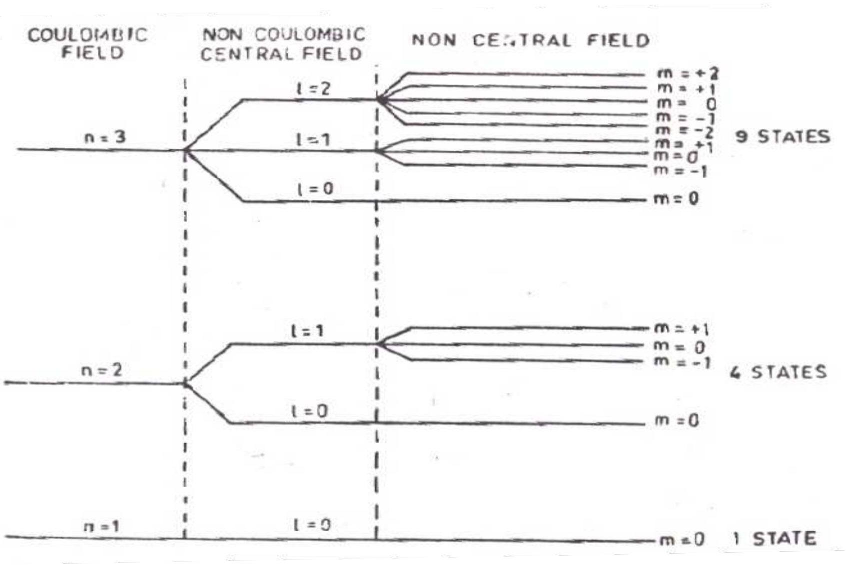

Fig. 10.8: Different eigenstates in hydrogen-like atom.

Hence for each value of *n*, *l* can take values from 0 to *n*–1 and for each of these values, *n*, can take values from –*l* to +*l*. Hence the total degeneracy may be put as follows:

$$\sum_{l=0}^{n-l}(2l+1)=\frac{2(n)(n-1)}{2}+n=n^2 \qquad \text{...(10.52)}$$

where $m=\ 0, \pm 1, \pm 2, \ldots \pm l$

$l = 0, 1, 2 \ldots (n-1)$

When $n=2$, l=0, m=0, [l=1, m=0] and l=1, m=±1 therefore yielding four wave functions or quantum states in all. For n=3 there are nine states and for n=4, there are sixteen states and so on.

10.6 The normal state of hydrogen atom:

For ground state of hydrogen atom, n=1, l=0 and m=0. Therefore, the wave function for such an atom may become as follows:

$$\psi_{1,0,0}=\sqrt{\left(\frac{1}{\pi a_0^{\ 3}}\right)}e^{-\rho/2}. \qquad \text{...(10.53)}$$

But,

$$\rho = \alpha r = \frac{2zr}{na_0} = \frac{2r}{a_0} \quad [\because \ n=1, z=1] \text{and} \, a_0 = \frac{h^2}{4\pi^2 \mu e^2}$$

$$\therefore \qquad \psi_{1,0,0} = \sqrt{\left(\frac{1}{\pi a_0{}^3}\right)\exp.\left[\frac{-r}{a_0}\right]} \qquad \text{...(10.54)}$$

and

$$\psi_{1,0,0}\psi^*{}_{1,0,0} = \frac{1}{\pi a_0{}^3}\exp.\left[\frac{-2r}{a_0}\right] \qquad \text{...(10.55)}$$

As the above equations are independent of θ and ϕ, it means that normal hydrogen atom will be spherically symmetric.

Suppose there is a small volume $dV=r^2 \sin \theta dr \, d\theta d\phi$. Now the probability of finding the electron in this volume is given as follows :

$$\psi_{1,0,0}\psi^*{}_{1,0,0} \, r^2 dr \sin\theta \, d\theta \, d\phi = \frac{1}{\pi a_0{}^3}\exp.\left[\frac{-2r}{a_0}\right] r^2 dr \sin \, \theta \, d\theta d\phi \qquad \text{...(10.56)}$$

For the whole surface of the sphere, the probability is given as follows :

$$= \frac{1}{\pi a_0{}^3}\exp.\left[\frac{-2r}{a_0}\right] r^2 dr \int_0^{\pi} \sin\theta d\theta \int_0^{2\pi} d\phi$$

$$= \frac{4}{a_0{}^3}\exp.\left[\frac{-2r}{a_0}\right] r^2 dr.$$

Hence the probability that the electron is lying between the distances *r* and *r+dr* from the nucleus may be put as follows :

$$P(r)dr = \frac{4}{a_0{}^3}\exp.\left[\frac{-2r}{a_0}\right] r^2 dr \qquad \text{...(10.57)}$$

The radial distribution function is given as follows :

$$P(r) = \frac{4}{a_0{}^3}\exp.\left[\frac{-2r}{a_0}\right] r^2 \qquad \text{...(10.58)}$$

The probability becomes maximum if *dP/dr=0.*

$$\therefore \quad \frac{dP}{dr} = \frac{4}{a_0^3}\left[r^2 . \left(-\frac{2}{a_0} \right) \exp . \left(\frac{-2r}{a_0} \right) + 2r \exp . \left(\frac{-2r}{a_0} \right) \right] = 0$$

or

$$\frac{4}{a_0^3} \exp . \left(\frac{2r}{a_0} \right) \left[2r - \frac{2r^2}{a_0} \right] = 0$$

or

$$2r - \frac{2r^2}{a_0} = 0$$

$$r = a_0 \qquad \text{...(10.59)}$$

From the above equation it is evident that in the normal state the maximum probability will be at a distance equal to the radius of the Bohr's first orbit.

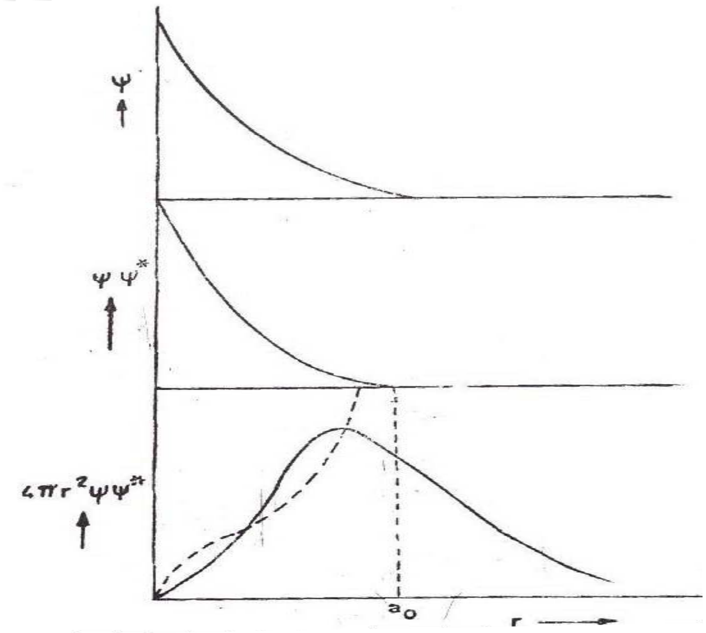

Fig. 10.9

The radial distribution function $P(r)\, dr$ is depicted in Fig. 10.9 together with $\psi_{100}$and ψ^2_{100}. The dotted curve is representing the probability distribution function for a Bohr orbit.

Example 10.1*: Consider two hypothetical spherical shells centred on the nucleus of a hydrogen atom with radii r and r+dr. What is the probability P(r) that the electron will lie between these shells, as a function of r? The motion of the electron in the atom is described by the wave function*

$$\Psi = \frac{1}{\sqrt{\pi} a_0^{3/2}} e^{-r/a_0} \cos \omega t.$$

Sol. The volume between the shells is

$$dV = 4\pi r^2 \, dr.$$

The probability of the electron being found between the shells is given by

$$P(r)dr = \Psi^2 \, dV$$

$$= \left(\frac{1}{\pi a_0^3} e^{-2r/a_0} \cos^2 \omega t \right) 4\pi r^2 \, dr.$$

The average probability is obtained by replacing $\cos^2 \omega t$ by its average value which is ½. Thus

$$\overline{P(r)} = \left\{ \frac{1}{\pi a_0^3} e^{-\frac{2r}{a_0}} \left(\frac{1}{2} \right) \right\} 4\pi r^2$$

$$= \frac{2r^2}{a_0^3} e^{-2r/a_0} .$$

Example 10.2:*Show that the degree of freedom of degeneracy of the nth energy level in the hydrogen atom in* n^2.

Sol. The energy values given by

$$E = -\frac{\mu e^4}{8\varepsilon_0^2 h^2} \left(\frac{1}{n^2} \right)$$

Depend only on *n*and hence are degenerate with respect to both *l*and m_l(that is, the states having same *n*but different *l's* or m_l*'s* or have same energy).

