

Elements of Quantum Mechanics & Atomic Spectra

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Chapter 1

Introduction to Quantum Mechanics

1.1 Introduction

At the end of eighteenth century, the edifice of classical theoretical physics - classical mechanics, maxwellian electromagnetic theory, statistical mechanics and thermodynamics seemed to be essentially complete and unshakable. These laws of physics described nature very well under most conditions, however, some measurements of the late 19th and early 20th century could not be understood, i.e., a few puzzles remained but it seemed eminently likely that they would be solved by the clever applications of known principles.

Classical mechanics- based on Newton's three laws is also known as Newtonian mechanics. Classical mechanics uses the concept of absolute mass and absolute time. Classical mechanics, no doubt has been capable in explaining the motion of macroscopic celestial (stars, planets etc.) and terrestrial bodies moving with non relativistic speeds i.e., bodies moving with velocity much less than the velocity of light. However classical mechanics could not explain the motion of microscopic bodies viz; atoms, electrons, protons etc. The problems with classical physics led to the development of quantum mechanics and special theory of relativity.

Classical physics / mechanics could not explain the following :-

1. Stability of atoms.
2. Observed spectrum of black body radiation
3. Observed variation of specific heat of solids
4. Origin of discrete spectra of atoms

Apart from this, classical mechanics could also not explain various phenomena viz. photoelectric effect, Compton effect, Raman effect, short wavelength limit of X-Ray spectra etc.

The failure of classical mechanics in explaining the above led to the development of quantum mechanics. Now we will discuss the inadequacy of classical mechanics for some of the above points in detail.

1.2 Inadequacy of Classical Mechanics

(1) Classical Physics could not explain the phenomenon of black body radiation.\

A black body is an ideal body which allows the whole of the incident radiation to pass into itself (without reflecting the energy) and absorbs within itself this whole incident radiation (without passing on the energy). This property is valid for radiation corresponding to all wavelengths and to all angles of incidence. Therefore, the black body is an ideal absorber of incident radiation.

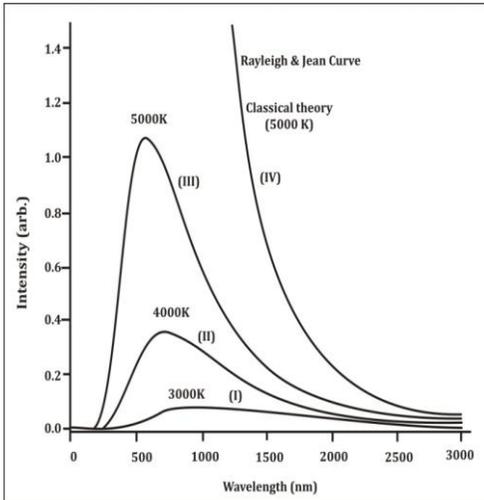


Fig. 1.1

Black body radiation spectral distribution-

Curves (I, II, III), experimentally obtained by Lummer & Pringsheim.

Curve (IV) was predicted theoretically on the basis of classical physics by Rayleigh and Jean.

One of the outstanding puzzles remaining concerned the spectral distribution of energy radiated from a “black body” a solid of ideal emissivity. This spectral distribution depends only on the temperature of the radiating body, and the experimentally observed distribution is shown for several temperatures in fig. 1.1 Classical electromagnetic theory, when applied to this problem, yielded the famous

Rayleigh-Jeans radiation formula- plotted as the black line in fig. 1.1 - proportional to the inverse fourth power of the wavelength, i.e; increasing without limit as the wavelength is decreased. The Rayleigh – Jeans formula fitted the experimental data in the long wavelength limit but gave patently ridiculous predictions for the short wavelength region.

Rayleigh & Jean tried to explain the above curves on the basis of classical theory of radiation which assumes that all values of energy are possible in the black body radiations.

As according to the classical theory, the average energy associated with the degree of freedom is KT , therefore the energy per unit volume in the frequency range ν and $\nu + d\nu$ is given as-

$$E_{\nu} d\nu = \frac{8 \pi \nu^2 k T}{c^2}$$

This is Rayleigh Jean’s radiation law derived from classical consideration.

Rayleigh & Jean plotted the following curve on the basis of theory of classical physics. It is obvious from the fig. 1.1 that there is no match between experimental curves (shown by magenta, green and blue lines in fig. 1.1) & theoretical curves drawn by Rayleigh and Jean (shown by red line).

It means that assumptions of classical physics according to which “the energy changes of radiators take place continuously”, was not capable in explaining the phenomenon of Black Body Radiations.

Max Planck explained the aforesaid phenomenon on the basis of his revolutionary quantum theory radiation, which was published on 14th Dec 1900 at Berlin Academy of Sciences.

Max Planck (1858-1947)

As a young German student, Planck came close to choosing music career rather than physics as his major interest. His long scientific career was devoted almost entirely to the fields of heat and thermodynamics. He discovered the quantized nature



of energy while he was professor in Berlin, Publishing his findings in a series of papers between 1897 and 1901. He developed a formula that agreed with his experimental data on heat radiation, and then he had to introduce the concept of energy gaps to explain his results. At first, Planck thought the success of his concept might be nothing more than a happy mathematical accident. As others made further important progress based on the concept, his doubts diminished, but he continued to look in vain for ways to reconcile quantum physics with the classical Newtonian view. By 1918, when he received the Noble prize, his pre-eminence as a scientist and teacher was well establish. In 1930, he became head of the Kasier Wilhelm Society, the most prestigious scientific organization in Germany, but was forced to resign in 1937 because of his opposition to Hitler's persecutions. his son was executed in 1944 after an attempt on Hitler's life. After the war, when he was nearly 90, Planck was reappointed head of the society, which was renamed the Max Planck Society in his honour.

The title of the paper in which he described his theory was "Theory of law of Distribution of Energy in the normal spectrum of Black Body Radiation."

Planck postulated from study of radiation from hot bodies that the radiating atoms can only radiate energy in discrete amounts— or that atoms exist only in discrete states, called Quantum states. Planck found that the black body could not radiate energy in a continuous fashion but only in discrete packets of energy i.e.; emission of radiation from a black body takes place in bundles of energy or quanta known as photons.

Planck found an empirical formula' based on the following assumptions to explain the experimentally observed distribution of energy in the spectrum of a black body-

- (i) A chamber containing black body radiations also contains simple harmonic oscillators or molecular dimensions which can vibrate with all possible frequencies.
- (ii) An oscillator can not have any energy ; but only energies given by

$$E = nh\nu$$

Where $n = 1,2,3, \dots$ and h is Planck's constant

$$E = 0, h\nu, 2h\nu, 3h\nu \dots\dots\dots$$

- (iii) The oscillators can not radiate or absorb energy continuously; but an oscillator of frequency ν can only radiate or absorb energy in units or quanta of $h\nu$. In other words it states that the exchanges of energy between radiation and matter can not take place continuously, but are limited to the discrete set of values $0, h\nu, 2h\nu, 3h\nu \dots\dots\dots$

Planck deduced the following relation of energy density belonging to the range $d\nu$:

$$E_\nu d\nu = \frac{8 \pi h\nu^3 k T}{c^2} \frac{d\nu}{e^{\frac{h\nu}{kT}} - 1}$$

The above relation is known as Planck’s radiation law and explains all experimentally observed facts.

(2) Classical physics could not explain stability of an atom

Rutherford said that electron revolve around the nucleus in circular orbits but according to the classical theory of electromagnetic radiation given by Maxwell of radiation every accelerating charge radiates electromagnetic energy. Since electron is performing circular motion therefore electron will experience centripetal acceleration. Consequently in accordance with the classical theory, the electron will radiate electromagnetic energy. Owing to which the decay of energy of electron will take place and thereby the radius of the circular orbit will

also be decreased and ultimately the electron would fall into the nucleus in a very short interval of time of the order of few nano seconds (Fig. 1.2). That is classical physics required that this atom is unstable electrons would fall into the nucleus in 10^{-7} sec. But this never happens in the actual practice. Therefore on the basis of classical theory,

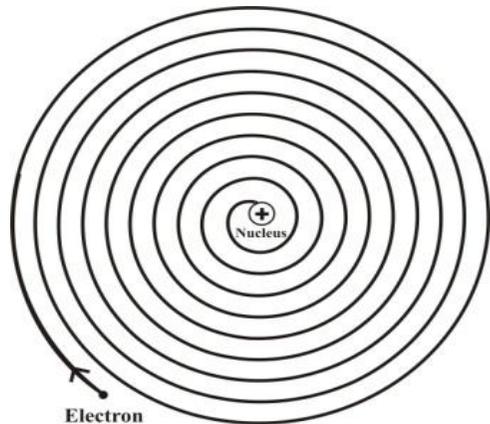


Fig. 1.2

stability of an atom can not be explained.

Neils Bohr on the basis of quantum mechanics explained the stability of an atom by applying the concepts of closed orbits and quantization of angular momentum.

ACCORDING TO Bohr's model electron can revolve only in those orbits in which its angular momentum is an integral multiple of $\frac{h}{2\pi}$, i.e.,

$$mvr = n \frac{h}{2\pi}$$

where m , v , r and h are the mass of the electron, velocity of the electron, radius of the orbit and planck,s constant respectively.

(3) Classical Physics could not explain the theory of specific heat of solids.

At room temperature, specific heat of solids at constant volume is given by the following Dulong & Peit law which is derived by the assumptions of the classical theoretical physics:

$$C_v = 3R \text{ cal/mol K}$$

The above relation can be derived on the basis of kinetic theory according to which mean kinetic energy per degree of freedom of a gas molecule at absolute temperature T is $\frac{3}{2}kT$, where k is Boltzmann's constant. For a monoatomic gas molecule, there are three degrees

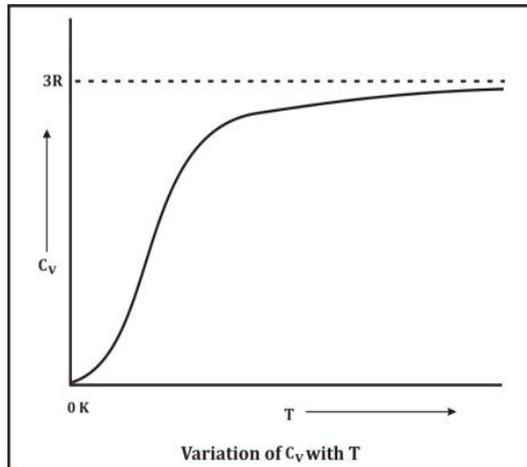


Fig. 1.3

of motion of translational motion. Therefore the total average kinetic energy per molecule is $\frac{3}{2}kT$. A solid may be supposed to consist of individual atoms which are bound to their neighbours, but they can resonate and vibrate freely when heated.

Therefore the kinetic energy of oscillation for 1 mol of atoms will be

$$N \left(\frac{3}{2}\right) kT = \left(\frac{3}{2}\right) RT \quad \left(\text{since } k = \frac{R}{N}\right)$$

The mean potential energy for each of the three components of vibrations is equal to $\frac{1}{2}kT$ since average kinetic energy is equal to average potential energy in simple harmonic motion.

Therefore the potential energy of oscillation for 1 mol of atoms will be

$$N \frac{3}{2} kT = \frac{3}{2} RT$$

Therefore the total energy of oscillation for 1 mol of atoms will be

$$E = \frac{3}{2} RT + \frac{3}{2} RT$$

Now by definition, the specific heat at constant volume is given as

$$C_v = \left(\frac{\partial E}{\partial t}\right)_v = 3R$$

According to this the specific heat of all solids should be constant and independent of temperature (Fig 1.3).

As the numerical value of R is 1.9856 cal/mol, therefore the numerical value of specific heat should be $3 \times 1.9856 = 5.96$ cal/mol.

This treatment was considered as a theoretical proof of early law of Dulong and Petit which states that the heat capacity per mol

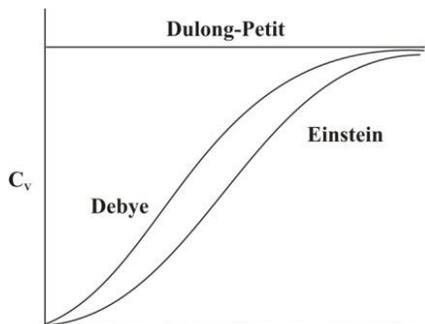


Fig. 1.4

atom of most solid substances is approximately 6. However the law fails completely when applied to light elements like carbon at low temperature since the specific heat varies with temperature tending to zero at absolute zero.

This failure of the law could not be explained by classical theory which assumes that a body absorbs heat continuously in indefinitely small amounts. Therefore it is clear that fundamental assumption of the classical theory is at fault.

Delong & Petit law however successfully explains the value of Specific heat of solids at constant volume at room temperature but the behaviour of specific heat of solids at low temperatures can not be explained by this law. In this connection this is important to note that specific heat of solids at low temperatures is directly proportional to cube of absolute temp, i.e., $C_v \propto T^3$, which is also known as cube law (Fig.1.4)

The first attempt to explain the variation of specific heat of solids with temperature was made by Einstein in 1907 on the quantum theory. According to quantum theory heat is radiated in the form discrete packets called the photons. Each photon has energy $h\nu$.

Einstein assumed :

- (1) The atoms of the solids are at rest under mutual attraction and repulsions. When the solid is heated, the atoms are set into simple harmonic motion about their positions of equilibrium. The frequency of these vibrations is same characteristic of the particular solid concerned.
- (2) Each atom of solid has three degree of freedom like a molecule of a monoatomic
- (3) The average energy per degree of freedom is not kT as given by law of equipartition of energy but is equal to $\frac{h\nu}{e^{kT} - 1}$ as calculated by Planck by the application of quantum theory.

On the basis of the above assumptions Einstein derived the following relation :

$$C_v = 3Nk \frac{e^{\frac{h\nu}{kT}}}{e^{\frac{h\nu}{kT}} - 1} \left(\frac{h\nu}{kT} \right)^2$$

The above relation however shows that specific heat of solids depend upon temperature. Though The Einstein theory predicts almost correctly the variation of specific heat with temperature, but it was observed in case of certain elements like copper, aluminium etc., the specific heat at low temperature decreases more rapidly than that predicted by Einstein's theory. This agreement is due to the neglecting mutual forces exerted by the atoms upon each other. Debye, Therefore modified Einstein's theory by assuming that any solid is capable of vibrating elastically in many varying frequencies of limited number of different modes.

Debye's theory gives excellent agreement with experiment over the whole observable temperature range.

(4) Classical physics could not explain the presence of various lines in the hydrogen spectrum.

According to classical physics the spectrum of hydrogen must be of continuous type. But the spectrum is experimentally observed as discrete, i.e.; the hydrogen spectrum is a line spectra consisting of large number of lines known as Lyman, Balmer, Paschen, Brackett & Pfund series (Fig. 1.5)

On the basis of classical physics the presence of Lyman, Balmer, Paschen, Brackett & Pfund series of hydrogen spectrum could not be explained. The presence of the aforesaid series was explained by Neils Bohr on the basis of quantum theory of radiation. Bohr derived the following equation to explain the presence of various series in hydrogen spectrum.

$$\frac{1}{\lambda} = R \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

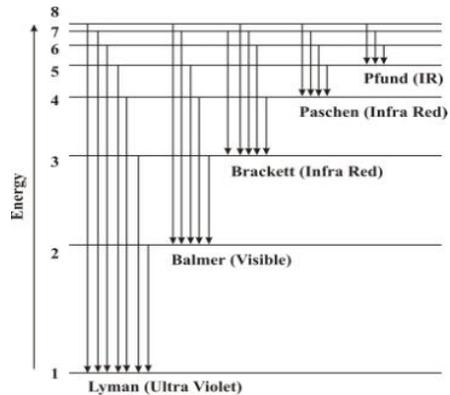


Fig. 1.5

For Lyman series $n_1 = 1$ and $n_2 = 2,3,4,5, \dots$

For Balmer series $n_1 = 2$ and $n_2 = 3,4,5,6, \dots$

For Paschen series $n_1 = 3$, and $n_2 = 4,5,6,7, \dots$

For Brackett series $n_1 = 4$, and $n_2 = 5,6,7,8, \dots$

For Pfund series $n_1 = 5$ and $n_2 = 6,7,8,9, \dots$

1.3 Classical mechanics vs Quantum mechanics

A beginning student usually has more difficulty in learning quantum mechanics than classical mechanics, although the complexities of the two theoretical approaches are not widely different. This difficulty is caused mostly by the fact that everyone is familiar with the concepts of classical mechanics than with those of quantum mechanics.

The evidence of experiments and authority of leading scientists support the necessity of using quantum mechanics for the description of atomic motion. The following table describes the difference between classical and quantum physics. The classical and quantum concept of energy of a particle is shown in and Fig 1.6 and Fig.1.7. The difference between classical mechanics, quantum mechanics, relativistic mechanics and quantum field theory has been represented in fig 1.8 (a) and 1.8 (b).

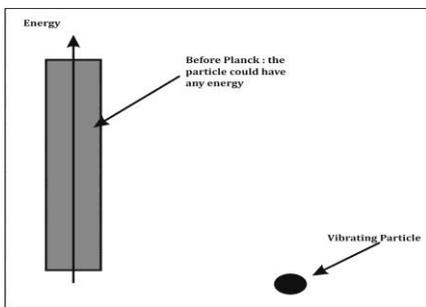


Fig.1.6

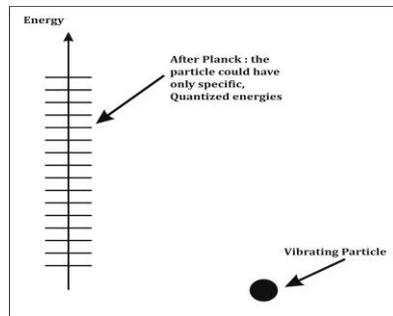


Fig.1.7

Classical World	Quantum world
It deals with macroscopic particles. In everyday life, quantum effects can be safely ignored This is because Planck's constant is so small	At atomic & subatomic scales, quantum effects are dominant & must be considered Laws of nature developed without consideration of quantum effects do not work for atoms
It is based upon Newton's law of motion.	It takes into account Heisenberg's uncertainty principle and de-Broglie's matter wave theory i.e. dual nature of matter(particle nature and wave nature)
It is based on Maxwell's electromagnetic wave theory, according to which any amount of energy may be emitted or absorbed continuously.	It is based on Planck's quantum theory of radiation, according to which only discrete values of energy are emitted or absorbed.
The state of a system is defined by specifying all the forces acting on the particle as well as their positions and velocities. The future state can then be predicted with certainty.	It gives probabilities of finding the particles at various locations in space.

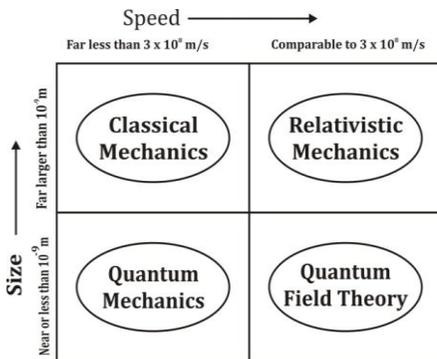


Fig. 1.8 (a)

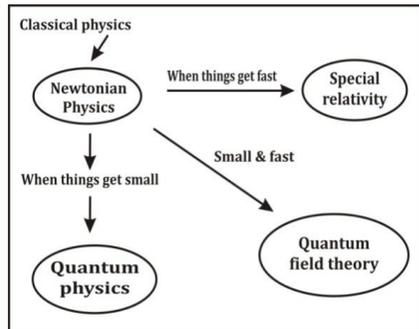


Fig. 1.8

1.4 A beautiful example to understand the rules of macroscopic and microscopic world

Macroscopic world:

- On the right side, we have a basket of cherries.
 - Many of them are identical.
 - We can see them and taste others.
- Taking one has negligible effect.
- **“Cherries are both red and good”.**



Fig. 1.9 (a)

Microscopic world

- Now on the right side, we have Single cherry.
- either we look at it without eating
- It is red.
- Or we eat it, it is good.
- ***We can not try both at the same time***
- ***“The cherry could not be good and red at the same time”.***



Fig. 1.9 (b)

1.5 The domain of quantum mechanics

A more accurate criterion for establishing the appropriate domain for quantum mechanics is based directly on Planck’s constant $h = 6.626 \times 10^{-34}$ joule.

second. Obviously the dimensions of Planck's constant is energy x time. In classical mechanics, a physical quantity known as "action" [defined by $\int_{t_2}^{t_1} L dt$, where L is the Lagrangian of the system ($L = T - V$, where T and V are kinetic energy and potential energy respectively)] also has the dimensions of energy x time i.e. $[ML^2T^{-1}]$. The dimensions of action can easily be shown to be also the same as angular momentum (momentum times distance) i.e. $[ML^2T^{-1}]$. It means the dimensions of Planck's constant, action and angular momentum are same. Therefore our criterion become self the action or angular momentum involved in a given physical event is of the order of Planck's constant, then we must use quantum mechanics to describe the event accurately. If the action or angular momentum involved in a physical event is of the order of magnitude larger than Planck's constant, classical mechanics will describe the event satisfactory accuracy.

1.6 Some applications of quantum mechanics

Without Quantum Mechanics, we could never have designed and built:

Semiconductor devices

Computers, Cell phones, etc.

Lasers

CD/DVD players, Bar-code scanners, Surgical applications

MRI (magnetic resonance imaging) technology

Nuclear reactors

Atomic clocks (e.g., GPS navigation), etc.

Physicists didn't embrace quantum mechanics because it was strange or unusual or novel. It's simply that the thing worked so well.

Exercise

Problem 1: What do you understand by inadequacy of classical mechanics? Briefly mention the phenomena which classical mechanics could not explain.

Problem 2: Under what circumstances will classical mechanics suffice and under what circumstances must we use quantum mechanics?

Problem 3: Under Quantum effects are not apparent in our everyday life, because Planck's constant h is so small. If it were a great deal larger we would be quite aware of such quantum effects. How large would h have to be before the allowed speeds of a bicycle would occur in increments of 10 km/hour.

Chapter 2

Particle properties of waves

2.1 Photo electric effect

In 1887, Heinrich Hertz observed that electrodes illuminated with ultraviolet light create electric sparks. This observation of Hertz paved the way of the development of the photoelectric effect. Photoelectric effect which is a quantum electronic phenomenon, is defined as-

“When a light ray of suitable frequency is incident on the metal plate then electrons are ejected.” This phenomenon is called photoelectric effect.

The aforesaid phenomenon cannot be explained on the basis of classical physics that is by Maxwell’s theory of electromagnetic waves.

Regarding photoelectric effect, the following points are worthy to note=

- (i) In 1905 Albert Einstein published a paper in which he explained experimental data from the photoelectric effect as the result of light energy being carried in discrete quantized packets, known as photons. This discovery led to the quantum revolution.
- (ii) In 1914, Robert Millikan's experiment confirmed Einstein's law on photoelectric effect.
- (iii) Einstein got the Nobel prize in 1921 for explaining the ‘photoelectric effect’ on the basis of Quantum theory of Radiation

2.2 Experimental Arrangement

For drawing various characteristics, the arrangement has been shown in the Fig. 2.1. K, P are cathode and plate respectively which are sealed in a high evacuated glass envelop.

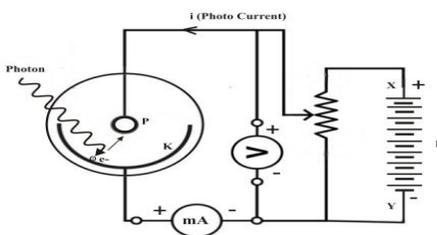


Fig. 2.1

Ordinarily cathode K and plate are maintained at negative and positive potential by means of a high tension battery B through a potential divider, Arrangement of the experiment is such that potentials can be reversed. Voltmeter V measures the potential difference between the plate and the cathode and milli ammeter mA measures the photo current it.

2.3 Experimental study of the photoelectric effect

Photoelectric current (i)

The electric current, flowing on account of photoelectrons in photoelectric effect is defined as photoelectric current.

On the basis of the experimental observations, we find the following facts.

- Intensity of the incident light
- Potential difference (V) applied between the cathode and the plate (anode)
- Nature of surface of the metal.

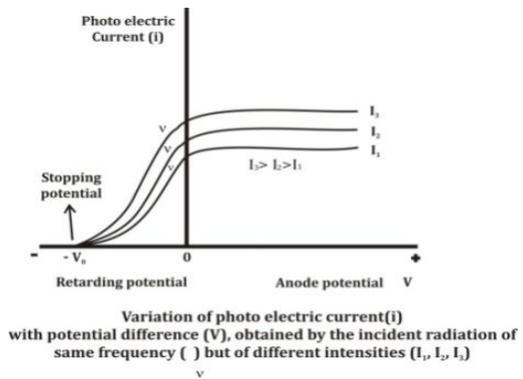


Fig. 2.2

Saturated photoelectric current (i_s)

The maximum constant value of photoelectric current is known as saturated photoelectric current. In saturation stage, the value of photoelectric current is inversely proportional to the square of the distance between the light source and the the metal surface. i.e.,

$$i_s \propto \frac{1}{d^2}$$

Stopping potential (V_0)

This is obvious from the Fig 2.2 that when negative potential on anode (plate) with respect to the cathode in a photocell is applied then at the certain value of this negative potential, photocurrent becomes zero. Therefore we can define stopping potential as-

The minimum value of the potential which is necessary to **stop** any electron (or, in other words, to **stop** even the electron with the maximum kinetic energy) from 'reaching the plate (anode).

Stopping potential is a measure of the maximum value of the kinetic energy of the electrons emitted as a result of the photoelectric effect.

$$\text{As } V = \frac{W}{q}$$

$$\text{Therefore } V_0 = \frac{K_{max}}{e}$$

$$\therefore K_{max} = eV_0$$

$$\therefore \frac{1}{2}mv_{max}^2 = eV_0$$

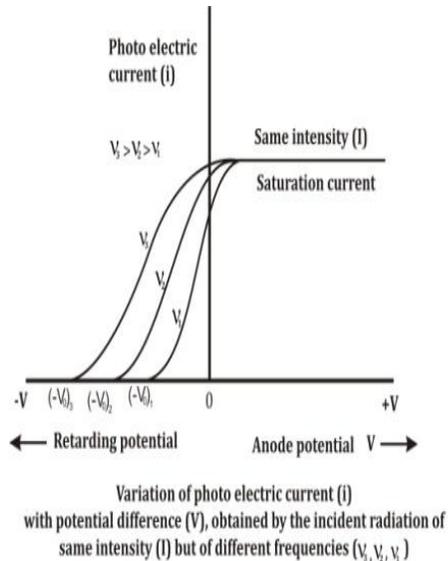


Fig. 2.3

From the Fig. 2.2 and Fig. 2.3, we conclude that-

Stopping potential depends on-

- (a) Frequency of the incident light
- (b) The nature of the cathode material

It is obvious that stopping potential does not depend on the intensity of light.

Work Function (W)

Minimum energy of the incident photon required to release an electron from the surface of a metal is called the work function of the metal.

Work function is given as

$$W = h\nu_0$$

or $= \frac{hc}{\lambda_0}$, where h is the planck's constant, ν_0 is the threshold frequency and λ_0

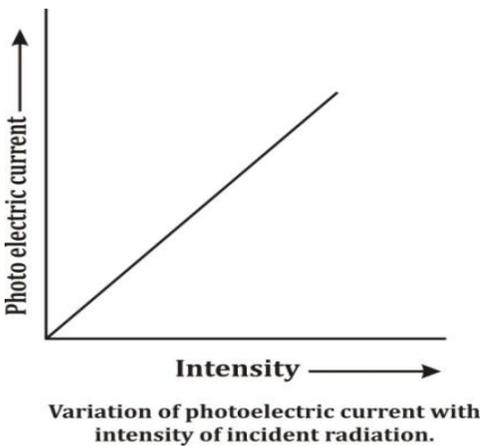


Fig. 2.4

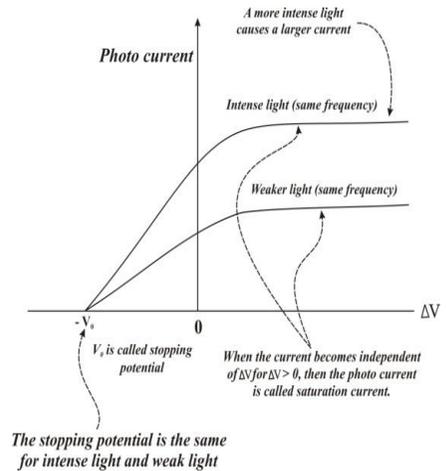


Fig. 2.5

2.4 Failure of (classical) electromagnetic theory in explaining photoelectric effect:

According to the Maxwell's electromagnetic theory of light, a substance exposed to light is subjected to an oscillatory electric field, the intensity of light is proportional to an oscillatory electric field. The intensity of light is proportional to the square of the amplitude of the electric vector. Due to interaction of the electrons of the substance with the electric field, the electrons gain kinetic energy. These electrons leave the substance as soon as their kinetic energy exceeds the binding

energy of the electron. The electromagnetic energy gained by the electron depends upon

1. Intensity of the incident light
2. Area of the surface ,exposed to the light
3. Time for which the surface is illuminated

If we consider the light falling on a sodium surface, a detectable photo-electric current will be obtained when 10^{-6} w m^{-2} of electromagnetic energy is absorbed by the surface. A layer of sodium, one atom thick and 1 m^2 in area has 10^{19} atoms. Each atom will receive an average amount of energy equal to 10^{-25} watts so that 1.6×10^6 seconds (nearly 2 weeks) will be required by an atom to have 1eV of energy and an electron in sodium will gain sufficient energy to be liberated in about 2 months.

Hence the electromagnetic theory fails to explain why there is no time lag between the instant the light falls and that of the emission of photoelectrons.

Secondly, according to electromagnetic theory , the the ejection of an electron should depend upon the intensity of light and not on frequency. In other words , there should be no threshold frequency for any material. This is contrary to the observed facts.

Moreover there is no limit on the maximum energy to be transferred to the electron i.e the electron can have any value of maximum energy. This is contrary to the observed facts. Hence classical theory *i.e.* electromagnetic theory of light fails to explain the basic facts of the photoelectric effect.

2.5 Einstein's photoelectric laws

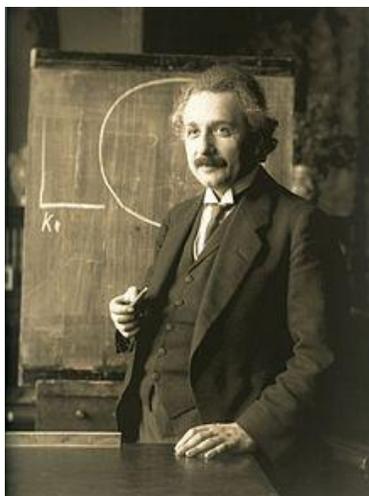
- (i) For each emitting surface, there exists a threshold frequency (ν_0) known as Threshold frequency (or Delhi frequency) at and above which electrons are emitted but below which no electron is emitted.
- (ii) The number of electrons emitted for a given surface of cathode per second is directly proportional to the intensity of incident light (not on the frequency of light).
- (iii) Maximum kinetic Energy of the photoelectrons increases with increase in frequency of incident light used, provided $\nu > \nu_0$. (Note : The value of the Maximum kinetic energy does not depend on the intensity of incident light).

(iv) The stopping potential for a given metal surface is proportional to the frequency of incident light but is independent of the intensity of light.

There is practically no time lagging between the incidence of light and ejection of photoelectron from the cathode. (Note: If we use intensity of light as 10^{-10} watt/m² then photoelectrons are emitted within a very short interval of time 3×10^{-9} sec).

Albert Einstein (1879 –1955)

Albert Einstein was born in Ulm, in the Kingdom of Württemberg in the German Empire. As a student, Einstein was unhappy in the rigid, militaristic school system of Germany, which was his native country. His interest in physics flourished after he moved to Zurich to complete his undergraduate studies. Despite excellent references, he could not get a teaching job and found work in the patent office instead, continuing his studies in theoretical physics in his spare time. At the age of 26, he published papers on Brownian motion, the photoelectric effect, and relativity. He received the



1921 Nobel Prize in Physics for his discovery of the law of the photoelectric effect. These famous studies were but the beginning of a long and brilliant career. He fled the persecutions of Hitler's Germany, and in 1940 he became an American citizen. Partly through his efforts, the United States assembled many of the world's best scientists to develop atomic bombs before Nazi Germany could do so. In addition to being the most famous modern scientist, Einstein was noted for his warm and compassionate personality and his deep interest in peace and social justice.

2.6 Einstein's Photoelectric Equation

When a photon of energy E is incident on a metal surface then a part of the energy of the photon is used to liberate the electron from the surface of the metal and the rest amount of the energy provides the maximum value of the kinetic energy (K_{max}) to the electron, i.e.

$$E = W + K_{max} \quad (1)$$

But $E = h\nu$ and $W = h\nu_0$ and K_{max} is the maximum value of the K.E., therefore from equation (1)

$$h\nu = h\nu_0 + K_{max} \quad (2)$$

$$\text{or} \quad h\nu = h\nu_0 + \frac{1}{2}mv_{max}^2 \quad (3)$$

$$\text{or} \quad h\nu = h\nu_0 + eV_0 \quad (4)$$

Where ν is the frequency of the incident photon and ν_0 is the threshold frequency, e is the charge on electron and V_0 is the stopping potential and $K_{max} = eV_0$

$$\therefore \quad \frac{hc}{\lambda} = \frac{hc}{\lambda_0} + eV_0 \quad (\text{since } \nu = \frac{c}{\lambda} \text{ and } \nu_0 = \frac{c}{\lambda_0}) \quad (5)$$

Where λ is the wavelength of the incident photon and λ_0 is the threshold wavelength.

Equations (1), (2), (3) and (4) are the various form of the Einstein's photoelectric equation.

Now from equation (2)

$$h\nu = h\nu_0 + K_{max}$$

$$\therefore K_{max} = h\nu - h\nu_0,$$

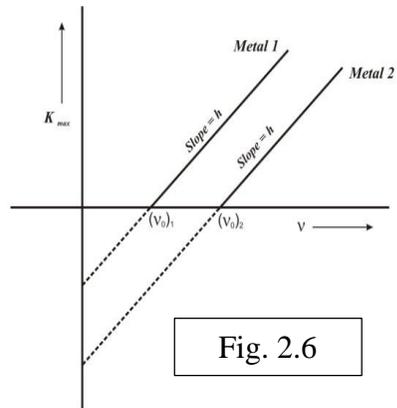


Fig. 2.6

Comparing the above equation with $y = mx + C$, we find that the slope of the straight line represented by $K_{max} = h\nu - h\nu_0$ is h (planck's constant). This is represented in the graph shown in Fig. 2.6.

2.7 Applications of the photoelectric effect

The Photoelectric effect has numerous applications, some of the applications are given below-

Night vision devices

In night vision devices, photons entering the device strike a plate which causes electrons to be emitted, these pass through a disk consisting of millions of channels, the current through these are amplified and directed towards a fluorescent screen which glows when electrons hit it. Image converters, image intensifiers, television camera tubes, and image storage tubes also take advantage of the point-by-point emission of the photocathode. In these devices an optical image incident on a semitransparent photocathode is used to transform the light image into an "electron image." The electrons released by each element of the photoemitter are focused by an electron-optical device onto a fluorescent screen, reconvertng it in the process again into an optical image.

Photoelectric Detectors

In one type of photoelectric device, smoke can block a light beam. In this case, the reduction in light reaching a photocell sets off the alarm. In the most common type of photoelectric unit, however, light is scattered by smoke particles onto a photocell, initiating an alarm. In this type of detector there is a T-shaped chamber with a light-emitting diode (LED) that shoots a beam of light across the horizontal bar of the T. A photocell, positioned at the bottom of the vertical base of the T, generates a current when it is exposed to light. Under smoke-free conditions, the light beam crosses the top of the T in an uninterrupted straight line, not striking the photocell positioned at a right angle below the beam. When smoke is present, the light is scattered by smoke particles, and some of the light is directed down the vertical part of the T to strike the photocell. When sufficient light hits the cell, the current triggers the alarm.

Solar panels

Solar panels are nothing more than a series of metallic plates that face the Sun and exploit the photoelectric effect. The light from the Sun will liberate electrons, which can be used to heat your home, run your lights, or, in sufficient enough quantities, power everything in your home.

Photodiodes and phototransistors

Solar cells (used in solar power) and light-sensitive diodes use a variant of the photoelectric effect, but not ejecting electrons out of the material. In semiconductors, light of even relatively low energy, such as visible photons, can kick

electrons out of the valence band and into the higher-energy conduction band, where they can be harnessed, creating electric current at a voltage related to the band gap energy.

Image sensors

Silicon image sensors, such as charge-coupled devices, widely used for photographic imaging, are based on a variant of the photoelectric effect, in which photons knock electrons out of the valence band of energy states in a semiconductor, but not out of the solid itself.

Photoelectron spectroscopy

Since the energy of the photoelectrons emitted is exactly the energy of the incident photon minus the material's work

function or binding energy, the work function of a sample can be determined by bombarding it with a monochromatic X-ray source or UV source (typically a helium discharge lamp), and measuring the kinetic energy distribution of the electrons emitted. Photoelectron spectroscopy is done in a high vacuum environment, since the electrons would be scattered by air.

A typical electron energy analyzer is a concentric hemispherical analyser (CHA), which uses an electric field to divert.

electrons different amounts depending on their kinetic energies. For every element and core (atomic orbital) there will be a different binding energy. The many electrons created from each will then show up as spikes in the analyzer, and can be used to determine the elemental composition of the sample.

Spacecraft

The photoelectric effect will cause spacecraft exposed to sunlight to develop a positive charge. This can get up to the tens of volts. This can be a major problem, as other parts of the spacecraft in shadow develop a negative charge (up to several kilovolts) from nearby plasma, and the imbalance can discharge through delicate electrical components. The static charge created by the photoelectric effect is self-limiting, though, because a more highly-charged object gives up its electrons less easily.

Moon dust

Light from the sun hitting lunar dust causes it to become charged through the photoelectric effect. The charged dust then repels itself and lifts off the surface of the Moon by electrostatic levitation. This manifests itself almost like an "atmosphere of dust", visible as a thin haze and blurring of distant features, and visible as a dim glow after the sun has set. This was first photographed by the Surveyor program probes in the 1960s. It is thought that the smallest particles are repelled up to kilometers high, and that the particles move in "fountains" as they charge and discharge

2.8 Important points regarding photoelectric effect

- I. In accordance with conservation of energy photoelectric effect represents conversion of light energy into electrical energy, reverse of what happens in an electric bulb.
- II. Photoelectric effect takes place only if the electron is loosely bound to the metal, i.e., photoelectric effect can never take place with completely free electron.
- III. In photoelectric effect all the emitted photoelectrons do not have the same kinetic energy. The emitted photoelectrons have kinetic energy in the range from 0 to K_{max} . K_{max} depends both on frequency of incident radiation and nature of metal.

- IV. With emission of photoelectrons the metal will become positively charged and if the metal plate is isolated then photoelectric effect will cease after some time when the potential (V) acquired by the metal such that $eV = K_{\max}$. In this situation any electron emitted by the metal will turn back to it by attractive force and will not escape.
- V. Apart from photoelectric emission, electrons can also be emitted from a metal by heating (thermionic emission), by applying a strong electric field (field emission) or by bombarding it with electrons (secondary emission).
- VI. Irradiation of substance by light under specific conditions instead of producing photoelectric effect may increase its electrical conductivity resulting in ‘photoconductive effect’ or may produce an EMF across it resulting in ‘photovoltaic effect’.
- VII. When electromagnetic wave interact with matter, then
- Photoelectric effect takes place if $E \sim eV$.
 - Compton effect takes place if $E \sim KeV$.
 - Pair production takes place if $E \sim MeV$.

(Viii) This is important to note here that the idea of quantum nature of radiation was first proposed by Planck to explain the black body radiation. According to him radiation is emitted or absorbed by atoms in discrete amounts ($E = nh\nu$) and not continuously. However, he treated the radiation itself as continuous, i.e., waves. However, according to Einstein, energy is not emitted or absorbed by atoms in quanta but also propagates in space as quanta each having energy $E = h\nu$.

If P is the power of radiation and E is the energy of a photon,

$$\text{Number of photons emitted per sec} = \frac{P}{E}$$

- (a) Energy crossing unit area normally per sec is called intensity, power density or energy flux and at a distance r from a point-source of power p is given by

$$I = \frac{U}{St} = \frac{P}{S} = \frac{P}{4\pi r^2}$$

Where U is the energy radiated in time t .

- (b) The number of photons crossing unit area normally per sec is called photon-flux and is given by

$$\text{Photon flux} = \frac{\text{Energy Flux}}{\text{Photon energy}} = \frac{I}{E}$$

- (x) For an electron in a metal, the momentum of incident photon is shared by both the electron and the lattice, while lattice due to its large mass (compared to that of electron) does not share the energy of the incident photon.

2.9 Compton effect

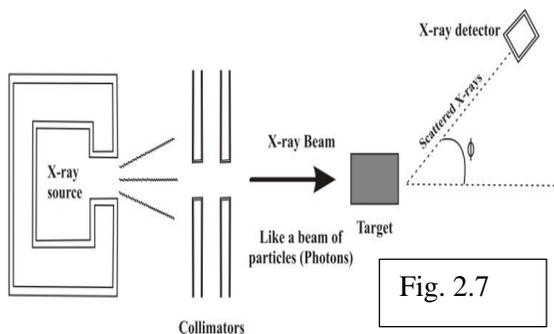
Compton in 1923 measured intensity of scattered X-rays from solid target, as function of wavelength for different angles. He won the 1927 Nobel prize When X-rays

radiations are incident on a crystal having low atomic weight like carbon then after scattering through the crystal, we get following two types of radiation:

- Unmodified radiation
- Modified radiation

(a) Unmodified radiation

In this type of the scattered radiation, the wavelength is equal to the wavelength of the incident X-rays. This is known as unmodified, or coherent or classical scattering.



(c) Modified radiation

In this type of the scattered radiation, the wavelength is greater than the wavelength of the incident X-rays. This is known as modified, or incoherent scattering. This phenomenon is called as Compton effect as it was first observed by A. H. Compton in 1924. This Phenomenon provides additional direct confirmation of the quantum nature of electromagnetic radiation.

Classical picture: oscillating electromagnetic field causes oscillations in positions of charged particles, which re-radiate in all directions at *same frequency and wavelength* as incident radiation.

Change in wavelength of scattered light is completely unexpected classically

Compton explained the presence modified radiations on the basis of Planck's quantum theory of radiation.

2.10 Expression for Compton shift

Compton calculated the increase in wavelength (Compton Shift) of the scattered photon by applying quantum theory and by making following assumptions:-

The X-rays of frequency ν (wavelength λ) consist of photons of energy $h\nu$ and momentum $h/\lambda = h\nu/c$.

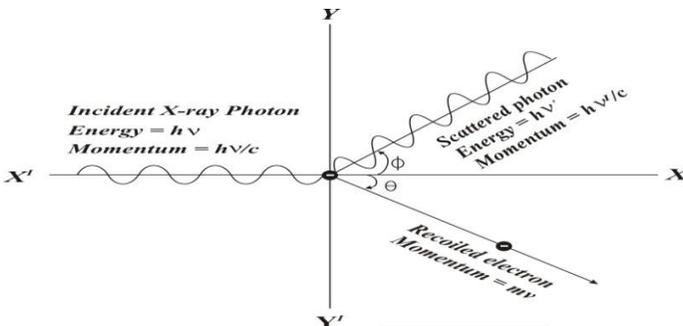


Fig. 2.8

1. The electrons are assumed to be free and stationary. It is so, because the binding energy of the electron to the atom is of the order of 10 eV which is very small as compared to the energy of X-ray photon which is of the order of 10 KeV'

The kinetic energy of the electron being of the same order as the binding energy it is comparatively at rest.

2. The collision between the high energy x-ray photon and the electron is perfectly elastic. The energy and momentum carried by the scattered photon and recoil electron is governed by the law of conservation of energy and momentum respectively.

Let a X-ray photon of energy $h\nu$ and momentum $\frac{h\nu}{c}$ strikes on an electron of the crystal of rest mass m_0 , then after scattering, X-ray photon is scattered through angle ϕ and the electron recoils with in the crystal by making angle θ from the x-axis as shown in the Fig.(2.8). The energy and momentum of the scattered photon are $h\nu'$ and $h\nu'/c$ respectively. The momentum of the recoiled electron is mv . Where m is the relativistic mass of the electron, moving with velocity v .

Now from the the law of conservation of energy

$$E_{\text{before collision}} = E_{\text{after collision}}$$

$$h\nu + m_0c^2 = h\nu' + mc^2 \quad (1)$$

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

Applying the law of conservation of momentum in X- direction,

$$\frac{h\nu}{c} + 0 = \frac{h\nu'}{c} \cos(+\phi) + mv \cos(-\theta)$$

$$\frac{h\nu}{c} + 0 = \frac{h\nu'}{c} \cos \phi + mv \cos \theta \quad [\text{since } \cos(-\theta) = \cos \theta]$$

$$h\nu = h\nu' \cos \phi + mvc \cos \theta$$

$$mvc \cos \theta = h(\nu - \nu') \cos \phi \quad (3)$$

Applying the law of conservation of momentum in Y- direction,

$$0 + 0 = \frac{h\nu'}{c} \sin(+\phi) + mv \sin(-\theta)$$

$$0 = \frac{h\nu'}{c} \sin \phi + mv \sin \theta \quad [\text{since } \sin(-\theta) = -\sin \theta]$$

$$mvc \sin \theta = hv' \sin \phi \quad (4)$$

By squaring and adding equations (3) & (4), we get,

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

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

$$\text{Or} \quad m^2 v^2 c^2 = h^2 v^2 + h^2 v'^2 - 2h^2 v v' \cos \phi \quad (5)$$

Now from equation (1)

$$mc^2 = h(v - v') + m_0 c^2$$

by squaring the above equation, we have

$$m^2 c^4 = h^2 (v - v')^2 + m_0^2 c^4 + 2hm_0 c^2 (v - v')$$

$$\text{Or} \quad m^2 c^4 = h^2 v^2 + h^2 v'^2 - 2h^2 v v' + m_0^2 c^4 + 2hm_0 c^2 (v - v') \quad (6)$$

subtracting equation (5) from equation (6), we have

$$m^2 c^4 - m^2 v^2 c^2 = h^2 v^2 + h^2 v'^2 - 2h^2 v v' + m_0^2 c^4 + 2hm_0 c^2 (v - v') - (h^2 v^2 + h^2 v'^2 - 2h^2 v v')$$

$$m^2 c^2 (c^2 - v^2) = m_0^2 c^4 + 2hm_0 c^2 (v - v') - 2h^2 v v' (1 - \cos \phi) \quad (7)$$

Now from equation (2)

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

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

$$\begin{aligned}\therefore m^2 &= \frac{m_0^2}{(c^2 - v^2)/c^2} \\ \therefore m^2(c^2 - v^2) &= m_0^2 c^2\end{aligned}\quad (8)$$

using equation (8) for equation (7)

$$m_0^2 c^4 = m_0^2 c^4 + 2hm_0 c^2(v - v') - 2h^2 v v'(1 - \cos \phi)$$

$$2hm_0 c^2(v - v') = 2h^2 v v'(1 - \cos \phi)$$

$$\frac{v - v'}{v v'} = \frac{h}{m_0 c^2} (1 - \cos \phi)$$

$$\frac{1}{v'} - \frac{1}{v} = \frac{h}{m_0 c^2} (1 - \cos \phi)$$

$$\frac{c}{v'} - \frac{c}{v} = \frac{h}{m_0 c} (1 - \cos \phi)$$

$$\lambda' - \lambda = \frac{h}{m_0 c} (1 - \cos \phi)\quad (9)$$

$$\Delta\lambda = \frac{h}{m_0 c} (1 - \cos \phi)\quad (10)$$

From equation (9), It is obvious that

$$\lambda' > \lambda$$

2.11 Compton wavelength

From equation (10), we have

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

It is obvious that $\frac{h}{m_0 c}$ has dimensions of wavelength, $\frac{h}{m_0 c}$ is called Compton wavelength.

$$\therefore \text{Compton wavelength} = \frac{h}{m_0 c}$$

Now value of Compton wavelength = $\frac{h}{m_0 c} =$

$$\frac{6.625 \times 10^{-34} \text{ joule.sec}}{9.1083 \times 10^{-31} \text{ kg} \times 3 \times 10^8 \text{ ms}^{-1}}$$

$$\frac{h}{m_0 c} = 0.0243 \text{ \AA} \approx 0.024 \text{ \AA}$$

Case (i) when $\phi = 0^\circ$

Then from equation (10)

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

$$\therefore \Delta\lambda = \frac{h}{m_0 c} (1 - \cos 0^\circ) \quad (\text{since } \cos \Phi = \cos 0^\circ = 1)$$

$$\therefore \Delta\lambda = \frac{h}{m_0 c} (1 - 1)$$

$$\therefore \Delta\lambda = 0$$

i.e., there is no change in wavelength of the X-rays, when X-ray photons are scattered through angle $\Phi = 0^\circ$

Case (ii) when $\phi = 90^\circ$

Then from (10)

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

$$\therefore \Delta\lambda = \frac{h}{m_0 c} (1 - \cos 90^\circ) \quad (\text{since } \cos \Phi = \cos 90^\circ = 0)$$

$$\therefore \Delta\lambda = \frac{h}{m_0c} (1 - 0)$$

$$\begin{aligned}\therefore \Delta\lambda &= \frac{h}{m_0c} \\ &= 0.024 \text{ \AA} = \text{Compton wavelength}\end{aligned}$$

i.e., when X-ray photons are scattered through angle $\Phi = 90^\circ$, then change in wavelength of X-rays is exactly equal to the Compton wavelength

Case (iii) when $\phi = 180^\circ$

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

$$\therefore \Delta\lambda = \frac{h}{m_0c} (1 - \cos 180^\circ)$$

$$\therefore \Delta\lambda = \frac{h}{m_0c} [1 - (-1)] \quad (\text{since}$$

$\cos 180^\circ = -1$)

$$\therefore \Delta\lambda = 2 \times 0.024 \text{ \AA}$$

$$= 0.048 \text{ \AA}$$

i.e., maximum change in wavelength of the X-rays is observed, when X-ray photons are scattered through angle $\Phi = 180^\circ$

2.12 Difference between photoelectric effect and Compton effect

Photoelectric Effect	Compton Effect
Photon is completely absorbed by the electron i.e., no photon remains after Collision of photon and electron.	Photon is not completely absorbed. A part of photon remains after the collision of photon and electron.

<p>Electron is assumed as tight bound.</p> <p>Reason: A free electron can never absorb full photon because if we assume that the electron is free in photo electric effect then</p> $h\nu = \frac{1}{2}mv^2 \quad (1)$ $\frac{h\nu}{c} = mv$ <p>or $mv c = h\nu \quad (2)$</p> <p>Now from Equations (1) and (2) $mv c = \frac{1}{2}mv^2$</p> <p>or $v = 2c$</p> <p>which is impossible, since according to the special theory of relativity, no object can move beyond the velocity of light.</p>	<p>The electron is assumed as free.</p>
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Solved Problems

Problem 1. Does the mass of a body change when it emits or absorbs photons?

Solution: Yes ; photon has energy $h\nu$ and according to ' theory of relativity' energy E is equivalent to a mass (E/c^2) ; so photon has a mass $(h\nu/c^2)$. So theoretically the mass of a body will decrease if it emits photons and will increase if it absorbs them. However, due to small value of h ($=6.6 \times 10^{-34}$ J-s) and large value of c ($=3 \times 10^8$ m/s) as the mass of an optical photon

$$m = \frac{6.6 \times 10^{-34}}{(3 \times 10^8)^2} \times 10^{15} \approx 10^{-35} \text{ kg}$$

is too small, the change in mass of a body due to emission or absorption of photons is practically negligible as compared to the mass of the body.

Problem 2. Show that a stream of photons impinging normally on a completely absorbing screen in vacuum exerts a pressure $P = (I/c)$ where I is the irradiance and c is the speed of light in free space

Solution : As pressure is defined as :

$$P = \frac{F}{S} = \frac{1}{S} \frac{\Delta P}{\Delta t} \left[\text{as } F = \frac{\Delta P}{\Delta t} \right] \quad \dots (1)$$

And for complete absorption of photons at normal incidence

$$\Delta p = p - 0 = (E/c) \quad [\text{as for photon } p = E/c] \quad \dots (2)$$

So substituting the value of Δp from Eqn. (2) in (1).

$$P = \frac{1}{c} = \frac{E}{S\Delta t} = \frac{I}{c} \quad [\text{as by definition } I = \frac{E}{S\Delta t}]$$

Note :

- (i) If the surface is perfectly reflecting, $\Delta p = p - (-p) = 2p$ and so

$$P = 2(I/c).$$

- (ii) Due to radiation pressure the tail of a comet, when it is approaching the sun, is always directed away from the sun.
-

Problem 3. Show that it is impossible for a photon to give up all its energy and momentum to a free electron. This is why photoelectric effect can not take place with completely free electrons.

Solution: If photon can transfer its whole energy and momentum to free electron, by conservation of momentum we have.

$$\frac{h\nu}{c} = 0 = p \quad \text{i. e.} \quad \frac{h\nu}{c} = p \quad \dots (1)$$

While conservation of energy implies ... (2)

$$h\nu + m_0c^2 = E$$

But according to ' Theory of relativity' ... (3)

$$E^2 = m_0^2c^4 + P^2c^2$$

So substituting the values of p and E from Eqns. (1) and (2), we get

$$(h\nu + m_0c^2)^2 = m_0^2c^4 + (h\nu/c)^2 \times c^2$$

i.e.
$$2(h\nu)(m_0c^2) = 0$$

which is not physically possible as both $h\nu$ and m_0c^2 are finite. So a photon can not transfer whole of its energy and momentum to a free electron.

Problem 4. Electrons with a kinetic energy of 6.023×10^4 J/mol are evolved from the surface of a metal, when exposed to a radiation of wavelength of 600 nm (photoelectric effect). What is The minimum amount of energy required to remove an electron from the metal atom ?

Solution

When a radiation is passed on to the surface of a metal, some amount of energy is used in overcoming the attraction force on the electron and knocks it out from the atom. The remaining part is converted to kinetic energy.

Therefore:

$$E = W + KE$$

Where:

W = work function or ionization energy required to remove the electron from the atom.

KE = kinetic energy

From the data:

$$KE \text{ for } 6.023 \times 10^{23} \text{ electrons (one mole)} = 6.023 \times 10^4 \text{ J}$$

$$\text{Therefore KE for one electron} = 6.023 \times 10^4 / 6.023 \times 10^{23} = 1 \times 10^{-19} \text{ J}$$

now

$$E = hc/\lambda = 6.626 \times 10^{-34} \text{ J s} \times 3.0 \times 10^8 \text{ m s}^{-1} / 600 \times 10^{-9} \text{ m} = 3.313 \times 10^{-19} \text{ J}$$

$$\text{Therefore } W = E - KE = (3.313 \times 10^{-19} \text{ J}) - (1 \times 10^{-19} \text{ J}) = 2.313 \times 10^{-19}$$

Problem 5. The work function (Φ) of some metals is listed below. The number of metals which will show photoelectric effect when light of 300nm wavelength falls on the metal is:

Metal	Li	Na	K	Mg	Cu	Ag	Fe	Pt	W
W (in eV)	2.4	2.3	2.2	3.7	4.8	4.3	4.7	6.3	4.75

(IIT JEE 2011)

Solution:

The energy of radiation must be equal to or greater than the work functions of metals to show photoelectric effect.

We need to convert wavelength of radiation into energy expressed in eV units.

$$E = hc/\lambda = 6.626 \times 10^{-34} \text{ J s} \times 3.0 \times 10^8 \text{ m s}^{-1} / 300 \times 10^{-9} \text{ m} = 6.626 \times 10^{-19} \text{ J}$$

Now convert this value into eV.

We know that:

$$1 \text{ J} = 6.24 \times 10^{18} \text{ eV}$$

Therefore:

$$6.626 \times 10^{-19} \text{ J} = 6.626 \times 10^{-19} \times 6.24 \times 10^{18} \text{ eV} = 4.134 \text{ eV}$$

Conclusion:

Since the work functions of only Li, Na, K and Mg fall below 4.134 eV, only these metals can show photoelectric effect upon exposure of radiation of 300nm wavelength.

The number of metals that can show photoelectric effect = 4.

Problem 6. Calculate the work function in electron-volts for a metal, given that the photoelectric threshold wavelength is 6800 Å.

Solution: Threshold wavelength $\lambda_0 = 6800 \text{ Å} = 6800 \times 10^{-10} \text{ meter}$. If ν_0 be the threshold frequency, then the work function for the metal is

$$\begin{aligned} W &= h\nu_0 = \frac{hc}{\lambda_0} \\ &= \frac{(6.6 \times 10^{-34} \text{ joule-sec}) \times (3.0 \times 10^8 \text{ m-sec}^{-1})}{6800 \times 10^{-10} \text{ m}} \\ &= 2.9 \times 10^{-10} \text{ joule.} \end{aligned}$$

Now $1 \text{ eV} = 1.6 \times 10^{-19} \text{ Joule}$

$$\therefore W = \frac{2.9 \times 10^{-19}}{1.6 \times 10^{-19}} = 1.8 \text{ eV.}$$

Problem 7. A photon of wavelength 3310 \AA falls on a photocathode and ejects an electron of maximum energy $3 \times 10^{-12} \text{ erg}$. Calculate the work function of the cathode material. ($h = 6.62 \times 10^{-27} \text{ erg-sec}$, $c = 3 \times 10^{10} \text{ cm/sec}$ and $1 \text{ eV} = 1.6 \times 10^{-12} \text{ erg}$.)

Solution: When a photon of frequency ν falls on a photocathode of work function W , the maximum kinetic energy K_{max} of the photoelectrons is given by the Einstein photoelectric equation:

$$K_{max} = h\nu - W$$

$$\text{Or } W = h\nu - K_{max}$$

$$= \frac{hc}{\lambda} - K_{max}.$$

Substituting the given values, we get

$$W = \frac{(6.62 \times 10^{-27} \text{ erg sec}) \times (3 \times 10^{10} \text{ cm sec}^{-1})}{(3310 \times 10^{-8} \text{ cm})} - (3 \times 10^{-12} \text{ erg})$$

Problem 8. The threshold frequency for photoelectron emission in copper is $1.1 \times 10^{15} \text{ sec}^{-1}$. Find the maximum energy of the photoelectrons when light of frequency $1.5 \times 10^{15} \text{ sec}^{-1}$ falls on copper surface. Also calculate the retarding potential. ($h = 6.62 \times 10^{-34} \text{ joule -sec}$)

(LU 95)

Solution: If ν_0 be the threshold frequency, then according to Einstein's equation, the maximum kinetic energy of the photoelectrons is

$$\begin{aligned} K_{max} &= h\nu - h\nu_0 \\ &= 6.62 \times 10^{-34} (1.5 \times 10^{15} - 1.1 \times 10^{15}) \\ &= 2.648 \times 10^{-19} \text{ joule.} \end{aligned}$$

But $1 \text{ eV} = 1.6 \times 10^{-19} \text{ joule}$.

$$\therefore K_{max} = \frac{2.648 \times 10^{-19}}{1.6 \times 10^{-19}} = 1.655 \text{ eV.}$$

The retarding potential V_0 is the potential which just stops the photoelectrons of maximum kinetic energy. Thus

$$V_0 = 1.655 \text{ volts.}$$

Problem 9.

The work function of a metal surface is 1.2 eV. Calculate the kinetic energy of the fastest and slowest photoelectrons and the retarding potential when light of frequency $5.5 \times 10^{14} \text{ sec}^{-1}$ falls on the surface.

($h = 6.62 \times 10^{-34} \text{ joule-sec}$).

Solution: Let K_{max} be the kinetic energy of the fastest photoelectrons. Then the photoelectric equation is

$$K_{max} = h\nu - W,$$

Where W is the work function and ν the incident frequency. Let us evaluate $h\nu$ in electron-volts. This is

$$\begin{aligned} h\nu &= (6.62 \times 10^{-34} \text{ joule sec}) (5.5 \times 10^{14} \text{ sec}^{-1}) \\ &= 3.64 \times 10^{-19} \text{ joule.} \end{aligned}$$

But $1 \text{ eV} = 1.60 \times 10^{-19} \text{ joule}$.

$$\therefore h\nu = \frac{3.64 \times 10^{-19}}{1.60 \times 10^{-19}} = 2.27 \text{ eV.}$$

Substituting this value of $h\nu$ and the given value of W (1.2 eV) in eq. (i), we get

$$K_{\max} = 2.27 - 1.2 = \mathbf{1.07 \text{ eV.}}$$

The kinetic energy of the slowest photoelectrons is **ZERO**.

The stopping potential V_0 is measured by the kinetic energy K_{\max} of the fastest photoelectrons which is 1.07 electron-volts.

$$\therefore \quad V_0 = \mathbf{1.07 \text{ volts.}}$$

Problem 10. A radiation of frequency 10^{15} Hz falls on a photocathode and ejects electrons with maximum energy of 4.22×10^{-19} J. If the frequency of radiation is changed to 5×10^{14} Hz, the maximum energy of ejected electrons becomes 0.9×10^{-19} J. Calculate Planck's constant, threshold frequency and work function of photocathode material.

Solution: The photoelectric equation is

$$K_{\max} = h\nu - W,$$

where ν is the incident frequency and W is the work function.

Substituting the given values in the two cases, we have

$$4.2 \times 10^{-19} \text{ J} = h (10 \times 10^{14} \text{ s}^{-1}) - W$$

.. (i)

And

$$0.9 \times 10^{-19} \text{ J} = h (5 \times 10^{14} \text{ s}^{-1}) - W$$

.. (ii)

Subtracting eq. (ii) from eq. (i), we get

$$3.3 \times 10^{-19} \text{ J} = h (5 \times 10^{14} \text{ s}^{-1})$$

Or

$$h = \frac{3.3 \times 10^{-19} \text{ J}}{5 \times 10^{14} \text{ s}^{-1}} = 6.6 \times 10^{-19} \text{ J} \cdot \text{s}$$

Putting this value of h in eq. (i) and solving, we get

$$W = 2.4 \times 10^{-19} \text{ J.}$$

$$\text{The threshold frequency is } \nu_0 = \frac{W}{h} = \frac{2.4 \times 10^{-19}}{6.6 \times 10^{-34} \text{ J-s}} = 3.6 \times 10^{-14} \text{ s}^{-1}$$

Problem 11. Light of wavelength 3000 \AA falls on a metal surface having a work function of 2.3 eV . Calculate the maximum velocity of the ejected electrons.

($h = 6.6 \times 10^{-34} \text{ joule sec}$, $c = 3.0 \times 10^8 \text{ m/sec}$, electronic mass $m = 9.1 \times 10^{-31} \text{ kg}$ and $1 \text{ eV} = 1.6 \times 10^{-19} \text{ joule}$).

Solution. The photoelectric equation is

$$\begin{aligned} K_{\max} &= h\nu - W = \frac{hc}{\lambda} - W \\ &= \frac{(6.6 \times 10^{-34} \text{ joule sec}) \times (3.0 \times 10^8 \text{ m sec}^{-1})}{3000 \times 10^{-10} \text{ m}} \\ &\quad - (2.3 \times 1.6 \times 10^{-19} \text{ joule}) \\ &= 6.6 \times 10^{-19} \text{ joule} - 3.7 \times 10^{-19} \text{ joule} \\ &= 2.9 \times 10^{-19} \text{ joule.} \end{aligned}$$

Now
$$K_{\max} = \frac{1}{2} m v_{\max}^2$$

$$\begin{aligned} \therefore v_{\max} &= \sqrt{\left[\frac{2 K_{\max}}{m} \right]} \\ &= \sqrt{\left[\frac{2 \times 2.9 \times 10^{-19}}{9.1 \times 10^{-31}} \right]} = 8 \times 10^5 \text{ m/sec.} \end{aligned}$$

Problem 12. (a) A stopping potential of 0.82 V is required to stop the emission of photoelectrons from the

surface of a metal for light of wavelength 4000\AA . For light of wavelength 3000\AA . The stopping potential is 1.85 V . Find the value of Planck's constant.

(b) At stopping potential, if wavelength of the incident light is kept fixed, at 4000\AA , but the intensity of light is doubled, will photoelectric current be observed? Give reason in support of your answer. [$c = 3 \times 10^8\text{ m/s}$ and $e = 1.6 \times 10^{-19}\text{ coulomb}$]

[M.N.R. 1993]

Ans. (a) According to Einstein equation for photoelectric effect,

$$K_{\max} = h\nu - W \quad \text{i.e.} \quad h\nu = K_{\max} + W$$

But as $\nu = (c/\lambda)$ and $K_{\max} = eV_0$ $\frac{hc}{\lambda} = eV_0 + W$

So that for wavelengths λ_1 and λ_2 ,

$$\frac{hc}{\lambda_1} = e(V_0)_1 + W \quad \text{and} \quad \frac{hc}{\lambda_2} = e(V_0)_2 + W$$

Or $hc = \left[\frac{1}{\lambda_1} - \frac{1}{\lambda_2} \right] = e [(V_0)_1 - (V_0)_2]$

i.e., $h = \frac{e}{c} \left[\frac{\lambda_1 \lambda_2}{\lambda_1 - \lambda_2} \right] [(V_0)_1 - (V_0)_2]$

or, $h = \frac{1.6 \times 10^{-19}}{3 \times 10^8} \left[\frac{(3 \times 10^{-7} \times 4 \times 10^{-7})}{(4-3) \times 10^{-7}} \right] [1.85 - 0.82]$

or, $h = 6.4 \times 1.03 \times 10^{-34} = 6.59 \times 10^{-34}\text{ J-s}$

(c) No; as at stopping potential (for a given wavelength and metal) no photo electrons will be emitted how intense the light may be. This is because kinetic

energy of emitted photoelectrons is independent of intensity of incident light but depends on nature of metal and wavelength of incident light.

Problem 13. When a surface is irradiated with light of wavelength 4950 \AA , a photocurrent appears which vanishes if a retarding potential greater than 0.6 V is applied across the photo tube. When a different source of light is used it is found that the critical retarding potential is changed to 1.1 V . Find the work function of the emitter surface and the wavelength of the second source. If the photoelectrons (after emission from the surface) are subjected to a magnetic field of 10 Tesla , what changes will be observed in the above two retarding potentials? [$h=6.6 \times 10^{-34} \text{ J-s}$; $c = 3 \times 10^8 \text{ m/s}$ and $e = 1.6 \times 10^{-19} \text{ C}$]

Solution : According to Einstein equation for photoelectric effect,

$$K_{\max} = h\nu - W$$

But as
$$K_{\max} = eV_0 \quad \text{and } \nu = (c/\lambda)$$

$$W = \frac{hc}{\lambda} - eV_0$$

So,
$$W = \left[\frac{6.6 \times 10^{-34} \times 3 \times 10^8}{4950 \times 10^{-10}} - 1.6 \times 10^{-19} \times 0.6 \right] \text{ J}$$

i.e.
$$W = \left(\frac{19.8}{4.95} - 0.96 \right) \times 10^{-19} = 3.04 \times 10^{-19} \text{ J}$$

or,
$$W = \frac{3.04 \times 10^{-19}}{1.6 \times 10^{-19}} \text{ eV} = 1.9 \text{ eV}$$

Now for the second source,

$$\frac{ch}{\lambda} = W + eV_0 = \left[3.04 \times 10^{-19} + 1.6 \times 10^{-19} \times 1.1 \right] \text{ J}$$

Or,
$$\lambda = \frac{3 \times 10^8 \times 6.6 \times 10^{-34}}{4.8 \times 10^{-19}} \text{ m}$$

Or,
$$\lambda = 4.125 \times 10^{-7} \text{ m} = 4125 \text{ \AA}$$

Now as retarding potential V_s is related to KE of the photoelectrons through the relation $eV_s = K_{\max}$ and as magnetic field does not affect the speed and hence, kinetic energy of the electrons, retarding potentials will remain unchanged.

Problem 14: Show that Compton shift is independent of wavelength of incident X-rays.

(LU 1996)

Solution: Compton shift is independent of wavelength of incident X-rays

Compton shift is given as-

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

this is known as Compton equation. It shows that the increase in wavelength of the X-rays or Compton shift is independent of the wavelength of the the incident X-rays as well as the nature of the scattering substance. It only depends upon the angle of scattering.

Problem 15: How do you account for the presence of unmodified component of X-rays in the study of Compton effect?

Solution : In deriving the relation for Compton shift it is assumed that the electron is free and stationary. But all the electrons do not satisfy this condition. When Compton scattering takes place from an electron tightly bound to the atom, the collision is in fact with the atom to which the electron is tightly bound, As the Compton wavelength $\lambda = h/m_0c$ is inversely proportional to the mass of the scattering particle. Its magnitude for an atom is nearly 10^{-4} times the value for an electron as calculated below for an atom of carbon of mass $m_0 = 2 \times 10^{-26}$ kg for which

$$\lambda_0 = \lambda = h/m_0c$$

Problem 16: Whether Compton effect can be observed by visible radiations ?

Solution: No.

Compton effect can not be detected in case visible radiations. The reason is illustrated in the following comparison table.

X-ray radiations	Visible radiations
<p>Wavelength range of X-rays radiations is from 1\AA to 100\AA</p> <p>let X-ray photon of wavelength $\lambda = 5\text{\AA}$ is incident on the electron and we know that maximum change in Compton shift</p> $(\Delta \lambda)_{\max} = 0.048\text{\AA} \cong 0.05\text{\AA}$ <p>% change in wavelength is given by :</p> $= \Delta \lambda / \lambda \times 100\%$ <p>therefore % change in wavelength</p> $= 0.05\text{\AA} / 5\text{\AA} \times 100$ $= 1\%$ <p>which is fairly large.</p> <p>Therefore Compton effect can be easily detected in case of X-ray radiations.</p>	<p>Wavelength range of visible Radiations is from 4000\AA - 7000\AA</p> <p>Let visible radiation photon of wavelength $\lambda = 5000\text{\AA}$ is incident on the electron</p> $(\Delta \lambda)_{\max} = 0.048\text{\AA} \cong 0.05$ <p>% change in wavelength is given by :</p> $= \Delta \lambda / \lambda \times 100\%$ <p>Therefore % change in wavelength</p> $= 0.05\text{\AA} / 5000\text{\AA} \times 100$ $= 0.$ <p>which is very small.</p> <p>Therefore Compton effect can not be detected in case visible radiations.</p>

Problem 17: Whether Compton Effect can be observed in case of γ radiations.

Solution : No

Compton effect can not be detected in case of γ radiations. The reason is given below.

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

when we will use γ radiations then due to intense energy of γ rays whole atom will recoil instead of electron of the atom. Therefore in equation we will have to replace m (mass of the atom) by m_0 (mass of the electron)

Then eqⁿ (x) will become

$$\Delta\lambda = \frac{h}{m c} (1 - \cos \phi)$$

Now since $m \gg m_0$

$$\text{therefore } \frac{h}{m c} \ll \frac{h}{m_0c} \ll 0.0243\text{\AA}^0$$

i.e.; $\Delta\lambda$ is undetectable\

Problem 18: In the Compton Effect photon is scattered through angle Φ and electron is scattered through angle Θ . Find the ratio of the K.E. of the recoiled electron to the total energy of the photon is equal to

$$\frac{x(1-\cos \phi)}{1+x(1-\cos \phi)}, \text{ where } x = \frac{h\nu}{m_0c^2}$$

Solution: The ratio of the Kinetic energy of the recoiled electron to the total energy of the photon is given by

$$\begin{aligned} \frac{(\text{K.E.})_{\text{electron}}}{E_{\text{total}}} &= \frac{h\nu - h\nu'}{h\nu} \\ &= \frac{\nu - \nu'}{\nu} \end{aligned}$$

$$\begin{aligned}
&= \frac{c/\lambda - c/\lambda'}{c/\lambda} \\
&= \frac{1/\lambda - 1/\lambda'}{1/\lambda} \\
&= \frac{\lambda' - \lambda}{\lambda'} \\
&= \frac{\Delta\lambda}{\lambda + \Delta\lambda} \quad (\text{since } \lambda' - \lambda = \Delta\lambda) \\
&= \frac{\frac{h}{m_0 c} (1 - \cos \phi)}{\lambda + \frac{h}{m_0 c} (1 - \cos \phi)} \\
&= \frac{\frac{h}{m_0 c} (1 - \cos \phi)}{\frac{c}{\nu} + \frac{h}{m_0 c} (1 - \cos \phi)}
\end{aligned}$$

multiplying numerator and denominator of the above equation by ν/c

$$\begin{aligned}
&= \frac{\frac{h\nu}{m_0 c^2} (1 - \cos \phi)}{1 + \frac{h}{m_0 c} (1 - \cos \phi)} \\
&= \frac{x(1 - \cos \phi)}{1 + x(1 - \cos \phi)} \quad \left(\text{as } x = \frac{h\nu}{m_0 c^2} \right)
\end{aligned}$$

Problem 19. A beam of γ -radiation having photon energy of 510 keV is incident on a foil of aluminium. Calculate wavelength of the radiation scattered at 90° and also the energy and direction of emission of the recoil electron.

Solution. The energy of the incident γ - radiation is

$$E = 510 \text{ keV} = 510 \times 10^3 \text{ eV}$$

$$= 510 \times 10^3 \times 1.6 \times 10^{-19} = 8.16 \times 10^{-14} \text{ joule}$$

Its wavelength is given by

$$\lambda = \frac{hc}{E} \frac{(6.62 \times 10^{-34} \text{ joule sec}) \times (3.0 \times 10^8 \text{ m/sec})}{8.16 \times 10^{-14} \text{ joule}}$$

$$= 2.43 \times 10^{-12} \text{ meter} = 0.0243 \text{ \AA}.$$

The Compton-shift in wavelength at scattering angle of 90° is given by

$$\Delta\lambda = 0.0243 (1 - \cos 90^\circ) = 0.0243 \text{ \AA}.$$

Hence the wavelength of the scattered radiation is

$$\lambda' = \lambda + \Delta\lambda = 0.0243 + 0.0243 = \mathbf{0.0486 \text{ \AA}}$$

The kinetic energy of the recoiling electron is given by

$$K = \frac{hc \Delta\lambda}{\lambda\lambda'}$$

$$\frac{(6.62 \times 10^{-34} \text{ joule sec}) \times (3.0 \times 10^8 / \text{sec}) (0.0243 \times 10^{-10} \text{ m})}{(0.0243 \times 10^{-10} \text{ m}) (0.0486 \times 10^{-10} \text{ m})}$$

$$= 4.1 \times 10^{-14} \text{ joule} = \frac{4.1 \times 10^{-14}}{1.6 \times 10^{-19}} = 2.56 \times 10^5 \text{ eV}$$

$$= \mathbf{256 \text{ keV}}.$$

The direction Φ of the

recoil electron for 90° -scattering is given by

$$\tan \Phi = \frac{v'}{v} = \frac{\lambda}{\lambda'} = \frac{0.0243}{0.0486} = 0.5$$

Exercise

(A) Descriptive type

Section I Photoelectric effect

(1) Explain the mechanism of photoelectric emission. Derive and explain the Einstein's photoelectric equation. How is it different from Compton Effect and thermionic emission?

(L.U. 2007)

(2) What is photoelectric effect? State the laws of photoemission. Discuss the effect of variation of frequency and intensity of incident radiation, on photocurrent.

(L.U. 2008)

(3) Explain the mechanism of photoelectric emission and derive Einstein's photo electric equation. The energy required to remove an electron from sodium is 2.3 eV. Does sodium show photoemission for light of wavelength 6800 Å.

(L.U. 2009)

(4) Explain the mechanism of photoelectric emission. Derive and explain Einstein's photoelectric equation. How is it different from Compton Effect and thermionic emission?

(L.U. 2007)

(5) Explain the mechanism of photoelectric emission. Derive and explain Einstein's photoelectric equation. How is it different from Compton effect and thermionic emission?

(L.U. 2011)

(6) Explain the mechanism of photoelectric emission and derive Einstein's photo electric equation. The energy required to remove an electron from sodium is 2.3 eV. Does sodium show photoemission for light of wavelength 6800 Å.