For each value of *n, l* can take *n* values from 0 to *n-1,* and for each value of *l* there are (*2l+1*) values of $m_l(=0, \pm 1, \pm 2, \ldots \ldots . \pm l)$. Therefore, the degeneracy of the nth energy level is

$$\sum_{l=0}^{n-1} (2l+1) = 1 + 3 + 5 \ldots \ldots . + (2n-1);$$

A total of *n* terms

$$= \frac{n}{2} [2(1) + (n-1)2] = n^2 .$$

Example 10.3: (a) *The 2s and 2p$_z$ orbitals for a hydrogen atom are*

$$\Psi_{2s} = \frac{1}{4\sqrt{2\pi a_0^{\frac{3}{2}}}}\left(2 - \frac{r}{a_0}\right) e^{-\frac{r}{2a_0}}$$

$$\Psi_{2p_z} = \frac{1}{4\sqrt{2\pi}\, a_0^{\frac{3}{2}}}\left(\frac{r}{a_0}\right) e^{-\frac{r}{2a_0}} \cos\theta$$

$$(a_0 = \text{Bohar radius} = 0.529\text{Å})$$

Using these orbitals write explicitly expressions for the two diagonal (sp) hybrid orbitals along the z-axis given by

$$D_{1,2} = \frac{1}{\sqrt{2}}\left(\Psi_{2s} \pm \Psi_{2p_z}\right).$$

(b) For either (not both) of your hybrid functions, calculate the probability density (modΨ^2) on the z-axis at z = $3a_0$ and z = -$3a_0$, in terms of a_0 and other universal constants.

(c) Make a same calculation separately for the 2s function and for the 2p$_z$ function.

Sol: (a)

$$D_{1,2} = \frac{1}{\sqrt{2}}\left(\Psi_{2s} \pm \Psi_{2p_z}\right)$$

$$= \frac{1}{8\sqrt{\pi}\, a_0^{\frac{3}{2}}}\left[2 + \frac{r}{a_0}(-1 \pm cos\theta)\right] e^{-\frac{r}{2a_0}}$$

(b) If z = $\pm 3a_0$, x=y=0, then

r = $3a_0, \theta = 0 \text{ or } \pi, cos\theta = \pm 1,$

$$D_1 = \frac{1}{8\sqrt{\pi}\, a_0^{\frac{3}{2}}}\left[2 + \frac{3a_0}{a_0}(-1 \pm 1)\right] e^{-\frac{3a_0}{2a_0}}$$

$$\text{or} D_1 = \frac{1}{8\sqrt{\pi}\, a_0^{\frac{3}{2}}}[(-1 \pm 3)] e^{-\frac{3}{2a_0}}$$

$$\text{mod}(D_1)^2 = \frac{{a_0}^{-3} e^{-8}}{64\pi}[(-1 \pm 3)^2]$$

$$\Rightarrow \left(D_1(\theta = \pi)\right)^2$$

$$= \frac{{a_0}^{-3}e^{-8}}{4\pi}$$

$$\text{and}(D_1(\theta = \pi))^2 = \frac{{a_0}^{-3}e^{-8}}{4\pi}.$$

(c) The functions

$$\Psi_{2s}(r = 3a_0) = \frac{-\mathrm{a_0}^{-\frac{3}{2}}}{4\sqrt{2\pi}}\mathrm{e}^{-\frac{3}{2}}$$

$$\mathrm{mod}(\Psi_{2s})^2 = \frac{{a_0}^{-3}e^{-8}}{32\pi}$$

$$\text{Similarly,}\,\Psi_{2p_z}(r = 3a_0, \theta = 0 \; or \; \pi) = \frac{\pm 3\mathrm{a_0}^{-\frac{3}{2}}}{4\sqrt{2\pi}}\mathrm{e}^{-\frac{3}{2}}$$

$$\mathrm{mod}\left(\Psi_{2p_z}\right)^2 = \frac{9{a_0}^{-3}e^{-8}}{32\pi}.$$

Example 10.4:*A three-dimensional isotropic harmonic oscillator has the energy eigen-values* $\hbar\omega\left(n + \frac{3}{2}\right)$ *where* $n = 0,1,2, \dots \dots$ *What is the degree of freedom of degeneracy of the quantum state n ?*

Sol. A state of the three dimensional oscillator is uniquely specified by the set of three numbers (n_1, n_2, n_3) with n_1, n_2, $n_3 \geq 0$and n_1+ n_2+n_3=n. The numbers n_1, n_2, n_3 are the harmonic oscillator quantum numbers for excitations along the x-, y-, z-axis respectively. For fixed n_3 and n, the number of pairs (n_1,n_2) for which n_1+ n_2 = n-n_3, is

$$\sum_{n_1=0}^{n-n_3} 1 = (n - n_3 + 1)$$

Finally summing over n_3 we obtain the total degeneracy, d_n,

$$d_n = \sum_{n_3=0}^{n} (n + 1 - n_3)$$

$$= (n+1)^2 - \frac{n(n+1)}{2} = \frac{(n+2)(n+1)}{2}.$$

Example 10.5:*Consider the one-dimensional Schroedinger equation with*

$$V(x) = \begin{cases} \frac{m}{2}\omega^2 x^2 & for\, x > 0, \\ +\infty & for\, x < 0. \end{cases}$$

Find the energy eigen values.

Sol. In the region $x>0$, ψ obeys the same differential equation as the two sided harmonic oscillator however, the only acceptable solutions are those that vanish at the origin.

Therefore, the eigen-values are those of the ordinary harmonic oscillator belonging to wave functions of odd parity. Now the parity of the S.H.O. wave functions alternates with increasing n, starting with an even-parity ground state. Hence,

$$E = \frac{(4n+3)h\omega}{2} \qquad \text{with } n = 0, 1, ...$$

10.7 Summary:

In this unit we have discussed the important applications of Schrödinger equation as the linear harmonic oscillator and the hydrogen atom. We have described the physical significant of linear harmonic oscillator and discrete eigen values. We also learned that the three dimensional spherical structure of hydrogen atoms and its quantised eigen valves & eigen states. Further, we learnt about the probability distribution of an electron in the hydrogen atom, and compare with the Bohr orbit.

10.8 Glossary:

Harmonic- relating to component frequencies of a complex oscillation or wave function

Oscillator - to move repeatedly from one position to another (like shaking, swinging and vibrating)

Asymptotic- asymptotic is a line that approaches a curve but never touches

Recursion- Recursion occurs when a thing is defined in terms of itself or of its type. Recursion is used in a variety of disciplines ranging from linguistics to logic.

Depicted- to show, to represent

10.9 References:

1. Beiser A., *Concepts of Modern Physics*, 6th Edition, McGraw Hill (2003) ISBN 0-07-244848-2.
2. ZettiliNouredine, *Quantum Mechanics: Concepts and Applications*, John Wiley and Son's Publishers, United Kingdom (2009) ISBN 978-0-470-02678-6.
3. Chatwal, G. R.; Anand, S. K.; Arora, M., *Quantum Mechanics,* Himalaya Publishing House (2007) ISBN 978-9-350-24732-7.

10.10 Suggested Reading:

1. Quantum Mechanics by E Merzbacher

2. Introduction to Quantum Mechanics by J Griffiths David

3. Quantum Mechanics: A Textbook for Undergraduates by Jain Mahesh

10.11 Terminal Questions:

Objective Type Questions:

a) According to wave mechanics, a free particle can possess-

(v) Discrete energies

(vi) Continuous energies

(vii) Only one single value of energy

(viii) None of these

b) A hydrogen atom remains in its ground state when electron-

(i) Resides inside the nucleus

(ii) Escape from the atom

(iii) Is in its first orbital

(iv) Does not orbit round but is stationary

c) The existence of zero-point energy for a linear harmonic oscillator is a consequence of-

(i) Pauli exclusive principle

(ii) Special theory of relativity

(iii) Matter waves

(iv) Uncertainty principle

d) According to the quantum mechanics, the most probable distance of electron from the nucleus in 1st state of hydrogen atom (a_0 is Bohr radius)-

(i) $3a_0/2$

(ii) $a_0/2$

(iii) a_0

(iv) Infinite

Short Answer Type Questions:

Q. 10.1 What is linear harmonic oscillator? Explain.

Q. 10.2 Determine the energy levels of a linear harmonic oscillator on the basis of the Schrödinger's equation.

Q. 10.3 What is the physical significant of zero-point energy in case of linear harmonic oscillator?

Q. 10.4 Calculate the zero-point energy of system consisting of a mass of 1 g.m. connected to a fixed point by a spring which is stretched 1 cm by a force of 10,000 dynes, the particle being constrained to move only along X-axis.

Q. 10.5 Discuss the complete wave function for one-dimension harmonic oscillator with its normalization constant.

Q. 10.6 Draw the graph of wave-functions and probabilities of harmonic oscillator for n = 0 to 5. How these are differing from the classical behaviours?

Q. 10.7 Define the four quantum numbers (n, l, m_l, and m_s).

Long Answer Type Questions:

Q. 10.8 Explain how one can solve the problem of the hydrogen atom quantum mechanically. Solve the radial part of the Schrödinger equation for hydrogen atom and obtain the energy eigen values.

Q. 10.9 Show that the energy-level spacing of a harmonic oscillator is in accord with the correspondence principle by finding the ratio $\Delta E_n/E_n$ between adjacent energy 1evels and seeing what happens to this ratio as $n \to \infty$.

Q. 10.10 What bearing would you think the uncertainty principle has on the existence of the zero-point energy of a harmonic oscillator?

Q. 10.11 Find the expectation values $<x>$ and $<x^2>$ for the first two states of a harmonic oscillator.

Q. 10.12 The potential energy of a harmonic oscillator is $U = \frac{1}{2}kx^2$. Show that the expectation value of $<U>$ of U is $E_0/2$ when the oscillator is in the $n = 0$ state. What is the expectation value of the oscillator's kinetic energy? How do these results compare with the classical values of $\acute{U}$ and $\acute{K}E$?

Q. 10.13 A pendulum with a 1.00-g bob has a massless string 250 mm long. The period of the pendulum is 1.00-s, (a) What is its zero-point energy? Would you expect the zero-point oscillations to be detectable? (b) The pendulum swings with a very small amplitude such that its bob rises a maximum of 1.00mm above its equilibrium position. What is the corresponding quantum number?

Q. 10.14 What is the ground state of the hydrogen atom? Derive it. And also calculate the probability for that.

Q. 10.15 Obtain and solve the radial equation for the hydrogen atom. Calculate the most probable distance of the electron from the nucleus.

Q. 10.16 Write the Schrödinger equation in the spherical co-ordinates for the electron in the hydrogen atom. Write down the expression for eigen functions. Calculate:

(a) The average distance of the electron from the proton in the ground state.

(b) The expectation value of kinetic energy for any state.

10.12 (a) Answers of Self Assessment Question (SAQ)

Ans.1: Refer section-10.3

Ans.2: $E = 2.5\ \hbar\omega$

Ans.3: $\nu = (E_3 - E_2)/\ h$

Ans.4: Refer section-10.4

(b) Answers of Terminal Questions:

Answer of objective questions: a) (i) **b)**(iii) **c)**(iv) **d)**(iii)
Ans.10.4 $E_0 = \frac{1}{2}\hbar\omega_0 = 5.25\times10^{-25}$ ergs.
Ans.10.11 $<x>=0$, and $<x^2>= E/k$ for both state.
Ans.10.13 (a) $2.07 \times 10^{-15}\ eV$, no (b) 1.48×10^{28}

Unit 11: Theory of Relativity

Structure

11.1 Introduction:

All the motions in nature are relative to each other. A motion cannot be described until we have a well define reference point or coordinate system. Simply, the motion of a train i.e. 80 km/h is defined with respect to an observer on earth. However, for another observer on train, the train is at rest. In the development of science, generally the physics in the period prior to 1900 is called classical physics. The mechanics of that period, i.e. classical mechanics was developed by Newton and also known as Newtonian mechanics. Classical mechanics is based on invariance of space, mass and time. Newton assumed that space, mass and time are absolute and remain unaffected in all circumstances. This concept explains satisfactory the ordinary motions in our physical world but this theory was not giving correct results when applied to object moving with higher speed.

In 1905, Albert Einstein showed that measurement of space (length), mass and time are affected by motion of observer and object. These measurements are not absolute velocity has no meaning. We always need a reference point or coordinate system to describe motions. Einstein's theory of relativity revolutionized science specially physics and astrophysics. In this chapter we discuss the theory of relativity and its consequences.

In 1905, Albert Eisenstein that the space (length), mass and time are affected by motion of object and observer. These are measurements not absolute. He also concluded that motions are related and absolute motion hah no meaning. Thus for describing the motion, we always need a reference point or coordinate system. Einstein theory of relativity revolutionized the science specially physics. In this chapter we discuss the theory of relativity and it consequences.

11.2 Objective:

After learning this unit we will able to

- Understand the meaning of relativity
- Understand frame of reference and its types
- Understand Michelson Morley experiment and its results
- Understand Special theory of relativity
- Lorentz Transformation
- Length transformation
- Consequences of relativity like length contraction, time dilation, variation of mass
- Relativistic velocity addition.
- Equivalence of mass and energy, relativistic momentum
- Basic of general theory of relativity.

11.3 Frame of reference:

As we know all motion are relative to each other. When we say that anything is moving, it means its position is changing relative to something. Thus to specify position and motion of any thing we need a coordinate system. A frame of reference is a coordinate system relative to which the position and events of body may be described. For example earth, laboratory, sun can be considered as a frame of reference. Generally, Cartesian coordinate system is used from denoting a frame of reference in which origin O is used for reference point. Position vector of a point P is given as

$$\vec{P} = \hat{\imath}x + \hat{\jmath}y + \hat{z}k$$

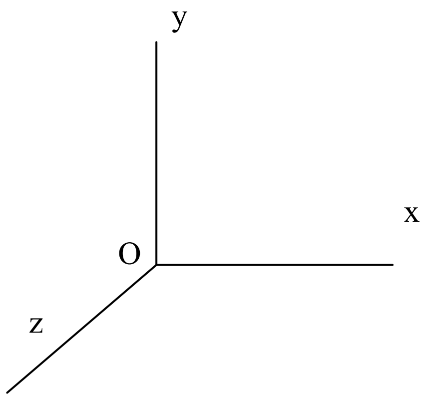

Figure 11.1 Cartesian coordinate system as frame of reference.

11.3.1 Inertial frame of reference:

Frame of reference in which Newton's 1^{st} and 2^{nd} law of motion hold is called inertial frame of reference. In such a frame, a body at rest remains at rest and a body in motion remains in motion until an external force is applied. A non-accelerating frame of reference is inertial frame of reference. All inertial frames of reference are equally valid. Any frame of reference, moving with constant velocity with reference to an inertial frame is itself an inertial frame. In 1905 Einstein published special theory of relativity which deals the problem that involved inertial frame of reference.

11.3.1 Non-inertial frame of reference:

Frame of reference in which Newton's 1^{st} and 2^{nd} law of motion do not hold is called Non-inertial frame of references. If a frame of reference is accelerating with respect to an inertial frame of reference such frame of reference is called non-inertial frame of reference. In fact all accelerating and rotating frames are non-inertial. In accelerating frame, a force which does not really act but appears due to acceleration (F=ma) of frame, is called fictitious or pseudo force.

11.4 Galilean Transformations:

Galilean transformations are used to transform the coordinates of one inertial frame to another inertial frame of reference. Simply there transformations are relation between two inertial frames of reference.

Let us consider two frames of reference S and S'. The second one S' moving with constant velocity v along x axis with respect the first frame of reference S. There are two observer O and O' at origins of frames of reference S and S' respectively as shown in figure 11.2.

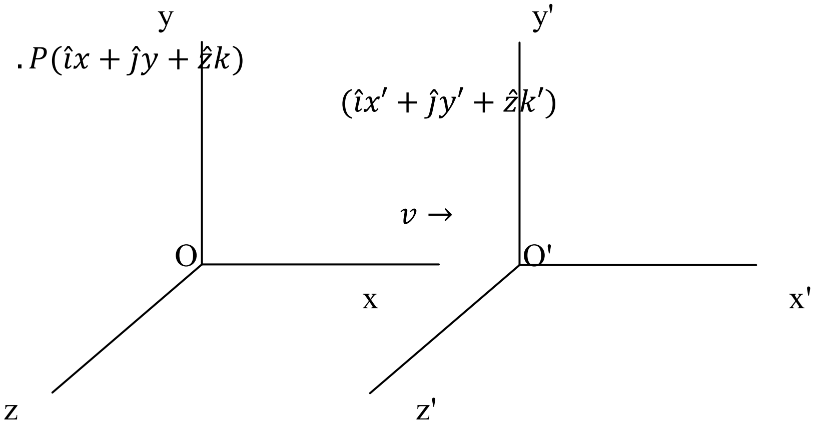

Figure 11.2: Galilean transformation

Let us consider a point P in space where an event is happened. The coordinates of point P are (x, y, z, t) and (x', y', z', t') with respect to frame S and S'respectively.

Since the S'is moving only along x axis with velocity v thus

Thus,
x'= x-vt
y'= y
z'= z
t'= t

These equations are called Galilean transformation equations.

Similarly the Galilean transformation for velocity can also be found out by differentiating with respect to time.

11.6 Michelson Morley Experiment:

In 19th century, scientist assumed that the whole space was filled with hypothetical medium named luminescent ether. This medium is perfectly transparent for propagation of light and material bodies may pass in this medium without any resistance. At that time scientist though that electromagnetic waves needed a medium for propagation. Ether remains fixed in space and considered as absolute frame of reference. It was also assumed that velocity of light should be different in the direction of motion of earth and perpendicular to the direction of motion of earth according to Galilean transformation.

Michelson Morley performed an experiment for the verification of existence of ether and relative motion between ether and earth. If ether is assumed to be at rest, the velocity of earth relative to ether medium will be equal to the orbital velocity of earth i.e., 3×10^4 m/s. The aim of this experiment was to find out this drift velocity and its effect.