(L.U. 2009)

(7) Explain the mechanism of photoelectric emission and derive Einstein's photoelectric equation.

(L.U. 2012)

Section II Compton effect

(8) An X-ray photon is scattered by a free electron. Prove that the change in its wavelength will be independent of its original wavelength.

(L.U. 2010)

(9) Show that 'Compton shift' is independent of wavelength of incident X-rays. How will you explain 'Normal scattering' by Compton's equation?

(L.U. 2012)

(10) What is Compton effect? Derive an expression for the Compton shift.

(L.U. 2013)

(11) Derive an expression for Compton shift.

(LU 2015)

(12) A photon of wavelength λ is scattered through angle θ by a free electron at rest. Show that the ratio of Kinetic energy of incident photon (E_ν) to that of recoiled electron (E_e) is

$$\frac{E_\nu}{E_e} = \left[1 + \frac{\gamma}{\frac{h}{m_0 c} (1 - \cos \theta)} \right]$$

(LU 2016)

(A) Short answer type

Section I Photoelectric effect

(1) How the maximum energy of ejected photoelectrons will be affected when :

(i) Intensity of light is increased **(L.U. 2010)**

(ii) Emitting material is changed **(L.U. 2010)**

(iii) Wavelength of light is increased? **(L.U. 2010)**

(2) Define Photoelectric effect. **(L.U. 2013)**

(3) Write laws of photoelectric emission and Einstein's photoelectric equation.

(L.U. 2015)

(4) Give physical significance of Einstein's Photoelectric equation.

(L.U. 2016)

(5) Explain why wave nature of radiation fails to explain Photoelectric Effect?

(L.U. 2016)

(6) Figure shows variation in kinetic energy (E_k) of fastest ejected photoelectrons with incident frequency (ν). What will be the effect on line OA if

- (i) Work function of metal is increased?
- (ii) Intensity of incident radiation is increased?
- (iii) Wavelength of radiation is increased?

(L.U. 2016)

Section II Compton effect

(7) What is the Compton Shift $\Delta\lambda$?

(L.U. 2009)

(8) Explain why Compton effect cannot be detected with visible light. **(L.U. 2009)**

(9) What kinetic energy is imparted to the recoil electron?

(L.U. 2009)

(10) What is Compton wavelength? .

(L.U. 2015)

(11) Why is it not possible to observe Compton effect with visible light?

(L.U. 2015)

(12) Account for the presence of unmodified wavelength in Compton scattering.

(L.U. 2010)

(13) For which angle of scattering, the Compton-shift will be half of Compton wavelength?

(L.U. 2016)

(C) Numerical problems

Section I Photoelectric effect

(1) Photons of energy 3.6 eV are incident on metal of work function 2.0 eV. Calculate the wavelength of fastest ejected photoelectrons.

(L.U. 2016)

(2) Find the energy y of a 7000 Å photon.

(L.U. 2007)

- (3) Show that the rest mass of a photon is zero. **(L.U. 2007)**
- (4) The work function of sodium metal is 2.3 eV. What is the longest wavelength of light that can cause photoelectron emission from sodium? **(L.U. 2007)**
- (5) The work function of sodium metal is 2.3 eV. What is the longest wavelength of light that can eject photoelectron from this metal? **(L.U. 2008)**
- (6) Light of wavelength 5000 Å is made of incident on a metal of work function 2.0 eV. Calculate minimum potential needed to stop emission. **(L.U. 2010)**

Section II Photoelectric effect

- (7) X-rays with $\lambda - 1 \text{ \AA}$ are scattered from a carbon block. The scattered radiation is viewed at 90° to the incident beam. . **(L.U. 2009)**
- (8) X-rays of wavelength 0.82 Å fall on a metal plate. Find the wavelength associated with the photoelectron emitted. Neglect the work function of the metal. **(L.U. 2012)**
- (9) 17. X-rays of $\lambda = 1.0 \text{ \AA}$ are Scattered at 60° from the free electrons. Calculate the shift in wavelength and the energy of the recoil electrons. **(Ans. 0.012 Å, 147 eV.)**
- (10) In Compton effect, if the incident photon has wavelength $2.0 \times 10^{-8} \text{ cm}$ and $\Phi = 90^\circ$, deduce (i) the wavelength of the scattered photon, (ii) the energy of the recoil electron, (iii) the angle at which the recoil electron appears. ($h = 6.62 \times 10^{-27} \text{ erg sec}$, $c = 3.0 \times 10^{10} \text{ cm sec}^{-1}$, $1 \text{ eV} = 1.6 \times 10^{-12} \text{ erg}$.) **(L.U. 91)**
- Ans. (i) 2.0243 Å. (ii) 74.4 eV, (iii) $\tan^{-1} (0.99)$.**
- (11) 22. In Compton scattering the incident radiation has a wavelength of 2 Å, and that scattered through 180° has 0.048 Å. Calculate **the energy of** recoil electron which scatters radiation through 90° . (Values of h , c and 1 eV same as above) **Ans. 37 eV**
-

Chapter 3

Wave mechanics -I

3.1 de-Broglie's concept of matter waves

There are some experimental phenomena of light such as reflection, refraction, interference, diffraction polarisation etc., which can be explained only on the basis of wave theory of light, i.e., these phenomena verify the wave nature of light. But some experimental phenomena of light like photo-electric effect and Compton effect can not be explained on the basis of wave theory light. These phenomena can be explained only when we assume that light has particle character, i.e., light consists of photons which are the discrete packets of energy, these photons, like particles impart momentum and energy while interacting with matter. On the basis of the above experimental phenomena, it was inferred that light does not have any definite nature, rather its nature depends upon the experiment. In some experiments, light behaves like waves while in some other experiments light behaves like particles. Therefore light has dual character, i.e., light sometimes behave like wave and some time behaves like particles. In this connection this is important to note that the wave nature and particle nature is not possible simultaneously.

Louis de Broglie in 1923 proposed that as nature loves symmetry, therefore matter particles should exhibit wave properties just as light waves exhibited particle properties. According to him, there must be a wave associated with a moving particle. He termed this wave as de-Broglie's wave or matter wave. These waves have very small wavelengths in most situations so that their presence was difficult to observe.

de-Broglie gave the above theory in the year 1923. These waves were observed a few years later by Davisson and G.P. Thomson with high energy electrons. These electrons show the same pattern when scattered from crystals as X-rays of similar wave lengths.

3.2 Expression for the wavelength of a de-Broglie wave

(a) Mass of a photon

From Einstein's energy - mass relation:

$$E = mc^2 \quad (1)$$

From the Max Planck's quantum theory of radiation, energy of a photon is given as

$$E = h\nu \quad (2)$$

Where h is Planck's constant and ν is frequency of the photon.

from (1) & (2)

$$h\nu = mc^2$$

$$\mathbf{m} = \frac{h\nu}{mc^2} \quad (3)$$

m is the mass of a photon moving with velocity c.

(a) Momentum of photon (P)

$$P = mc$$

$$= \left(\frac{h\nu}{mc^2} \right) c$$

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

$$\therefore \mathbf{P} = \frac{h}{\lambda} \quad (\text{since } c = \nu\lambda, \text{ therefore } \nu/c = 1/\lambda) \quad (4)$$

Eqⁿ (4) represents momentum of a photon,

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

if a particle is moving with velocity v then $p = mv$, Now from (4),

$$\lambda = \frac{h}{mv} \quad (5)$$

3.3 Wavelength of a de-Broglie wave for a moving electron

(Non- relativistic case)

Let an electron moves from point A to point B. If the potential difference between A and B is V , then

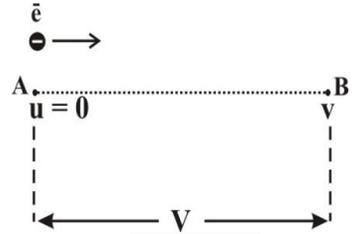


Fig.3.1

From the definition of potential difference

$$V = \frac{W}{q}$$

$$\text{Or } V = \frac{W}{e} \quad (\text{since } q = e)$$

$$\therefore W = eV$$

$$\therefore \frac{1}{2}mv^2 = eV \quad (\text{since } W = \frac{1}{2}mv^2)$$

$$\therefore v^2 = \frac{2eV}{m}$$

$$\therefore v = \sqrt{\frac{2eV}{m}}$$

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

$$= \frac{h}{m\sqrt{2eV/m}}$$

$$= \frac{h}{\sqrt{2me}} \times \frac{1}{\sqrt{V}}$$

$$= \frac{6.6 \times 10^{-34} \text{ Joule. sec}}{\sqrt{22 \times 9.1083 \times 10^{-31} \text{ kg} \times 1.6 \times 10^{-19} \text{ C}}} \times \frac{1}{\sqrt{V}}$$

$$\therefore \lambda = \sqrt{\frac{150}{V}} \text{ \AA}$$

$$\text{or } \lambda = \frac{12.27}{\sqrt{V}} \text{ \AA}$$

3.4 Wavelength of a de- Broglie for a moving electron (relativistic case)

The total energy of a particle of rest mass m_0 , moving with velocity v is given by the following relativistic equation-

$$E^2 = m_0^2 c^4 + p^2 c^2 \quad (1)$$

Proof of $E^2 = m_0^2 c^4 + p^2 c^2$

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

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

Now $E = mc^2$
 $= \frac{m_0 c^2}{\sqrt{1 - p^2/m^2 c^2}}$

$$\therefore E^2 = \frac{m_0^2 c^4}{1 - p^2 c^2 / m^2 c^2}$$

$$\therefore m_0^2 c^4 = E^2 (1 - p^2 c^2 / E^2)$$

$$\text{or } m_0^2 c^4 = E^2 - p^2 c^2$$

$$\therefore E^2 = m_0^2 c^4 + p^2 c^2$$

The total energy E of a particle of rest mass m_0 (relativistic mass m ,

$(m = \frac{m_0}{\sqrt{1 - v^2/c^2}})$, moving with kinetic energy E_k is given as-

$$E = E_k + m_0 c^2 \quad (2)$$

If a charged particle having charge q is accelerated through a potential difference of V volt, then

$$V = \frac{E_k}{q}$$

$$\therefore E_k = qV \quad (3)$$

From (2)

$$E = qV + m_0c^2 \quad (4)$$

From equations (4) & (1)

$$(qV + m_0c^2)^2 = m_0^2c^4 + p^2c^2$$

$$q^2V^2 + m_0^2c^4 + 2qVm_0c^2 = m_0^2c^4 + p^2c^2$$

$$\text{or } p^2c^2 = q^2V^2 + 2qVm_0c^2$$

$$\begin{aligned} \text{or } p^2 &= \frac{q^2V^2 + 2qVm_0c^2}{c^2} \\ &= 2qVm_0 \left(\frac{q^2V^2}{2m_0c^2} + 1 \right) \end{aligned}$$

$$\therefore p = \sqrt{2qVm_0 \left(\frac{q^2V^2}{2m_0c^2} + 1 \right)}$$

Now De-Broglie wavelength is given by

$$\begin{aligned} \lambda &= \frac{h}{p} \\ \therefore \lambda &= \frac{h}{\sqrt{2qVm_0 \left(\frac{q^2V^2}{2m_0c^2} + 1 \right)}} \end{aligned}$$

If charged particle is electron, then $q = e$

3.5 Experimental evidence of existence of matter waves

Direct confirmation of de-Broglie's supposition was obtained 1927 by C.J. Davisson and L.H. Germer. G.P. Thomson in 1928 performed experiments with thin gold foil and again confirmed the wave nature of electrons. This is interesting to mention that J.J. Thomson father of G.P. Thomson ascertained that fast moving electrons of cathode rays are particles .

3.6 Davisson & Germer Experiment

Electrons are emitted by a hot filament 'F' by thermionic emission. They are passed between the anode and the cathode, which accelerates the electrons. These accelerated electrons were made to fall on a nickel crystal normally. A diffraction effect from the surface layer of the crystal acting as plane grating is produced. From each azimuth of the crystal, The beam of electrons is diffracted by the crystal and received at an angle θ by a faraday cylinder synchronised with a detector. The intensity of the diffracted electrons is measured by the detector as a function of angle θ and also the scattered electron current. The detector is moved to various positions on the scale and the galvanometer deflection at each position is noted. This deflection gives the measure of the intensity of the diffracted beam of the electrons.

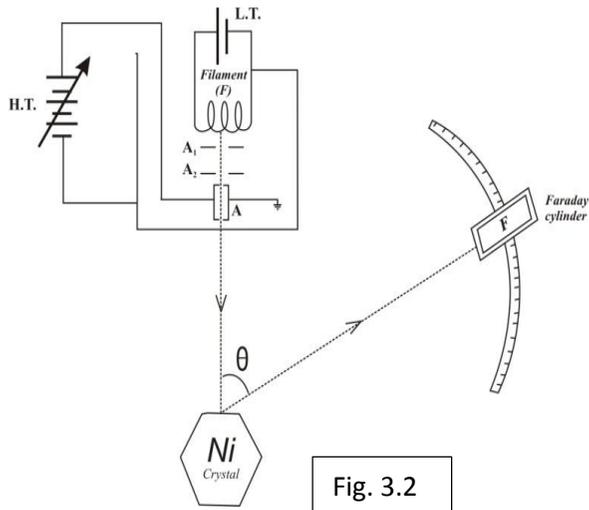


Fig. 3.2

$$\therefore \lambda = \frac{h}{\sqrt{2eVm_0\left(\frac{e^2v^2}{2m_0c^2} + 1\right)}}$$

The galvanometer deflection is plotted against the angle between the incident beam and the beam entering the detector. The observations are repeated for different accelerating voltage and a number of curves are drawn. The graph remains fairly smooth, till the value of accelerating voltage equals to 44V and a spur appears on the curve. As the accelerating voltage is increased, the length of the spur increases, till it reaches a maximum at 54V at an angle of 50° .

The occurrence of a pronounced spur or bump at 50° at 54V is the result of the constructive interference of waves associated with the accelerating electrons, scattered in this direction, from the regularly spaced parallel planes in the crystal. The peak value in the graph can be explained by Bragg's formula.

Polar graphs

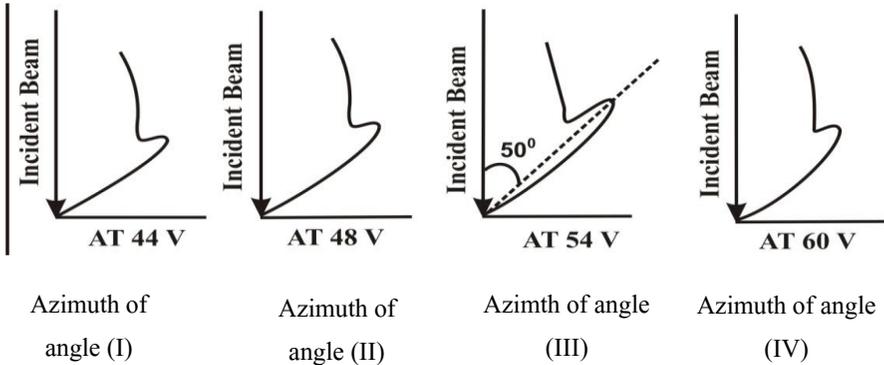


Fig. 3.3

Calculations

From (III) graph

$$\lambda = 12.2 \text{ \AA}^0$$

$$\sqrt{V}$$

Putting $V = 54 \text{ V}$

$$\lambda = 12.2 \text{ \AA}^0$$

$$\sqrt{54}$$

$\lambda = 1.66 \text{ \AA}^0$ From (III) graph

$$\lambda = 12.2 \text{ \AA}^0$$

$$\sqrt{V}$$

Putting $V = 54 \text{ V}$

$$\lambda = 12.2 \text{ \AA}^0$$

$$\sqrt{54}$$

$$\lambda = 1.66 \text{ \AA}$$

Now from Bragg's Law

$$2d \sin \theta = n \lambda \quad (i)$$

Where d is interatomic spacing,

and n is the order of diffraction

now for the first order of diffraction, when we use X-rays

$$\theta = 50^\circ$$

$$2d = 2.15 \text{ \AA}$$

$$n = 1$$

then from (i)

$$2.15 \sin (50^\circ) = 1 \times \lambda$$

$$\lambda = 1.65 \text{ \AA}$$

It is obvious that two values determined by independent methods closely agrees which establishes the wave nature of particle.

3.7 G.P. Thomson Experiment

The wave like nature of electrons was confirmed by G.P. Thomson by his famous electron diffraction experiment. The sketch diagram of the experimental arrangement has been shown in Fig. 3.4. The diffraction pattern obtained by passing a beam of electrons of velocity v through a thin gold foil was exactly similar to that obtained from X-rays of wavelength $\lambda = \frac{h}{mv}$. The electrons are produced by passing an electric current through a positive potential of the order of 50000 volts to the anode. The whole apparatus is kept highly evacuated. The electron beam passes through a fine hole in a metal block B and falls on a gold foil

of thickness of the order of 10^{-8} m. The electrons suffer diffraction and are recorded on a photographic plate giving rise to diffraction rings exactly similar to those obtained by diffraction through a small circular hole.

To rule out the possibility that cathode ray beam produced X-rays on striking the film and these X-rays produced the diffraction pattern, the experiment was repeated by introducing a magnetic induction field between the film and the photographic plate. It was found that diffraction pattern was exactly similar but moved as a whole to one side due to the effect of the magnetic field, showing that the diffraction pattern was due to the charged particles (electrons), all of them having the same velocity.

On removing the gold foil only central spot is obtained on the photographic plate without any diffraction pattern.

Further experiment showed that not only electrons but also protons, neutrons and molecules behave like waves under suitable conditions.

Note: *This is noteworthy that G.P. Thompson, who shared the 1937 Nobel Prize with Davisson for the experiments which established that electrons possess wave nature, is the son of J.J. Thompson who received the Nobel Prize in 1906 for proving that cathode rays (Electron beams) were actually Particles. This is quite interesting to note in this connection that that they were both right.*

The diffraction rings are associated with electron diffraction from the interplanar spacing within tiny crystallites in the gold foil. The continuous rings arise because the tiny crystallites are randomly oriented in the foil. we know that diffraction is the

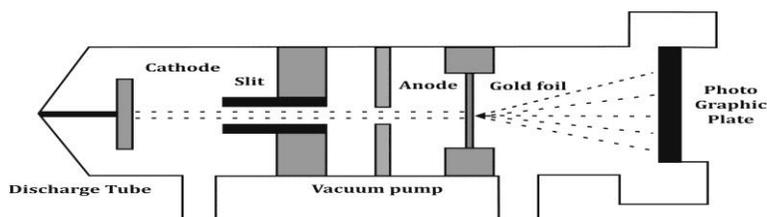


Fig. 3.4

proof for establishing wave nature. Therefore it is concluded that cathode rays (fast moving electrons) behave like a wave G.P. Thomson calculated the wavelength of fast moving electrons (electron beam) by the following way

Calculation of wavelength from radii of rings

Gold foil is a poly-crystalline film. In such a film there are some crystals set at the correct angle to give Bragg's reflection. If there are sufficient number of crystals at random, Bragg reflection will form a series of rings as shown in Fig. 3.6 arising from the intersection of the cones of diffraction with the photographic plate shown in the Fig. 3.7.

Let AB be the incident beam passing through the film at B . After suffering Bragg reflection at some crystal, the reflected beam goes along BE and meets the photographic plate at E . Let $OE = R$ where O is the central point. The distance from the film to the plate $BO = L$ and $\angle EBO = 2\theta$, where θ is the glancing angle given by Bragg's law.

Now from Bragg's formula

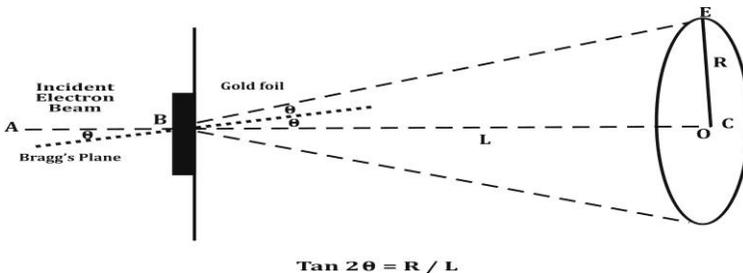
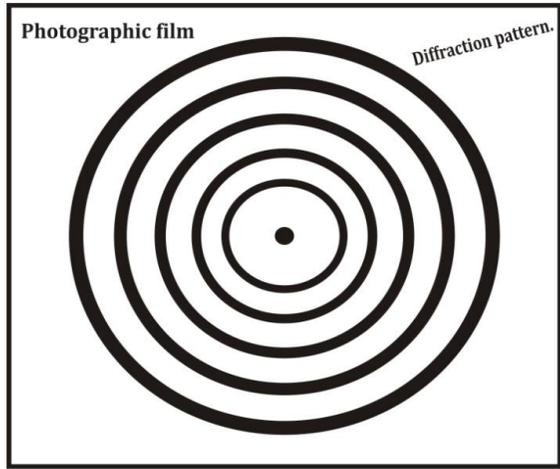


Fig. 3.6

$$2d \sin\theta = n\lambda \quad (1)$$



Diffraction of electron beam by gold foil

Fig. 3.5

For 1st order, $n = 1$

$$\therefore 2d \sin\theta = \lambda \quad (2)$$

Since θ is very small, $\therefore \sin\theta \approx \theta$, therefore, from equation (2),

$$2d\theta = \lambda$$

or $(2\theta)d = \lambda \quad (3)$

Now from Δ BOE $\tan 2\theta = \frac{R}{L} \quad (4)$

Since θ is very small, $\therefore \tan 2\theta \approx 2\theta$, therefore, from equation (4),

$$2\theta = \frac{R}{L} \quad (5)$$

Using equation (5) for equation (4), we have

$$\lambda = \left(\frac{R}{L}\right) d \quad (6)$$

From relativistic consideration λ can be calculated theoretically as

$$\lambda = \frac{h}{\sqrt{2eVm_0\left(\frac{e^2v^2}{2m_0c^2} + 1\right)}} \quad (7)$$

After performing the above experiment, the following points were noted-

- (i) The values of λ obtained by equations (6) & (7) agree.
- (ii) If X-ray are used in place of electron beam then value of λ , obtained by Bragg's formula again agrees with equation (2)

3.8 Some fundamentals regarding wave motion

(a) Difference between the waves and particles

S.N.	waves	particles
1.	A wave is a disturbance which takes place in a medium and it is specified by its frequency, wavelength, phase, amplitude and intensity	A particle or matter has mass and it is located at a some definite point and it is specified by its mass, velocity, momentum and energy.

2.	Waves can pass through each other ! As they pass through each other they can enhance or cancel each other Later they regain their original form	When particles collide they cannot pass through each other ! They can bounce or they can shatter Before collision. After collision Another after collision state shatter.
3.	Waves Spread in space and time Wavelength.	Particles Localized in space and time.

(b) Wave velocity or Phase velocity (v_p)

When a monochromatic wave (wave of a single frequency and wavelength) travels in a medium, its velocity of advancement in the medium is called the ‘ wave velocity’. Wave velocity is also called as ‘phase velocity’.

As obvious from the standard statement of the definition of velocity, the distance covered by a monochromatic wave in unit time will be known as wave velocity.

$$v_p = \frac{dx}{dt}$$

It can be shown that wave velocity is the ratio of angular frequency to the propagation constant, i.e.,

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

Where ω is the angular frequency ($\omega = 2 \pi n$, where n is the linear frequency or simply frequency)

And k is the propagation constant ($k = 2 \pi / \lambda$, where λ is the wavelength.)

(a) Alternative definition of wave velocity or phase velocity (v_p)

The phase velocity of a wave is the rate at which the phase of the wave propagates in space. This is the velocity at which the phase of any one frequency component

of the wave travels. For such a component, any given phase of the wave (for example, the crest) will appear to travel at the phase velocity.

or

The velocity by which the planes of constant phase advance in the medium is called wave velocity or Phase velocity.

The equation of a simple plane progressive wave moving along + x direction is given as-

$$y = a \sin(\omega t - kx)$$

In the above equation

y is the displacement of a particle of the medium situated at distance x from the reference point at time t

a is the displacement amplitude or simply amplitude

ω is the angular frequency ($\omega = 2\pi n$, where n is the linear frequency or simply frequency)

k is the propagation constant ($k = 2\pi/\lambda$)

$(\omega t - kx)$ is the phase.

Now from the alternative definition of wave velocity (phase velocity),

$$(\omega t - kx) = \text{constt.}$$

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

differentiating the above equation with respect to 't', we have,

$$\frac{dx}{dt} = \frac{\omega}{k}$$

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

$$= \frac{2\pi n}{2\pi/\lambda} \quad \left(\omega = 2\pi n \text{ and } k = \frac{2\pi}{\lambda} \right)$$

$$v_p = n\lambda \quad (k \text{ is called propagation constant})$$

Note: AS already mentioned, the term of wave velocity or phase velocity (v_p) is used only for a monochromatic wave only.

- (a) **Propagation constant (k)** It is defined as the phase difference between the nearest particles separated by unit distance.

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

(b) **Group velocity (v_g)**

We are much familiar to pulse rather than monochromatic waves. A pulse consists of a number of waves differing slightly from one another in frequency. A superposition of these waves is called a 'wave packet' or a 'wave group'. For example white light consists of a continuous visible wavelength spectrum ranging from about 3000\AA in the violet to about 7000\AA in the red region. When such a group travels in a medium, the phase velocities of its different components are different. The observed velocity is however, the velocity with which the maximum amplitude of the group advances in the medium. This is called the 'group velocity'.

Thus group velocity is the velocity with which the energy in the group is transmitted.

In Fig.3.8 are two plane harmonic waves of equal amplitude but slightly different frequencies, travelling from left to right have been shown. The wave represented by dotted lines has lower frequency and is travelling faster. At a certain instant the two waves are in phase at the point P. Therefore, at this instant, the maximum amplitude of the group formed by them also lies at P. At a later instant the maximum will be built up a little to the left of P. i.e., maximum will move to the left with time relative to the waves. As a result, the group velocity will be lower than the wave velocities.

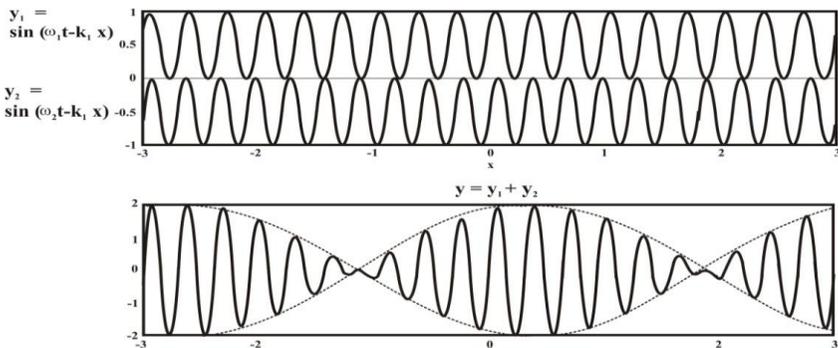


Fig. 3.7

The group velocity can also be defined in the following way:

The velocity with which the slowly varying envelop of the modulated pattern due to a group of waves travels in a medium is known as the group velocity.

Mathematically group velocity is defined as

$$\mathbf{v}_g = \frac{d\omega}{dk}$$

(c) Expression for the group velocity

Let us consider a wave group consisting of two wave components of equal amplitudes a but slightly different angular frequencies ω_1 and ω_2 and propagation constants k_1 and k_2 . Let the displacements of the wave components are y_1 and y_2 , then

$$y_1 = a \sin(\omega_1 t - k_1 x) \quad (1)$$

$$y_2 = a \sin(\omega_2 t - k_2 x) \quad (2)$$

from the principle of superposition

$$y = y_1 + y_2 \quad (3)$$

Using equations (1) and (2) for equation (3), we have

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

This represent a wave system with a frequency $(\omega_1 + \omega_2) / 2$ which is very close to the frequency of either component, but with an amplitude given by

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

Thus the amplitude of the wave group is modulated both in space and time by a very- slowly varying envelope of frequency $(\omega_1 - \omega_2) / 2$ and propagation constant $(k_1 - k_2) / 2$, and has a maximum value of $2a$. This envelope is represented by the dotted curves in Fig. 3.7.

The velocity with which this envelope moves, i.e., the velocity of maximum amplitude of the group is given by

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

If a group consists a number of frequency components in an infinitely small frequency interval, then the expression for the group velocity may be written as

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

(d) Relationship between v_p & v_g

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

Explanation:

$$\begin{aligned} v_g &= \frac{d\omega}{dk} \\ &= \frac{d(v_p k)}{dk} \quad (\text{Since } v_p = \omega/k) \end{aligned}$$

$$\begin{aligned} v_g &= v_p + k \frac{d(v_p)}{dk} \\ &= v_p + \frac{2\pi}{\lambda} \frac{d(v_p)}{d(\frac{2\pi}{\lambda})} \\ &= v_p + \frac{1}{\lambda} \frac{d(v_p)}{d(\frac{1}{\lambda})} \end{aligned}$$

$$\begin{aligned}
 &= v_p + \frac{1}{\lambda} \frac{d(v_p)}{(-\frac{1}{\lambda^2})d\lambda} \\
 &= v_p - \lambda \frac{dv_p}{d\lambda}
 \end{aligned}$$

3.9 Velocity of a de-Broglie wave

(a) Wave velocity or phase velocity (v_p) of a de-Broglie wave.

Let us calculate the wave velocity or phase velocity (v_p) of a de-Broglie wave.

We know that phase velocity (v_p) is given as

$$v_p = \frac{\omega}{k} \quad (1)$$

where $\omega = 2\pi \nu$ (2)

$$k = \frac{2\pi}{\lambda} \quad (3)$$

From (2)

$$\omega = 2\pi \nu$$

But $E = h \nu$

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

$$\nu = \frac{mc^2}{h} \quad (4)$$

using (4) for (2)

$$\omega = \frac{2\pi mc^2}{h} \quad (5)$$

Now from eq. (3)

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

But de-Broglie wavelength is given by

$$\lambda = \frac{h}{mv} \quad (6)$$

using eq. (3) for eq. (6)

$$k = \frac{2\pi mv}{h} \quad (7)$$

Using (5) & (7) for (1)

$$v_p = \frac{2\pi mc^2/h}{2\pi mv/h}$$

$$v_p = \frac{c^2}{v} \quad (8)$$

Where v_p = Phase velocity
 v = Particle velocity
 c = velocity of light

As the velocity of the particle will always less than the velocity of light ($v < c$), therefore it is obvious from equation (8),

$$v_p > c$$

i.e. phase velocity is greater than the velocity of light which is impossible. As we know that the term of phase velocity is applied only in the case of a monochromatic wave, therefore we conclude that a De- Broglie wave cannot be monochromatic wave

(b) Group velocity (v_g) of a de-Broglie wave.

Now we must treat a de-Broglie wave as pulse i.e. a group of number of waves having slightly different frequencies. We know that group (V_g) is given as

$$v_g = \frac{d\omega}{dk} \quad (9)$$

$$\omega = 2\pi \nu$$

But $E = h \nu$

$$\begin{aligned} \therefore \nu &= \frac{E}{h} \\ \nu &= \frac{mc^2}{h} \end{aligned} \quad (4)$$

Using equation (4) for equation (2)

$$\omega = \frac{2\pi mc^2}{h} \quad (5)$$

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

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

differentiating equation (6) with respect to 'v' we have,

$$\begin{aligned} \frac{d\omega}{dv} &= \frac{2\pi m_0 c^2}{h} \frac{d}{dv} \left(\frac{1}{\sqrt{1-v^2/c^2}} \right) \\ &= \frac{2\pi m_0 c^2}{h} \left(\frac{\left(\sqrt{1-v^2/c^2} \right) \frac{d}{dv} (1) - 1x \frac{d}{dv} \left(\frac{1}{\sqrt{1-v^2/c^2}} \right)}{\left(\sqrt{1-v^2/c^2} \right)^2} \right) \\ &= \frac{2\pi m_0 c^2}{h} \left(\frac{\left(\sqrt{1-v^2/c^2} \right) (0) - 1x \frac{d}{dv} \left(\frac{1}{\sqrt{1-v^2/c^2}} \right)}{1-v^2/c^2} \right) \end{aligned}$$

$$\begin{aligned}
&= \frac{2\pi m_0 c^2}{h} \left(\frac{0 - \left(-\frac{1}{2}\right) (1-v^2/c^2)^{-1/2} \left(-\frac{2v}{c^2}\right)}{1-v^2/c^2} \right) \\
&= \frac{2\pi m_0 v}{h (1-v^2/c^2)^{3/2}}
\end{aligned}$$

Now as $k = \frac{2\pi}{\lambda}$ and de-Broglie wavelength is $\lambda = \frac{h}{mv}$, therefore,

$$k = \frac{2\pi mv}{h} \quad (7)$$

$$= \frac{2\pi m_0 v}{h\sqrt{1-v^2/c^2}} \quad (6) \quad \left(\text{since } m = \frac{m_0}{\sqrt{1-v^2/c^2}}\right)$$

differentiating equation (7) with respect to 'v' we have,

$$\begin{aligned}
\frac{dk}{dv} &= \frac{2\pi m_0}{h} \frac{d}{dv} \left(\frac{v}{\sqrt{1-v^2/c^2}} \right) \\
&= \frac{2\pi m_0}{h} \left(\frac{\left(\sqrt{1-v^2/c^2} \right) \frac{d}{dv} (v) - v \frac{d}{dv} \left(\frac{1}{\sqrt{1-v^2/c^2}} \right)}{\left(\sqrt{1-v^2/c^2} \right)^2} \right) \\
&= \frac{2\pi m_0}{h} \left(\frac{\left(\sqrt{1-\frac{v^2}{c^2}} \right) (1) - \left(-\frac{1}{2}\right) (1-v^2/c^2)^{-1/2} \left(-\frac{2v}{c^2}\right)}{\left(\sqrt{1-v^2/c^2} \right)^2} \right) \\
&= \frac{2\pi m_0}{h} \left(\frac{\left(\sqrt{1-\frac{v^2}{c^2}} \right) (1) + \frac{v^2/c^2}{\sqrt{1-v^2/c^2}}}{\left(\sqrt{1-v^2/c^2} \right)^2} \right) \\
&= \frac{2\pi m_0}{h} \left(\frac{\frac{1-v^2}{c^2} + \frac{v^2}{c^2}}{\left(\sqrt{1-v^2/c^2} \right)^2} \right)
\end{aligned}$$

$$= \frac{2\pi m_0}{h} \left(\frac{1}{(\sqrt{1-v^2/c^2})^{3/2}} \right)$$

$$\therefore \frac{dk}{dv} = \frac{2\pi m_0}{h (1-v^2/c^2)^{3/2}} \quad (8)$$

The group velocity v_g associated with the particle is

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

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

Therefore dividing equation (7) by equation (8), we get

$$v_g = v$$

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

3.10 de-Broglie waves show dispersion in vaccum

In free space or vaccum the velocity of de-Broglie waves depends upon wavelength. As a result, de-Broglie waves of different wavelngts have different phase velocities. Thus, vaccum is a dispersive medium so far as de-Broglie waves are concerned but is not a dispersive medium for the electromagnetic waves as in their case the waves of all wavelength travel with the same velocity in vaccum.

Relation between phase velocity and group velocity in case of de-Broglie waves

(a) For dispersive medium

The relation between the phase velocity and group velocity is given as

$$v_g = v_p - \lambda \frac{dv_p}{d\lambda}$$

i.e., $v_p = f(\lambda)$

usually we find that $dv_p/d\lambda$ is positive (Case of normal dispersion)

$$V_g < v_p$$

This is the case for de-Broglie waves.

(b) For non-dispersive medium

The relation between the phase velocity and group velocity is given as

$$V_g = v_p - \lambda \frac{dv_p}{d\lambda}$$

For a non-dispersive medium

$$\frac{dv_p}{d\lambda} = 0$$

$$\text{i.e., } v_p \neq f(\lambda)$$

$$V_g = v_p$$

3.11 Wave mechanics implies quantum mechanics

Wave mechanics is also referred as quantum mechanics. This can be understood by the following article-

Resonance in de-broglie waves; stationary states

When we study waves along a stretched string and sound waves along organ pipes, we see that resonance phenomenon is of great importance. This is also true for de-broglie waves. Let us examine a simple situation in which de-broglie wave resonance should occur.

A particle in a tube or box

Let us consider a particle of mass m is confined in a narrow tube of length L . If the particle behaves like a wave then its de- Broglie wave should resonate in the tube. This resonance is called a stationary state , because the particle can not go beyond

the closed ends, where nodes are formed. Here this is important to note that de-Broglie waves tell us where the particle is likely to be found.

Therefore the particle will resonate within the tube when its de-broglie wave has the wavelengths, given by the following conditions-

$$L = \frac{1}{2}\lambda_1 \quad \text{or} \quad L = 2\left(\frac{1}{2}\lambda_2\right) \quad \text{or} \quad L = 3\left(\frac{3}{2}\lambda_2\right)$$

or in general, a stationary state for the particle will occur when

$$\lambda_n = \frac{2L}{n} \quad \text{where } n = 1, 2, 3, \dots \quad (1)$$

This is quite obvious that the particle will resonate only in the tube when its resonance wavelength will be given by the above condition.

As only at the condition of resonance the amplitude of the wave is large, otherwise negligible. Now as amplitude of the wave is a measure of where the particle is likely to be found, we expect that the particle to be found in the tube at the antinodes under resonance conditions. The more surprising fact is that the particle will never be found at the nodes. This contradicts classical physics, which tells that the possibility of the finding the particle is equal everywhere in the tube.

Now let us calculate the energy E_n of the particle at the nth resonance state

$$\begin{aligned} E_n &= \frac{1}{2}mv_n^2 \\ &= \frac{p_n^2}{2m} \end{aligned} \quad (2)$$

However the particle's de-Broglie wavelength is

$$\lambda_n = \frac{h}{p_n} \quad (3)$$

Using Equation (3) for (2), we have

$$E_n = \frac{h^2}{2m\lambda_n^2} \quad (4)$$

Now using equation (1) for (4), we have

$$E_n = \frac{n^2 h^2}{8mL^2} \quad (5)$$

From equation (5), we find that particle's energy in the tube is quantised, which contradicts classical mechanics. Classical mechanics predicts that a particle in a tube can have all values of kinetic energies including zero.