11.6.1 Experimental setup:

Michelson and Morley designed an interferometer as shown in figure 11.3. A monochromatic beam of light is fall on a half silvered glass plate G. Some part of light is transmitted from glass plate G and after passing through another glass plate G'falls on mirror M_2 and reflected back. Similarly some part of light reflected from the Glass plate P called reflected (transverse) part and fall on mirror M_1 and reflected back. The light reflected from mirror M_1 and mirror M_2 finally reach in the direction along the telescope PT and produce interference pattern.

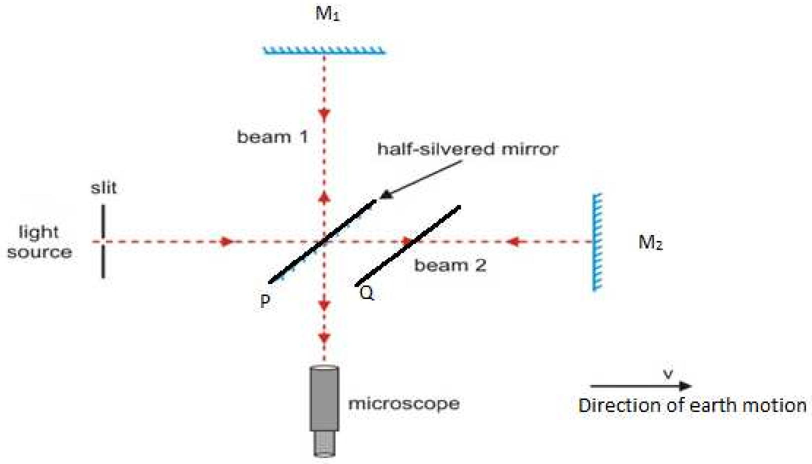

Figure 11.3. Michelson-Morley experiment

In this experiment the light is travelling in the direction of earth motion. Due to motion of apparatus with earth, the optical path travelled by both reflected and transmitted light are not same as velocity is different in both directions.

If l is the distance between plate P to M_1 and P to M_2 , and t is time period in which the light reaches from point P to A then according to figure 11.4.

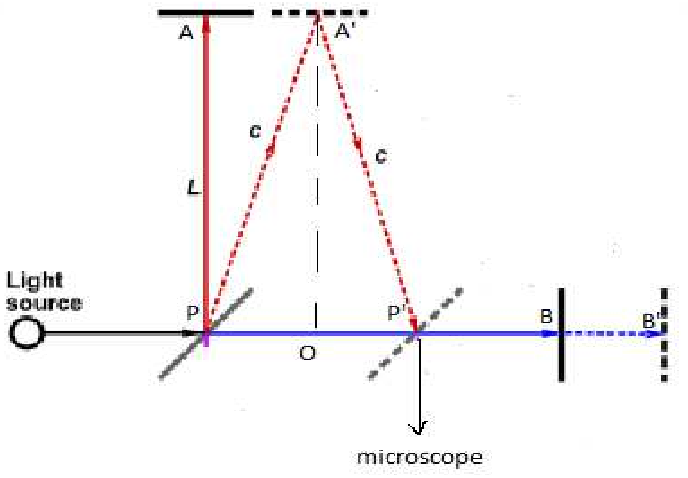

Figure 11.4: Optical path of reflected light

Total path travelled by reflected light = P A'P'

= 2 PA'

Since velocity along direction of motion of apparatus (along x axis) is v

then PA'= ct and A A'=vt

$(PA')^2 = (PQ)+(OA')^2$

$$c^2t^2 = v^2t^2 + l^2$$

$$t = \frac{l}{(c^2-v^2)^{1/2}}$$

If t_1 is time taken by reflected light to travel the total path l

$$t_1 = 2t = \frac{2l}{\sqrt{c^2-v^2}} = \frac{2l}{(c^2-v^2)^{1/2}} = \frac{2l}{c\left(1-\frac{v^2}{c^2}\right)^{1/2}}$$

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

Now the transmitted light has velocity (c-v) relative to apparatus from P to B and (c+v) from B'to P'.

Total time taken by transmitted light to travel total path t_2

$$t_2 = \frac{l}{c-v} + \frac{l}{c+v} = \frac{2lc}{c^2-v^2} = \frac{2lc}{c^2}\left[1-\frac{v^2}{c^2}\right]^{-1} = \frac{2l}{c}\left[1+\frac{v^2}{c^2}\right]$$

Time difference $\Delta t = t_2 - t_1 = \frac{2l}{c}\left[1+\frac{v^2}{c^2}\right] - \frac{2l}{c}\left[1+\frac{v^2}{2c^2}\right] = \frac{2l}{c}\frac{v^2}{2c^2} = \frac{lv^2}{c^3}$

Thus the path difference between two rays $= c.\Delta t = \frac{l\,v^2}{c^2}$

If λ is the wavelength of light used, the path difference in terms of fring shift

$$\Delta x = n\lambda$$

or $n = \frac{\Delta x}{\lambda} = \frac{lv^2}{\lambda c^2}$

In This experiment l = 1m, λ = 6×10^{-5}m, v =3×10^4 m/s, c=3×10^8m/c then the calculated values of $n \approx 0.37$

Thus if apparatus is at rest and start motion there should be a fringe shift of $\frac{lv^2}{\lambda c^2}$. But it is not possible to make earth at rest. The problem was resolved by using a concept that if whole apparatus of Michelson Morley experiment was turn through 90°. The fringe shift should be observed. The experiment was performed by many scientists, many times but fringe shift was not observed. This is called negative result of Michelson Morley experiment and it shows:

1. The existence of stationary ether medium is disproved.
2. There is no any absolute frame of reference.
3. The speed of light is same in all directions.

11.6.1 Einstein's explanations:

In 1905, Einstein proposed an explanation of negative result of Michelson Morley experiment. He argued that the velocity of light is same in all directions thus velocity of light is invariant. This is one of the postulates of special theory of relativity.

11.7 Special Theory of Relativity:

After the negative result of Michelson-Morley experiment, Einstein felt that there was no such thing which can be an absolute or fixed frame of reference. He worked on the absence of such absolute frame of reference and examined the consequences of such theory. On the basis of this revolutionary idea, in 1905 he published his special theory of relativity which deals the problems that involve inertial frame of reference. After 10 year later, in 1915 he also proposed second part of his theory of relativity which was more complex in the form of general theory of relativity which deals the problems that involve non inertial frame of reference.

Postulates of special theory of relativity:

1. The laws of physics are same in all inertial frames of reference.
2. The velocity of light in free reference is same in all frames of reference.

According to 2nd postulate the velocity of light (c) is invariant to transform from one inertial frame to another but according to Galilean transformation the velocity of light is not invariant. For example if c be the velocity of light in a frame S, and another frame $S'$is moving with velocity v with respect to S, then according to Galilean transformation the velocity of light in frame S'must be $c' = c - v$, however we have $c' = c$. Thus after new postulate, there was a variance with Galilean transformation. After this concept, we look for a new transformation system called Lorentz transformation.

11.8 Lorentz transformation:

Let us consider there are two inertial frames of reference S and S, S′having a uniform velocity v relative to S.

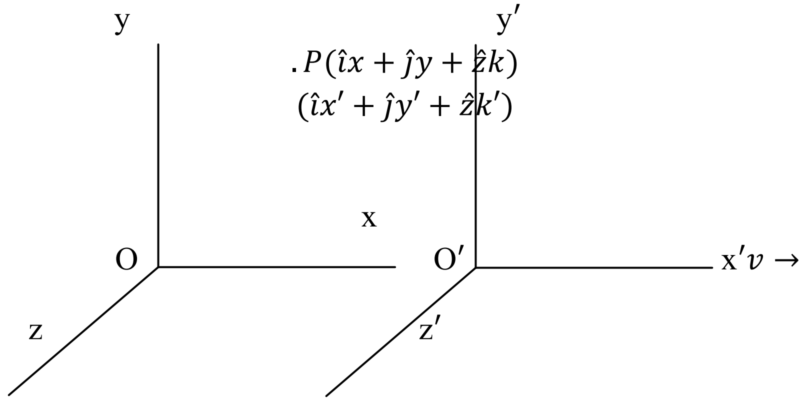

Figure 11.5: Lorentz transformation

An event at P is determined by the coordinates (x, y, z, t) and (x′, y′, z′, t′) by observers at O′ and O′. Let a light pulse produced at t=0, which will spread out a glowing sphere. Then the coordinate of this event for observer O in S frame:

$$x^2 + y^2 + z^2 = c^2t^2$$

$$\text{or } x^2 + y^2 + z^2 - c^2t^2 = 0 \qquad (1)$$

Similarly the coordinate of same event for observer O′ in S′ frame is

$$x'^2 + y'^2 + z'^2 = c^2t'^2$$

$$\text{or } x'^2 + y'^2 + z'^2 - c^2t'^2 = 0 \qquad (2)$$

by equation (1) and (2)

$$x^2 + y^2 + z^2 - c^2t^2 = \lambda({x'}^2 + {y'}^2 + {z'}^2 - c^2{t'}^2) \qquad (3)$$

Where λ is undetermined constant.

Since S′ is moving along x axis thus $y = y'$ and $z = z'$ thus λ=1. Then equation (3) becomes

$$x^2 - c^2t^2 = {x'}^2 - c^2{t'}^2$$

Now consider a linier transformation equation which relates x and x′ as

$$x' = \gamma(x - vt)$$

Where γ is constant.

If we assume that S is moving related to S' with velocity –v then

$$x = \gamma(x' + vt')$$

Putting the value of x' in this equation

$$x = \gamma[\gamma(x - vt) + vt']$$

$$= \gamma^2(x - vt) + \gamma vt'$$

$$\gamma vt' = x - \gamma^2(x - vt)$$

$$t' = \frac{x}{\gamma v} - \frac{\gamma}{v}(x - vt)$$

$$t' = \gamma\left[\frac{x}{\gamma^2 v} - \frac{x}{v} + t\right]$$

$t' = \gamma\left[t - \frac{x}{v}\left(1 - \frac{1}{\gamma^2}\right)\right]$ (6)

Put the value of x' and t' in equation (4)

$$x^2 - c^2t^2 = \gamma^2(x - vt)^2 - c^2\gamma^2\left[t - \frac{x}{v}\left(1 - \frac{1}{\gamma^2}\right)\right]^2$$

$$x^2 - c^2t^2 - \gamma^2(x^2 + v^2t^2 - 2xvt) + c^2\gamma^2\left[t^2 + \frac{x^2}{v^2}\left(1 - \frac{1}{\gamma^2}\right)^2 - \frac{2xt}{v}\left(1 - \frac{1}{\gamma^2}\right)\right] = 0$$

Since equation is an identity thus the coefficients of , t, x^2, t^2 and xt must be zero. Comparing the coefficients of xt

$$\gamma^2.2v + c^2\gamma^2\left[-\frac{2}{v}\left(1 - \frac{1}{\gamma^2}\right) = 0\right]$$

$$v - \frac{c^2}{v}\left(1 - \frac{1}{\gamma^2}\right) = 0$$

$$v^2 - c^2\left(1 - \frac{1}{\gamma^2}\right) = 0$$

$$v^2 - c^2 + \frac{c^2}{\gamma^2} = 0$$

$$\gamma = \sqrt{\frac{c^2}{c^2 - v^2}}$$

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

Putting this equation in (6)

$$t' = \gamma \left[t - \frac{x}{v}\left(1 - 1 + \frac{v^2}{c^2}\right)\right]$$

$$= \gamma \left[t - \frac{xv}{c^2}\right]$$

$$t' = \frac{t - \frac{xv}{c^2}}{\sqrt{1 - \frac{v^2}{c^2}}}$$

Thus the set of transformations:

$$x' = \frac{x - vt}{\sqrt{1 - \frac{v^2}{c^2}}}\ ; \quad y' = y\ ; \quad z' = z\ ; \quad t' = \frac{t - \frac{xv}{c^2}}{\sqrt{1 - \frac{v^2}{c^2}}}$$

Which is called Lorentz transformation.

Lorentz transformation is relativistic and Lorentz first time showed that this transformation have same form for law of electricity and magnetism in inertial frames of reference.

It can also observed that when v<<c or v/c→ 0. We have $\gamma = \frac{1}{\sqrt{1 - v^2/c^2}} \approx 1$, in this case the Lorentz relativistic transformation reduces to Galilean transformation. Thus it can be stated that the Galilean or Newtonian physics is a particular case of relativistic physics. In our daily life in planet earth the concern velocities are very small even the speed of earth motion is 29.6 km/sec. which is approximately $1/1000$ of c, thus Newtonian of Galilean physics is perfectly valid our particular cases. But when the value of v is very high and comparable to c in cases of electron, proton, neutrons etc. then only relativistic physics is valid.

Inverse Lorentz transformation:

If we exchange the frame S and S' (or S moves with a velocity-v) the Lorentz transformation becomes:

$$x = \frac{x\prime + vt\prime}{\sqrt{1-\frac{v^2}{c^2}}} ; \quad y = y' ; \quad z = z' ; \quad t = \frac{t\prime + \frac{x\prime v}{c^2}}{\sqrt{1-\frac{v^2}{c^2}}}$$

This set of transformation is called inverse Lorentz transformation which is also equally valid. Now we will examine some consequences of relativistic effect which can be obtained with the help of Lorentz transformation.

11.9 Length contraction:

Consider a rod is laid along the x axis in a frame of references S′. The rod is at rest with respect to an observer O′ in S′ frame. The length of rod, as measured in S′ frame of reference at rest by an observer O′is called proper length L_0 as shown in figure 11.6. If $x_1'$and x_2' are the coordinates of rod's ends with respect to O′ then paper length of rod

$$L_o = x_2' - x_1'$$

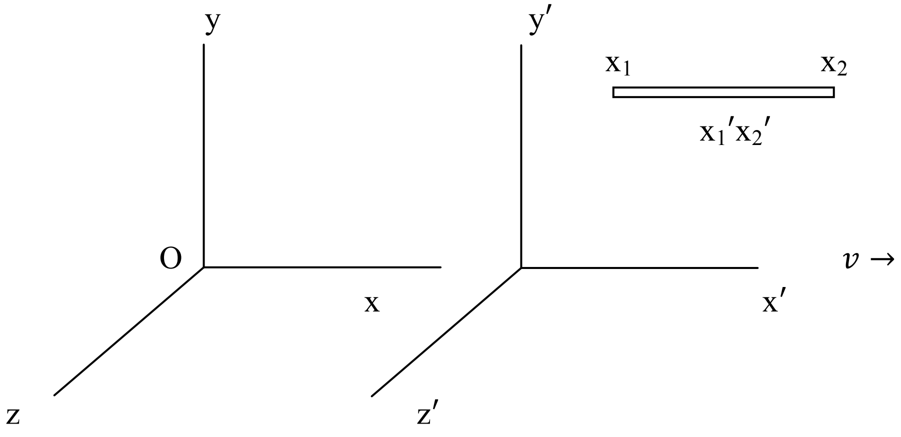

Figure 11.6: Length contraction of a rod in moving frame.

Similarly the coordinates of its ends with respect to observer O are x_2 and x_1. Consider frame S' is moving with velocity v along x axis with respect to S and we are interested to find out the length of rod when observed from frame S.

According to inverse Lorentz transformation:

$$x = \frac{x' + vt'}{\sqrt{1-\frac{v^2}{c^2}}}$$

Putting the value of t' from Lorentz transformation equation $t' = \frac{t-\frac{xv}{c^2}}{\sqrt{1-\frac{v^2}{c^2}}}$ we have

$$x = \frac{x' + v\frac{t-\frac{xv}{c^2}}{\sqrt{1-\frac{v^2}{c^2}}}}{\sqrt{1-\frac{v^2}{c^2}}}$$

$$x = \frac{x'}{\sqrt{1-\frac{v^2}{c^2}}} + \frac{vt}{1-\frac{v^2}{c^2}} - \frac{v^2x}{c^2(1-\frac{v^2}{c^2})}$$

$$x\left[1+\frac{\frac{v^2}{c^2}}{1-\frac{v^2}{c^2}}\right] = \frac{x'}{\sqrt{1-\frac{v^2}{c^2}}} + \frac{vt}{1-\frac{v^2}{c^2}}$$

$$\frac{x}{1-\frac{v^2}{c^2}} = \frac{x'}{\sqrt{1-\frac{v^2}{c^2}}} + \frac{vt}{1-\frac{v^2}{c^2}}$$

$$x = x'\sqrt{1-\frac{v^2}{c^2}} + vt$$

Thus the coordinate of end points of rods are

$$x_1 = x_1{}'\sqrt{1-\frac{v^2}{c^2}} + vt$$

$$x_2 = x_2{}'\sqrt{1-\frac{v^2}{c^2}} + vt$$

or

$$x_2 - x_1 = (x_2{}' - x_1{}')\sqrt{1-\frac{v^2}{c^2}}$$

If $x_2 - x_1 = L$ and $x_2{}' - x_1{}' = L_o$(proper length)

$$L = L_0\sqrt{1-\frac{v^2}{c^2}}$$

It is clear that $L<L_0$ and if v is higher or rod is moving faster then the length is observed shorter in comparison to proper length. This is called length contraction. It can also be noticed that there is no contraction along y and z axis as the rod is moving only along x axis. In another case if the rod moves with speed of light c, its length would be zero.

11.10 Time Dilation:

Consider two frame of references S and S', S'is moving with velocity v along x axis as shown in figure 11.5. Let a clock is situated at point P in S' gives signal at time interval Δt with respect to S and Δt' with respect to S'. Using inverse Lorentz transformation

$$t_1 = \frac{t_1{}' + \frac{x'v}{c^2}}{\sqrt{1-\frac{v^2}{c^2}}}$$

$$t_2 = \frac{t_2{}' + \frac{x'v}{c^2}}{\sqrt{1-\frac{v^2}{c^2}}}$$

$$t_2 - t_1 = \frac{t_2{}' - t_1{}'}{\sqrt{1-\frac{v^2}{c^2}}}$$

$$\Delta t = \frac{\Delta t'}{\sqrt{1-\frac{v^2}{c^2}}}$$

Δt is time measured by observer is S frame and $\Delta t'$ proper time. It can be noticed that $\Delta t > \Delta t'$ as $\sqrt{1 - {v^2}/{c^2}}$ is always less than 1.