It is for this reason that wave mechanics is often referred to as quantum mechanics.

3.12 Quantum condition for the stationary orbits

The de-Broglie wave associated with the electron of mass 'm' moving in an orbit with velocity 'v' will be given as

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

The electron will be in a stable state or in a stationary state in which it will not radiate electromagnetic energy when its de-Broglie wave resonates in the orbit. For resonance, the orbit length $2\pi r$, must be a whole number of wavelengths long. i.e.,

$$\begin{aligned} n\lambda &= 2\pi r \\ \text{where} \\ &= 1, 2, 3, \dots \end{aligned} \quad (2)$$

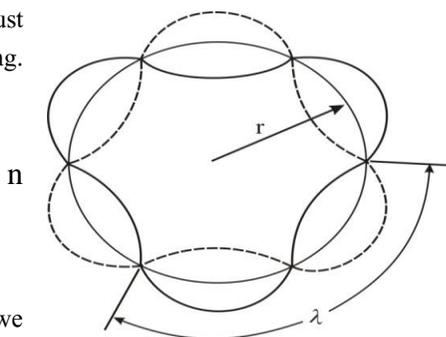


Fig. 3.8

Using equation (1) for equation (2), we have

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

Or
$$mvr = n \left(\frac{h}{2\pi} \right)$$

Which is the well known quantum condition for the motion of electrons in a stationary orbit. This is worth mentioning here that although Bohr used the same criterion to select the stable orbits, he however could give no physical justification for it.

3.13 Some remarks on de Broglie wave

(1) Practical observation of matter waves is possible only when the wavelength of matter waves is greater than the size of the particle ($\lambda \gg a$).

- (2) Matter waves propagate in the form of wave packets with group velocity.
- (3) The wavelength of matter waves does not depend on the nature and charge of the particle.
- (4) Matter waves travel in vacuum, hence these are not mechanical waves.
- (5) These waves are also associated with electrically neutral particles hence these can not be the electromagnetic waves even
- (6) Actually matter waves are probabilistic waves because these waves represent the probability of finding a particle in space.
- (7) True understanding of nature required that physical objects, whatever they are, are neither exclusively particles or waves
- (8) No experiment can ever measure both aspects at the same time, so we never see a mixture of particle and wave.
- (9) When one observes a physical phenomenon involving a physical object, the behaviour we will observe – whether particle like or wave like – depends on our method of observation.
- (10) True understanding of nature required that physical objects are neither exclusively particles or waves. No experiment can ever measure both aspects at the same time, therefore we never see a mixture of particle and wave simultaneously.
- (11) **Note :** *Classical mechanics becomes invalid when the wavelength of the wave associated with the moving particle is comparable or larger than the smallest dimensions of the experiment. This is likely to happen only when we are dealing with the particles that are atomic in size or smaller. In particular the wave effects of the electrons within the atoms can be easily noticed. Under these conditions classical mechanics is replaced by wave mechanics.*

3.14 Heisenberg's Uncertainty Principle

The wave nature of the moving particles leads to a great philosophical principle which is known as Heisenberg uncertainty principle.

Before the knowledge of above principle, scientists were not of the same opinion about the complete determination of the fate of the universe. This was a most relevant question of that time whether the position, speed and energy of all the particles in the universe could be determined with accuracy so that the course all future events could be predicted. The answer of this question is negative in the light of the wave nature of the moving particles.

Heisenberg in 1927 gave the following principle- "It is impossible to obtain correct measurements of two physical quantities which are canonically conjugate to each other with unlimited accuracy simultaneously."

The pairs of canonically conjugate physical quantities are –

- (i) Position and momentum (x, P)
- (ii) Angular displacement and angular momentum (θ , J)
- (iii) Energy and time. (E, t)

Heisenberg uncertainty principle also says that the product of uncertainties in the measurement of position & momentum of a body is greater than or equal to $h/4\pi$ i.e.

$$\Delta x. \Delta p_x \geq \frac{\hbar}{2} \quad (1a) \text{ [where } \hbar = h / 2\pi, h \text{ is planck's constant]}$$

$$\text{or } \Delta x. \Delta p_x \geq \frac{h}{4\pi} \quad (1b)$$

Δx is uncertainty in the measurement of position.

and Δp is uncertainty in the measurement of momentum.

For angular displacement & angular momentum Heisenberg Principle can be written as-

$$\Delta \theta. \Delta J \geq \frac{\hbar}{2} \quad (2a)$$

$$\text{or } \Delta \theta. \Delta J \geq \frac{h}{4\pi} \quad (2b)$$

For energy & time, Heisenberg's principle is written as

$$\Delta E. \Delta t \geq \frac{\hbar}{2} \quad (3a)$$

$$\text{Or} \quad \Delta E. \Delta t \geq \frac{\hbar}{4\pi} \quad (3b)$$

Note: Canonically conjugate quantities

Those quantities, the dimensions of whose product are equivalent to those of action (i.e. joule.sec) are defined as canonically conjugate quantities.. In classical mechanics, a physical quantity known as “action” [defined by $\int_{t_2}^{t_1} L dt$, where L is the Lagrangian of the system ($L = T - V$, where T and V are kinetic energy and potential energy respectively)] also has the dimensions of energy x time i.e.[ML^2T^{-1}]. The dimensions of action can easily be shown to be also the same as angular momentum (momentum times distance) i.e. [ML^2T^{-1}]. It means the dimensions of Planck’s constant, action and angular momentum are same.

Note: 1. Heisenberg’s uncertainty principle is neither related with the inaccuracy of measuring instruments nor it is connected with the quality of experimental methods.

2. Heisenberg’s uncertainty principle is the result of the matter wave properties of the moving particles. Even with perfect instruments and techniques, the uncertainty is inherent in the nature of things.

3. The abstract of Heisenberg’s uncertainty principle is as following:”

‘Act of measurement influences the particle - gives it a kick and it is no longer where it was’.

3.15 Explanation of Heisenberg’s uncertainty principle

Let us consider how we would locate the position, speed and kinetic energy of an object or a particle . In order to know the position of the particle, we must either touch it with another particle or look at it in a beam of light. Let us make the light beam as weak as momentum will not disturb the object at which we are looking. To that end, we look at the object by using a single photon. Or if

we choose, we touch the object with a single, extremely small particle. We call the photon or particle that we use to investigate the object the *probe particle*. To minimize the disturbance the probe particle will

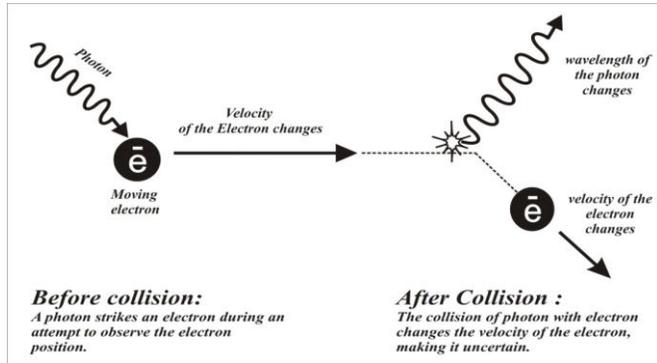


Fig. 3.9

cause, we use as low an energy as we can. There is however, a lower limit on this energy, because the wavelength of this probe particle must be smaller than the object we are looking at. Otherwise interference and diffraction effects will cause the waves associated with the probe particle to cast extremely blurred images of the object. As we know that the finest detail we can see using waves (either light or particle waves) is detail of the same size as the wavelength. Hence the position of the object at which we are looking may be in error by an amount $\Delta x \approx \lambda$. Moreover, the momentum of the probe particle (whether photon or material) is given by $p = h/\lambda$. When it touches the object we are looking at, some of this momentum is transferred to the object, and this disturbance may alter the momentum of the object. The uncertainty in the momentum of the object $\Delta p \approx \frac{h}{\lambda}$.

If we multiply the expressions for Δp and Δx , we find

$$\Delta x \Delta p \approx h$$

A second form of the uncertainty principle can be obtained through similar reasoning. As the probe particle passes by the object we are looking at, the position of the object is uncertain to within a distance of about λ , as we have just seen. If speed of the probe particle is v , the time taken for the particle to pass through this

distance of uncertainty is λ/v . Therefore, the exact amount of time during which the object is at a particular position is uncertain by an amount

$$\Delta t \approx \frac{\lambda}{v}$$

In addition, the energy of the probe is partly lost to the object under observation when the two come into contact. As a result, the uncertainty in the energy of the object is of the order of the probe particle's energy. Therefore $\Delta E = \frac{hv}{\lambda}$

If we multiply the expressions for ΔE and Δt , we find

$$\Delta E \Delta t \approx h$$

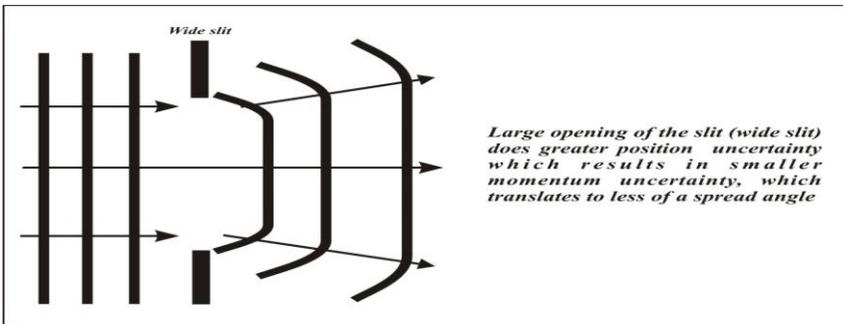


Fig. 3.10 (a)

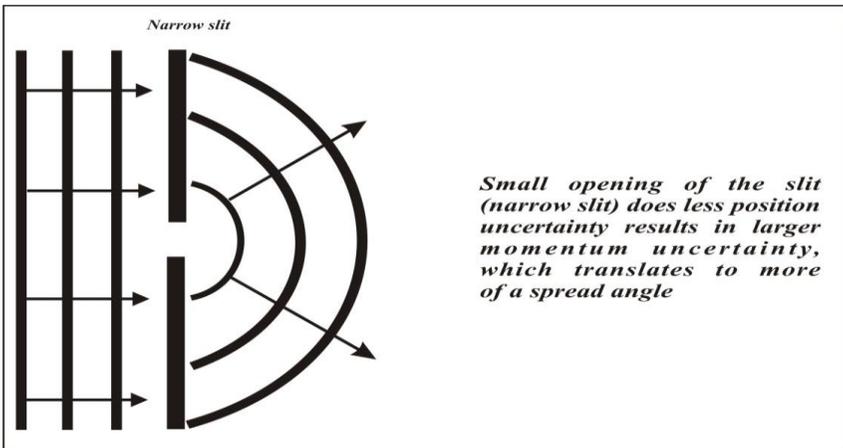


Fig. 3.10 (b)

3.14 To prove that $\Delta x \Delta p$ equals to $\Delta \theta \Delta J$

We know that

$$\Delta \theta = \frac{\Delta x}{r} \quad (1)$$

And $p = mv$

And $J = rp = mvr$

$$\therefore \Delta J = m\Delta vr \quad (2)$$

Multiplying equations (1) and (2), we have

$$\Delta \theta \Delta J = \Delta x \Delta p$$

3.15 To prove that $\Delta x \Delta p$ equals to $\Delta E \Delta t$

Kinetic energy (E) of a particle is defined as

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

$$\therefore \frac{dE}{dv} = \frac{1}{2}m \cdot 2v$$

$$\therefore \frac{dE}{dv} = mv$$

or $dE = mv dv$

or $dE = v (mdv)$

or $dE = v dp$

or $\Delta E = v \Delta p$

$$\text{or } \Delta p = \frac{\Delta E}{v} \quad (1)$$

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

$$\text{or } \Delta x = v \Delta t \quad (2)$$

Multiplying equations (1) and (2), we have

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

3.16 Validity of Heisenberg's uncertainty principle

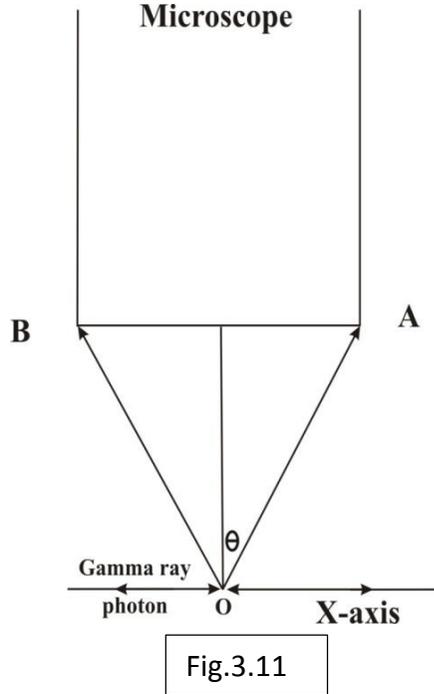
The validity of Heisenberg's uncertainty principle may be illustrated very well by the following hypothetical experiment.

(a) Heisenberg's gamma ray microscope

Heisenberg's principle can be understood by a hypothetical experiment in which γ ray microscope is used. The method of this experiment was suggested by Bohr and fully developed by Heisenberg. Let O be the electron, λ be the wavelength of γ rays and θ be semi vertex angle of the cone of the rays that enter the microscope objective from the object (here electron).

The resolving power of the microscope is given by the following relation.

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



Where Δx is the shortest distance between two points in the field of view which can be distinguished as separate. In other words, if the position of the electron O changes by an amount equal to or less than Δx , the microscope will not be able to detect it or the uncertainty in the measurement of the position of electron is Δx .

The electron is seen by the γ radiation scattered by it into the microscope. During this scattering. The electron will recoil and there will be change in the momentum. In order that this change may be as small as possible consider a single γ ray photon incident on it along the X-axis, then a scattered photon of wavelength λ will enter the objective anywhere between OA and OB .

The momentum of the scattered photon is $\frac{h}{\lambda}$.

If it enters the objective along OA, its component along X-axis is $\frac{h}{\lambda} \sin \theta$

Hence momentum imparted to the electron in the X-direction

$$= \frac{h}{\lambda'} - \frac{h}{\lambda} \sin \theta \quad (1)$$

Where λ' is the wavelength of the γ radiation before scattering.

If the scattered photon enters the objective along OB, its component along X-axis

$$\text{is } -\frac{h}{\lambda} \sin \theta$$

Hence momentum imparted to the electron in the X-direction

$$\begin{aligned} &= \frac{h}{\lambda'} - \left(-\frac{h}{\lambda} \sin \theta \right) \\ &= \frac{h}{\lambda'} + \frac{h}{\lambda} \sin \theta \quad (2) \end{aligned}$$

The momentum given to the electron can, therefore, have any value between those given by equations (1) and (2). The uncertainty or the error involved in the measurement of the momentum of the electron, therefore is given by

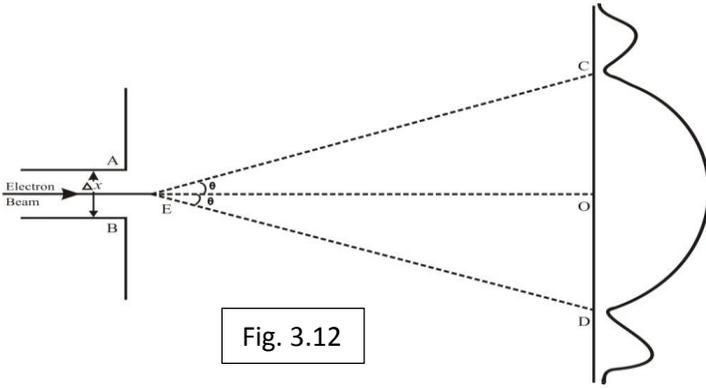
$$\begin{aligned} \Delta P_x &= \left(\frac{h}{\lambda'} - \frac{h}{\lambda} \sin \theta \right) - \left(\frac{h}{\lambda'} + \frac{h}{\lambda} \sin \theta \right) = \frac{2h}{\lambda} \sin \theta \\ \therefore \Delta x \cdot \Delta P_x &= \frac{\lambda}{2 \sin \theta} \frac{2h}{\lambda} \sin \theta = h \end{aligned}$$

However, a more rigorous treatment gives $\Delta x \cdot \Delta P_x = \frac{h}{2}$

(b) Diffraction of a beam of electrons by a slit

Let us consider a narrow slit AB of width Δx as shown in the Fig 3.10. Let a beam of electrons fall on this slit. After passing through the slit the electron beam spread out i.e., it suffers diffraction. The first minimum of the diffraction pattern is given by the relation $d \sin \theta = n\lambda$, where $d = \Delta x$, $n = 1$, and θ is the angle through which the electron beam is diffracted

$$\Delta x \sin\theta = \lambda \quad (1)$$



It is very difficult to locate the exact position of the slit at which the beam of electrons enters the slit. Therefore, the uncertainty in the measurement of the position of the electron beam in the slit. In a direction perpendicular to the direction of incident beam is equal to the width of the slit

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

Let \vec{P} be the momentum of the electron. If the electron moves in the direction EC after diffraction, then momentum of the electron in a direction perpendicular to the initial direction of the electron i.e., along $OC = \vec{P} \sin\theta$. If the electron after diffraction goes in the direction ED, then momentum of the electron in the direction $OD = -\vec{P} \sin\theta$. As the electron may be anywhere within the diffraction pattern from angle $-\theta$ to $+\theta$, the perpendicular component of the momentum of the electron may be anywhere between $-\vec{P} \sin\theta$ to $+\vec{P} \sin\theta$.

\therefore Uncertainty in the measurement of momentum of the electron

$$\Delta P = \vec{P} \sin\theta - (-\vec{P} \sin\theta) = 2\vec{P} \sin\theta$$

$$= 2\vec{P} \sin\theta$$

$$\text{But } \lambda = \frac{h}{P} \quad \text{or } P = \frac{h}{\lambda} \quad \therefore \Delta P = 2 \frac{h}{\lambda} \sin\theta \quad (3)$$

From (2) and (3), we have,

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

3.17 Consequences of uncertainty principle

(a) Non-existence of electrons in the nucleus

If an electron is to exist within the nucleus then the uncertainty in its position in the nucleus should not exceed the radius of the nucleus which is of the order of 10^{-14} m.

$$\text{i.e., } \Delta x \geq 10^{-14}$$

according to Heisenberg's uncertainty principle

$$\Delta x \cdot \Delta P_x = \frac{\hbar}{2}$$

Where ΔP_x is the uncertainty in the x component of momentum and $\hbar = \frac{h}{2\pi}$

\therefore Uncertainty in the momentum of the electron, if it is to exist in the nucleus

$$\Delta P_x \geq \frac{\hbar}{2\Delta x} = \frac{6.6 \times 10^{-34}}{2 \times 2\pi \times 10^{-14}} = 5.3 \times 10^{-21} \text{ kg ms}^{-1}$$

This means that the total momentum of the electron in the nucleus must be at least of the order of $5.3 \times 10^{-21} \text{ kg ms}^{-1}$.

Hence the above value of the momentum is relativistic as a non-relativistic relation for momentum gives a value of $v > c$.

According to the theory of relativity, the total relativistic energy of the electron is given as

$$E = [m_0^2 c^4 + p^2 c^2]^{1/2}$$

$$E = [(9.1 \times 10^{-31})^2 \times (3 \times 10^8)^4 + (5.3 \times 10^{-21})^2 \times (3 \times 10^8)^2]^{1/2}$$

$$= 16 \times 10^{-31} \text{ Joule} = 16 \times 10^{-31} / 1.6 \times 10^{-19} = 10 \text{ MeV}$$

Thus the kinetic energy of a free electron confined within a nucleus should have a minimum value of 10 MeV. The rest mass energy of an electron is only about 0.5 MeV and experimentally, the highest value of the kinetic energy of a β particle

emitted spontaneously by a nucleus is found to be about 4 MeV. Since this is much less than the calculated value of minimum kinetic energy which the electron, if it exists inside the nucleus, should possess, we come to the conclusion that electrons can not be constituents of the atomic nucleus.

(b)- Existence of protons, neutrons and α particles in the nucleus

If a proton or a neutron or an α particle is to exist within the nucleus then the uncertainty in its position in the nucleus should not exceed the radius of the nucleus which is of the order of 10^{-14} m.

$$\text{i.e., } \Delta x \geq 10^{-14}$$

according to Heisenberg's uncertainty principle

$$\Delta x \cdot \Delta P_x = \frac{\hbar}{2}$$

Where ΔP_x is the uncertainty in the x component of momentum and $\hbar = \frac{h}{2\pi}$

\therefore Uncertainty in the momentum of the electron, if it is to exist in the nucleus

$$\Delta P_x \geq \frac{\hbar}{2\Delta x} = \frac{6.6 \times 10^{-34}}{2 \times 2\pi \times 10^{-14}} = 5.3 \times 10^{-21} \text{ kg ms}^{-1}$$

This means that the total momentum of the electron in the nucleus must be at least of the order of 5.3×10^{-21} kg ms⁻¹.

The rest mass of the proton or neutron is of the order of 1.67×10^{-27} kg. Hence the value of momentum 5.3×10^{-21} kg ms⁻¹ as calculated above is non-relativistic as the value of v comes out to be $5.3 \times 10^{-21} / 1.67 \times 10^{-27} = 3.1 \times 10^6$ ms⁻¹

The corresponding value of kinetic energy is given as

$$\begin{aligned} E_k &= \frac{p^2}{2m_0} = \frac{(5.3 \times 10^{-21})^2}{2 \times 1.67 \times 10^{-27}} = 8.4 \times 10^{-15} \text{ Joule} \\ &= 8.4 \times 10^{-15} / 1.6 \times 10^{-19} = 52 \text{ KeV} \end{aligned}$$

The rest mass of α particle is nearly four times the proton mass. Thus, the α particle should have a minimum kinetic energy of 13 keV. Since the energy carried

by the protons or neutrons emitted by the nuclei are greater than 52 keV and for α particles more than 13 keV, these particles can exist in the nuclei.

(c)- Uncertainty in the frequency of radiation emitted by an atom.

On transition from a higher energy state the nucleus, atoms and molecules emit characteristic electromagnetic radiation. In the case of nucleus, these radiations are gamma rays and in the case of atoms, these are in the ultraviolet and visible regions. For molecules these fall in the infrared region.

An excited system has a small finite life time ΔT and the uncertainty for this interval is of same value. The energy of the excited state is therefore also uncertain. If ΔE is the uncertainty in energy of the state, then

$$\Delta E \cdot \Delta T \geq \frac{\hbar}{2}$$

$$\Delta E \geq \frac{\hbar}{2\Delta T} = \frac{h}{4\pi\Delta T}$$

As $E = h\nu$, the uncertainty in the frequency of the emitted photon $\Delta\nu$ is given by $\Delta E = h\Delta\nu$

$$\text{or } \Delta\nu = \frac{\Delta E}{h} = \frac{h}{4\pi\Delta T} \frac{1}{h} = \frac{1}{4\pi\Delta T}$$

Now the average life time for an excited atom is 10^{-8} seconds or $\Delta T = 10^{-8}$ sec.

$$\therefore \Delta\nu = 1/4\pi \times 10^{-8} = 0.8 \times 10^7 \text{ Hz.}$$

As a result the radiation from an excited atom does not a precise value ν but has a range from $\nu - \Delta\nu$ to $\nu + \Delta\nu$.

(d)- A beam of short wavelength gives accurately their position of a particle.

According to Heisenberg's principle

$$\Delta x \cdot \Delta p = \frac{\hbar}{2}$$

To determine the position of a particle accurately, the value of Δx must be small.

As $\Delta P \cdot \Delta x = \text{constant}$, ΔP should be large.

Now the wavelength associated with a moving particle is given by

$$\lambda = h / mv = h/P$$

$$\therefore P = h/\lambda$$

Therefore for large P (or ΔP), λ should be small. Therefore short wavelength beam will give more accurately the position of the particle.

3.18 Complimentary principle

According to complimentary principle the wave and particle aspects of matter and light are complimentary rather than contradictory, that is we need both these aspects to obtain a complete picture of the same system.

3.19 Comments on Heisenberg's uncertainty principle

- 1) The particle & wave properties are strictly complementary. A material particle cannot behave as a particle & a wave at the same instant of time. If we devise an experiment showing wave properties of the matter, we cannot see its particle property and vice-versa. This means that we can observe either the wave nature or the particle behavior of radiation.
- 2) The uncertainty principle prevents us from observing both type of properties together. \
- 3) Uncertainty principle makes predictions only of probable behavior of the particles.
- 4) Material particle in motion is equivalent to a group of waves or a wave packet.
- 5) Wave packet plus guiding wave possess the properties of a particle moving with velocity v and also exhibit interference and diffraction phenomenon.
- 6) The following scheme shows the equivalence between the wave and particle properties of the matter.

Particle Property	Wave Property	Formula
Momentum	Wavelength	$P = h/\lambda$
Energy	frequency	$E = h \nu$

- 7) Classical world is deterministic that is by knowing the position and velocity of all objects at a particular time and then using the laws of force and Newton's laws of motion , the future can be predicted with cent percent accuracy.
- 8) Quantum world is probabilistic that is it is impossible to know position and velocity with certainty at a time. Only probability of future state can be predicted using the laws of force and equations of quantum mechanics. Quantum Mechanics is a probabilistic theory of nature.
- 9) The object is described by mathematical Functions which are measures of probability,
- 10) Note: Since in quantum mechanics a particle is recognized by a wave packet which moves with particle velocity i.e. group velocity of a particle is equal to the particle velocity.
- 11) In a wave packet the position of the particle can only be found by probability concept. Therefore it is almost impossible to find the correct position of the particle exactly in the same way as is done in classical mechanics

In 1933, in the Copenhagen interpretation of Bohr and Heisenberg , this was resolved that "it is impossible in principle for our world to be deterministic". However Einstein, a founder of quantum mechanics was uncomfortable with this interpretation, he said "God does not play dice" !

Solved Problems

Problem 1. Show that rest mass of the photon is zero. (L.U. 1996, 2009)

Solution: In a relativistic case the total energy of a de-Broglie waves associated with a moving particle of rest mass m_0 , having a momentum p is given by the following relation-

$$E = [m_0^2 c^4 + p^2 c^2]^{1/2}$$

$$\begin{aligned} \text{Now phase velocity } v_p = E/P &= [(m_0^2 c^4 + p^2 c^2) / p^2]^{1/2} \\ &= c [m_0^2 c^2 / p^2 + 1]^{1/2} \\ &= c [m_0^2 c^2 \lambda^2 / h^2 + 1]^{1/2} \dots\dots\dots(1) \end{aligned}$$

Now consider de-Broglie wave travelling with velocity c . This corresponds to the propagation of electromagnetic waves. The velocity of the associated particle i.e. the photon is also c . Substituting $v_p = c$ in eq. (1), we have,

$$\begin{aligned} c &= c [m_0^2 c^2 \lambda^2 / h^2 + 1]^{1/2} \\ m_0^2 c^2 \lambda^2 / h^2 &= 0 \\ \text{or } m_0 &= 0 \end{aligned}$$

Thus the rest mass of the photon is zero.

Problem 2. Find The de-Broglie wavelength associated with

- (a) A 46 gm golf ball with velocity 36 ms^{-1}
- (b) An electron with a velocity 10^7 ms^{-1}

which of these two show wave character and why?

Solution:

(a) Since the velocity of the golf ball $v \ll c$, therefore we can take the mass of the golf ball as rest mass., i.e., $m = m_0$.

Hence
$$\lambda = \frac{h}{mv} = \frac{6.62 \times 10^{-34}}{.046 \times 36} = 4.0 \times 10^{-34} \text{ m}$$

This is obvious that the wavelength associated with golf ball is much smaller in comparison to its dimension. Therefore the golf ball will not exhibit the wave character.

(b) again the given velocity (v) of the electron is much less than the velocity of light, i.e., $v \ll c$, therefore we can take the mass of the electron as rest mass., i.e.,

$$m = m_0 = 9.11 \times 10^{-31}$$

Hence
$$\lambda = \frac{h}{mv} = \frac{6.62 \times 10^{-34}}{9.11 \times 10^{-31} \times 10^7} = 7.3 \times 10^{-11} \text{ m}$$

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

Problem 3. Calculate the de-broglie wavelength of 1 MeV electron. Mass of the electron = $9.11 \times 10^{-31} \text{ kg}$; $h = 6.62 \times 10^{-34} \text{ Js}$ (L.U. 1992)

Solution: Given: $K.E. = 1 \text{ MeV} = 1 \times 1.6 \times 10^{-19} \times 10^6 = 10^{13} \text{ joule}$

Now from $K.E. = \frac{1}{2}mv^2$

$$\therefore v = \sqrt{\frac{2(K.E.)}{m}} = \sqrt{\frac{2 \times 10^{13} \times 1.6 \times 10^{-19}}{9.11 \times 10^{-31}}} = 5.927 \times 10^8 \text{ ms}^{-1}$$

Which is not possible as the velocity can not be greater than the velocity of light.

Therefore instead of applying non relativistic equation $E = \frac{1}{2}mv^2$, we should apply relativistic equation.

Let m_0 is the rest mass of the electron and m is the mass of the moving electron

$$mc^2 = m_0c^2 + K.E.$$

$$\therefore m \times (3 \times 10^8)^2 = 9.11 \times 10^{-31} \times (3 \times 10^8)^2 + 1.6 \times 10^{-13}$$

$$\therefore m = \frac{9.11 \times 10^{-31} \times (3 \times 10^8)^2 + 1.6 \times 10^{-13}}{(3 \times 10^8)^2}$$

$$= \frac{9.11 \times 10^{-31} \times 9 \times 10^{16} + 1.6 \times 10^{-13}}{9 \times 10^{16}}$$

$$= 26.88 \times 10^{-31} \text{ kg}$$

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

Or $1 - \frac{v^2}{c^2} = \left(\frac{m_0}{m}\right)^2$

Or $1 - \frac{v^2}{c^2} = \left(\frac{9.11 \times 10^{-31}}{26.88 \times 10^{-31}}\right)^2$

or $1 - \frac{v^2}{c^2} = (0.3389)^2 = 0.1149$

or $\frac{v^2}{c^2} = 1 - 0.1149 = 0.8851$

or $\frac{v}{c} = 0.9407$

or $\frac{v}{3 \times 10^8} = 0.9407$

or $v = 0.9407 \times 3 \times 10^8 = 2.822 \times 10^8 \text{ ms}^{-1}$

hence de-Broglie wavelength

$$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}}{26.88 \times 10^{-31} \times 2.822 \times 10^8}$$

$$= 0.0087 \times 10^{-10}$$

$$= 0.0087 \text{ \AA}$$

Problem 4. What voltage must be applied to an electron microscope to produce electrons of wavelength $\lambda = 1.0 \text{ \AA} = 10^{-10}$ meter ?

(Meerut - 2011)

Solution : de-Broglie wavelength of electron is given by,

$$\lambda = \sqrt{\frac{150}{V}} \text{ \AA}$$

But

$$\lambda = 1.0 \text{ \AA}$$

$$1.0 \text{ \AA} = \sqrt{\frac{150}{V}} \text{ \AA}$$

$$V = 150 \text{ volt}$$

Problem 5. What voltage must be applied to an electron microscope to produce electrons of wavelength $\lambda = 1.0 \text{ \AA} = 10^{-10}$ meter ?

(Meerut - 2007)

Solution : The de-Broglie wavelength of a particle of mass m moving with velocity v is given by

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

Ignoring relativistic effect, i.e., $m = m_0$

$$\lambda = \frac{h}{m_0 v}$$

K.E. is given by

$$K = \frac{1}{2} m_0 v^2 \quad (2)$$

From equation (1)

$$v = \frac{h}{m_0 \lambda}$$

Putting the value of v in equation (2), we get

$$K = \frac{m_0 h^2}{2m_0^2 \lambda^2} = \frac{h^2}{2m_0 \lambda^2} = \frac{(6.63 \times 10^{-34})^2}{2 \times (9.1 \times 10^{-31}) \times (5896 \times 10^{-10})^2}$$

$$= 6.95 \times 10^{-25} \text{ Joule}$$

$$K = \frac{6.95 \times 10^{-25}}{1.6 \times 10^{-19}} = 4.34 \times 10^{-6} \text{ eV}$$

$$(\because 1\text{eV} = 1.6 \times 10^{-19} \text{ Joule})$$

Problem 6. Free electron cannot exist inside nucleus Justify.
(L.U. 2010)

Solution: If an electron is to exist within the nucleus then the uncertainty in its position in the nucleus should not exceed the radius of the nucleus which is of the order of 10^{-14} m.

$$\text{i.e., } \Delta x \geq 10^{-14}$$

according to Heisenberg's uncertainty principle

$$\Delta x \cdot \Delta P_x = \frac{\hbar}{2}$$

Where ΔP_x is the uncertainty in the x component of momentum and $\hbar = \frac{h}{2\pi}$

\therefore Uncertainty in the momentum of the electron, if it is to exist in the nucleus

$$\Delta P_x \geq \frac{\hbar}{2\Delta x} = \frac{6.6 \times 10^{-34}}{2 \times 2\pi \times 10^{-14}} = 5.3 \times 10^{-21} \text{ kg ms}^{-1}$$

This means that the total momentum of the electron in the nucleus must be at least of the order of 5.3×10^{-21} kg ms⁻¹.

Hence the above value of the momentum is relativistic as a non-relativistic relation for momentum gives a value of $v > c$.

According to the theory of relativity, the total relativistic energy of the electron is given as

$$E = [m_0^2 c^4 + p^2 c^2]^{1/2}$$

$$E = [(9.1 \times 10^{-31})^2 \times (3 \times 10^8)^4 + (5.3 \times 10^{-21})^2 \times (3 \times 10^8)^2]^{1/2}$$

$$= 16 \times 10^{-31} \text{ Joule} = 16 \times 10^{-31} / 1.6 \times 10^{-19} = 10 \text{ MeV}$$

Thus the kinetic energy of a free electron confined within a nucleus should have a minimum value of 10 MeV. The rest mass energy of an electron is only about 0.5 MeV and experimentally, the highest value of the kinetic energy of a β particle emitted spontaneously by a nucleus is found to be about 4 MeV. Since this is much less than the calculated value of minimum kinetic energy which the electron, if it exists inside the nucleus, should possess, we come to the conclusion that electrons can not be constituents of the atomic nucleus.

Problem 7. The electron in hydrogen atom may be thought as confined as a nucleus of radius = 5×10^{-11} metre. Calculate the minimum uncertainty in the momentum of the electron. Also calculate the minimum kinetic energy of the electron.

Given: $m_e = 9.11 \times 10^{-31} \text{ kg}$, $h = 6.62 \times 10^{-34} \text{ Js}$

Solution: According to Heisenberg's principle

$$\Delta x \cdot \Delta P \geq \frac{\hbar}{2} \geq \frac{h}{4\pi} \quad (1)$$

Where Δx is the uncertainty in position and ΔP is the uncertainty in the of a particle.

As the electron is confined to a radius of 5×10^{-11} metre, the uncertainty in the position of the electron

$$\Delta x = 5 \times 10^{-11} \text{ metre}$$

Now from equation (1)

$$\Delta P \geq \frac{h}{4\pi \Delta x} \geq \frac{6.62 \times 10^{-34}}{4\pi \times 5 \times 10^{-11}} = 1.054 \times 10^{-24} \text{ kg. ms}^{-1}$$

Now kinetic energy $E = \frac{p^2}{2m}$

$$\therefore \Delta E = \frac{\Delta P^2}{2m} \geq \frac{(1.054 \times 10^{-24})^2}{2 \times 9.11 \times 10^{-31}} \geq 6.142 \times 10^{-19} \text{ j}$$

Problem 8. The average time that an atom retains excess excitation energy before re-emitting it in the form of electromagnetic radiations is 10^{-8} sec. Calculate the limit of accuracy with which the excitation energy of the emitted radiation can be determined.

Solution : According to uncertainty principle $\nabla E \cdot \nabla t \approx \hbar$, where ∇E is the uncertainty in energy and ∇t that in time.

$$\text{Given } \Delta t = 10^{-8} \text{ sec.}$$

$$\begin{aligned}
 \therefore \Delta E &= \frac{\hbar}{\Delta t} = \frac{1.05 \times 10^{-34} \text{ joule} - \text{sec.}}{10^{-8}} \\
 &= 1.05 \times 10^{-26} \text{ joule} - \text{sec.} \\
 &= \frac{1.05 \times 10^{-26}}{1.6 \times 10^{-19}} \text{ eV} = 6.56 \times 10^{-8} \text{ eV.}
 \end{aligned}$$

\therefore Uncertainty in energy = **$6.56 \times 10^{-8} \text{ eV}$** .

Problem 9. The uncertainty in the location of a particle moving with a velocity of $7.28 \times 10^7 \text{ m/s}$ is double of its de-Broglie wavelength. Find out the uncertainty in measuring the velocity.

Solution : The de-Broglie wavelength associated with particle

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

$$\therefore \text{Uncertainty in position } \Delta x = 2\lambda = \frac{2h}{mv} \quad (1)$$

$$\text{From uncertainty principle } \Delta x \Delta p \approx \hbar. \quad (2)$$

$$\text{As } p = mv$$

$$\therefore \Delta p = \Delta(mv) = m(\Delta v) \quad (3)$$

Using (1), (2) and (3) and by putting $\hbar = h/2\pi$, we get

$$\frac{2h}{mv} \cdot m(\Delta v) = \frac{h}{2\pi}.$$

Uncertainty in velocity,

$$\therefore \Delta v = \frac{v}{4\pi} = \frac{7.28 \times 10^7}{4 \times 3.14} \text{ m/s} = \mathbf{5.96 \times 10^6 \text{ m/s.}}$$

Exercise

(A) Descriptive type

Section I- de-Broglie wave

- (1) What is wave particle duality? Derive an expression for wavelength of matter waves. Differentiate between 'group velocity' and 'phase velocity'.
(L.U. 2011)
- (2) State and explain wave-particle duality. Discuss one experiment each to demonstrate the wave and particle nature of matter.
(L.U. 2013)
- (3) Discuss the de-Broglie's matter wave hypothesis and hence explain the absence of matter wave in macroscopic world.
(L.U. 2014)
- (4) Find de-Broglie wavelength of neutron thermally excited to 327°C.
(L.U. 2016)
- (5) Prove that wavelength of electron accelerated to V volt will be

$$\lambda = \frac{12.27}{\sqrt{V}} \text{ \AA}$$
(LU 2016)
- (6) Find the expression for group velocity of matter waves.
(LU 2015)

Section II- Heisenberg's uncertainty principle

- (7) State and explain Heisenberg's uncertainty principle. Explain how its validity is supported by the gamma-ray microscope experiment.
(L.U. 2007)
- (8) State, Explain and prove Heisenberg uncertainty principle.
(L.U. 2008)
- (9) State the Heisenberg's Uncertainty Principle. Explain its significance with the help of examples. .
(L.U. 2015)

(10) Express 'Uncertainty principle' in its different forms.