Thus the measurements of time interval are affected by relative motion between and observer and object, if a clock moves with respect to an observer the clock get slower, all the processes in such moving frame occur more slowly. The biological process and life period are also become slower in such a moving frame if observed from a different inertial frame.

11.10.1 Twin paradox:

Consider there are two identical twin brothers. One of them goes to a long space journey in a spaceship at a speed near to speed of light (c) and second one stay behind on earth. The clock in the moving space ship will appear to go slower and biological processes of his body also go slower. When the first one returns to the earth he will find himself younger than second who stayed on earth. This phenomenon due to time dilation is called twin paradox.

11.11 Velocity Addition:

Suppose we have two frames of reference S and S'. S' is moving with a uniform velocity v along x axis with respect to S. Suppose a particle is moving in x axis with velocity u as measured by frame S and u' as measured by frame S'.

In S frame $u = u_x + u_y + u_z$ (1)

In S' frame $u' = u_x' + u_y' + u_z'$ (2)

The velocity measured by frame S and frame S' are $u_x = \frac{dx}{dt}$ and $u_x' = \frac{dx'}{dt'}$

Differentiate Lorentz transformation

$$dx' = \frac{dx - vdt}{\sqrt{1-\frac{v^2}{c^2}}} \ ; dt' = \frac{dt - \frac{v}{c^2}dx}{\sqrt{1-\frac{v^2}{c^2}}} \ ; \ dy' = dy \ ; \ dz' = dz \qquad (3)$$

Dividing above transformation relations for $dx', dy' and\ dz'$ by dt'

$$\frac{dx'}{dt'} = \frac{dx - vdt}{dt - \frac{v}{c^2}dx} \quad \text{or} \quad u_x' = \frac{u_x - v}{1 - \frac{v}{c^2}u_x} \qquad (4)$$

$$\frac{dy'}{dt'} = \frac{dy\sqrt{1-\frac{v^2}{c^2}}}{dt - \frac{v}{c^2}dx} \quad \text{or} \quad u_y' = \frac{u_y\sqrt{1-\frac{v^2}{c^2}}}{1 - \frac{v}{c^2}u_x} \qquad (5)$$

$$\frac{dz'}{dt'} = \frac{dz\sqrt{1-\frac{v^2}{c^2}}}{dt - \frac{v}{c^2}dx} \quad \text{or} \quad u_z' = \frac{u_z\sqrt{1-\frac{v^2}{c^2}}}{1 - \frac{v}{c^2}u_x} \qquad (6)$$

These equations (4), (5) and (6) are the relation for relativistic velocity additions.

If a photon is moving with velocity c in S'frame, $u_x' = c$ and this frame is also moving with velocity c, i.e., v=c then the velocity of this photon when observed from S frame can be calculated by above relation:

or $u_x' = \frac{u_x - v}{1 - \frac{v}{c^2}u_x}$ here $u_x' = c$, v=c

or c= $\frac{u_x - c}{1 - \frac{c}{c^2}u_x}$ or $u_x = c$

Thus this particular velocity c remains same in all frames of reference and remains invariant. By using inverse Lorentz transformation (replacing v by -v) the above relativistic velocity equations (4), (5) and (6) becomes:

or $u_x = \frac{u'_x+v}{1+\frac{v}{c^2}u_x}$; $u_y = \frac{u_y'\sqrt{1-\frac{v^2}{c^2}}}{1+\frac{v}{c^2}u_x'}$; $u_z = \frac{u_z'\sqrt{1-\frac{v^2}{c^2}}}{1+\frac{v}{c^2}u_x'}$

11.12 The relativity of mass (mass variation):

The mass of moving body also varies like length and time its variation is direct consequence of time dilation. Let us consider two frames of references S and S' as shown in figure 11.7. S' is moving with a constant velocity v relative to S. Suppose there are two balls A and B of equal masses m in S' frame, both balls are approaches toward each other at equal speeds u and –u. after collision, the balls coalesce into one body.

If S' frame according to conservation of momentum:

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

mu-mu = momentum of coalesce mass = 0

Thus coalesced mass must be at rest in S'frame. In S frame if u_1 and u_2 are the velocity of two balls A and B then

$$u_1 = \frac{u+v}{1+{uv}/{c^2}} \tag{1}$$

$$u_2 = \frac{-u+v}{1-{uv}/{c^2}} \tag{2}$$

Since frame S'is moving with velocity v and therefore after collision coalesced mass have velocity v with respect to S. if m_1 and m_2 are mass of balls A and B measured from S frame then according to conservation of momentum;

$$m_1u_1 + m_2u_2 = (m_1+m_2)v \tag{3}$$

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

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

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

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

Using equation (1)

$$1-\frac{{u_1}^2}{c^2} = 1-\frac{(u+v)^2}{c^2\left(1+{uv}/{c^2}\right)^2} = \frac{1+\frac{u^2v^2}{c^4}+\frac{2uv}{c^2}-\frac{u^2}{c^2}-\frac{v^2}{c^2}-\frac{2uv}{c^2}}{\left(1+{uv}/{c^2}\right)^2}$$

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

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

Similarly using equation (2) we get

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

Dividing equation (6) by equation (5)

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

$$\frac{1+{uv}/{c^2}}{1-{uv}/{c^2}} = \frac{\sqrt{1-\frac{{u_2}^2}{c^2}}}{\sqrt{1-\frac{{u_1}^2}{c^2}}}$$

Putting this value in equation (4)

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

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

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

m_0 is constant and is called rest mass of the body. $m_1$and m_2 are the masses at velocities u_1 and u_2 respectively. Similarly if m_0 is mass of body in S' frame of reference when it is moving with velocity v with respect to S, and m is mass of this body in S frame, then

$m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$ (7)

This is the relation for mass variation. If the velocity of particle becomes c i.e. v→ c then m = $\frac{m_0}{o}$=∞. Thus if a particle moves with velocity of light its mass becomes infinity. But in actual no material body have velocity equal to c.

11.12.1 Experimental verification of mass variation:

In 1906 Kaufman experimentally verified the increase in mass with velocity. He observed that during β decay from a radioactive material, when the velocities of β particles are high, their masses were found is greater than actual rest mass corresponding to velocities. Similarly In particle accelerator (a device used to accelerate particles) when proton or electrons are accelerated to a high velocities, their masses increased as predicted by relativistic mass formula.

11.13 Equivalence of Mass and Energy:

Einstein obtained his most famous mass energy relation (E=mc^2) from the postulates of special theory of relativity.

Derivation:

We know that the work is define as $W = F.s$

If there is no other external forces act on an object, and object starts with rest and acquire a velocity v then all the work done on it becomes it kinetic energy.

$$KE = \int_0^v F.ds$$

Relativistic 2nd law of motion $F = \frac{d}{dt}(mv)$

$$KE = \int_0^v \frac{d}{dt}(mv).ds$$

Since m is not constant and vary with velocity then

$$KE = \int_0^v d(mv).\frac{ds}{dt}$$

$$KE = \int_0^v v.d(mv)$$

$KE = \int_0^v v.d\left(\frac{m_0 v}{\sqrt{1-\frac{v^2}{c^2}}}\right)$(1)

Integrating above equation by integration by part as

$$\int x\,dy = xy - \int dx\,y$$

$$KE = \left[v.\frac{m_0 v}{\sqrt{1-\frac{v^2}{c^2}}} - \int_0^v dv\left(\frac{m_0 v}{\sqrt{1-\frac{v^2}{c^2}}}\right)\right] \quad (2)$$

Second part of the integration can be solved by substitution as

$$1-\frac{v^2}{c^2} = t^2$$

$$-\frac{2v\,dv}{c^2} = 2t\,dt$$

Now integration $\int_0^v dv\left(\frac{m_0 v}{\sqrt{1-\frac{v^2}{c^2}}}\right)$ becomes

I (say) = $\int_1^{\sqrt{1-\frac{v^2}{c^2}}} \frac{-m_0 c^2 t\,dt}{t} \;=\; -m_0 c^2 [t]_1^{\sqrt{1-\frac{v^2}{c^2}}}$

I = $-m_0 c^2\left[\sqrt{1-\frac{v^2}{c^2}} - \;1\right] = m_0 c^2\sqrt{1-\frac{v^2}{c^2}} + \; m_0 c^2$

Putting this value in equation (2)

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

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

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

$$KE = mc^2 - m_0 c^2 \qquad (3)$$

Total Energy E = KE + rest mass energy

$$E = mc^2 - m_0c^2 + m_0c^2$$

$$E = mc^2$$

Thus the classic law of conservation of mass and energy combined in to a single principle of mass and energy equivalence.

11.14 Relativistic momentum and energy relationship:

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

Relativistic Momentum $p = mv = \frac{m_0 v}{\sqrt{1-\frac{v^2}{c^2}}}$

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

Now we calculate a quantity

$$p^2c^2 + {m_0}^2c^4 = \frac{{m_0}^2v^2c^2}{1 - \frac{v^2}{c^2}} + {m_0}^2c^4$$

$$= \frac{{m_0}^2v^2c^2 + {m_0}^2c^4 - {m_0}^2v^2c^2}{1 - \frac{v^2}{c^2}}$$

$$= \frac{{m_0}^2c^4}{1 - \frac{v^2}{c^2}} = E^2$$

$$E^2 = p^2c^2 + {m_0}^2c^4$$

This is the relation between energy and momentum.

For mass less particles $E^2 = p^2c^2$ or E= pc

11.14.1 Kinetic speed at low speed:

According to relativistic kinetic energy

$$KE = mc^2 - m_0c^2 = \frac{m_0c^2}{\sqrt{1-\frac{v^2}{c^2}}} - m_0c^2$$

$$= m_0c^2\left(1 - \frac{v^2}{c^2}\right)^{-1/2} - m_0c^2$$

$= m_0c^2\left(1 + \frac{1v^2}{2c^2}\right) - m_0c^2$ (using binomial theorem) $= \frac{1}{2}m_0v^2$

Thus at v << c the formula for relativistic KE reduce to classical formula.

11.15 General theory of relativity:

Einstein special theory of relativity deals the motion and events in inertial frames. In 1915, Einstein published general theory of relativity which deals with motions and events in accelerating frame. Thus the general theory of relativity is generalization of theory of relativity regardless of their state of motion whether accelerating or non-accelerating. General relativity provides a unified description of Newton’s laws of motion, laws of gravitation, gravity, special relativity, geometrical properties of space and time. After unification of all theories, the law of physics may be expressed by Einstein field equations, a system of partial differential equations.

Some predictions of general theory of relativity differ significantly from classical physics, like concerning the passage of time, geometry of space, propagation of electromagnetic wave, etc. some new phenomenon like gravitational time dilation, gravitational Lansing, gravitational red shift. Gravitational time delay is consequences of general theory of relativity. The predictions of general theory of relativity have been confirmed in observation and experiments. Einstein theory has improved astrophysics and different other events taking place in universe like black hole, massive starts, nova, super nova, quasar, gravitational waves etc. The more details of this theory is an advance course and will be studies in higher advanced books.

Example 11.1: The length of a rod as is measured in different frames is 20.0 cm, 19.8 cm, 19.9 cm. In which frame the rod is at rest. Explain why.

Solution: The rod will be at rest in the frame in which its length is maximum, and maximum measured lengths 10.1 cm. It is because in a moving frame length contraction takes place and it appears that length decreases. So the frame at rest is that in which the length has the highest values.

Example 11.2: A rod of 1 m long is moving along its length with a velocity 0.6 c. Calculate its length as it appears to (i) an observer on the earth (ii) moving with the rod itself.

Solution: The length of the rod in the moving (S') frame i.e. proper length is

$$L_0 = 1 \text{ m}$$

If the observer moving with the rod itself, then there will be no relative motion and length appears to be 1 meter. As the rod is moving when observed by an observer on the earth, the length of the rod appears to be shorter, then

$$L = L_0\sqrt{1-\frac{v^2}{c^2}} = 1\sqrt{1-(0.6)^2} = \sqrt{1-0.36} = \sqrt{0.64}$$

$$L = 0.8 \text{ m}$$

Example 11.3: A rod has a length of 2m. Find its length when carried in a rocket with a speed 2.7×10^8 m/s.

Solution: The length of the rod is given by

$$L = L_0\sqrt{1-\frac{v^2}{c^2}} = 2\sqrt{1-\left(\frac{2.7\times10^8}{3\times3\times^8}\right)^2} = 2\sqrt{1-0.81}$$

$$= 2\times\sqrt{0.19} = 2\times 0.436 = 0.872\text{m}$$

Example 11.4: The apparent length of a rod in the direction of motion moving with a velocity 2×10^8 m/s is 1 meter. What is the proper length of the rod at rest?

Solution: Length of rod at rest, $L_0 = \frac{L}{\sqrt{1-\frac{v^2}{c^2}}}$

$$= \frac{1}{\sqrt{1-\frac{(2\times10^8)}{(3\times10^8)^2}^2}} = 1.34 \text{ m}$$

Example 11.5: The length of a spaceship is 90 m when measured on the earth. It length when it was flying was 80m measured by an observer on the earth. Find out the velocity of spacecraft.

Solution: The length of a spaceship is given by

$$L = L_0\sqrt{1-\frac{v^2}{c^2}}$$

$$80 = 90\sqrt{1 - \frac{v^2}{3 \times 3 \times 10^{16}}}$$

$$1 - \left(\frac{v^2}{3 \times 3 \times 10^{16}}\right) = \frac{80 \times 80}{90 \times 90}$$

$$\left(\frac{v^2}{3 \times 3 \times 10^{16}}\right) = 1 - \frac{80 \times 80}{90 \times 90} = 0.2098$$

$v = 0.4580 \times 3 \times 10^8 = 1.37 \times 10^8 \text{m/s}$

Example 11.6: A rod is placed in a spacecraft moving with a velocity .8c with respect to earth along the direction (i) parallel to earth and (ii) along a direction 30^0 with the length of rod. Calculate the percentage contraction in the length of rod in both cases.

Solution: (i) In case rod is moving parallel to the length (say along x axis), then the measured length L of the rod with proper length L_0 is given as

$$L = L_0\sqrt{1 - \frac{v^2}{c^2}}$$

$$L = L_0\sqrt{1 - \frac{(.8c)^2}{c^2}} = L_0\sqrt{1 - .64} = L_0\sqrt{.36} = .6L_0$$

Percentage contraction in the length of rod $= \frac{L_0 - .6L_0}{L_0} \times 100 = 40\%$

(ii) In case rod is moving in a direction along 30^0 with the length of rod (along x axis), then the length of rod along direction of motion (along x axis) $= L_0 \cos 30^0 = \frac{\sqrt{3}}{2} L_0$

The observed length L' along the direction of motion (along x axis) as rod is moving with .6c

$L' = \frac{\sqrt{3}}{2} L_0\sqrt{1 - \frac{(.8c)^2}{c^2}} = \frac{\sqrt{3}}{2} L_0 \times .6 = 0.52L_0$ (1)

The length of rod along direction perpendicular to motion (along y axis) $= L_0 \sin 30^0 = 0.5L_0$

The observed length L'' along the direction perpendicular to motion (along y axis) remains same as rod is moving perpendicular to this direction.

Thus the observed length L'' along the y axis $L'' = 0.5L_0$ (2)

Using eq. (1) and eq. (2) we can find the total observed length of rod as

$$L = \sqrt{L'^2 + L''^2} = \sqrt{(0.52L_0{}^2 + \ (0.5L_0)^2} = 0.72L_0$$

Percent contraction $= \frac{L_0 - 0.72L_0}{L_0} \times 100 = 22.72\%$

Example 11.7: Mass of a moving particle becomes 3 times of its rest mass. Find out the speed of the particle.

Solution: The mass of a moving body m is given as

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

$$3m_0 = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$$

$$\sqrt{1 - \frac{v^2}{c^2}} = \frac{1}{3}$$

$$1 - \frac{v^2}{c^2} = \frac{1}{9}$$

$$\frac{v^2}{c^2} = 1 - \frac{1}{9} = \frac{8}{9}$$

$$v = .94c$$

Example 11.8: In the laboratory there are two particles moving in opposite to each other with the velocities 2.8×10^8 m/s. Calculate their relative velocities.

Solution: We can consider one particle is placed in S' frame which is moving with velocity $v = -2.8 \times 10^8$ m/s (say along –x axis) and the velocity of particle is $u = 2.8 \times 10^8$ m/s. For relative velocity u' we have to calculate velocity of particle with respect to S by using Lorentz velocity transformation as

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

$$u' = \frac{2.8 \times 10^8 - (-2.8 \times 10^8)}{1 - \frac{2.8 \times 10^8 \times 2.8 \times 10^8}{c^2}}$$

$u' = \frac{(5.6\times10^8)}{1.87}$= 2.995×$10^8$ m/s

Thus the velocity relative to each other is 2.995×10^8 m/s.

Example 11.9: Two β particles are emitted by a radioactive source. The particles are moving in opposite direction to each other with velocity 0.9c. Calculate their relative velocity.

Solution: We can consider two particles A and B. Particle A is placed in frame S' which is moving with velocity -0.9c with respect to S. Thus the velocity of particle A is -0.9c with respect to S. If the particle B has velocity 0.9c with respect to S, then

velocity of particle A = v = -0.9c

velocity of particle B = u = 0.9c

According to Lorentz velocity transformation the relative velocity of a and B is u' and given as

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

$$u' = \frac{.9\mathrm{c} - (-.9c)}{1 - \frac{.9\mathrm{c} \times (-.9c)}{c^2}}$$

$u' = \frac{(1.8c)}{1.81}$=0.994c= 2.98×10^8 m/s

Example 11.10: An electron moves with velocity 0.6×10^8 m/s If its rest mass is 9×10^{-31} kg Calculate it's mass.