(L.U. 2016)

(11) Write down the three Heisenberg uncertainty relations and its consequences.

(L.U. 2014)

(12) Heisenberg uncertainty principle and its consequences.

(L.U. 2013)

Short answer type

(1) What do you understand by wave particle duality?

(L.U. 2010)

(2) Free electron cannot exist inside nucleus Justify.

(L.U. 2010)

(3) Free electron cannot exist inside nucleus Justify.

(L.U. 2010)

(4) Show that phase velocity is greater than the velocity of light.

(L.U. 2010)

(5) Distinguish clearly between the phase velocity and the group velocity of a wave packet.

(L.U. 2013)

(6) What is meant by a wave packet?

(L.U. 2011)

(7) What is meant by a wave packet ?

(L.U. 2007)

(8) Show that the rest mass of a photon is zero.

(L.U. 2009)

(9) Show that phase velocity of a matter wave is greater than velocity of light.

(L.U. 2014)

(10) Discuss the probabilistic description of photon.

(L.U. 2014)

(11) What is the importance of de-Broglie's matter waves?

(LU 2015)

(12) Explain, why free electron cannot exist inside nucleus.

(L.U. 2011)

(13) Show that wavelength of electron cannot exist inside nucleus. **(L.U. 2010)**

(14) State 'Heisenberg's uncertainty principle'. **(L.U. 2012)**

(A) Numericals

(B) Find the de-Broglie wavelength associated with a 50 gm. Golf ball moving at 40 ms^{-1} . **(L.U. 2007)**

(C) Calculate the kinetic energy of neutron star in electron volts whose de-Broglie wavelength is 1 \AA . **(L.U. 2008)**

(D) Find the De-Broglie wavelength of 15 eV proton. **(L.U. 2009)**

(E) Calculate the Kinetic energy of neutron star in electron volts, whose de-Broglie wavelength is 1 \AA . **(L.U. 2011)**

(F) Calculate de-Broglie's wavelength of thermal neutrons at 300 K . **(L.U. 2014)**
(Mass of neutron = $1.675 \times 10^{-34} \text{ g}$)

(G) Show that de-Broglie wavelength of an electron moving with velocity 0.707 times the velocity of light in vacuum is equal to Compton wavelength. **(L.U. 2010)**

(H) A proton is confined to a nucleus of radius $5 \times 10^{-15} \text{ m}$. Calculate the maximum uncertainty in its momentum and maximum kinetic energy, the proton should have. **(L.U. 2008)**

(I) Average life-time of an excited atomic state is 10^{-8} second. Find the uncertainty in the energy of the photon. **(L.U. 2009)**

Chapter 4

Wave mechanics –II

4.1 Postulates of Quantum Mechanics

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

Physical Quantity	Classical definition	Quantum operator
Position	\vec{r}	\vec{r}
Linear momentum	\vec{P}	$-i\hbar\vec{\nabla}$
Angular momentum	$\vec{r} \times \vec{P}$	$\vec{r} \times -i\hbar\vec{\nabla}$
Kinetic Energy	$\frac{P^2}{2m}$	$\frac{\hbar^2 \nabla^2}{8\pi^2 m}$
Potential Energy	V	V
Total Energy	$\frac{P^2}{2m} + V$	$\frac{\hbar^2 \nabla^2}{8\pi^2 m} + V$

1. A linear Eigen value equation can be always linked with each operator.

Let the equation is

$$P\psi = \lambda \psi \quad (1)$$

Where

$P \Rightarrow$ operator

$\psi \Rightarrow$ Eigen function

$\lambda \Rightarrow$ Eigen value of the operator P associated with Eigen function

2. In general, when a measurement of a dynamical quantity 'a' is made on a particle for which the wave function is ψ , we get different values of a during

different trials. This is in conformity with the uncertainty principle. The most probable value of 'a' is given by

$$\langle a \rangle = \int \psi^* \hat{A} \psi d\tau \quad (2)$$

Where \hat{A} is the operator associated with the quantity a and ψ^* is the complex conjugate of ψ then quantity $\langle a \rangle$ is called expectation value of \hat{A} .

4.2 Schrödinger equation

The quantity that characterizes the de-Broglie wave is called the wave function. It is denoted by ψ . It may be a complex function. A particle is equivalent to a wave-packet. The size of packet is large as compared to particle. To locate the particle within the wave packet, Schrodinger in 1926 gave an equation called the guiding wave equation. The Schrödinger equation is the fundamental equation of wave mechanics in the same sense as the Newton's second law of motion of classical mechanics.

Erwin Schrödinger (1887-1961)

Erwin Schrödinger was an Austrian physicist whose groundbreaking equation of wave mechanics changed the face of quantum theory. He was a brilliant and charming Austrian, one of the greatest scientists of the twentieth century, and a man with passionate interests in people and ideas.

Born on August 12, 1887, in Vienna, Austria, Erwin Schrödinger went on to become a noted theoretical physicist and scholar who came up with a groundbreaking wave equation known as Schrödinger's wave equation, was made at the end of this epoch-during the first half of 1926, for electron movements.



He went on to enter the University of Vienna, where he focused primarily on the study of physics and was strongly influenced by another young physicist, Fritz

Hasenöhl, and graduated with a Ph.D. in physics in 1910. From 1906 to 1910 he was a student at the University of Vienna, during which time he came under the strong influence of Fritz Hasenöhl, who was Boltzmann's .It came as a result of his dissatisfaction with the quantum condition in Bohr's orbit theory and his belief that atomic spectra should really be determined by some kind of Eigen value problem. For this work he shared with Dirac the Nobel Prize for 1933.

In 1927 Schrödinger moved to Berlin as Planck's successor. he was also the author of the well-known little book "What is Life?". He remained greatly interested in the foundations of atomic physics. He died on the 4th of January, 1961, after a long illness, survived by his faithful companion, Annemarie Bartle, whom he married in 1920.

(a)Time independent form of Schrödinger equation

Let us consider a system of stationary wave to be associated with a particle. Let $\psi(\vec{r}, t)$ be the wave displacement for the de-Broglie waves at any location $\vec{r} = \hat{i}x + \hat{j}y + \hat{k}z$ at time 't'. Then the differential equation of wave motion in three dimensions in accordance with Maxwell's wave equation can be written as

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{u^2} \frac{\partial^2 \psi}{\partial t^2} \quad (1)$$

eqn (1) can also be written as

$$\nabla^2 \psi = \frac{1}{u^2} \frac{\partial^2 \psi}{\partial t^2} \quad (2)$$

$$\text{where } \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (3)$$

$$(\nabla^2 = \vec{\nabla} \cdot \vec{\nabla})$$

$\vec{\nabla}$ is defined by

$$\vec{\nabla} = \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z},$$

where \hat{i} , \hat{j} and \hat{k} are unit vectors along x, y and z directions and u is the wave velocity (Phase velocity).

Note :Derivation of differential equation of wave motion

$$y = a \sin (\omega t - kx) \quad (1)$$

In the above equation

y is the displacement of a particle of the medium situated at distance x from the reference point at time t

a is the displacement amplitude or simply amplitude

ω is the angular frequency ($\omega = 2 \pi n$, where n is the linear frequency or simply frequency)

k is the propagation constant ($k = 2 \pi / \lambda$)

$(\omega t - kx)$ is the phase

$$y = a \sin (\omega t - kx) \quad (1)$$

Differentiating equation (1), partially with respect to 't', we have

$$\frac{\partial y}{\partial t} = a \omega \cos (\omega t - kx) \quad (2)$$

Differentiating equation (2), partially with respect to 't', we have

$$\frac{\partial^2 y}{\partial t^2} = -a \omega^2 \sin (\omega t - kx) \quad (3)$$

partially differentiating equation (1) with respect to 'x', we have

$$\frac{\partial y}{\partial x} = -ak \cos (\omega t - kx) \quad (4)$$

Differentiating equation (4), partially with respect to x

$$\frac{\partial^2 y}{\partial x^2} = -ak^2 \sin(\omega t - kx) \quad (5)$$

Dividing equation (3) by equation (4). We have,

$$\begin{aligned} \frac{\frac{\partial^2 y}{\partial t^2}}{\frac{\partial^2 y}{\partial x^2}} &= \frac{-a\omega^2 \sin(\omega t - kx)}{-ak^2 \sin(\omega t - kx)} \\ \text{or } \frac{\frac{\partial^2 y}{\partial t^2}}{\frac{\partial^2 y}{\partial x^2}} &= \frac{\omega^2}{k^2} \\ \text{or } \frac{\frac{\partial^2 y}{\partial t^2}}{\frac{\partial^2 y}{\partial x^2}} &= u^2 \\ \therefore \frac{\partial^2 y}{\partial t^2} &= u^2 \frac{\partial^2 y}{\partial x^2} \\ \text{or } \frac{\partial^2 y}{\partial x^2} &= \frac{1}{u^2} \frac{\partial^2 y}{\partial t^2} \end{aligned} \quad (6)$$

Putting $y = \psi$ in the above equation

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{u^2} \frac{\partial^2 \psi}{\partial t^2} \quad (7)$$

Equation (7) is the differential equation of wave motion in one dimension.

Differential equation of wave motion in three dimensions is given by

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{u^2} \frac{\partial^2 \psi}{\partial t^2} \quad (8)$$

Equation (8) can also be written as

$$\nabla^2 \psi = \frac{1}{u^2} \frac{\partial^2 \psi}{\partial t^2} \quad (9)$$

The solution of equation (1) is given as

$$\psi(\vec{r}, t) = \psi_0(\vec{r}, t) e^{-i\omega t} \quad (4)$$

Where ψ is the wave function of the de-Broglie wave associated with the moving particle, situated at \vec{r} position vector at time 't'. The position vector \vec{r} is defined as

$$\vec{r} = \hat{i}x + \hat{j}y + \hat{k}z \quad (5)$$

Equation (4), in concise form can be written as

$$\psi = \psi_0 e^{-i\omega t} \quad (6)$$

partially differentiating equation (6) with respect to 't', we get,

$$\frac{\partial \psi}{\partial t} = (-i\omega) \psi_0 e^{-i\omega t} \quad (7)$$

partially differentiating equation (7) with respect to 't', we get

$$\frac{\partial^2 \psi}{\partial t^2} = (-i\omega)(-i\omega) \psi_0 e^{-i\omega t} \quad (8)$$

$$\text{or} \quad \frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi_0 e^{-i\omega t} \quad (9)$$

$$\text{or} \quad \frac{\partial^2 \psi}{\partial t^2} = -\omega^2 \psi \quad (\text{since } \psi = \psi_0 e^{-i\omega t}) \quad (10)$$

Using equation (1) for equation (2), We have,

$$\begin{aligned} \text{Or} \quad \nabla^2 \psi &= -\frac{\omega^2}{u^2} \psi \\ \text{or} \quad \nabla^2 \psi + \frac{\omega^2}{u^2} \psi &= 0 \end{aligned} \quad (11)$$

Now $\omega = 2\pi\nu$

But $E = h\nu$ or $\nu = E/h$

$$\therefore \quad \omega = \frac{2\pi E}{h} \quad (12)$$

Also $u = \nu\lambda$

$$\text{but } \nu = \frac{E}{h} \quad \text{and} \quad \lambda = \frac{h}{m\nu}$$

$$\therefore \quad \mathbf{u} = \frac{E}{mv} \quad (13)$$

Dividing equation (12) by equation (13), we get,

$$\frac{\omega}{u} = \frac{2\pi mv}{h} \quad (14)$$

By squaring equation (14), we have,

$$\frac{\omega^2}{u^2} = \frac{4\pi^2 m^2 v^2}{h^2} \quad (15)$$

Using equation (15) for equation for (11), we have,

$$\nabla^2 \psi + \frac{4\pi^2 m^2 v^2}{h^2} \psi = 0 \quad (16)$$

$$\text{or} \quad \nabla^2 \psi + \frac{8\pi^2 m \left(\frac{1}{2} mv^2\right)}{h^2} \psi = 0 \quad (17)$$

Now $\frac{1}{2} mv^2 = \text{Kinetic energy, which is denoted by } T$

And if total energy and potential energy is denoted by E and V respectively, the $E = T + V$

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

$$\frac{1}{2} mv^2 = E - V \quad (18)$$

Using (18) for (17), we have,

$$\nabla^2 \psi + \frac{8\pi^2 m(E-V)}{h^2} \psi = 0 \quad (19)$$

$$\text{or} \quad \nabla^2 \psi + \frac{2m}{h^2/4\pi^2} (E - V) \psi = 0 \quad (20)$$

$$\text{or} \quad \nabla^2 \psi + \frac{2m}{(h/2\pi)^2} (E - V) \psi = 0 \quad (21)$$

$$\text{or} \quad \nabla^2 \psi + \frac{2m}{h^2} (E - V) \psi = 0 \quad (22)$$

Equation (22) is called time independent form of the **Schrödinger equation**.

(b) Time dependent form of Schrödinger equation

Differential equation of wave motion in three dimensions is given by

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{1}{u^2} \frac{\partial^2 \psi}{\partial t^2} \quad (1)$$

Equation (1) can also be written as

$$\nabla^2 \psi = \frac{1}{u^2} \frac{\partial^2 \psi}{\partial t^2} \quad (2)$$

The solution of equation (1) or equation (2) is given as

$$\psi(\vec{r}, t) = \psi_0(\vec{r}, t) e^{-i\omega t} \quad (3)$$

Where ψ is the wave function of the de-Broglie wave associated with the moving particle, situated at \vec{r} position vector at time 't'. The position vector \vec{r} is defined as

$$\vec{r} = \hat{i}x + \hat{j}y + \hat{k}z \quad (4)$$

Equation (4), in concise form can be written as

$$\psi = \psi_0 e^{-i\omega t} \quad (5)$$

partially differentiating equation (5) with respect to 't', we get,

$$\frac{\partial \psi}{\partial t} = (-i\omega) \psi_0 e^{-i\omega t} \quad (6)$$

$$= (-i) (2\pi\nu) \psi_0 e^{-i\omega t} \quad (7)$$

(Since $\omega = 2\pi\nu$)

$$= (-i) \left(2\pi \frac{E}{h} \right) \psi \quad (8)$$

(Since $E = h\nu$, $\psi = \psi_0 e^{-i\omega t}$)

$$= (-i) \times \frac{i}{i} \left(\frac{E}{h} \right) \psi \quad \left(\text{since } \hbar = \frac{h}{2\pi} \right) \quad (9)$$

$$\text{or} \quad \frac{\partial \psi}{\partial t} = \frac{1}{i} \left(\frac{E}{\hbar} \right) \psi \quad (10)$$

$$\left(\text{Since } \hbar = \frac{h}{2\pi} \right)$$

$$\text{or} \quad E\psi = i\hbar \frac{\partial \psi}{\partial t} \quad (11)$$

Now from time independent Schrödinger equation

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

$$\text{or} \quad \nabla^2 \psi + \frac{2m}{\hbar^2} (E\psi - V\psi) = 0 \quad (12)$$

Substituting the value of $E\psi$ from equation (11) in equation (12), we have

$$\nabla^2 \psi + \frac{2m}{\hbar^2} \left[i\hbar \frac{\partial \psi}{\partial t} - V\psi \right] = 0$$

Multiplying the above equation by $-\frac{\hbar^2}{2m}$, we have

$$-\frac{\hbar^2}{2m} \nabla^2 \psi - \left[i\hbar \frac{\partial \psi}{\partial t} - V\psi \right] = 0$$

$$\text{or} \quad \left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \psi = i\hbar \frac{\partial \psi}{\partial t} \quad (13)$$

Equation (11) is called time dependent form of the Schrödinger equation.

(c)- Schrödinger equation in terms of operators

From equation (13)

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] \psi = i\hbar \frac{\partial \psi}{\partial t}$$

the operator $\left[-\frac{\hbar^2}{2m} \nabla^2 + V \right]$ is called Hamiltonian and is represented by \hat{H} ;

while operator $i\hbar \frac{\partial \psi}{\partial t}$, operating on ψ gives \hat{E} , which can be seen from equation (11). Therefore equation (13) can be written as

$$\hat{H}\psi = \hat{E}\psi \quad (14)$$

(d)- Schrödinger equation for a free particle

From time independent Schrödinger equation

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

For a free particle, $V = 0$, since in the absence of external forces, a particle can be treated as free particle. If no external force is acting on the particle then its potential energy (V) will be zero.

i.e., for a free particle,

$V = 0$, substituting this value of potential energy in the above equation, we have

$$\nabla^2 \psi + \frac{2m}{\hbar^2} E \psi = 0 \quad (15)$$

Note: The forms of the Schrödinger equation, derived in the above sub articles (a), (b) and (c) describes the motion of a non-relativistic material particle.

4.3 Interpretation of the wave function

Background

Millikan said that wave function is merely an auxiliary mathematical quantity for doing calculations for the experimental results.

Schrödinger attempted to interpret the wave function as charge density wave function. Since the particle density is directly proportional to ψ^2 , therefore charge density can be obtained by multiplying the particle density ψ^2 by the charge on the particle. The quantity ψ^2 , therefore is a measure of charge density, this interpretation, given by Schrödinger, however gave satisfactory results when wave mechanics was applied in the cases of stable states of Bohr's atom, emission of spectral lines, intensity distribution of Compton scattering etc. but there were some difficulties in connection with dissipation of the wave packets with time etc.

Satisfactory interpretation

A satisfactory interpretation of the wave function ψ associated with a moving particle was given by Max Born in 1926 and then developed by Bohr, Dirac, Heisenberg & others. Max Born postulated that the square the magnitude of

the wave function, $[\psi]^2$ or $(\psi \psi^*$ if ψ is complex). Evaluated at a particular pt represents the probability of finding the particle at that pt. $[\psi]^2$ is called probability density and ψ is probability amplitude.

According to this interpretation the probability of finding the particle with in an element of volume $d\tau$ is $[\psi]^2 d\tau$. Therefore $\psi \psi^* = [\psi]^2$ represents probability density of the particle in the state ψ . Then the probability of finding the particle in a volume element $d\tau = dx dy dz$ about any point \vec{r} at time 't' is expressed as

$$P(\vec{r}, t) = |\psi(\vec{r}, t)|^2 d\tau$$

Since the particle is certainly somewhere; The integral of $d\tau$ over the whole space must be unity.

$$\int_{-\infty}^{+\infty} |\psi(\vec{r}, t)|^2 d\tau = 1$$

A wave function that obeys the above eqⁿ is said to be normalized besides being normalisable, an acceptable wave function ψ must full fill the following requirement

- (a) It must be finite everywhere.
- (b) It must be single valued.
- (c) It must be continuous & must have a continuous 1st derivative everywhere.

(d)4.4 Normalized wave function

According to interpretation of wave function (ψ), $\psi\psi^* d\tau$ or $|\psi|^2 d\tau$ signifies the probability of locating the particle in the volume element $d\tau$.

There are several situations in which we find that the particle is bound to move in a limited region, e.g. the electron in an atom i.e., a particle in a box with in penetrable walls. In this situation , the probability $P(\vec{r}, t)$ of finding the particle in the bounded region or in the entire space will be unity, i.e.,

$$P(\vec{r}, t) = \int |\psi(\vec{r}, t)|^2 d\tau = 1$$

$$\int |\psi(\vec{r}, t)|^2 d\tau = 1 \quad (1)$$

or
$$\int \psi(\vec{r}, t) \psi^*(\vec{r}, t) d\tau = 1 \quad (2)$$

Therefore a wave function is said to be normalized when:

$$\int \psi(\vec{r}, t) \psi^*(\vec{r}, t) d\tau = 1$$

Or simply

$$\int \psi \psi^* d\tau = 1$$

If there are two wave functions ψ_i & ψ_j , then they will be called normalised wavefunctions, provided:

$$\int \psi_i \psi_i^* d\tau = 1$$

and

$$\int \psi_j \psi_j^* d\tau = 1$$

This is important to note here that if the particle is bound in the limited region then the probability of finding the particle at infinite distance will be zero.

$$\text{If } \int \psi \psi^* d\tau = N \quad (3)$$

then obviously ψ is not a normalised wave function, however from equation (3), we can obtain a normalised wave function as

$$\int \psi \psi^* d\tau = N$$

$$\text{i.e. } \frac{1}{N} \int \psi \psi^* d\tau = 1$$

$$\int \frac{\psi}{\sqrt{N}} \frac{\psi^*}{\sqrt{N}} d\tau = 1 \quad (4)$$

From equation (4), this is evident that normalised wave function with respect to equation (3) is $\frac{\psi}{\sqrt{N}}$ and the normalising factor is $\frac{1}{\sqrt{N}}$.

4.5 Orthogonal wave functions

If ψ_i & ψ_j are two different wave functions then ψ_i & ψ_j will be called orthogonal wavefunctions provided, they fulfil the following conditions:

$$\int \psi_i \psi_j^* d\tau = 0 \quad \left| \quad \text{For } i \neq j \right.$$

and $\int \psi_j \psi_i^* d\tau = 0$

i.e. the integral $\int \psi_i \psi_j^* d\tau$ and $\int \psi_j \psi_i^* d\tau$ vanishes over entire space

Note: We know that if two vectors are orthogonal then their scalar product is zero. in the similar fashion, wave function ψ which is a infinite dimensional vector, under certain condition may give orthogonality condition

4.6 Expectation value

The exact value of a dynamical quantity defined by the wave function can not be calculated as wave function ψ has probabilistic interpretation. Therefore it is essential to calculate the expectation value (or average value) of such dynamical quantities.

The expectation value of a dynamical quantity is defined as

“The expectation value of a dynamical quantity is the average of the result of a large number of measurements on independent systems”.

Mathematically, the expectation value of any quantity $f(\vec{r}, t)$ is defined as

$$\begin{aligned} \langle f(\vec{r}, t) \rangle &= \int P(\vec{r}, t) f(\vec{r}, t) d\tau \\ &= \int \psi^*(\vec{r}, t) f(\vec{r}, t) \psi(\vec{r}, t) d\tau \quad (1) \end{aligned}$$

(1) Expectation value of position $\langle \vec{r} \rangle$

The expectation value of the position vector (\vec{r}) , defined as

$\vec{r} = \hat{i}x + \hat{j}y + \hat{k}z$ is given as

$$\langle \vec{r} \rangle = \int \psi^*(\vec{r}, t) \vec{r} \psi(\vec{r}, t) d\tau$$

and in terms of components –

$$\langle x \rangle = \int \psi^*(\vec{r}, t) x \psi(\vec{r}, t) d\tau$$

$$\langle y \rangle = \int \psi^*(\vec{r}, t) y \psi(\vec{r}, t) d\tau$$

$$\langle z \rangle = \int \psi^*(\vec{r}, t) z \psi(\vec{r}, t) d\tau$$

where $\langle x \rangle$, $\langle y \rangle$ and $\langle z \rangle$ are the expectation values of the co-ordinates x, y and z of the particle respectively.

(2) Expectation value of Potential $\langle V \rangle$

The expectation value of the potential (V) is defined

$$\langle V \rangle = \int \psi^*(\vec{r}, t) V(\vec{r}, t) \psi(\vec{r}, t) d\tau$$

(3) Expectation value of Energy $\langle E \rangle$

The time dependent schrödinger equation is given as

$$E\psi = i\hbar \frac{\partial \psi}{\partial t} \quad (1)$$

so that the total energy can be represented by differential operator that acts on the wave function ψ , i.e.,

$$\hat{E} = i\hbar \frac{\partial}{\partial t} \quad (2)$$

where \hat{E} is energy operator

Therefore the expectation value of energy is defined as

$$\begin{aligned} \langle E \rangle &= \int \psi^* \hat{E} \psi d\tau \\ &= \int \psi^* i\hbar \frac{\partial}{\partial t} \psi d\tau \\ &= i\hbar \int \psi^* \frac{\partial \psi}{\partial t} d\tau \end{aligned} \quad (3)$$

(4) Expectation value of momentum $\langle \vec{P} \rangle$

As

Total energy = kinetic energy + potential energy

$$\text{i.e.,} \quad E = T + V$$

$$\text{or} \quad E = \frac{P^2}{2m} + V$$

$$\text{or} \quad \langle E \rangle = \left\langle \frac{P^2}{2m} \right\rangle + \langle V \rangle \quad (1)$$

now from the time independent schrödinger equation, which is given as

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

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

$$\therefore -\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi = E \psi$$

$$\text{or} \quad E \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi$$

$$\text{or} \quad E = -\frac{\hbar^2}{2m} \nabla^2 + V$$

$$\text{or} \quad \langle E \rangle = \left\langle -\frac{\hbar^2}{2m} \nabla^2 \right\rangle + V \quad (2)$$

Comparing equations (1) and (2), we have,

$$\left\langle \frac{P^2}{2m} \right\rangle = \left\langle -\frac{\hbar^2}{2m} \nabla^2 \right\rangle$$

$$\text{or} \quad \frac{P^2}{2m} = -\frac{\hbar^2}{2m} \nabla^2$$

$$\text{or} \quad P^2 = -\hbar^2 \nabla^2$$

$$\text{or} \quad P^2 = \frac{\hbar^2}{i^2} \nabla^2$$

$$\text{or} \quad \vec{P} = -i\hbar \vec{\nabla} \quad (3)$$

Equation (3) suggests that momentum can be represented by a differential operator $-i\hbar\vec{\nabla}$,

i.e. $\hat{P} = -i\hbar\vec{\nabla}$ (where \hat{P} is the momentum operator)

therefore the expectation value of momentum is defined as

$$\begin{aligned}\langle P \rangle &= \int \psi^* \hat{P} \psi \, d\tau \\ &= \int \psi^* (-i\hbar\vec{\nabla}) \psi \, d\tau \\ &= \int \psi^* (-i\hbar\vec{\nabla}) \psi \, d\tau \\ &= -i\hbar \int \psi^* \vec{\nabla} \psi \, d\tau\end{aligned}\quad (4)$$

Equation (4) is equivalent to the following three component equations

$$\begin{aligned}\langle P_x \rangle &= -i\hbar \int \psi^* \frac{\partial \psi}{\partial x} \, d\tau \\ \langle P_y \rangle &= -i\hbar \int \psi^* \frac{\partial \psi}{\partial y} \, d\tau \\ \langle P_z \rangle &= -i\hbar \int \psi^* \frac{\partial \psi}{\partial z} \, d\tau\end{aligned}\quad (7)$$

Where $\langle P_x \rangle$, $\langle P_y \rangle$ and $\langle P_z \rangle$ are the expectation values of the components along x, y and z axes respectively.

Note: The above equations of expectation values are valid only if the wave function ψ is normalized. If the wave function ψ is not normalized then the expectation value of any quantity 'f' will be defined as

$$\langle f \rangle = \frac{\int \psi^* f \psi \, d\tau}{\int \psi^* \psi \, d\tau}$$

4.7 Ehrenfest's theorem

Statement:

Schrödinger wave equation leads to the results which satisfy the classical law of motion on the average.

Or

“The average motion of a wave packet is in agreement with the motion of the corresponding classical particle”.

For example according to Newtonian mechanics or classical mechanics

$$\frac{d\vec{P}}{dt} = -\vec{\nabla} V \quad (1)$$

$$\text{And} \quad \frac{d\vec{r}}{dt} = \frac{\vec{P}}{m} \quad (2)$$

or in terms of components, equation (1) can be written as

$$\frac{dP_x}{dt} = -\frac{\partial V_x}{\partial x} \quad (3A)$$

$$\frac{dP_y}{dt} = -\frac{\partial V_y}{\partial y} \quad (3B)$$

$$\frac{dP_z}{dt} = -\frac{\partial V_z}{\partial z} \quad (3C)$$

similarly in terms of components, equation (2) can be written as

$$\frac{dx}{dt} = \frac{P_x}{m} \quad (4A)$$

$$\frac{dy}{dt} = \frac{P_y}{m} \quad (4B)$$

$$\frac{dz}{dt} = \frac{P_z}{m} \quad (4C)$$

But according to the statement of the Ehrenfest's Theorem, in quantum mechanics, the equations (1) and (6) will be respectively written as

$$\frac{d}{dt} \langle \vec{P} \rangle = \langle -\vec{\nabla} V \rangle \quad (5)$$

$$\frac{d}{dt} \langle \vec{r} \rangle = \frac{\langle \vec{P} \rangle}{m} \quad (6)$$

and the equations (3A), (3B) and (3C) will be written respectively as

$$\frac{d}{dt} \langle P_x \rangle = \left\langle -\frac{\partial V}{\partial x} \right\rangle \quad (7A)$$

$$\frac{d}{dt} \langle P_y \rangle = \left\langle -\frac{\partial V}{\partial y} \right\rangle \quad (7B)$$

$$\frac{d}{dt} \langle P_z \rangle = \left\langle -\frac{\partial V}{\partial z} \right\rangle \quad (7C)$$

and the equations (4A), (4B) and (4C) will be written respectively as

$$\frac{d}{dt} \langle x \rangle = \frac{\langle P_x \rangle}{m} \quad (8A)$$

$$\frac{d}{dt} \langle y \rangle = \frac{\langle P_y \rangle}{m} \quad (8B)$$

$$\frac{d}{dt} \langle z \rangle = \frac{\langle P_z \rangle}{m} \quad (8C)$$

Proof of $\frac{d}{dt} \langle \vec{r} \rangle = \frac{\langle \vec{P} \rangle}{m}$

The x component of velocity may be defined at the time rate of change of expectation value of x component of position

$$\begin{aligned} \frac{d}{dt} \langle x \rangle &= \frac{d}{dt} \int \psi^* x \psi d\tau \\ &= \int \psi^* x \frac{\partial \psi}{\partial t} d\tau + \int \frac{\partial \psi^*}{\partial t} x \psi d\tau \end{aligned} \quad (9)$$

Now from time dependent Schrödinger equation –

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi \quad (10A)$$

$$\therefore \frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} \left[-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi \right] \quad (10B)$$

Complex conjugate of time dependent Schrödinger equation is

$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi^* + V\psi^* \quad (11A)$$

$$\therefore \frac{\partial \psi^*}{\partial t} = \frac{1}{-i\hbar} \left[-\frac{\hbar^2}{2m} \nabla^2 \psi^* + V\psi^* \right] \quad (11B)$$

Substituting the values of $\frac{\partial \psi}{\partial t}$ and $\frac{\partial \psi^*}{\partial t}$ from equations (10B) and (11B) in equation (9), we get

$$\begin{aligned}
\frac{d}{dt} \langle x \rangle &= \int \psi^* x \left\{ \frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi \right) \right\} d\tau \\
&+ \int \left\{ \frac{1}{-i\hbar} \left(-\frac{\hbar^2}{2m} \nabla^2 \psi^* + V\psi^* \right) \right\} x\psi d\tau \\
&= \frac{1}{i\hbar} \int \left[\psi^* x \left(-\frac{\hbar^2}{2m} \nabla^2 \psi \right) + \psi^* x V\psi + \left(\frac{\hbar^2}{2m} \nabla^2 \psi^* \right) x\psi \right. \\
&\quad \left. - V\psi^* x\psi \right] d\tau \\
&\quad - \frac{\hbar}{2im} \int [\psi^* x (\nabla^2 \psi) - (\nabla^2 \psi^*) x\psi] d\tau \\
&= -\frac{\hbar}{2im} \int \psi^* x (\nabla^2 \psi) d\tau + \frac{\hbar}{2im} \int (\nabla^2 \psi^*) x\psi d\tau \quad (12)
\end{aligned}$$

$$\therefore \frac{d}{dt} \langle x \rangle = -\frac{\hbar}{2im} I_1 + \frac{\hbar}{2im} I_2 \quad (13)$$

Where

$$I_1 = \int \psi^* x (\nabla^2 \psi) d\tau \quad (14)$$

$$I_2 = \int (\nabla^2 \psi^*) x\psi d\tau \quad (15)$$

Now we will simplify I_2 as

$$\begin{aligned}
I_2 &= \int (\nabla^2 \psi^*) x\psi d\tau \\
&= \int \vec{\nabla} \cdot (\vec{\nabla} \psi^*) x\psi d\tau
\end{aligned}$$

$$\therefore I_2 = \int x\psi \vec{\nabla} \cdot (\vec{\nabla} \psi^*) d\tau \quad (16)$$

Now we know that

$$\text{div } S\vec{A} = S \text{div } \vec{A} + \vec{A} \cdot \text{grad } S$$

$$\text{or } \vec{\nabla} \cdot (S\vec{A}) = S \vec{\nabla} \cdot \vec{A} + \vec{A} \cdot \vec{\nabla} S \quad (17)$$

Let $S = x\psi$ and $\vec{A} = \vec{\nabla}\psi^*$, then from (17), we get

$$\begin{aligned} \vec{\nabla} \cdot (x\psi \vec{\nabla}\psi^*) &= x\psi \vec{\nabla} \cdot (\vec{\nabla}\psi^*) + \vec{\nabla}\psi^* \cdot \vec{\nabla}S \\ &= x\psi \vec{\nabla} \cdot (\vec{\nabla}\psi^*) = \vec{\nabla} \cdot (x\psi \vec{\nabla}\psi^*) - \vec{\nabla}\psi^* \cdot \vec{\nabla}x\psi \\ &= \int x\psi \vec{\nabla} \cdot (\vec{\nabla}\psi^*) x\psi d\tau = \int \vec{\nabla} \cdot (x\psi \vec{\nabla}\psi^*) d\tau - \int \vec{\nabla}\psi^* \cdot \vec{\nabla}x\psi d\tau \end{aligned}$$

Now from Gauss divergence theorem ($\int_V \vec{\nabla} \cdot \vec{A} dV = \int_S \vec{A} \cdot d\vec{S}$), we can write

$$\int \vec{\nabla} \cdot (x\psi \vec{\nabla}\psi^*) d\tau = \int (x\psi \vec{\nabla}\psi^*) \cdot d\vec{A}$$

$$\text{But } \int (x\psi \vec{\nabla}\psi^*) \cdot d\vec{A} = 0$$

Since the wave packet ψ vanishes at great distances, as the integral has been taken over normal component of $x\psi \vec{\nabla}\psi^*$ over infinite bounding surface A, therefore,

$$\begin{aligned} &= \int x\psi \vec{\nabla} \cdot (\vec{\nabla}\psi^*) x\psi d\tau = \int (x\psi \vec{\nabla}\psi^*) \cdot d\vec{A} - \int \vec{\nabla}\psi^* \cdot \vec{\nabla}x\psi d\tau \\ &= \int x\psi \vec{\nabla} \cdot (\vec{\nabla}\psi^*) x\psi d\tau = 0 - \int \vec{\nabla}\psi^* \cdot \vec{\nabla}x\psi d\tau \\ &= \int x\psi \vec{\nabla} \cdot (\vec{\nabla}\psi^*) x\psi d\tau = - \int \vec{\nabla}\psi^* \cdot \vec{\nabla}x\psi d\tau \\ I_2 &= \int (\nabla^2 \psi^*) x\psi d\tau = \int x\psi \vec{\nabla} \cdot (\vec{\nabla}\psi^*) x\psi d\tau \\ &= - \int \vec{\nabla}\psi^* \cdot \vec{\nabla}x\psi d\tau \end{aligned}$$

$$\therefore I_2 = \int (\nabla^2 \psi^*) x\psi d\tau = - \int \vec{\nabla}\psi^* \cdot \vec{\nabla}x\psi d\tau \quad (18)$$

Now from the following vector identity

$$\text{div}(U \text{ grad } W) = U \nabla^2 W + (\text{ grad } U) \cdot (\text{ grad } W)$$

Putting $U = \psi^*$ and $W = x\psi$ in the above vector identity, we get

$$\text{div}(\psi^* \text{ grad } x\psi) = \psi^* \nabla^2 x\psi + (\text{ grad } \psi^*) \cdot (\text{ grad } x\psi)$$

$$\vec{\nabla} \cdot (\psi^* \vec{\nabla} x \psi) = \psi^* \nabla^2 x \psi + \vec{\nabla} \psi^* \cdot \vec{\nabla} x \psi$$

$$\vec{\nabla} \psi^* \cdot \vec{\nabla} x \psi = \vec{\nabla} \cdot (\psi^* \vec{\nabla} x \psi) - \psi^* \nabla^2 x \psi$$

$$\therefore \int \vec{\nabla} \psi^* \cdot \vec{\nabla} x \psi \, d\tau = \int \vec{\nabla} \cdot (\psi^* \vec{\nabla} x \psi) \, d\tau - \int \psi^* \nabla^2 x \psi \, d\tau$$

Now from Gauss divergence theorem ($\int_V \vec{\nabla} \cdot \vec{A} \, dV = \int_S \vec{A} \cdot d\vec{S}$),

$$\therefore \int \vec{\nabla} \cdot (\psi^* \vec{\nabla} x \psi) \, d\tau = \int (\psi^* \vec{\nabla} x \psi) \, dA$$

$$\text{But} \quad \int (\psi^* \vec{\nabla} x \psi) \, dA = 0$$

Since the wave packet ψ vanishes at great distances, as the integral has been taken over normal component of $x\psi \vec{\nabla} \psi^*$ over infinite bounding surface A, therefore,

$$\int \vec{\nabla} \psi^* \cdot \vec{\nabla} x \psi \, d\tau = 0 - \int \psi^* \nabla^2 x \psi \, d\tau$$

$$\therefore \int \vec{\nabla} \psi^* \cdot \vec{\nabla} x \psi \, d\tau = - \int \psi^* \nabla^2 x \psi \, d\tau \quad (19)$$

Using equation (19) for equation (18), we get

$$I_2 = \int (\nabla^2 \psi^*) x \psi \, d\tau = \int \psi^* \nabla^2 x \psi \, d\tau \quad (20)$$

Using equations (20) and (14) for equation (13), we get

$$\begin{aligned} \frac{d}{dt} \langle x \rangle &= -\frac{\hbar}{2im} \int \psi^* x (\nabla^2 \psi) \, d\tau + \frac{\hbar}{2im} \int \psi^* \nabla^2 x \psi \, d\tau \quad (21) \\ &= -\frac{\hbar}{2im} \left[\int \psi^* x (\nabla^2 \psi) \, d\tau - \int \psi^* \nabla^2 x \psi \, d\tau \right] \end{aligned}$$

Taking x component of the above equation

$$\begin{aligned} &= -\frac{\hbar}{2im} \left[\int \psi^* x \left(\frac{\partial^2 \psi}{\partial x^2} \right) \, d\tau - \int \psi^* \frac{\partial^2}{\partial x^2} (x\psi) \, d\tau \right] \\ &= -\frac{\hbar}{2im} \left[\int \psi^* x \left(\frac{\partial^2 \psi}{\partial x^2} \right) \, d\tau - \int \psi^* \frac{\partial}{\partial x} \left\{ \frac{\partial}{\partial x} (x\psi) \right\} \, d\tau \right] \end{aligned}$$

$$\begin{aligned}
&= -\frac{\hbar}{2im} \left[\int \psi^* x \left(\frac{\partial^2 \psi}{\partial x^2} \right) d\tau - \int \psi^* \frac{\partial}{\partial x} \left\{ x \frac{\partial \psi}{\partial x} + \psi \frac{\partial x}{\partial x} \right\} d\tau \right] \\
&= -\frac{\hbar}{2im} \left[\int \psi^* x \left(\frac{\partial^2 \psi}{\partial x^2} \right) d\tau - \int \psi^* \frac{\partial}{\partial x} \left\{ x \frac{\partial \psi}{\partial x} + \psi \right\} d\tau \right] \\
&= -\frac{\hbar}{2im} \left[\int \psi^* x \left(\frac{\partial^2 \psi}{\partial x^2} \right) d\tau - \int \psi^* \left\{ \frac{\partial}{\partial x} \left(x \frac{\partial \psi}{\partial x} \right) + \frac{\partial \psi}{\partial x} \right\} d\tau \right] \\
&= -\frac{\hbar}{2im} \left[\int \psi^* x \left(\frac{\partial^2 \psi}{\partial x^2} \right) d\tau - \int \psi^* \left\{ \left(x \frac{\partial}{\partial x} \left(\frac{\partial \psi}{\partial x} \right) + \frac{\partial \psi}{\partial x} \frac{\partial x}{\partial x} \right) + \frac{\partial \psi}{\partial x} \right\} d\tau \right] \\
&= -\frac{\hbar}{2im} \left[\int \psi^* x \left(\frac{\partial^2 \psi}{\partial x^2} \right) d\tau - \int \left\{ \psi^* x \left(\frac{\partial^2 \psi}{\partial x^2} \right) + 2\psi^* \frac{\partial \psi}{\partial x} \right\} d\tau \right] \\
&= -\frac{\hbar}{2im} \left[\int \left\{ \psi^* x \left(\frac{\partial^2 \psi}{\partial x^2} \right) d\tau - \psi^* x \left(\frac{\partial^2 \psi}{\partial x^2} \right) - 2\psi^* \frac{\partial \psi}{\partial x} \right\} d\tau \right] \\
&= -\frac{\hbar}{2im} \int \left(-2\psi^* \frac{\partial \psi}{\partial x} \right) d\tau \\
&= \frac{\hbar}{im} \int \psi^* \frac{\partial \psi}{\partial x} d\tau \\
&= \frac{-i\hbar}{m} \int \psi^* \frac{\partial \psi}{\partial x} d\tau \\
&= \frac{-i\hbar}{m} \int \psi^* \frac{\partial \psi}{\partial x} d\tau \\
&= \frac{-i\hbar \int \psi^* \frac{\partial \psi}{\partial x} d\tau}{m} \quad (\text{since } \langle P_x \rangle = -i\hbar \int \psi^* \frac{\partial \psi}{\partial x} d\tau)
\end{aligned}$$

$$\therefore \frac{d}{dt} \langle x \rangle = \frac{\langle P_x \rangle}{m}$$

Similarly, we can prove

$$\frac{d}{dt} \langle x \rangle = \frac{\langle P_x \rangle}{m}$$

$$\frac{d}{dt} \langle y \rangle = \frac{\langle P_y \rangle}{m}$$

$$\frac{d}{dt} \langle Z \rangle = \frac{\langle P_z \rangle}{m}$$

i.e.
$$\frac{d}{dt} \langle \vec{r} \rangle = \frac{\langle \vec{P} \rangle}{m}$$

Proof of
$$\frac{d}{dt} \langle \vec{P} \rangle = \langle -\vec{\nabla} V \rangle$$

The time rate of change of momentum along x- axis can be written as

$$\begin{aligned} \frac{d}{dt} \langle P_x \rangle &= \frac{d}{dt} \int \psi^* \left(-i\hbar \frac{\partial \psi}{\partial x} \right) d\tau \\ &= -i\hbar \int \frac{d}{dt} \left(\psi^* \frac{\partial \psi}{\partial x} \right) d\tau \\ &= -i\hbar \left[\int \psi^* \frac{\partial}{\partial t} \left(\frac{\partial \psi}{\partial x} \right) d\tau + \int \frac{\partial \psi^*}{\partial t} \frac{\partial \psi}{\partial x} d\tau \right] \\ &= -i\hbar \int \psi^* \frac{\partial}{\partial x} \left(\frac{\partial \psi}{\partial t} \right) d\tau + \int \frac{\partial \psi^*}{\partial t} \frac{\partial \psi}{\partial x} d\tau \\ &= - \int \psi^* \frac{\partial}{\partial x} \left(i\hbar \frac{\partial \psi}{\partial t} \right) d\tau + \int \left(-i\hbar \frac{\partial \psi^*}{\partial t} \right) \frac{\partial \psi}{\partial x} d\tau \quad (22) \end{aligned}$$

Using time dependent Schrödinger equation (10A) and its complex conjugate equation (11A) for equation (22)

$$\begin{aligned} &= - \int \psi^* \frac{\partial}{\partial x} \left(- \frac{\hbar^2}{2m} \nabla^2 \psi + V\psi \right) d\tau + \int \left(- \frac{\hbar^2}{2m} \nabla^2 \psi^* + V\psi^* \right) \frac{\partial \psi}{\partial x} d\tau \\ &= - \int \psi^* \left[\frac{\partial}{\partial x} (V\psi) - V \frac{\partial \psi}{\partial x} \right] d\tau \\ &= - \int \psi^* \left[V \frac{\partial \psi}{\partial x} + \psi \frac{\partial V}{\partial x} - V \frac{\partial \psi}{\partial x} \right] d\tau \\ &= - \int \psi^* \frac{\partial V}{\partial x} \psi d\tau \\ &= \int \psi^* \left(- \frac{\partial V}{\partial x} \right) \psi d\tau \end{aligned}$$

$$= \left\langle -\frac{\partial V}{\partial x} \right\rangle$$

i.e.,
$$\frac{d}{dt} \langle P_x \rangle = \left\langle -\frac{\partial V}{\partial x} \right\rangle$$

Similarly, we can prove that,

$$\frac{d}{dt} \langle P_y \rangle = \left\langle -\frac{\partial V}{\partial y} \right\rangle$$

$$\frac{d}{dt} \langle P_z \rangle = \left\langle -\frac{\partial V}{\partial z} \right\rangle$$

$$\therefore \frac{d}{dt} \langle \vec{P} \rangle = \langle -\vec{\nabla} V \rangle$$

Solved problems

Problem 1. Show that the function $\psi = \cos ax \cos by \cos cz$ is an eigen function of the Laplacian operator. What is the corresponding eigen value?

Solution. Laplacian operator $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$. Hence

$$\begin{aligned} \nabla^2 \psi &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} (\cos ax \cos by \cos cz) \\ &= (\cos by \cos cz \frac{\partial^2}{\partial x^2} (\cos ax) + \cos ax \cos cz \frac{\partial^2}{\partial y^2} (\cos by) + \cos ax \cos by \frac{\partial^2}{\partial z^2} (\cos cz)) \\ &= \cos by \cos cz (-a^2 \cos ax) + \cos ax \cos cz (-b^2 \cos by) + \cos ax \cos by (-c^2 \cos cz) \\ &\left[\because \frac{\partial^2}{\partial x^2} (\cos ax) = \frac{\partial}{\partial x} (-a \sin ax) = -a^2 \cos ax \text{ and so on} \right] \\ &= -(a^2 + b^2 + c^2) \cos ax \cos by \cos cz = -(a^2 + b^2 + c^2) \psi \end{aligned}$$

As $(a^2 + b^2 + c^2)$ is constant, hence the given function is an eigen function of Laplacian operator. Further eigen value = $-(a^2 + b^2 + c^2)$.

Problem 2. A particle is in motion along a line between $x = 0$ and $x = a$ with zero potential energy. At points for which $x < 0$ and $x > a$, the potential energy is infinite. The wave function for the particle in the n th state is given by $\psi_n = A \sin \frac{n\pi x}{a}$. find the expression for the normalized wave function.

Solution. The probability of finding the particle between x and $x + dx$ for n th state is given by

$$P_n \cdot dx = |\psi_n(x)|^2 \cdot dx$$

But the particle reside between $x = 0$ to $x = a$

Hence,
$$\int P_n dx = \int_0^a |\psi_n(x)|^2 dx = 1$$

Given
$$\psi_n(x) = A \sin \frac{n\pi x}{a}$$

$$\int P_n dx = \int_0^a A^2 \sin^2 \frac{n\pi x}{a} dx = 1$$

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

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

$$\therefore \frac{A^2}{2} \left[x - \frac{a}{2n\pi} \sin \frac{2n\pi x}{a} \right]_0^a = 1$$

$$\therefore \frac{A^2}{2} \cdot a = 1$$

$$\therefore A^2 \frac{2}{a}, A = \sqrt{\frac{2}{a}}$$

So the normalized wave function is

$$\psi_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

Problem 3. The normalized state of the free particle is represented by a wave function.

$$\psi(x) = N e^{-(x^2/2a^2)} e^{ikx}$$

I. Calculate normalization constant.

II. In what region of space, the probability of finding the particle is maximum?

Solution: (i) Normalisation condition can be written as

$$\int_{-\infty}^{+\infty} \psi^*(x)\psi(x) dx = 1$$

$$\therefore |N|^2 \int_{-\infty}^{+\infty} (e^{-x^2/2a^2} e^{-ikx})(e^{-x^2/2a^2} e^{-ikx}) dx = 1$$

$$\therefore |N|^2 \int_{-\infty}^{+\infty} (e^{-x^2/a^2}) dx = 1$$

$$\therefore |N|^2 a\sqrt{\pi} = 1$$

$$[\text{Since } \int_{-\infty}^{+\infty} e^{-x^2/a^2} dx = a\sqrt{\pi}]$$

$$\therefore |N|^2 = \frac{1}{a\sqrt{\pi}}$$

$$\therefore N = \frac{1}{\sqrt{a\sqrt{\pi}}}$$

Problem 4. What is the lowest energy that a neutron (mass 1.67×10^{-27} kg) can have if confined to move along the edge of an impenetrable box of length 10^{-14} meter? ($h=6.63 \times 10^{-34}$ joule-sec).

Solution. The quantised energies of a particle of mass m in a one-dimensional box of length L are given by

$$E_n = \frac{n^2 h^2}{8mL^2} \quad n = 1, 2, 3, \dots$$

The lowest energy corresponds to $n = 1$, and is thus

$$E_1 \frac{h^2}{8mL^2}$$

Substituting the given values, we have

$$\begin{aligned} E_1 &= \frac{(6.63 \times 10^{-34} \text{ joule} - \text{sec})^2}{8 \times (1.67 \times 10^{-27} \text{ kg}) \times (10^{-14} \text{ meter})^2} \\ &= 3.29 \times 10^{-13} \text{ joule} \\ &= \frac{3.29 \times 10^{-13}}{1.6 \times 10^{-13}} \\ &(\because \text{MeV} = 1.6 \times 10^{-12} \text{ joule}) \\ &= \mathbf{2.06 \text{ Mev.}} \end{aligned}$$

Problem 5. 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 is 9.1×10^{-31} kg and $h = 6.63 \times 10^{-34}$ joule-sec).

Solution. 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

$$L = n \frac{\lambda}{2}, \quad n = 1, 2, 3, \dots$$

or
$$\lambda = \frac{2L}{n}.$$

Here
$$L = 10^{-9} \text{ meter} = 10 \text{ \AA}$$

$$\therefore \lambda = \frac{2 \times 10 \text{ \AA}}{n}, \quad n = 1, 2, 3, \dots$$

$$= 20 \text{ \AA}, 10 \text{ \AA}, 6.7 \text{ \AA}, \dots$$

The corresponding energies are given by

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

Here $m = 9.1 \times 10^{-31}$ kg and $L = 10^{-9}$ meter.

$$\begin{aligned} \therefore E_n &= \frac{(6.63 \times 10^{-34})^2 n^2}{8 \times (9.1 \times 10^{-31}) \times (10^{-9})^2} \\ &= 6.04 \times 10^{-20} n^2 \text{ joule} \\ \frac{6.04 \times 10^{-20} n^2}{1.6 \times 10^{-19}} &= 0.38 n^2 \text{ eV.} \end{aligned}$$

For $n = 1, 2, 3$, we have

$$E_1 = 0.38 \text{ eV}, E_2 = 1.52 \text{ eV}, E_3 = 3.42 \text{ eV}.$$

Problem 6. Find the probabilities of finding a particle trapped in a box of length L in the region from $0.45 L$ to $0.55 L$ for the ground state and the first excited state.

Solution. The eigenfunctions of a particle trapped in a box of length L are

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

The probability of finding the particle between x_1 and x_2 , when it is in the n th state, is

$$\begin{aligned} P &= \int_{x_1}^{x_2} |\psi_n|^2 dx \\ &= \frac{2}{L} \int_{x_1}^{x_2} \sin^2 \frac{n\pi x}{L} dx \\ &= \frac{2}{L} \int_{x_1}^{x_2} \frac{1}{2} \left(1 - \cos \frac{2n\pi x}{L}\right) dx \\ &= \frac{1}{L} \left[x - \frac{L}{2n\pi} \sin \frac{2n\pi x}{L} \right]_{x_1}^{x_2} \end{aligned}$$

Here $x_1 = 0.45L$, $x_2 = 0.55L$ and for the ground state, $n = 1$,

$$\begin{aligned}
 \therefore \quad P &= \frac{1}{2} \left[x - \frac{L}{2\pi} \sin \frac{2\pi x}{L} \right]_{0.22L}^{0.45L} \\
 &= \frac{1}{2} \left[\left(0.55L - \frac{L}{2\pi} \sin 1.10 \pi \right) - \left(0.45L - \frac{L}{2\pi} \sin 0.90 \pi \right) \right] \\
 &= \left[\left(0.55 - \frac{1}{2\pi} \sin 198^\circ \right) - \left(0.45 - \frac{1}{2\pi} \sin 162^\circ \right) \right] \\
 &= (0.55 - 0.45) - \frac{1}{2\pi} (\sin 198^\circ - \sin 162^\circ) \\
 &= (0.55 - 0.45) - \frac{1}{2\pi} (\sin 198^\circ - \sin 162^\circ) \\
 &= 0.10 - \frac{1}{\pi} (\cos 180^\circ \sin 18^\circ) \\
 &= 0.10 + \frac{0.3090}{3.14} = 0.198 = \mathbf{19.8 \%}.
 \end{aligned}$$

For the first excited state ($n=2$), we shall have **P=065% (Try)**.

Exercise

(A) Descriptive type

- (1) Write down Schrodinger's time independent equation for a particle of energy E and mass m . Explain the restrictions imposed on the Eigen functions before they are accepted as valid solutions.
(L.U. 2007)
- (2) An electron is confined to move between two rigid walls separated by 10^{-9} m. Find the de-Broglie wavelengths representing the first three allowed energy states of the electron and the corresponding energies.
(L.U. 2014)
- (3) Explain the term 'Normalisation'. What is meant by the Expectation Value of a dynamical variable? Give its physical meaning.
(L.U. 2007)
- (4) Explain physical significance of wave function. What are orthogonal wave functions?
(L.U. 2008)
- (5) Explain physical significance of wave function. What are orthogonal wave functions?
(L.U. 2009)
- (6) Establish the time independent form of Schrodinger wave equation.
(L.U. 2009)
- (7) Explain physical significance of the wave function.
(L.U. 2010)
- (8) Establish the time independent form the Schrodinger wave equation.
(L.U. 2011)
- (9) State and prove Ehrenfest's theorem.
(LU 2015)

- (10) Find the value of A for which wave function : $\psi = A \sin \left[\frac{n\pi x}{a} \right]$ is normalized in the region $0 \leq x \leq a$
(L.U. 2010)
- (11) Explain the physical significance of the wave function ψ . What are orthogonal wave functions?
(L.U. 2012)
- (12) Establish the time independent form of Schrodinger wave equation.
(L.U. 2012)
- (13) Describe the concept of wave function and its physical significance. Also derive equation of motion for wave function ψ . transmission through barrier.
(L.U. 2014)
- (14) Establish three dimensional time dependent form of Schrodinger wave equation for particle moving in a potential field.
(L.U. 2014)
- (15) What are limitations of classical mechanics? Give an account of eigen functions and eigen values.
(L.U. 2014)

Short answer type

- (1) Write down postulates of quantum mechanics.
(L.U. 2011)
- (2) Write down postulates of quantum mechanics. (vi) Write down operator equivalent for energy.
(L.U. 2010)
- (3) State Ehrenfest Theorem.
(L.U. 2009)
- (4) Write down operator equivalent for energy and momentum.
(L.U. 2011)
- (5) State Ehrenfest Theorem.
(L.U. 2011)

- (6) What is quantum mechanical tunneling? (L.U. 2011)
- (7) Show that the wave function $\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$ is orthogonal. (L.U. 2011)
- (8) Explain physical significance of wave function. (L.U. 2011)
- (9) What do you mean by normalization of wave function? (L.U. 2011)
- (10) State 'Ehrenfest theorem'. (L.U. 2012)
- (11) Write down the quantum operator for kinetic energy of a system. (L.U. 2012)
- (12) List the postulates of quantum mechanics. (L.U., 2014)
- (13) Write down the energy and momentum operator. (L.U. 2008)
- (14) State the various conditions for the acceptability of a wave function. (L.U. 2014)
- (15) State Ehrenfest theorem. (L.U. 2008)
- (16) Show that we wave function $\psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi X}{L}$ are orthogonal. (L.U. 2008)
- (17) What do you mean by :
- (i) Expectation value of a dynamical variable. (L.U. 2008)
 - (ii) Normalisation of a wave function? (L.U. 2008)
- (18) Give mathematical expression of a wave equivalent of an unrestricted particle of total energy E and momentum P moving in the +X direction. (L.U. 2009)
- What do you mean by Eigen function and Eigen value? (L.U. 2010)

- (19) Write down the three-dimensional time dependent Schrödinger wave equation for a particle moving in potential field. **(L.U. 2010)**
- (20) What do you mean by normalization of wave function? **(L.U. 2010)**
- (21) Explain the term 'Normalisation'. **(L.U. 2012)**
- (22) Discuss the principle of superposition. **(L.U. 2013)**
- (23) What is meant by an orthonormal set of Eigen functions? **(L.U. 2013)**
- (24) Derive the stationary state Schrodinger equation. **(L.U. 2013)**
- (25) Find the expectation value of the linear momentum of the particle. **(L.U. 2013)**
- (26) What are eigen values and eigen functions? **(L.U. 2015)**
- (27) What are expectation values.? **(L.U. 2015)**
- (28) What to you mean by Normalisation of wave function? **(L.U. 2016)**
- (29) Find the lowest energy of a neutron confined to a box of 10^{-15} m side. **(LU 2016)**

Chapter 5

Applications of Schrödinger equation

5.1 Particle in a Box

A particle is trapped in a box with infinitely hard walls. The particle is restricted to move along x axis between $x = 0$ and $x = L$. The particle is bouncing back and forth within the box by colliding infinitely hard walls of the box. Since the particle will not lose energy by colliding with such walls, therefore the total energy of the particle remains constant. We are considering the one dimensional case of the problem.

The potential function inside & outside the box is defined as-

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

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

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

for this particle we have to calculate the wave function associated with the wave packet of the moving particle & eigen values of energy for the particle.

Schrodinger equation for the particle in a box can be written as

$$\frac{d^2\psi}{d\psi^2} + \frac{2mE}{\hbar^2}\psi = 0 \quad (1)$$

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

$$\text{where } k^2 = \frac{2mE}{\hbar^2} \quad (3)$$

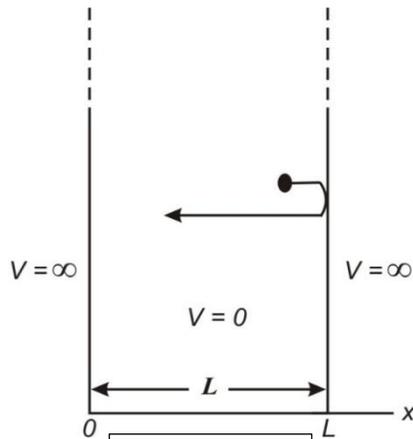


Fig. 5.1

The solution of equation (1) is given as

$$\psi = A \sin kx + B \cos kx \quad (4)$$

The constants A and B can be evaluated by the following boundary conditions.

Boundary conditions are

$$\psi = 0 \text{ at } x = 0 \quad (5a)$$

$$\psi = 0 \text{ at } x = L \quad (5b)$$

using (5a) for equation (4), we have

$$0 = A \sin kx_0 + B \cos kx_0$$

$$\therefore 0 = A \sin 0 + B \cos 0$$

$$\therefore B = 0 \quad (6)$$

Using equation (7) for equation (4), we have

$$\psi = A \sin kx \quad (7)$$

using boundary condition (6b) for equation (7)

$$A \sin kL = 0$$

$$\text{or } \sin kL = 0$$

$$\text{or } \sin kL = \sin n\pi$$

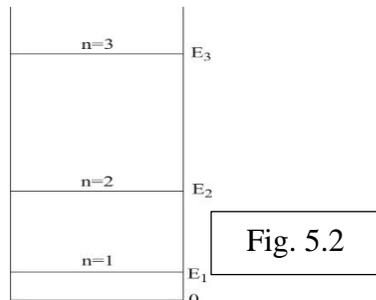
$$\text{or } kL = n\pi$$

$$k = \frac{n\pi}{L} \quad (8)$$

Using (9) for (3)

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

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



Writing E_n for E in the above equation, we have

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

Equation (9) shows that in a deep potential well, the particle can not take any value of energy but can have certain discrete values of energy corresponding to $n = 1, 2, 3, \dots$. These values of energy are called eigen values of the particle and constitute energy levels of the system. n is called quantum numbers.

Calculation for the wave function

From equation (7)

$$\psi = A \sin kx$$

Since the particle will be found definitely within the box, therefore the probability of finding the particle within the box will be unity i.e.

$$\int_0^L \psi^* \psi dx = 1 \quad (10)$$

Here $\psi = A \sin kx$

$$\text{and } \psi^* = A^* \sin kx$$

\therefore from equation (10)

$$\int_0^L (A \sin kx) (A^* \sin kx) dx = 1$$

$$\text{or } \int_0^L AA^* \sin^2 kx dx = 1$$

$$\text{or } AA^* \int_0^L \sin^2 kx dx = 1$$

$$\text{or } |A|^2 \int_0^L \left(\frac{1 - \cos 2kx}{2} \right) dx = 1$$

$$\text{or } \frac{|A|^2}{2} \int_0^L (1 - \cos 2kx) dx = 1$$

$$\text{or } \frac{|A|^2}{2} \left(x - \frac{\sin 2kx}{2} \right)_0^L = 1$$

or $\frac{A^2}{2} \left[L - \frac{\sin(2n\pi/L)L}{2} \right] = 1$

or $\frac{A^2}{2} [L - \sin n\pi] = 1$

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

or $\frac{A^2}{2} L = 1$

$\therefore A = \sqrt{\frac{2}{L}}$ (11)

Using (9) and (12) for equation (8), we get

$$\Psi = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

Writing Ψ_n for Ψ in the above equation, we have

$$\Psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \quad (12)$$

Since Ψ_n is normalised, therefore $|\Psi_n|^2$ represents the probability of finding the particle inside the box at a particular place and at a particular time. Three graphs corresponding to $n = 1, 2, 3$, as shown in Fig... are obtained when $|\Psi_n|^2$ is plotted with x .

This is obvious from the graphs that-

- (a) $|\Psi_n|^2 = 0$ at $x = 0$ and at $x = L$, i.e., $|\Psi_n|^2 = 0$ at the boundaries of the box.
- (b) $|\Psi_1|^2$ has its maximum value of $2/L$ in the middle of the box, i.e., a

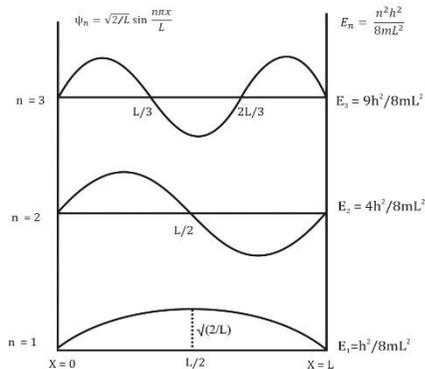


Fig. 5.3

particle in the lowest energy level of $n = 1$ is most likely in the middle of the box.

- (c) $|\Psi_2|^2 = 0$ in the middle of the box, i.e, a particle corresponding to energy level $n = 2$ is never present in the middle of the box.

This is noteworthy here that-

- (a) According to classical physics, the probability of finding the particle inside the box will be same everywhere which is contrary to the predictions of quantum mechanics.
- (b) Under the similar conditions, the forms and results in connection with waves formed in a stretched string and the matter wave associated with the particle trapped in 'the box' are same.

5.2 Step Potential

One dimensional Step potential is defined by the following conditions

$$V(x) = 0 \text{ for } x < 0$$

$$V(x) = V_0 \text{ for } x > 0$$

Case I $E > V_0$

The particle moves like a free particle in the region $x < 0$ but it approached the step potential towards the right i.e. $x > 0$, it has to face a potential hill or step or barrier of height (potential energy) $V(x) = V_0$. A one-dimensional potential step or barrier is shown in the Fig. 5.4.

There is a discontinuity at $x = 0$.

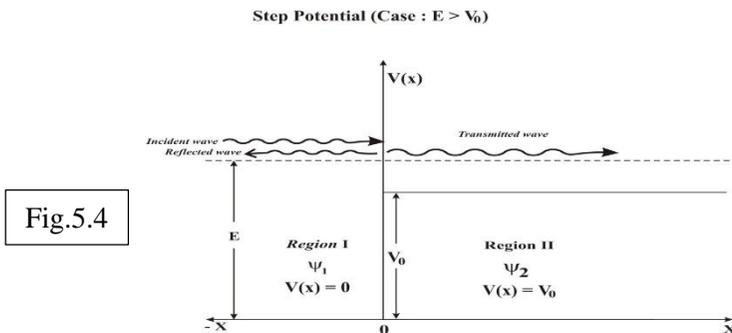


Fig.5.4

Classical view point.

According to classical mechanics the particle in having energy $E > V_0$ travelling in region I in the +ve x - direction will experience a retarding force $F = -dV/dx$ at the point $x = 0$, this force will slow down the motion of the particle in the +ve direction of x but the particles will keep moving and enter the region II i.e. $x > 0$.

The momentum of the particles in region I ($x < 0$) is given by

Total energy = kinetic energy + Potential ener

$$E = T + V$$

$$E = T + 0$$

(since in the first region, $V = 0$)

$$\therefore E = T = \frac{1}{2} m v_1^2 = \frac{m^2 v_1^2}{2m} = \frac{P_1^2}{2m}$$

where p_1 and v_1 are momentum and velocity of the particles respectively in the I region.

$$\therefore E = \frac{P_1^2}{2m}$$

$$\text{or } P_1 = \sqrt{2mE} \quad (1)$$

The momentum of the particles in region I ($x > 0$) is given by

Total energy = kinetic energy + Potential energy

$$E = T + V$$

$$E = T + V_0$$

(since in the first region, $V = V_0$)

$$\therefore T = E - V_0 = \frac{1}{2} m v_2^2 = \frac{m^2 v_2^2}{2m} = \frac{P_2^2}{2m}$$

$$\therefore E - V_0 = \frac{P_2^2}{2m}$$

$$P_2 = \sqrt{2m(E - V_0)} \quad (2)$$

where P_2 and v_2 are momentum and velocity of the particles respectively in the II region.

It is obvious that $P_2 < P_1$

According to classical mechanics, The velocity of particle in region II will be less than that in region I but the particle with $E < V_0$ will always be transmitted.

The change in potential from 0 to V_0 at $x = 0$ only provides a retarding force which reduces the speed of the particle

Quantum Mechanical View point

According to Quantum Mechanics the motion of the particle is governed by Schrodinger wave equation for region I & II. As the potential V_0 is independent of time we have to solve Schrödinger time independent wave equation to analyse the behaviours of the particle.

Schrodinger wave equation in one dimension is given by

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

Region I

Equation (3) for the I region can be written as

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2} \psi = 0 \quad (\text{since in the I region } V = 0) \quad (4)$$

$$\frac{\partial^2 \psi}{\partial x^2} + k_1^2 \psi = 0 \quad (5)$$

where $k_1^2 = \frac{2mE}{\hbar^2}$ (k_1 is the propagation constant in the I region)

$$k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$k_1 = \frac{P_1}{\hbar} \quad (\text{since in the I region, } P_1 = \sqrt{2mE}) \quad (6)$$

Region II

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V_0) \psi = 0 \quad (\text{since in the II region } V = V_0) \quad (7)$$

$$\text{or} \quad \frac{\partial^2 \psi}{\partial x^2} + k_2^2 \psi = 0 \quad (8)$$

where $k_2^2 = \frac{2m(E - V_0)}{\hbar^2}$ (k_2 is the propagation constant in the II region)

$$k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar}$$

$$k_2 = \frac{P_2}{\hbar} \quad (\text{since in the I region, } P_1 = \sqrt{2mE})$$

The solutions of equations (5) & (7) can be expressed as

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x} \quad (10)$$

$$\psi_2 = Ce^{ik_2x} + De^{-ik_2x} \quad (11)$$

In equation (10)

Ae^{ik_1x} → Represents incident wave moving along +ve x - direction in the I region.

Be^{-ik_1x} → Represents reflected wave from $x = 0$, moving along -ve x - direction in the I region.

In equation (11)

Ce^{ik_2x} → Represents transmitted wave from $x = 0$, moving along +ve x-direction in the II region.

$De^{-ik_2x} = 0$, since there is no reflected wave in the II region.

Therefore eqⁿ (11) becomes

$$\psi_2 = Ce^{ik_2x} \quad (12)$$

Since infinite energy and mass does not exist in nature. Therefore from eqⁿ (5) & (7) ψ_1 & ψ_2 must be finite & continuous. If ψ_1 & ψ_2 are continuous then their derivatives with respect to x must also be continuous. In the light of above facts we can write boundary conditions as following.

$$\psi_1 = \psi_2 \text{ at } x = 0 \quad (13)$$

$$\frac{\partial \psi_1}{\partial x} = \frac{\partial \psi_2}{\partial x} \quad \text{at } x = 0 \quad (14)$$

Applying boundary condition (13) for equations (10) and (12), we have,

$$A + B = C \quad (15)$$

Differentiating equations (10) and (12) with respect to x , we have,

$$\frac{\partial \psi_1}{\partial x} = ik_1 A e^{ik_1 x} - ik_1 B e^{-ik_1 x} \quad (16)$$

$$\frac{\partial \psi_2}{\partial x} = ik_2 C e^{ik_2 x} \quad (17)$$

Applying boundary condition (14) for equations (16) and (17), we have,

$$\left(\frac{\partial \psi_1}{\partial x} \right)_{x=0} = \left(\frac{\partial \psi_2}{\partial x} \right)_{x=0} \quad (18)$$

$$ik_1 A e^{ik_1 x 0} - ik_1 B e^{-ik_1 x 0} = ik_2 C e^{ik_2 x 0}$$

$$k_1(A - B) = k_2 C \quad (19)$$

$$A - B = \frac{k_2}{k_1} C \quad (20)$$

Solving equations (15) & (20)

$$A + B = C \quad (15)$$

$$A - B = \frac{k_2}{k_1} C \quad (20)$$

Adding eq. (15) and eq.(20), we have,

$$2A = \left[1 + \frac{k_2}{k_1} \right] C$$

$$\begin{aligned}\therefore 2A &= \left[\frac{k_1+k_2}{k_1} \right] C \\ \therefore C &= \left[\frac{2k_1}{k_1+k_2} \right] A\end{aligned}\quad (21)$$

Subtracting eq. (20) from eq.(15), we have,

$$\begin{aligned}2B &= \left[1 - \frac{k_2}{k_1} \right] C \\ \therefore 2B &= \left[\frac{k_1-k_2}{k_1} \right] C \\ \therefore C &= \left[\frac{2k_1}{k_1-k_2} \right] B\end{aligned}\quad (22)$$

Using (22) for (21), we have,

$$\begin{aligned}\left[\frac{2k_1}{k_1+k_2} \right] A &= \left[\frac{2k_1}{k_1-k_2} \right] B \\ \therefore B &= \left[\frac{k_1-k_2}{k_1+k_2} \right] A\end{aligned}\quad (23)$$

Reflectance (R)

Reflectance (R) is defined as

$$R = \frac{\text{Magnitude of the reflected probability density current } (S_{re})}{\text{Magnitude of the incident probability density current } (S_{in})} \quad (24)$$

$$\text{or} \quad R = \frac{S_{re}}{S_{in}} \quad (25)$$

Transmittance (T)

Transmittance (T) is defined as

$$T = \frac{\text{Magnitude of the transmitted probability density current } (S_{tr})}{\text{Magnitude of the incident probability density current } (S_{in})} \quad (26)$$

$$\text{or} \quad T = \frac{S_{tr}}{S_{in}} \quad (27)$$

Probability current density is defined by

$$S = v \psi \psi^* \quad (28)$$

Where v is particle velocity

Ψ is the wave function

ψ^* is the complex conjugate of the wave function

Incident probability current density is defined by

$$S_{in} = v_1 \psi_{in} \psi_{in}^* \quad (29)$$

Where v_1 is particle velocity

ψ_{in} is the wave function corresponding to the incident beam of the particles

ψ_{in}^* is the complex conjugate of the ψ_{in}

Reflected probability current density is defined by

$$S_{re} = v_1 \psi_{re} \psi_{re}^* \quad (30)$$

Where v_1 is particle velocity in the I region

ψ_{re} is the wave function corresponding to the reflected beam of the particles

ψ_{re}^* is the complex conjugate of the ψ_{re}

Transmitted probability current density is defined by

$$S_{tr} = v_2 \psi_{tr} \psi_{tr}^* \quad (31)$$

Where v_2 is particle velocity in the II region

ψ_{tr} is the wave function corresponding to the reflected beam of the particles

ψ_{tr}^* is the complex conjugate of the ψ_{tr}

Note; Probability current density is also defined as

$$S = \frac{\hbar}{2im} [\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^*] \quad (32)$$

From equation (10)

$$\psi_{in} = Ae^{ik_1x} \quad (32)$$

$$\Psi_{in}^* = A^* e^{-ik_1 x} \quad (33)$$

$$\Psi_{re} = B e^{-ik_1 x} \quad (34)$$

$$\Psi_{re}^* = B^* e^{ik_1 x} \quad (35)$$

From equation (12)

$$\Psi_{tr} = C e^{ik_2 x} \quad (36)$$

$$\Psi_{tr}^* = C^* e^{-ik_2 x} \quad (37)$$

Using equations (32), (33) for equation (29), we have,

$$\begin{aligned} S_{in} &= v_1 \Psi_{in} \Psi_{in}^* \\ S_{in} &= v_1 (A e^{ik_1 x}) (A^* e^{-ik_1 x}) \\ S_{in} &= v_1 A A^* \end{aligned} \quad (38)$$

Using equations (34), (35) for equation (30), we have,

$$\begin{aligned} S_{re} &= v_1 \Psi_{re} \Psi_{re}^* \\ S_{re} &= v_1 (B e^{-ik_1 x}) (B^* e^{ik_1 x}) \\ S_{re} &= v_1 B B^* \end{aligned} \quad (39)$$

Using equations (36), (37) for equation (31), we have,

$$\begin{aligned} S_{tr} &= v_2 \Psi_{tr} \Psi_{tr}^* \\ S_{tr} &= v_2 (C e^{ik_2 x}) (C^* e^{-ik_2 x}) \\ S_{tr} &= v_2 C C^* \end{aligned} \quad (40)$$

Using equations (38), (39) for equation (25), we have,

$$\begin{aligned} R &= \frac{S_{re}}{S_{in}} \\ \therefore R &= \frac{v_1 B B^*}{v_1 A A^*} \end{aligned}$$

$$\therefore R = \frac{|B|^2}{|A|^2} \quad (41)$$

Using equation (23) for equation (41)

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 \quad (42)$$

Using equations (38), (40) for equation (27), we have,

$$\begin{aligned} T &= \frac{S_{tr}}{S_{in}} \\ \therefore T &= \frac{v_2 CC^*}{v_1 AA^*} \\ \therefore T &= \frac{P_2/m(CC^*)}{P_1/m(AA^*)} \\ \therefore T &= \frac{P_2 CC^*}{P_1 AA^*} \\ \therefore T &= \frac{P_2 |C|^2}{P_1 |A|^2} \\ \therefore T &= \frac{\hbar k_2 |C|^2}{\hbar k_1 |A|^2} \\ \therefore T &= \frac{k_2 |C|^2}{k_1 |A|^2} \end{aligned}$$

Using equation (21) for equation (41)

$$\begin{aligned} T &= \frac{k_2}{k_1} \left(\frac{2k_1}{k_1 + k_2} \right)^2 \\ T &= \frac{4k_1 k_2}{(k_1 + k_2)^2} \quad (43) \end{aligned}$$

The above analysis shows that there is some probability of reflection from $x = 0$, as far as Quantum Mechanical considerations are concerned as $R \neq 0$ from (24) & (25).