Solution: We know $m_0 = 9 \times 10^{-31}$ kg

$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{9 \times 10^{-31}}{\sqrt{1 - \frac{.6 \times 10^8 \times .6 \times 10^8}{3 \times 10^8 \times 3 \times 10^8}}} = 9.18 \times 10^{-31}\ kg$$

Example 11.11: Calculate the ratio of mass of an electron to its rest mass if it is moving with kinetic energy 9.5MeV. The rest mass of electron is nearly 0.5MeV.

Solution: We know that

$$KE = mc^2 - m_0c^2$$

$$KE = mc^2 - m_0c^2 = 9.5\ MeV$$

$$mc^2 = 9.5 + 0.5 = 10\ MeV$$

$$\frac{m}{m_0} = \frac{mc^2}{m_0c^2} = \frac{10}{.5} = 20$$

11.16 Summary:

1. A frame of reference is a coordinate system relative to which the position and events of body may be described. For example earth, laboratory, sun can be considered as a frame of reference.

2. Frame of reference in which Newton's 1st and 2nd law of motion hold is called inertial frame of reference. A non-accelerating frame of reference is inertial frame of reference.

3. Frame of reference in which Newton's 1st and 2nd law of motion do not hold is called Non-inertial frame of references. If a frame of reference is accelerating with respect to an inertial frame of reference such frame of reference is called non-inertial frame of reference. In fact all accelerating and rotating frames are non-inertial.

4. Galilean transformations are used to transform the coordinates of one inertial frame to another inertial frame of reference.

5. Michelson Morley performed an experiment for the verification of existence of ether and relative motion between ether and earth. The negative result of Michelson Morley experiment and it shows:

4. The existence of stationary ether medium is disproved.
5. There is no any absolute frame of reference.
6. The speed of light is same in all directions.

6. Postulates of special theory of relativity:

3. The laws of physics are same in all inertial frames of reference.
4. The velocity of light in free reference is same in all frames of reference.

7. Lorentz transformation is relativistic and Lorentz first time showed that this transformation have same form for law of electricity and magnetism in inertial frames of reference. The set of transformations:

$$x' = \frac{x-vt}{\sqrt{1-\frac{v^2}{c^2}}}\ ; \quad y' = y\ ; \quad z' = z\ ; \quad t' = \frac{t-\frac{xv}{c^2}}{\sqrt{1-\frac{v^2}{c^2}}}$$

7. If we exchange the frame S and S' (or S moves with a velocity-v) the Lorentz transformation becomes inverse Lorentz transformation which is also equally valid.

$$x = \frac{x\prime + vt\prime}{\sqrt{1-\frac{v^2}{c^2}}}\,; \quad y = y'\,; \quad z = z'\,; \quad t = \frac{t\prime + \frac{x\prime v}{c^2}}{\sqrt{1-\frac{v^2}{c^2}}}$$

8. If a rod is laid along the x axis in a frame of references S' and this frame is moving with velocity v with respect to another frame S. When an observer in S frame observes the length L of this moving rod, it is observed shorter in comparison to proper length L_0. This is called length contraction.

$$L = L_0\sqrt{1-\frac{v^2}{c^2}}$$

9. The measurements of time interval are affected by relative motion between and observer and object, if a clock moves with respect to an observer the clock get slower, all the processes in such moving frame occur more slowly. This is called time dilation. Δt is time measured by observer is rest(in S frame) and $\Delta t'$ time period measured in moving frame called proper time.

$$\Delta t = \frac{\Delta t'}{\sqrt{1-\frac{v^2}{c^2}}}$$

10. If we have two frames of reference S and S'. S' is moving with a uniform velocity v along x axis with respect to S. Suppose a particle is moving in x axis with velocity u ($u = u_x + u_y + u_z$) as measured by frame S and u' ($u' = u_x{}' + u_y{}' + u_z{}'$)as measured by frame S'. Then the relations for relativistic velocity addition are:

$$u_x{}' = \frac{u_x - v}{1-\frac{v}{c^2}u_x} \;\; ; \; u_y{}' = \frac{u_y\sqrt{1-\frac{v^2}{c^2}}}{1-\frac{v}{c^2}u_x} \;\; ; \; u_z{}' = \frac{u_z\sqrt{1-\frac{v^2}{c^2}}}{1-\frac{v}{c^2}u_x}$$

$$\text{or } \; u_x = \frac{u_x' + v}{1+\frac{v}{c^2}u_x} \;\; ; \; u_y = \frac{u_y\prime\sqrt{1-\frac{v^2}{c^2}}}{1+\frac{v}{c^2}u_x\prime} \;\; ; \; u_z = \frac{u_z\prime\sqrt{1-\frac{v^2}{c^2}}}{1+\frac{v}{c^2}u_x\prime}$$

11. If m_0 is mass of body in S' frame of reference when it is moving with velocity v with respect to S, and m is mass of this body in S frame, then

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

This is the relation for mass variation.

12. Kinetic energy is given as $KE = mc^2 - m_0c^2$

Total Energy $E =$ KE + rest mass energy= $mc^2 - m_0c^2 + m_0c^2 = mc^2$

The classic law of conservation of mass and energy combined in to a single principle called mass and energy equivalence.

13. Relativistic Momentum $p = mv = \frac{m_0 v}{\sqrt{1-\frac{v^2}{c^2}}}$

14. Relation between energy and momentum:

$$E^2 = p^2c^2 + {m_0}^2c^4$$

11.17 Glossary:

1. Frame of reference : an specified space define by a coordinate system
2. Inertial : non accelerating
3. non-inertial : accelerating
4. Transformation : correlation from one system to another
5. ether : A hypothetical medium

11.18 References:

1. Modern physics, A. Beiser, Tata Mc Graw-Hill
2. Mechanics, D.S. Mathur, S Chand and Co., N Delhi
3. Modern Physics, R.Murugeshan and K Sivaprasath, S Chand and co. N. Delhi.

11.19 Suggested Reading:

1. What is relativity, L D Landall, G.B. Rumer
2. The theory of relativity and other essays. Albert Einstein.

11.19 Terminal Questions:

11.19.1 Short answer type question

Q1. Define inertial and non inertial frame of reference.

Q2. What is the negative result of Michelson Morley experiment?

Q3. Explain is Earth is an inertial Frame of reference?

Q4. Deduce the Galilean transformation equations.

Q5. What is Newtonian relativity? Give the basic assumption of Newtonian mechanics.

Q6. State the postulates of special theory of relativity.

Q7. What do you mean by velocity of light is absolute?

Q8. Why Lorentz transformation is needed?

Q10. What do you mean by proper length and length contraction?

Q11. What is meant by twin paradox?

Q12. Explain the time dilation.
Q13. State Einstein's velocity addition formula.
Q14. What is mass energy equivalence relation?
Q15. What is rest mass? Show that the rest mass of photon is zero.

11.20.2 Essay type question:

Q1. What is Michelson- Morley experiment? Why this experiment was performed? Explain its result.
Q2. State and explain the special theory of relativity. What are the consequences of this theory?
Q3. Deduce Lorentz transformation equation.
Q4. Define proper length and length contraction. On the basis of Lorentz transformation obtain a relation for length contraction.
Q5. What is time dilation? On the basis of Lorentz transformation obtain a relation for time dilation. Explain why moving clock appears to go slow.
Q6. What do you mean by twin paradox?
Q7. Deduce Einstein's velocity addition formula and show that speed of light remains same.
Q8. Deduce the formula for relativistic variation of mass.
Q9. Deduce Einstein's mass energy equivalence relation.
Q10. Give basic idea about general theory of relativity.

11.20.3 Numerical question:

Q1. An electron is moving with velocity 0.8c. The mass of electron is 9.1×10^{-31} kg. What is the mass of electron when it is observed? (Ans. 1.5×10^{-30} kg)
Q2.A rocket has rest mass 100kg. When is moving its mass changes by 1kg. Calculate the velocity of rocket. (Ans. 4.2×10^{7} m/s)

Q3. A clock keeps correct time. What should be speed of this clock so that it delayed by 1 second in 24 hours? (Ans. 0.11×10^{8} m/s)

Q4. A rod of length 2m is moving with velocity 2.7×10^{8} m/s with respect to earth in the direction along its length. Find out the length of the rod when observed from earth.
(Ans. 0.87 m)
Q5. Calculate the percent contraction in the length of a rod in a frame of reference moving with velocity 0.8 m/s along the direction of length. (Ans. 40%)
Q6. A clock seems to be slow by 1 minute in one hour. Calculate the speed of the clock.
(Ans. 0.1819c)
Q7. In the laboratory, the life time of a moving particle is 2×10^{-7} sec. The particle is moving with velocity 2.8×10^{8} m/s. Find out the proper life time of the particle.
(Ans. 7.17×10^{-3} s)

Q8. Two spacecrafts A and B are moving away from earth in the same direction with velocities 0.8c and 0.6c. respectively. Find out the velocity of b with respect to A.

(Ans. 0.38c)

Q9. At what speed the mass of a proton is exceeded by 1% ? What will be kinetic energy of this particle in eV? (Ans. 4.2×10^{7} m/s , 9.3×10^{7} eV)