It is obvious that-

$$R + T = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 + \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

$$R + T = \frac{(k_1 - k_2)^2 - 4k_1 k_2}{(k_1 + k_2)^2}$$

$$= \frac{(k_1 + k_2)^2}{(k_1 + k_2)^2} = 1$$

$$\therefore R + T = 1 \quad (44)$$

Case II when $E < V_0$

As discussed in the previous case, one dimensional Step potential is defined by the following conditions.

$$V(x) = 0 \text{ for } x < 0$$

$$V(x) = V_0 \text{ for } x > 0$$

We will discuss this problem when the total energy of the particle is less than that of the height of the potential barrier-

Step Potential (Case : $E < V_0$)

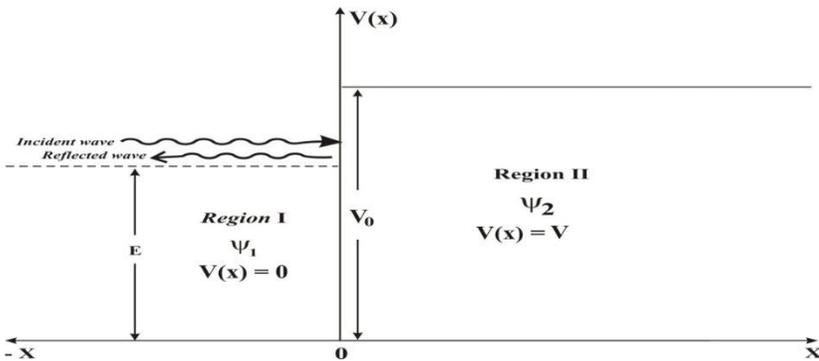


Fig. 5.5

The momentum of the particles in region I ($x < 0$) is given by

Total energy = kinetic energy + Potential energy

$$E = T + V$$

$$E = T + 0$$

(since in the first region, $V = 0$)

$$\therefore E = T = \frac{1}{2} m v_1^2 = \frac{m^2 v_1^2}{2m} = \frac{P_1^2}{2m}$$

where P_1 and v_1 are momentum and velocity of the particles respectively in the I region.

$$\therefore E = \frac{P_1^2}{2m}$$

$$\text{or } P_1 = \sqrt{2mE} \quad (1)$$

The momentum of the particles in region I ($x > 0$) is given by

Total energy = kinetic energy + Potential energy

$$E = T + V$$

$$E = T + V_0$$

(since in the first region, $V = 0$)

$$\therefore T = E - V_0 = \frac{1}{2} m v_2^2 = \frac{m^2 v_2^2}{2m} = \frac{P_2^2}{2m}$$

But as $E < V_0$, therefore $E - V_0$ will be -ve, i.e., T (K.E.) is -ve which is not possible, therefore in this case we will write the following equation for the K.E.

$$T = V_0 - E$$

$$\therefore V_0 - E = \frac{P_2^2}{2m}$$

$$\therefore P_2 = \sqrt{2m(V_0 - E)} \quad (2)$$

where P_2 and v_2 are momentum and velocity of the particles respectively in the II region.

It is obvious that $P_2 < P_1$

According to classical mechanics, The velocity of particle in region II will be less than that in region I but the particle with $E < V_0$ will always be transmitted.

The change in potential from 0 to V_0 at $x = 0$ only provides a retarding force which reduces the speed of the particle

Classical mechanical view point

According to classical mechanics the particle in having energy $E < V_0$ travelling in region I in the +ve x - direction will experience a retarding force $F = -dV/dx$ in the x direction, this force will slow down the motion of the particle in the +ve direction of x . Moreover since $E < V_0$, therefore according to classical mechanics, the particle can not penetrate into region II. This is because in region II

$$\therefore T = E - V_0 = \frac{1}{2} m v_2^2 = \frac{m^2 v_2^2}{2m} = \frac{P_2^2}{2m}$$

Since $E < V_0$, therefore,

$$\frac{P_2^2}{2m} < 0,$$

The above relation implies that kinetic energy is -ve which is meaningless, moreover $P_2^2 < 0$, which means P_2 or momentum of the particle in the II region is an imaginary quantity, which is again meaningless. Therefore this is obvious that that the particle can not enter in the II region and will be completely reflected at $x = 0$.

Quantum Mechanical View point

According to Quantum Mechanics the motion of the particle is governed by Schrodinger wave equation for region I & II. As the potential V_0 is independent of time we have to solve Schrödinger time independent wave equation to analyse the behaviours of the particle.

Schrodinger wave equation in one dimension is given by

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

Region I

Equation (3) for the I region can be written as

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2} \psi = 0 \quad (\text{since in the I region } V = 0) \quad (4)$$

$$\therefore \frac{\partial^2 \psi}{\partial x^2} + k_1^2 \psi = 0 \quad (5)$$

where $k_1^2 = \frac{2mE}{\hbar^2}$ (k_1 is the propagation constant in the I region)

$$\therefore k_1 = \frac{\sqrt{2mE}}{\hbar}$$

$$k_1 = \frac{P_1}{\hbar} \quad (\text{since in the I region, } P_1 = \sqrt{2mE}) \quad (6)$$

Region II

Equation (3) for the region II will be written as

$$\frac{\partial^2 \psi}{\partial x^2} - \frac{2m}{\hbar^2} (V_0 - E) \psi = 0 \quad (7) \quad (\text{since in the II region } V = V_0)$$

$$\therefore \frac{\partial^2 \psi}{\partial x^2} - k_2^2 \psi = 0 \quad (8)$$

where $k_2^2 = \frac{2m(V_0 - E)}{\hbar^2}$ (k_2 is the propagation constant in the II region)

$$\therefore k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \quad (9)$$

$$\therefore k_2 = \frac{P_2}{\hbar} \quad (\text{since in the I region, } P_1 = \sqrt{2mE})$$

The solutions of equations (5) & (7) can be expressed as

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x} \quad (10)$$

$$\psi_2 = Ce^{-k_2x} + De^{k_2x} \quad (11)$$

In equation (10)

$Ae^{ik_1x} \rightarrow$ Represents incident wave moving along +ve x - direction in the I region.

$Be^{-ik_1x} \rightarrow$ Represents reflected wave from $x = 0$, moving along $-ve x$ - direction in the I region.

In equation (11)

Where C and D are arbitrary constants. The wave function ψ_2 becomes infinite as $x \rightarrow \infty$ due to presence of De^{k_2x} , in order that ψ_2 may remain finite, we must have $D = 0$. Substituting $D = 0$ in equation (11), we get

$$\psi_2 = Ce^{-k_2x} \quad (12)$$

Since infinite energy and mass does not exist in nature. Therefore from eqⁿ (5) & (7) ψ_1 & ψ_2 must be finite & continuous. If ψ_1 & ψ_2 are continuous then their derivatives with respect to x must also be continuous. In the light of above facts we can write boundary conditions as following.

$$\psi_1 = \psi_2 \text{ at } x = 0 \quad (13)$$

$$\frac{\partial\psi_1}{\partial x} = \frac{\partial\psi_2}{\partial x} \text{ at } x = 0 \quad (14)$$

Applying boundary condition (13) for equations (10) and (12), we have,

$$A + B = C \quad (15)$$

Differentiating equations (10) and (12) with respect to x , we have,

$$\frac{\partial\psi_1}{\partial x} = ik_1Ae^{ik_1x} - ik_1Be^{-ik_1x} \quad (16)$$

$$\frac{\partial\psi_2}{\partial x} = -k_2Ce^{-k_2x} \quad (17)$$

Applying boundary condition (14) for equations (16) and (17), we have,

$$\left(\frac{\partial\psi_1}{\partial x}\right)_{x=0} = \left(\frac{\partial\psi_2}{\partial x}\right)_{x=0} \quad (18)$$

$$\therefore ik_1Ae^{ik_1x0} - ik_1Be^{-ik_1x0} = -k_2Ce^{-k_2x0}$$

$$\therefore ik_1(A - B) = -k_2C \quad (19)$$

$$\therefore A - B = \frac{-k_2}{ik_1} C$$

$$\therefore A - B = i \frac{k_2}{k_1} C \quad (20)$$

Solving equations (15) & (20)

$$A + B = C \quad (15)$$

$$A - B = i \frac{k_2}{k_1} C \quad (20)$$

Adding equations (15) and (20), we have,

$$2A = \left[1 + i \frac{k_2}{k_1}\right] C$$

$$\therefore 2A = \left[\frac{k_1 + ik_2}{k_1}\right] C$$

$$C = \left[\frac{2k_1}{k_1 + ik_2}\right] A$$

$$\therefore C = \left[\frac{2ik_1}{ik_1 - k_2}\right] A \quad (21)$$

Subtracting eq. (20) from eq. (15), we have,

$$2B = \left[1 - i \frac{k_2}{k_1}\right] C$$

$$\therefore 2B = \left[\frac{k_1 - ik_2}{k_1}\right] C$$

$$\therefore 2B = \left[\frac{ik_1 + k_2}{ik_1}\right] C$$

$$\therefore C = \left[\frac{ik_1}{ik_1 + k_2}\right] B \quad (22)$$

Using (22) for (21), we have,

$$\therefore \left[\frac{2ik_1}{ik_1 - k_2}\right] A = \left[\frac{ik_1}{ik_1 + k_2}\right] B$$

$$\therefore B = \left[\frac{ik_1 + k_2}{ik_1 - k_2}\right] A \quad (23)$$

Using equations (21) and (23) for equations (10) and (11), we get,

$$\psi_1 = Ae^{ik_1x} + A \left[\frac{ik_1+k_2}{ik_1-k_2} \right] e^{-ik_1x} \quad (24)$$

$$\& \quad \psi_2 = A \left[\frac{2ik_1}{ik_1-k_2} \right] e^{-k_2x} \quad (25)$$

Reflectance (R)

Reflectance (R) is defined as

$$R = \frac{\text{Magnitude of the reflected probability density current } (S_{re})}{\text{Magnitude of the incident probability density current } (S_{in})} \quad (26)$$

$$\text{or} \quad R = \frac{S_{re}}{S_{in}} \quad (27)$$

Probability current density is defined by

$$S = v \psi \psi^* \quad (28)$$

Where v is particle velocity

Ψ is the wave function

Ψ^* is the complex conjugate of the wave function

Incident probability current density is defined by

$$S_{in} = v_1 \psi_{in} \psi_{in}^* \quad (29)$$

Where v_1 is particle velocity

ψ_{in} is the wave function corresponding to the incident beam of the particles

ψ_{in}^* is the complex conjugate of the ψ_{in}

Reflected probability current density is defined by

$$S_{re} = v_1 \psi_{re} \psi_{re}^* \quad (30)$$

Where v_1 is particle velocity in the I region

ψ_{re} is the wave function corresponding to the reflected beam of the particles

ψ_{re}^* is the complex conjugate of the ψ_{re}

From equation (12)

$$\Psi_{\text{in}} = A e^{ik_1 x} \quad (31)$$

$$\Psi_{\text{in}}^* = A^* e^{-ik_1 x} \quad (32)$$

$$\Psi_{\text{re}} = A \left[\frac{ik_1 + k_2}{ik_1 - k_2} \right] e^{-ik_1 x} \quad (33)$$

$$\Psi_{\text{re}}^* = A^* \left[\frac{-ik_1 + k_2}{-ik_1 - k_2} \right] e^{-ik_1 x} \quad (34)$$

Using equations (31), (32) for equation (29), we have,

$$\begin{aligned} S_{\text{in}} &= v_1 \Psi_{\text{in}} \Psi_{\text{in}}^* \\ S_{\text{in}} &= v_1 (A e^{ik_1 x}) A^* e^{-ik_1 x} \\ S_{\text{in}} &= v_1 A A^* \end{aligned} \quad (35)$$

Using equations (33), (34) for equation (30), we have,

$$\begin{aligned} S_{\text{re}} &= v_1 \Psi_{\text{re}} \Psi_{\text{re}}^* \\ S_{\text{re}} &= v_1 \left(A \left[\frac{ik_1 + k_2}{ik_1 - k_2} \right] e^{-ik_1 x} \right) \left(A^* \left[\frac{-ik_1 + k_2}{-ik_1 - k_2} \right] e^{ik_1 x} \right) \\ S_{\text{re}} &= v_1 A A^* \left[\frac{ik_1 + k_2}{ik_1 - k_2} \right] \left[\frac{-ik_1 + k_2}{-ik_1 - k_2} \right] \end{aligned} \quad (36)$$

Using equations (35), (36) for equation (25), we have,

$$\begin{aligned} R &= \frac{S_{\text{re}}}{S_{\text{in}}} \\ R &= \frac{v_1 A A^* \left[\frac{ik_1 + k_2}{ik_1 - k_2} \right] \left[\frac{-ik_1 + k_2}{-ik_1 - k_2} \right]}{v_1 A A^*} \\ R &= 1 \end{aligned} \quad (37)$$

Which implies that the particle incident on the step potential with $E < V_0$ is always reflected. Thus in this case the predictions of quantum Mechanics and class mechanics are same.

Note: It is important to note that some particle will penetrate through the barrier. Penetration (or leakage) through the potential barrier.

Penetration or leakage through the potential barrier

Although the reflection coefficient is unity i.e. incident particle with $E < V_0$ is always reflected, the wave function ψ_2 in region II has a finite value given by

$$\psi_2 = Ce^{-k_2x} \quad (38)$$

$$\text{Where } C = \left[\frac{2ik_1}{ik_1 - k_2} \right] A$$

This waves function does not become zero at $x = 0$ but decays exponentially. The particle thus penetrates into region II but is always finally reflected.

Leakage Probability

The probability per unit length of finding the particle in II region is given as

$$\begin{aligned} P &= \psi_2 \psi_2^* \\ &= [Ce^{-k_2x}][C^* e^{-k_2x}] \\ &= CC^* e^{-2k_2x} \\ &= A \left[\frac{2ik_1}{ik_1 - k_2} \right] A^* \left[\frac{-2ik_1}{-ik_1 - k_2} \right] e^{-2k_2x} \\ &= |A|^2 \left[\frac{4k_1^2}{k_1^2 + k_2^2} \right] e^{-2k_2x} \end{aligned} \quad (39)$$

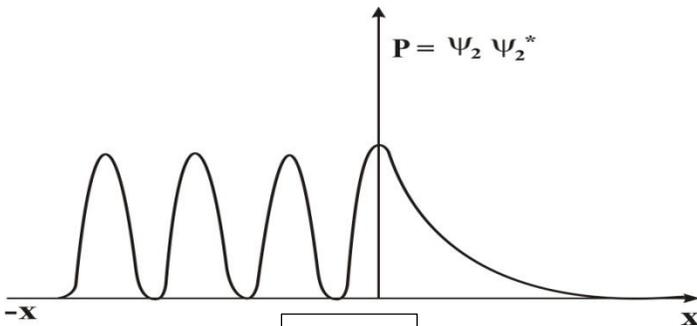


Fig. 5.6

Thus there is a finite probability of finding in the II region i.e. $x > 0$, due to leakage. This is in sharp contrast to the classical mechanics. This phenomenon is known as penetration of the classically excluded region.

Penetration distance

It is defined as the distance in which the wave function ψ_2 reduces to $1/e$ of its value at $x = 0$.

i.e., by definition,

$$\psi_2(\Delta x) = \frac{1}{e} \psi_2(x = 0)$$

$$C e^{-k_2 \Delta x} = \frac{1}{e} C \quad \text{[from equation (9)]}$$

$$e^{-k_2 \Delta x} = \frac{1}{e}$$

Taking log both the side, we get

$$-k_2 \Delta x = -1$$

$$\Delta x = \frac{1}{k_2}$$

$$\Delta x = \frac{\hbar}{\sqrt{2m(V_0 - E)}} \quad \text{[from equation]}$$

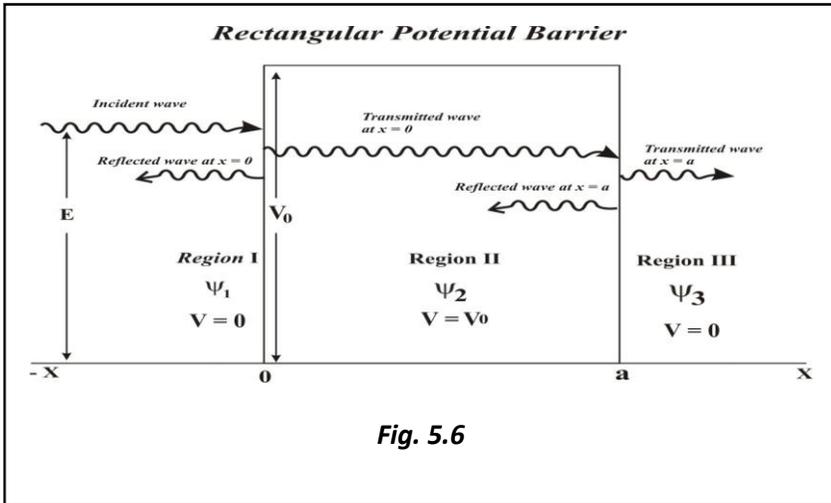
5.3 Rectangular Potential Barrier

Rectangular potential barrier is defined as-

$$V(x) = 0 \text{ for } x < 0$$

$$V(x) = V_0 \text{ for } 0 < x < a$$

$$V(x) = 0 \text{ for } x > a$$



Classical view point

According to classical mechanics, the particles of total energy $E < V_0$ in region I ($x < 0$) cannot overcome a barrier of height V_0 and penetrate into region II. It cannot therefore appear in region III. This means that the particle will always be reflected back.

Quantum Mechanical View Point

According to quantum mechanics the motion of the particle is governed by Schrodinger wave equation for I, II, & III rd region. As the potential V_0 is independent of time, we have to solve Schrodinger time independent wave equation to analysis the behaviours of the particle. It is given by

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0 \quad (1)$$

Region I

Equation (3) for the I region can be written as

$$\frac{\partial^2 \psi_1}{\partial x^2} + \frac{2mE}{\hbar^2} \psi_1 = 0 \quad (\text{since in the I region } V = 0) \quad (2)$$

$$\frac{\partial^2 \psi_1}{\partial x^2} + k_1^2 \psi_1 = 0 \quad (3)$$

where $K_1^2 = \frac{2mE}{\hbar^2}$ (k_1 is the propagation constant in the I region)

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \quad (4)$$

$$k_1 = \frac{P_1}{\hbar} \quad (\text{since in the I region, } P_1 = \sqrt{2mE}) \quad (5)$$

Region II

$$\frac{\partial^2 \psi_2}{\partial x^2} - \frac{2m}{\hbar^2} (V_0 - E) \psi_2 = 0 \quad (6) \quad (\text{since in the II region } V = V_0)$$

$$\frac{\partial^2 \psi_2}{\partial x^2} - k_2^2 \psi_2 = 0 \quad (7)$$

where $K_2^2 = \frac{2m(V_0 - E)}{\hbar^2}$ (k_2 is the propagation constant in the II region)

$$k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \quad (8)$$

$$k_2 = \frac{P_2}{\hbar} \quad (\text{since in the I region, } P_1 = \sqrt{2mE})$$

Region III

Equation (1) for the III region can be written as

$$\frac{\partial^2 \psi_3}{\partial x^2} + \frac{2mE}{\hbar^2} \psi_3 = 0 \quad (\text{since in the I region } V = 0) \quad (9)$$

$$\frac{\partial^2 \psi_3}{\partial x^2} + k_1^2 \psi_3 = 0 \quad (10)$$

where $K_1^2 = \frac{2mE}{\hbar^2}$ (k_1 is the propagation constant in the I region)

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \quad (11)$$

$$k_1 = \frac{P_1}{\hbar} \quad (\text{since in the I region, } P_1 = \sqrt{2mE}) \quad (12)$$

The solutions of equations (3) & (7) and (10) can be expressed as

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x} \quad (13)$$

$$\psi_2 = Ce^{-k_2x} + De^{k_2x} \quad (14)$$

$$\psi_3 = Fe^{ik_1x} + Ge^{-ik_1x} \quad (15)$$

In equation (13)

Ae^{ik_1x} → Represents incident wave moving along +ve x - direction in the I region.

Be^{-ik_1x} → Represents reflected wave from $x = 0$, moving along -ve x - direction in the I region.

In equation (14)

Where C and D are arbitrary constants.

In equation (15)

Fe^{ik_1x} → Represents incident wave moving along +ve x - direction in the III region.

Ge^{-ik_1x} → Represents reflected wave from $x = 0$, moving along -ve x - direction in the III region. But there is no reflected wave in the III region, therefore, $G = 0$,

substituting $G = 0$ in equation (15), we get,

$$\psi_3 = Fe^{ik_1x} \quad (16)$$

Since infinite energy and mass does not exist in nature. Therefore from eqⁿ (3), (7) and (10) ψ_1 , ψ_2 and ψ_3 must be finite & continuous. If ψ_1 , ψ_2 and ψ_3 are continuous then their derivatives with respect to x must also be continuous. In the light of above facts we can write boundary conditions as following.

$$(\psi_1)_{x=0} = (\psi_2)_{x=0} \quad (16)$$

$$(\psi_2)_{x=a} = (\psi_3)_{x=a} \quad (17)$$

$$\left(\frac{\partial\psi_1}{\partial x}\right)_{x=0} = \left(\frac{\partial\psi_2}{\partial x}\right)_{x=0} \quad (18)$$

$$\left(\frac{\partial \Psi_1}{\partial x}\right)_{x=a} = \left(\frac{\partial \Psi_2}{\partial x}\right)_{x=a} \quad (19)$$

Differentiating equations (13), (14) and (15) with respect to x , we have,

$$\frac{\partial \Psi_1}{\partial x} = ik_1 A e^{ik_1 x} - ik_1 B e^{-ik_1 x} \quad (20)$$

$$\frac{\partial \Psi_2}{\partial x} = -k_2 C e^{-k_2 x} + k_2 D e^{k_2 x} \quad (21)$$

$$\frac{\partial \Psi_3}{\partial x} = ik_1 F e^{ik_1 x} \quad (22)$$

Applying boundary condition (16) for equations (20) and (21), we have,

$$A e^{ik_1 x^0} + B e^{-ik_1 x^0} = C e^{-k_2 x^0} + D e^{k_2 x^0}$$

$$\therefore A + B = C + D \quad (23)$$

Applying boundary condition (17) for equations (14) and (15), we have,

$$C e^{-k_2 a} + D e^{k_2 a} = F e^{ik_1 a} \quad (24)$$

Applying boundary condition (18) for equations (20) and (21), we have,

$$ik_1 A e^{ik_1 x^0} - ik_1 B e^{-ik_1 x^0} = -k_2 C e^{-k_2 x^0} + k_2 D e^{k_2 x^0}$$

$$ik_1 A - ik_1 B = -k_2 C + k_2 D$$

$$ik_1 (A - B) = -k_2 (C - D)$$

$$(A - B) = -\frac{k_2}{ik_1} (C - D)$$

$$(A - B) = \frac{ik_2}{k_1} (C - D) \quad (25)$$

Applying boundary condition (19) for equations (21) and (22), we have,

$$-k_2 C e^{-k_2 a} + k_2 D e^{k_2 a} = ik_1 F e^{ik_1 a}$$

$$-C e^{-k_2 a} + D e^{k_2 a} = \frac{ik_1}{k_2} F e^{ik_1 a} \quad (26)$$

Adding equations (24) and (26), we get,

$$D = \frac{F}{2} e^{ik_1 a} \left[1 + \frac{ik_1}{k_2} \right] e^{-k_2 a} \quad (27)$$

subtracting equation (26) from equation (24), we get,

$$C = \frac{F}{2} e^{ik_1 a} \left[1 - \frac{ik_1}{k_2} \right] e^{k_2 a} \quad (28)$$

Adding equations (28) and (27), we get,

$$\begin{aligned} \therefore C + D &= \frac{F}{2} e^{ik_1 a} \left[1 + \frac{ik_1}{k_2} \right] e^{-k_2 a} + \frac{F}{2} e^{ik_1 a} \left[1 - \frac{ik_1}{k_2} \right] e^{k_2 a} \\ \therefore C + D &= \frac{F}{2} e^{ik_1 a} \left[(e^{k_2 a} + e^{-k_2 a}) - \frac{ik_1}{k_2} (e^{k_2 a} - e^{-k_2 a}) \right] \\ \therefore C + D &= Fe^{ik_1 a} \left[\frac{(e^{k_2 a} + e^{-k_2 a})}{2} - \frac{ik_1}{k_2} \frac{(e^{k_2 a} - e^{-k_2 a})}{2} \right] \\ \therefore C + D &= Fe^{ik_1 a} \left[\cosh(k_2 a) - \frac{ik_1}{k_2} \sinh(k_2 a) \right] \quad (29) \end{aligned}$$

$$[\text{since } \cosh x = \frac{(e^x + e^{-x})}{2} \text{ and } \sinh x = \frac{(e^x - e^{-x})}{2}]$$

subtracting equation (27) from equation (28), we get,

$$\begin{aligned} C - D &= \frac{F}{2} e^{ik_1 a} \left[1 - \frac{ik_1}{k_2} \right] e^{k_2 a} - \frac{F}{2} e^{ik_1 a} \left[1 + \frac{ik_1}{k_2} \right] e^{-k_2 a} \\ \therefore C - D &= \frac{F}{2} e^{ik_1 a} \left[(e^{k_2 a} - e^{-k_2 a}) - \frac{ik_1}{k_2} (e^{k_2 a} + e^{-k_2 a}) \right] \\ \therefore C - D &= Fe^{ik_1 a} \left[\frac{(e^{k_2 a} - e^{-k_2 a})}{2} - \frac{ik_1}{k_2} \frac{(e^{k_2 a} + e^{-k_2 a})}{2} \right] \\ \therefore C - D &= Fe^{ik_1 a} \left[\sinh(k_2 a) - \frac{ik_1}{k_2} \cosh(k_2 a) \right] \quad (30) \end{aligned}$$

Using equation (29) for equation (23), we get

$$A + B = Fe^{ik_1 a} \left[\cosh(k_2 a) - \frac{ik_1}{k_2} \sinh(k_2 a) \right] \quad (31)$$

Using equation (30) for equation (25), we get

$$A - B = Fe^{ik_1 a} \left[\frac{ik_2}{k_1} \sinh(k_2 a) - \frac{ik_2}{k_1} \frac{ik_1}{k_2} \cosh(k_2 a) \right]$$

$$\therefore A - B = Fe^{ik_1 a} \left[\frac{ik_2}{k_1} \sinh(k_2 a) + \cosh(k_2 a) \right] \quad (32)$$

Adding equations (31) and (32), we get,

$$2A = Fe^{ik_1 a} \left[2 \cosh(k_2 a) + i \left(\frac{k_2}{k_1} - \frac{k_1}{k_2} \right) \sinh(k_2 a) \right]$$

$$\therefore A = Fe^{ik_1 a} \left[\cosh(k_2 a) + \frac{i}{2} \left(\frac{k_2}{k_1} - \frac{k_1}{k_2} \right) \sinh(k_2 a) \right] \quad (33)$$

subtracting equation (32) from equation (31), we get,

$$\therefore B = -\frac{i}{2} Fe^{ik_1 a} \left[\left(\frac{k_2}{k_1} + \frac{k_1}{k_2} \right) \sinh(k_2 a) \right] \quad (34)$$

Reflectance (R)

Reflectance (R) is defined as

$$R = \frac{\text{Magnitude of the reflected probability density current } (S_{re})}{\text{Magnitude of the incident probability density current } (S_{in})} \quad (35)$$

$$\text{or} \quad R = \frac{S_{re}}{S_{in}} \quad (36)$$

The reflection coefficient (R) is a measure of the probability that the particle is reflected from the barrier.

Probability current density is defined by

$$S = v \psi \psi^* \quad (37)$$

Where v is particle velocity

Ψ is the wave function

Ψ^* is the complex conjugate of the wave function

Incident probability current density is defined by

$$S_{in} = v_1 \Psi_{in} \Psi_{in}^* \quad (38)$$

Ψ_{in} is the wave function corresponding to the incident beam of the particles

and Ψ_{in}^* is the complex conjugate of the Ψ_{in}

$$S_{in} = v_1 A e^{ik_1 x} A^* e^{-ik_1 x} \quad (39)$$

Where v_1 is particle velocity in the I region.

Reflected probability current density is defined by

$$S_{re} = v_1 \Psi_{re} \Psi_{re}^* \quad (40)$$

Ψ_{re} is the wave function corresponding to the reflected beam of the particles

and Ψ_{re}^* is the complex conjugate of the Ψ_{re}

$$\therefore S_{re} = v_1 B e^{ik_2 x} B^* e^{-ik_2 x} \quad (41)$$

Where v_1 is particle velocity in the I region

Therefore using equations (39) and (40) for equation (35), we get,

$$R = \frac{\text{Magnitude of the reflected probability density current } (S_{re})}{\text{Magnitude of the incident probability density current } (S_{in})}$$

$$R = \frac{S_{re}}{S_{in}}$$

$$R = \frac{v_1 B e^{ik_2 x} B^* e^{-ik_2 x}}{v_1 A e^{ik_1 x} A^* e^{-ik_1 x}}$$

$$R = \frac{BB^*}{AA^*} \quad (42)$$

Using equations (33) and (34) for equation (42), we get

$$R = \frac{-\frac{i}{2} F e^{ik_1 a} \left[\left(\frac{k_2 + k_1}{k_1 + k_2} \right) \sinh(k_2 a) \right] X \frac{i}{2} F^* e^{ik_1 a} \left[\left(\frac{k_2 + k_1}{k_1 + k_2} \right) \sinh(k_2 a) \right]}{F e^{ik_1 a} \left[\cosh(k_2 a) + \frac{i}{2} \left(\frac{k_2 - k_1}{k_1 + k_2} \right) \sinh(k_2 a) \right] F^* e^{-ik_1 a} \left[\cosh(k_2 a) - \frac{i}{2} \left(\frac{k_2 - k_1}{k_1 + k_2} \right) \sinh(k_2 a) \right]}$$

$$R = \frac{\frac{1}{4} \left(\frac{k_2 + k_1}{k_1 + k_2} \right)^2 \sinh^2(k_2 a)}{\cosh^2(k_2 a) + \left(\frac{k_2 - k_1}{k_1 + k_2} \right) \sinh^2(k_2 a)} \quad (43)$$

Transmittance (T)

Transmittance (T) is defined as

$$T = \frac{\text{Magnitude of the transmitted probability density current } (S_{tr})}{\text{Magnitude of the incident probability density current } (S_{in})} \quad (44)$$

$$\text{or} \quad T = \frac{S_{tr}}{S_{in}} \quad (45)$$

Where v_1 is particle velocity in the I region.

transmitted probability current density is defined by

$$S_{tr} = v_1 \Psi_{tr} \Psi_{tr}^* \quad (46)$$

Ψ_{tr} is the wave function corresponding to the reflected beam of the particles

and Ψ_{tr}^* is the complex conjugate of the Ψ_{tr}

$$\therefore S_{tr} = v_1 F e^{ik_1 x} F^* e^{-ik_1 x} \quad (47)$$

Where v_1 is particle velocity in the I region

Therefore using equations (39) and (47) for equation (45), we get,

$$T = \frac{\text{Magnitude of the transmitted probability density current } (S_{tr})}{\text{Magnitude of the incident probability density current } (S_{in})}$$

$$\begin{aligned} \text{or} \quad T &= \frac{S_{tr}}{S_{in}} \\ T &= \frac{v_1 F e^{ik_1 x} F^* e^{-ik_1 x}}{v_1 A e^{ik_1 x} A^* e^{-ik_1 x}} \\ T &= \frac{FF^*}{AA^*} \end{aligned} \quad (48)$$

Using equation (33) equation (48), we get

$$\begin{aligned} T &= \frac{1}{\cosh^2(k_2 a) + \left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)^2 \sinh^2(k_2 a)} \\ \therefore T &= \frac{1}{1 + \sinh^2(k_2 a) + \left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)^2 \sinh^2(k_2 a)} \end{aligned}$$

$$\therefore T = \frac{1}{1 + \left(1 + \frac{(k_2^2 - k_1^2)}{2k_1 k_2}\right)^2 \sinh^2(k_2 a)}$$

$$\therefore T = \frac{1}{1 + \left(\frac{(k_2^2 + k_1^2)}{2k_1 k_2}\right)^2 \sinh^2(k_2 a)}$$

Substituting the values of k_2^2 and k_1^2 , we get

$$T = \frac{1}{1 + \left(\frac{\left(\frac{2m(V_0 - E)}{\hbar^2} + \frac{2mE}{\hbar^2}\right)^2}{2\frac{\sqrt{2mE}}{\hbar}\sqrt{2m(V_0 - E)}}}\right)^2 \sinh^2\left(\frac{\sqrt{2m(V_0 - E)}}{\hbar}a\right)}$$

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2\frac{\sqrt{2m(V_0 - E)}}{\hbar}a} \quad (49)$$

Quantum mechanical tunnelling or Tunnel effect

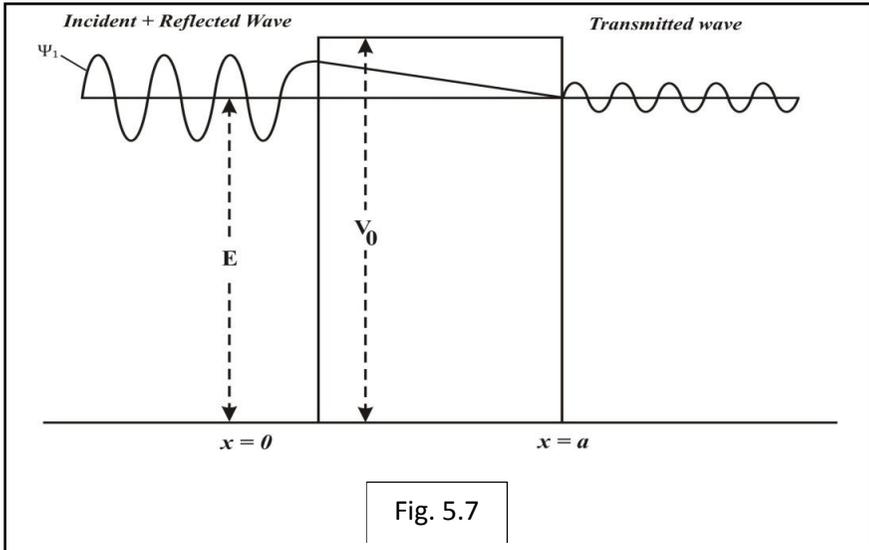
The transmission co-efficient T is a measure of the probability that the particle will be transmitted through the barrier. From relation (49), we see that $T \neq 0$. This shows that there is some probability that the particle may penetrate through the barrier and appear in the region III even when its energy $E < V_0$. This prediction of quantum theory is contrary to the classical behaviour of the particle.

The phenomenon of transmission of a particle through a potential barrier of finite width and height, even when its energy is less than the barrier height is called **quantum mechanical tunnelling**.

Explanation:

The property of barrier penetration is entirely due to the wave nature of matter and is very similar to the total internal reflection of the waves. If two plates of glass are placed very close to each other with a layer of air as a medium between them, the light will be transmitted from one plate to another, even though the angle of incidence is greater than the critical angle. However, the intensity of the transmitted wave will decrease exponentially with the increase in thickness of the layer of air. In this case the intensity of electron waves decreases exponentially with the

increase in thickness of the barrier. The wave function has the form more or less as shown in the Fig. 5.7



Significance:

The theory of tunnel effect is used to explain α -decay. There are so many examples of tunnelling of electrons in the solid state physics. Tunnel effect is specifically important in thermionic emission and field emission.

Note: The probability of transmission depends upon V_0 & 'a'. If the barrier is very high or quite thick, the probability of penetration becomes small.

5.4 Square well potential

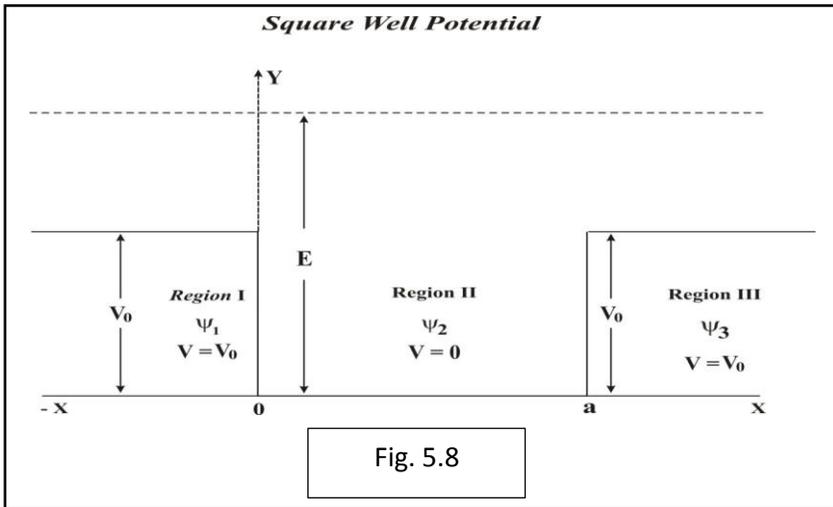
A square well potential defined by-

$$V = V_0 \quad \text{for} \quad -\infty < x < 0$$

$$V = 0 \quad \text{for} \quad 0 \leq x \leq a$$

$$V = V_0 \quad \text{for} \quad a < x < \infty$$

We will calculate the value of transmission coefficient, when $E > V_0$



Classical view point :

Both reflection & transmission will take place.

Quantum Mechanical View Point:

The motion of the particle is governed by Schrodinger eqⁿ and to the wave nature, the particle transmission in the IIIrd region will also take place.

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0 \quad (1)$$

Region I

Equation (1) for the I region can be written as

$$\frac{\partial^2 \psi_1}{\partial x^2} + \frac{2m}{\hbar^2} (E - V_0) \psi_2 = 0 \quad (2) \text{ (since in the II region } V = V_0)$$

$$\frac{\partial^2 \psi_1}{\partial x^2} + k_1^2 \psi_2 = 0 \quad (3)$$

where $K_1^2 = \frac{2m(E-V_0)}{\hbar^2}$ (k_1 is the propagation constant in the I region)

$$k_1 = \frac{\sqrt{2m(E-V_0)}}{\hbar} \quad (4)$$

Region II

Equation (1) for the III region can be written as

$$\frac{\partial^2 \psi_2}{\partial x^2} + \frac{2mE}{\hbar^2} \psi_2 = 0 \quad (\text{since in the I region } V = 0) \quad (5)$$

$$\frac{\partial^2 \psi_2}{\partial x^2} + k_2^2 \psi_2 = 0 \quad (6)$$

where $K_2^2 = \frac{2mE}{\hbar^2}$ (k_1 is the propagation constant in the I region)

$$k_2 = \frac{\sqrt{2mE}}{\hbar} \quad (7)$$

$$k_2 = \frac{P_2}{\hbar} \quad (\text{since in the II region, } P_2 = \sqrt{2mE}) \quad (8)$$

Region III

Equation (1) for the III region can be written as

$$\frac{\partial^2 \psi_3}{\partial x^2} + \frac{2mE}{\hbar^2} \psi_3 = 0 \quad (\text{since in the III region } V = V_0) \quad (9)$$

$$\frac{\partial^2 \psi_3}{\partial x^2} + k_1^2 \psi_3 = 0 \quad (10)$$

where $K_1^2 = \frac{2mE}{\hbar^2}$ (k_1 is the propagation constant in the III region)

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \quad (11)$$

$$k_1 = \frac{P_1}{\hbar} \quad (\text{since in the I region, } P_1 = \sqrt{2mE}) \quad (12)$$

The solutions of equations (3) & (6) and (10) can be expressed as

$$\psi_1 = Ae^{ik_1x} + Be^{-ik_1x} \quad (13)$$

$$\psi_2 = Ce^{ik_2x} + De^{-ik_2x} \quad (14)$$

$$\psi_3 = Fe^{ik_1x} + Ge^{-ik_1x} \quad (15)$$

In equation (13)

Ae^{ik_1x} → Represents incident wave moving along +ve x - direction in the I region.

Be^{-ik_1x} → Represents reflected wave from $x = 0$, moving along -ve x - direction in the I region.

In equation (14)

Ce^{ik_2x} → Represents transmitted wave at $x = 0$, moving along +ve x - direction in the II region.

De^{-ik_2x} → Represents reflected wave from $x = 0$, moving along -ve x - direction in the I region.

In equation (15)

Fe^{ik_1x} → Represents transmitted wave from $x = a$, moving along +ve x - direction in the III region.

Ge^{-ik_1x} → Represents reflected in the III region. But there is no reflected wave in the III region, but since there is no reflected wave in the III region, therefore, $G = 0$,

substituting $G = 0$ in equation (15), we get,

$$\psi_3 = Fe^{ik_1x} \quad (16)$$

Since infinite energy and mass does not exist in nature. Therefore from eqⁿ (3), (6) and (10) ψ_1 , ψ_2 and ψ_3 must be finite & continuous. If ψ_1 , ψ_2 and ψ_3 are continuous then their derivatives with respect to x must also be continuous. In the light of above facts we can write boundary conditions as following.

$$(\psi_1)_{x=0} = (\psi_2)_{x=0} \quad (17)$$

$$(\psi_2)_{x=a} = (\psi_3)_{x=a} \quad (18)$$

$$\left(\frac{\partial\psi_1}{\partial x}\right)_{x=0} = \left(\frac{\partial\psi_2}{\partial x}\right)_{x=0} \quad (19)$$

$$\left(\frac{\partial \Psi_1}{\partial x}\right)_{x=a} = \left(\frac{\partial \Psi_2}{\partial x}\right)_{x=a} \quad (20)$$

Differentiating equations (13), (14) and (16) with respect to x , we have,

$$\frac{\partial \Psi_1}{\partial x} = ik_1 A e^{ik_1 x} - ik_1 B e^{-ik_1 x} \quad (21)$$

$$\frac{\partial \Psi_2}{\partial x} = ik_2 C e^{ik_2 x} - ik_2 D e^{-ik_2 x} \quad (22)$$

$$\frac{\partial \Psi_3}{\partial x} = ik_1 F e^{ik_1 x} \quad (23)$$

Applying boundary condition (17) for equations (13) and (14), we have,

$$\begin{aligned} A e^{ik_1 x 0} + B e^{-ik_1 x 0} &= C e^{-k_2 x 0} + D e^{k_2 x 0} \\ A + B &= C + D \end{aligned} \quad (24)$$

Applying boundary condition (18) for equations (14) and (15), we have,

$$C e^{ik_2 a} + D e^{-ik_2 a} = F e^{ik_1 a} \quad (25)$$

Applying boundary condition (19) for equations (20) and (21), we have,

$$\begin{aligned} ik_1 A e^{ik_1 x 0} - ik_1 B e^{-ik_1 x 0} &= ik_2 C e^{ik_2 x 0} - ik_2 D e^{-ik_2 x 0} \\ \therefore k_1 A - k_1 B &= k_2 C - k_2 D \\ \therefore k_1 (A - B) &= k_2 (C - D) \\ \therefore (A - B) &= \frac{k_2}{k_1} (C - D) \end{aligned} \quad (26)$$

Applying boundary condition (20) for equations (22) and (23), we have,

$$\begin{aligned} ik_2 C e^{ik_2 a} - ik_2 D e^{-ik_2 a} &= ik_1 F e^{ik_1 a} \\ \therefore C e^{ik_2 a} - D e^{-ik_2 a} &= \frac{k_1}{k_2} F e^{ik_1 a} \end{aligned} \quad (27)$$

Adding equations (25) and (27), we get,

$$C = \frac{F}{2} e^{-ik_2 a} \left[1 + \frac{k_1}{k_2} \right] e^{ik_1 a} \quad (27)$$

Subtracting equation (27) from equation (25), we get,

$$D = \frac{F}{2} e^{ik_1 a} \left[1 - \frac{k_1}{k_2} \right] e^{ik_2 a} \quad (28)$$

Adding equations (27) and (28), we get,

$$\begin{aligned} \therefore C + D &= \frac{F}{2} e^{-ik_2 a} \left[1 + \frac{k_1}{k_2} \right] e^{ik_1 a} + \frac{F}{2} e^{ik_1 a} \left[1 - \frac{k_1}{k_2} \right] e^{ik_2 a} \\ \therefore C + D &= \frac{F}{2} e^{ik_1 a} \left[(e^{ik_2 a} + e^{-ik_2 a}) + \frac{k_1}{k_2} (e^{-ik_2 a} - e^{ik_2 a}) \right] \\ \therefore C + D &= Fe^{ik_1 a} \left[\frac{(e^{ik_2 a} + e^{-ik_2 a})}{2} - \frac{ik_1 (e^{ik_2 a} - e^{-ik_2 a})}{2i} \right] \\ \therefore C + D &= Fe^{ik_1 a} \left[\cos(k_2 a) - \frac{ik_1}{k_2} \sin(k_2 a) \right] \quad (29) \end{aligned}$$

$$[\text{since } \cos x = \frac{(e^{ix} + e^{-ix})}{2} \text{ and } \sin x = \frac{(e^{ix} - e^{-ix})}{2i}]$$

Subtracting equation (28) from equation (27), we get,

$$\begin{aligned} C - D &= \frac{F}{2} e^{-ik_2 a} \left[1 + \frac{k_1}{k_2} \right] e^{ik_1 a} - \frac{F}{2} e^{ik_1 a} \left[1 - \frac{k_1}{k_2} \right] e^{ik_2 a} \\ C - D &= \frac{F}{2} e^{ik_1 a} \left[(e^{-ik_2 a} + e^{ik_2 a}) + \frac{k_1}{k_2} (e^{ik_2 a} + e^{-ik_2 a}) \right] \\ C - D &= Fe^{ik_1 a} \left[\frac{(e^{-ik_2 a} + e^{ik_2 a})}{2} + \frac{k_1 (e^{ik_2 a} + e^{-ik_2 a})}{2} \right] \\ C - D &= Fe^{ik_1 a} \left[-i \sin(k_2 a) + \frac{k_1}{k_2} \cos(k_2 a) \right] \quad (30) \end{aligned}$$

Using equation (29) for equation (24), we get

$$A + B = Fe^{ik_1 a} \left[\cos(k_2 a) - \frac{ik_1}{k_2} \sin(k_2 a) \right] \quad (31)$$

Using equation (30) for equation (26), we get

$$A - B = \frac{k_2}{k_1} Fe^{ik_1 a} \left[-i \sin(k_2 a) + \frac{k_1}{k_2} \cos(k_2 a) \right]$$

$$\begin{aligned} \therefore A - B &= Fe^{ik_1a} \left[-i \frac{k_2}{k_1} \sin(k_2a) + \frac{k_2 k_1}{k_1 k_2} \cos(k_2a) \right] \\ \therefore A - B &= Fe^{ik_1a} \left[-i \frac{k_2}{k_1} \sin(k_2a) + \cos(k_2a) \right] \end{aligned} \quad (32)$$

Adding equations (31) and (32), we get,

$$\begin{aligned} 2A &= Fe^{ik_1a} \left[2 \cos(k_2a) - i \left(\frac{k_2}{k_1} + \frac{k_1}{k_2} \right) \sin(k_2a) \right] \\ \therefore A &= Fe^{ik_1a} \left[\cos(k_2a) - \frac{i}{2} \left(\frac{k_2}{k_1} + \frac{k_1}{k_2} \right) \sin(k_2a) \right] \end{aligned} \quad (33)$$

\therefore Subtracting equation (32) from equation (31), we get,

$$\therefore B = -\frac{i}{2} Fe^{ik_1a} \left[\left(\frac{k_1}{k_2} - \frac{k_2}{k_1} \right) \sin(k_2a) \right] \quad (34)$$

Transmittance (T)

Transmittance (T) is defined as

$$T = \frac{\text{Magnitude of the transmitted probability density current } (S_{tr})}{\text{Magnitude of the incident probability density current } (S_{in})} \quad (35)$$

$$\text{or} \quad T = \frac{S_{tr}}{S_{in}} \quad (36)$$

Where v_1 is particle velocity in the I region.

transmitted probability current density is defined by

$$S_{tr} = v_1 \Psi_{tr} \Psi_{tr}^* \quad (37)$$

Ψ_{tr} is the wave function corresponding to the reflected beam of the particles

and Ψ_{tr}^* is the complex conjugate of the Ψ_{tr}

$$\therefore S_{tr} = v_1 Fe^{ik_1x} F^* e^{-ik_1x} \quad (38)$$

Where v_1 is particle velocity in the I region

Therefore using equations (39) and (47) for equation (45), we get,

$$T = \frac{\text{Magnitude of the transmitted probability density current } (S_{tr})}{\text{Magnitude of the incident probability density current } (S_{in})}$$

$$\begin{aligned} \text{or } T &= \frac{S_{tr}}{S_{in}} \\ T &= \frac{v_1 F e^{ik_1 x} F^* e^{-ik_1 x}}{v_1 A e^{ik_1 x} A^* e^{-ik_1 x}} \\ T &= \frac{FF^*}{AA^*} \end{aligned} \quad (39)$$

Using equation (33) for equation (39), we get

$$\begin{aligned} T &= \frac{FF^*}{F e^{ik_1 a} \left[\cos(k_2 a) - \frac{i}{2} \left(\frac{k_2}{k_1} + \frac{k_1}{k_2} \right) \sin(k_2 a) \right] F^* e^{-ik_1 a} \left[\cos(k_2 a) + \frac{i}{2} \left(\frac{k_2}{k_1} + \frac{k_1}{k_2} \right) \sin(k_2 a) \right]} \\ T &= \frac{1}{\cos^2(k_2 a) + \frac{1}{4} \left(\frac{k_2}{k_1} + \frac{k_1}{k_2} \right)^2 \sin^2(k_2 a)} \\ T &= \frac{1}{1 - \sin^2(k_2 a) + \frac{1}{4} \left(\frac{k_2}{k_1} + \frac{k_1}{k_2} \right)^2 \sin^2(k_2 a)} \\ T &= \frac{1}{1 + \frac{1}{4} \left(\frac{k_2}{k_1} - \frac{k_1}{k_2} \right)^2 \sin^2(k_2 a)} \\ T &= \frac{1}{1 + \frac{1}{4} \left(\frac{k_2^2 - k_1^2}{k_1 k_2} \right)^2 \sin^2(k_2 a)} \end{aligned}$$

Substituting the values of k_2^2 and k_1^2 , we get

$$\begin{aligned} T &= \frac{1}{1 + \frac{1}{4} \left(\frac{\left(\frac{2mE}{\hbar^2} - \frac{2m(E-V_0)}{\hbar^2} \right)}{\frac{\sqrt{2mE}\sqrt{2m(E-V_0)}}{\hbar}} \right)^2 \sin^2 \frac{\sqrt{2mE}}{\hbar} a} \\ T &= \frac{1}{1 + \frac{V_0^2}{4E(E-V_0)} \sinh^2 \frac{\sqrt{2mE}}{\hbar} a} \end{aligned} \quad (40)$$

Eqⁿ (30) shows a very interesting property that the transmission coefficient series and falls as the energy E is increased. The value of T = 1,

When $\sqrt{2mE} \cdot a / \hbar$ is an integral multiple of π because then $\sin \sqrt{2mE} \cdot a / \hbar = 0$

The reason for the variation of I with E is that the wave function and its

Solved Problems

Problem 1. What is the lowest energy that a neutron (mass 1.67×10^{-27} kg) can have if confined to move along the edge of an impenetrable box of length 10^{-14} meter? ($h=6.63 \times 10^{-34}$ joule-sec).

Solution. The quantised energies of a particle of mass m in a one-dimensional box of length L are given by

$$E_n = \frac{n^2 h^2}{8mL^2} \quad n = 1, 2, 3, \dots$$

The lowest energy corresponds to $n = 1$, and is thus

$$E_1 = \frac{h^2}{8mL^2}$$

Substituting the given values, we have

$$\begin{aligned} E_1 &= \frac{(6.63 \times 10^{-34} \text{ joule} - \text{sec})^2}{8 \times (1.67 \times 10^{-27} \text{ kg}) \times (10^{-14} \text{ meter})^2} \\ &= 3.29 \times 10^{-13} \text{ joule} \\ &= \frac{3.29 \times 10^{-13}}{1.6 \times 10^{-13}} \quad (\because \text{MeV} = 1.6 \times 10^{-12} \text{ joule}) \\ &= 2.06 \text{ Mev.} \end{aligned}$$

Problem 2. 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 is 9.1×10^{-31} kg and $h = 6.63 \times 10^{-34}$ joule-sec).

Solution. 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

$$L = n \frac{\lambda}{2}, \quad n = 1, 2, 3, \dots$$

or
$$\lambda = \frac{2L}{n}.$$

Here
$$L = 10^{-9} \text{ meter} = 10 \text{ \AA}$$

$$\begin{aligned} \therefore \lambda &= \frac{2 \times 10 \text{ \AA}}{n}, \quad n = 1, 2, 3, \dots \\ &= 20 \text{ \AA}, 10 \text{ \AA}, 6.7 \text{ \AA}, \dots \end{aligned}$$

The corresponding energies are given by

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

Here $m = 9.1 \times 10^{-31}$ kg and $L = 10^{-9}$ meter.

$$\begin{aligned} \therefore E_n &= \frac{(6.63 \times 10^{-34})^2 n^2}{8 \times (9.1 \times 10^{-31}) \times (10^{-9})^2}, \\ &= 6.04 \times 10^{-20} n^2 \text{ joule} \end{aligned}$$

$$\frac{6.04 \times 10^{-20} n^2}{1.6 \times 10^{-19}} = 0.38 n^2 \text{ eV.}$$

For $n = 1, 2, 3$, we have

$$E_1 = 0.38 \text{ eV}, E_2 = 1.52 \text{ eV}, E_3 = 3.42 \text{ eV}.$$

Problem 3. 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.

Solution. The eigenfunctions of a particle trapped in a box of length L are

$$\psi_x(x) = \sqrt{\left(\frac{2}{L}\right) \sin \frac{n\pi x}{L}}.$$

The probability of finding the particle between x_1 and x_2 , when it is in the n th state, is

$$\begin{aligned} P &= \int_{x_1}^{x_2} |\psi_n|^2 dx \\ &= \frac{2}{L} \int_{x_1}^{x_2} \sin^2 \frac{n\pi x}{L} dx \\ &= \frac{2}{L} \int_{x_1}^{x_2} \frac{1}{2} \left(1 - \cos \frac{2n\pi x}{L}\right) dx \\ &= \frac{1}{L} \left[x - \frac{L}{2n\pi} \sin \frac{2n\pi x}{L} \right]_{x_1}^{x_2} \end{aligned}$$

Here $x_1 = 0.45L$, $x_2 = 0.55L$ and for the ground state, $n = 1$,

$$\begin{aligned} \therefore P &= \frac{1}{2} \left[x - \frac{L}{2\pi} \sin \frac{2\pi x}{L} \right]_{0.45L}^{0.22L} \\ &= \frac{1}{2} \left[\left(0.55L - \frac{L}{2\pi} \sin 1.10\pi\right) - \left(0.45L - \frac{L}{2\pi} \sin 0.90\pi\right) \right] \\ &= \left[\left(0.55 - \frac{1}{2\pi} \sin 198^\circ\right) - \left(0.45 - \frac{1}{2\pi} \sin 162^\circ\right) \right] \\ &= (0.55 - 0.45) - \frac{1}{2\pi} (\sin 198^\circ - \sin 162^\circ) \end{aligned}$$

$$\begin{aligned}
&= (0.55 - 0.45) - \frac{1}{2\pi} (\sin 198^\circ - \sin 162^\circ) \\
&= 0.10 - \frac{1}{\pi} (\cos 180^\circ \sin 18^\circ) \\
&= 0.10 + \frac{0.3090}{3.14} = 0.198 = \mathbf{19.8 \%}.
\end{aligned}$$

For the first excited state (n=2), we shall have **P=065% (Try)**.

Problem 4. The lowest energy possible for a certain particle entrapped in a box is 40 eV. What are the next higher energies the particle can have?

Solution: For a particle in a one dimensional box

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

The lowest possible energy corresponds to n=1 and is given by

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2} = 40eV$$

The next higher energy corresponds to n=2 and is given by

$$E_2 = 2^2 \frac{\pi^2 \hbar^2}{2mL^2} = 4 \times 40eV = 160eV$$

Similarly for n=3

$$E_3 = 3^2 \frac{\pi^2 \hbar^2}{2mL^2} = 9 \times 40eV = 360eV$$

Similarly for n=4

$$E_4 = 4^2 \frac{\pi^2 \hbar^2}{2mL^2} = 16 \times 40eV = 640eV$$

Problem 5. Calculate the value of lowest energy of an electron in one dimensional force free region of length 4A

Solution: for a particle in one dimensional force free region of length l, the energy is given as

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

$$= \frac{n^2 h^2}{8mL^2} \quad (\text{since } \hbar = \frac{h}{2\pi})$$

The lowest energy state corresponds to n=1. i.e.,

$$E_1 = \frac{n^2 h^2}{8mL^2}$$

$$= \frac{(6.62 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (4 \times 10^{-10})^2}$$

$$= 3.78 \times 10^{-19} \text{ J}$$

$$= \frac{3.78 \times 10^{-19}}{1.6 \times 10^{-19}} = 2.36 \text{ eV}$$

Problem 6. An electron and a proton of same energy (E) approach a potential barrier of height V, greater than E. Do they have the same probability of getting through? Explain'

Solution: The probability of a particle getting through the barrier and finding it on the other sides is given by

$$P = A^2 \left[\frac{4k_1^2}{k_1^2 + k_2^2} \right] e^{-2k_2x}$$

$$= 4A^2 \left[\frac{k_1^2}{1 + \frac{k_1^2}{k_2^2}} \right] e^{-2k_2x} 21q1$$

Now $\frac{k_2^2}{k_1^2} = \frac{2m(V_0 - E)}{\hbar^2} \cdot \frac{\hbar^2}{2mE}$

$= \frac{V_0 - E}{E}$, which is independent of the mass of the particle. The only factor which depends upon mass is e^{-2k_2x} , because

$$e^{-2k_2x} = e^{-2\sqrt{2m(V_0 - E)}x}$$

From the above expression, This is obvious that the larger the value of m , smaller the value of $e^{-2\sqrt{2m(V_0 - E)}x}$ and smaller is the probability. As the proton has a greater mass in comparison to the mass of the electron. The probability of the proton getting through the barrier is much smaller than that of the electron.

Exercise

(A) Descriptive type

- (1) Write down Schrodinger's time independent equation for a particle of energy E and mass m , moving in one-dimension. If this particle encounters a potential

$$\text{step: } V_x = \begin{cases} 0, & x \leq 0 \\ V, & x > 0 \end{cases}$$

Solve the Schrodinger's equation for its motion and discuss the results.

(L.U. 2011).

- (2) Solve the Schrödinger equation for a particle of mass m in a square potential well defined by :

$$V_x = \begin{cases} V_0 & , & \text{for } x < -a \\ 0 & , & \text{for } -a < x < a \\ V_0 & , & \text{for } x > a \end{cases}$$

Where the particle's total energy, $E < V_0$.

(L.U. 2010)

- (3) Solve the Schrodinger equation for a particle of mass 'm' in a square potential well defined by : $V(x) = V_0$, for $x < -a$

$$V(x) = 0, \text{ for } -a < x < a$$

$$V(x) = V_0, \text{ for } x > a.$$

(L.U. 2012)

- (4) Consider the transmission of a particle through a rectangular potential barrier of length L and height V , with $E < V$. Derive expressions for the reflection and transmission coefficient.

(L.U. 2013)

- (5) A particle of fixed energy E_0 moving along X-axis strikes a rectangular step potential barrier represented by function.

$$V_x = \begin{cases} 0, & \text{for } x < 0 \\ V_0. & \text{for } x > 0 \end{cases}$$

Discuss this situation for their reflection and transmission coefficient. Also explain which one has greater probability of Solve the Schrodinger wave equation for a particle in a square well potential defined by :

$$V(x) = 0 \text{ for } x < -a$$

$$V(x) = V_0 \text{ for } -a < x < a \quad \text{(L.U. 2015)}$$

(6) Particle of mass m and energy E and moving towards a step potential of height V_0 as shown in the diagram. Solve the Schrodinger wave equation for $E > V_0$ and $E < V_0$. Compute the fraction of particle reflected and transmitted. .

(L.U. 2009)

(B) Short answer type

(1) What is meant by infinite – Potential barrier?

(L.U. 2013)

(2) What is quantum mechanical tunneling ?

(L.U. 2008)

(3) What is meant by step potential

(L.U. 2014)

(4) Is there any possibility for a particle to exist outside the potential well.?

(L.U. 2015)

(5) Find the value of A for which wave function.

$$\Psi = A \sin \left(\frac{n\pi X}{a} \right)$$

is normalized in region $0 \leq X \leq a$.

(L.U. 2008)

(6) Given the wave function of a particle $\Psi(x) = \sqrt{\frac{2}{L}} \sin \left(\frac{\pi x}{L} \right)$. $0 < x < L$
 $= 0$, otherwise.

(L.U. 2013)

(7) An electron is moving in one-dimensional box of infinite height and width 1 \AA . Find the minimum energy of electron. ($h = 6.6 \times 10^{-34} \text{ J}$, $m = 9.1 \times 10^{-31} \text{ kg}$)

(L.U. 2008)

Chapter 6

The atom models

6.1 Spectroscopy

Spectroscopy is that branch of physics which deals with the observation and interpretation of radiation emitted and absorbed by atoms and molecules, and throws light on their structure. It provides information not only about the arrangement and motion of the outer electrons (optical spectroscopy) and about the angular momentum, magnetic moment, distribution of charge and magnetism of the nucleus (study of hyperfine structure, nuclear magnetic resonance, etc.)

Spectroscopy was originated by Newton when he showed that a prism refracts blue light more than red light, thus forming a band of colours known as 'spectrum'. Today we know that the visible spectrum is a very small part of the broad electromagnetic spectrum ranging from the gamma rays to the radio waves.

6.2 Thomson atomic model

J.J. Thomson, a British physicist in 1898 proposed an atomic model which was based on the following assumptions-

- (a) The atom is electrically neutral since positive charge present in the atom is equal to the negative charge of electrons present in the atom.
- (b) Atom is a positively charged solid sphere of radius approximately equal to 10^{-10} m in which electrons are embedded in between like raisins in a fruitcake.
- (c) The positive charge and the whole mass of the atom is uniformly distributed throughout the sphere.

Defects of Thomson atomic model

- (a) The spectrum of atom can not be explained
- (b) Scattering of α particles can not be explained with the help of this model.

Because Thomson had played an important role in discovering the electron, his idea was taken very seriously. But the real atom turned out to be quite different. The Rutherford scattering experiment showed it to be incorrect.

6.3 Rutherford atomic model

Ernest Rutherford in 1911, proposed an atomic model which is also known as ‘**Rutherford nuclear atom model**’ on the basis of his famous α scattering experiment. The important features of this model are as following-

- (a) The whole positive charge and almost whole mass of the atom is concentrated in a small part of radius, ranging from 10 m to 15 m which is known as nucleus.
- (b) Electrons revolve round the nucleus in circular orbits and are distributed in the hollow sphere of radius 10-10 m.
- (c) Atoms are electrically neutral because the total positive charge of nucleus present in the atom.

Defects of Rutherford atomic model

- (a) This model could not explain the stability of the atom. This is due to the fact that the revolving electron will experience a centripetal acceleration. Now it is a well known fact that an accelerated charge emits energy in the form of electromagnetic waves. Consequently the energy of an electron revolving around the nucleus should continuously decrease and it will come closer and closer to the nucleus until it will collapse with the nucleus.
- (b) According to this model the spectrum of atom must be continuous whereas practically it is a line spectrum.
- (c) This model did not explain the distribution of electrons outside nucleus.

6.4 Bohr’s theory of the atom

In order to explain the spectrum of hydrogen, Niels Bohr in 1913 formulated a theory. This theory is based on the following four postulates –

Postulate 1 (Stationary states)

Postulate 2 (Dynamics of Stationary orbits)

Postulate 3 (Quantum Conditions)**Postulate 4** (Frequency condition or Energy Emission)**Postulate 1**

An electron in the field of nucleus can revolve only in a certain privileged orbits in which it does not radiate energy. These privileged orbits are known as stationary orbits.

Bohr's first postulate provided stability to the atomic model.

Postulate 2

Electrons in an atom revolve round the nucleus in circular orbits so that coulomb force of attraction between electron and positive nucleus is balanced by centrifugal force. As the mass of the nucleus is much greater than that electron, therefore nucleus will be assumed in the rest state.

$$\frac{mv^2}{r} = \frac{1}{4\pi\epsilon_0} \frac{(Ze)(e)}{r^2}$$

Where m, v, r and e are mass, velocity, radius and charge of electron. Z is atomic number and Ze is the charge on the nucleus. R is the radius of the orbit.

$1/4\pi\epsilon_0 = 9 \times 10^9 \text{ Nm}^2\text{C}^{-2}$ (ϵ_0 is permittivity of the free space)

Postulate 3

The stationary orbit are those orbit for which angular momentum of electron is an integral multiple of $h/2\pi$ i.e.

$$mvr = n \frac{h}{2\pi}$$

Postulate 4

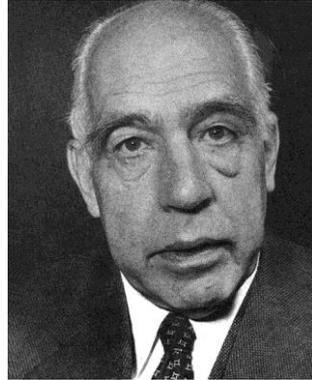
Whenever an electron jumps- from a high orbit of energy E_i to lower orbit of energy E_f , it emits the energy difference in the form of a photon.

If ν be the frequency of this photon then-

$$h\nu = E_i - E_f$$

Niels Bohr (1885-1962)

Bohr was born in Copenhagen, Denmark, on 7 October 1885. He received his Ph.D. degree from the University of Copenhagen in 1911. He went to Manchester to work in Rutherford's laboratory, where he understood the quantum ideas of Planck and Einstein. These ideas were applied by him in making the assumption that electron orbits are quantised in his revolutionary atomic theory. In 1913, Bohr returned to Copenhagen to become the first director of the Institute for Theoretical Physics. This



Copenhagen School soon became a meeting place for the scientists. During the second world war, he escaped from Denmark and became part of the team to develop the fission reactor and atomic bomb. After the war he worked for the peaceful development of the atomic power.

Radius of the orbit

The Coulomb force of attraction between the nucleus and electron provides the necessary centripetal force.

$$\frac{mv^2}{r} = \frac{1}{4\pi\epsilon_0} \frac{(Ze)(e)}{r^2}$$

$$\frac{mv^2}{r} = \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r^2}$$

(1)

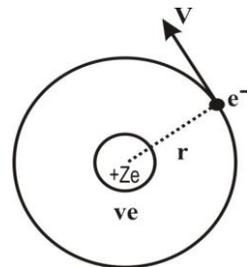


Fig. 6.1

According to the quantum condition

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

$$m^2 v^2 r^2 = \frac{n^2 h^2}{4\pi^2} \quad (3)$$

From equation (1) and equation (3), we have

$$r = \frac{n^2 h^2 \epsilon_0}{m \pi Z e^2} \quad (4)$$

For hydrogen

since $Z = 1$, therefore from (4)

$$r = \frac{n^2 h^2 \epsilon_0}{m \pi e^2} \quad (4)$$

$$\text{or } r = n^2 r_1 \quad (5)$$

For first orbit

$n = 1$ and $r = r_1$, therefore from equation (4), we have

$$\begin{aligned} r_1 &= \frac{h^2 \epsilon_0}{m \pi e^2} \\ r_1 &= \frac{(6.6 \times 10^{-34})^2 \times 8.85 \times 10^{-12}}{9.1 \times 10^{-31} \times (3.14)^2 (1.6 \times 10^{-19})^2} \\ &= 0.53 \text{ \AA} \end{aligned} \quad (6)$$

For second orbit

$n = 2$ and $r = r_2$, therefore from equation (5), we have

$$r_2 = 4r_1 \quad (7)$$

For third orbit

$n = 3$ and $r = r_3$, therefore from equation (5), we have

$$r_3 = 9r_1 \quad (8)$$

And so on.

Velocity of the electron in n^{th} orbit of hydrogen atom

From equation (2)

$$mvr = n \frac{h}{2\pi}$$

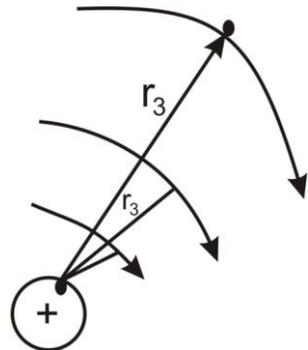


Fig. 6.2

Writing v_n which is the velocity of the electron in nth orbit, in place of v in the above equation, we get,

$$v_n = \frac{nh}{2\pi mr} \quad (9)$$

Substituting the value of r, from equation (4) in equation (9)

$$v_n = \frac{nh}{2\pi m \frac{n^2 h^2 \epsilon_0}{m \pi Z e^2}}$$

Substituting the values of m,h, ϵ_0 ,e and π in the above equation, we get

$$v_n = \frac{3 \times 10^8}{137} \frac{Z}{n} \text{ ms}^{-1}$$

$$\therefore v_n = \frac{c}{137} \frac{Z}{n} \text{ ms}^{-1} \quad (10)$$

where c = velocity of light in vaccum = $3 \times 10^8 \text{ ms}^{-1}$

for hydrogen Z=1, therefore from equation (10), we have,

$$v_n = \frac{c}{137} \frac{1}{n} \text{ ms}^{-1}$$

$$\therefore v_n = \frac{2.2 \times 10^6}{n} \text{ ms}^{-1} \quad (11)$$

For the first orbit, n = 1, therefore from equation (11), we have,

$$v_1 = 2.2 \times 10^6 \text{ ms}^{-1}$$

For the second orbit, n = 2, therefore from equation (11), we have,

$$v_2 = \frac{v_1}{2} \text{ ms}^{-1}$$

For the third orbit, n = 3, therefore from equation (11), we have,

$$v_3 = \frac{v_3}{2} \text{ ms}^{-1}$$

Energy of the electron in nth orbit

The total energy of electron in a orbit is the sum of its potential energy in the electric field of nucleus and its kinetic energy.

Kinetic energy

$$\begin{aligned}
 K.E. &= \frac{1}{2}mv^2 \\
 &= \frac{1}{2} \left[\frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r^2} \right] \quad [\text{from equation (1)}] \quad (12)
 \end{aligned}$$

Potential energy

$$\begin{aligned}
 P.E. &= \int_{\infty}^r \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r^2} dr \\
 &= \frac{Ze^2}{4\pi\epsilon_0} \int_{\infty}^r \frac{1}{r^2} dr \\
 &= \frac{Ze^2}{4\pi\epsilon_0} \left[-\frac{1}{r} \right]_{\infty}^r \\
 &= -\frac{Ze^2}{4\pi\epsilon_0 r} \\
 &\quad - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \quad (13)
 \end{aligned}$$

Total energy (E)

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

\therefore from (9) and (10)

$$\begin{aligned}
 E &= \frac{1}{2} \left[\frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \right] - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \\
 E &= -\frac{1}{2} \left[\frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \right] \quad (14)
 \end{aligned}$$

Using equation (4) for equation (14)

$$E = -\frac{1}{2} \left[\frac{1}{4\pi\epsilon_0} \frac{Ze^2}{\left(\frac{n^2 h^2 \epsilon_0}{m\pi Ze^2} \right)} \right] \quad (15)$$

$$\therefore E = -\frac{mZ^2 e^4}{8n^2 h^2 \epsilon_0^2}$$

$$\therefore E = -\frac{mZ^2 e^4}{8h^2 \epsilon_0^2} \left[\frac{1}{n^2} \right] \quad (16)$$

6.5 Bohr's theory of hydrogen Spectrum

From Bohr's IVth Postulate, whenever an electron jumps from a higher orbits of energy E_{n_2} to E_{n_1} then from the Planck's quantum theory,

$$E_{n_2} - E_{n_1} = h\nu \quad (17)$$

Now from equation (16), we have

$$E_{n_1} = -\frac{mZ^2e^4}{8h^2\epsilon_0^2} \left[\frac{1}{n_1^2} \right] \quad (18A)$$

$$E_{n_2} = -\frac{mZ^2e^4}{8h^2\epsilon_0^2} \left[\frac{1}{n_2^2} \right] \quad (18B)$$

Now from equations (18A) and (18B), we have,

$$E_{n_2} - E_{n_1} = \frac{mZ^2e^4}{8h^2\epsilon_0^2} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \quad (19)$$

Now from equations (17) and (19), we have,

$$\begin{aligned} h\nu &= \frac{mZ^2e^4}{8h^2\epsilon_0^2} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \\ \therefore \nu &= \frac{mZ^2e^4}{8h^3\epsilon_0^2} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \\ \therefore \frac{c}{\lambda} &= \frac{mZ^2e^4}{8h^3\epsilon_0^2} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \\ \therefore \frac{1}{\lambda} &= \frac{mZ^2e^4}{8ch^3\epsilon_0^2} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \\ \therefore \frac{c}{\lambda} &= \frac{mZ^2e^4}{8h^3\epsilon_0^2} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \\ \therefore \frac{c}{\lambda} &= \frac{mZ^2e^4}{8h^3\epsilon_0^2} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \\ \frac{1}{\lambda} &= Z^2 \left(\frac{me^4}{8ch^3\epsilon_0^2} \right) \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \end{aligned}$$

$$\therefore \frac{c}{\lambda} = \frac{mZ^2e^4}{8h^3\epsilon_0^2} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

$$\therefore \frac{1}{\lambda} = Z^2 R \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \quad (21)$$

$$\text{where } R = \frac{me^4}{8ch^3\epsilon_0^2} \quad (22)$$

R is called Rydberg constant. Rydberg constant was named after the Swedish physicist Johannes Rydberg.

$$R = \frac{9.1083 \times 10^{-31} \times (1.6 \times 10^{-16})^4}{8 \times 3 \times 10^8 \times (6.6 \times 10^{-34})^3 \times (8.85 \times 10^{-12})^2}$$

$$R = 1.0973 \times 10^7 \text{ m}^{-1}$$

Equation (22) can also be written as

$$\bar{\nu} = Z^2 R \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \quad (23)$$

Where $\bar{\nu} = \frac{1}{\lambda}$, $\bar{\nu}$ is called wave number

Various series of hydrogen spectrum

From equation (21)

$$\frac{1}{\lambda} = Z^2 R \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

For hydrogen $Z=1$, therefore from the above equation,

$$\frac{1}{\lambda} = R \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \quad (23)$$

On the basis of equation (19) we can define various spectral series such as Lyman, Balmer, Paschen, Brackett and Pfund.

$$\frac{1}{\lambda} = R \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

Lyman series

For Lyman series $n_1 = 1,$ $n_2 = 2,3,4,5,\dots$

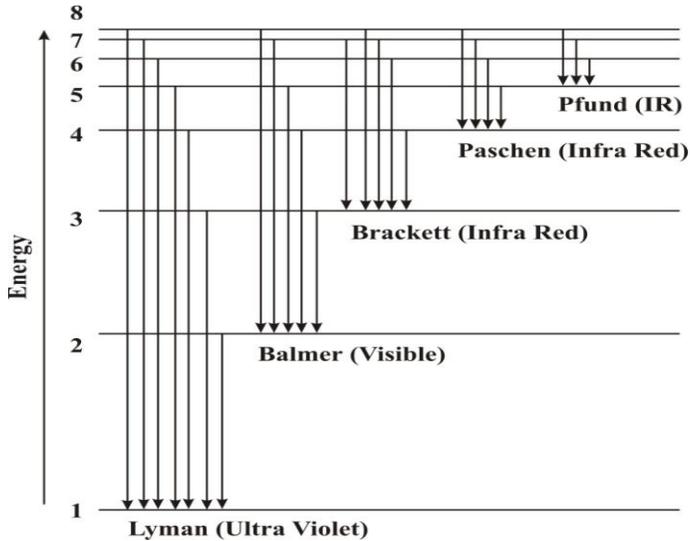


Fig. 6.3

Balmer series

For Balmer series $n_1 = 2,$ $n_2 = 3,4,5,6,\dots$

Paschen series

For Paschen series $n_1 = 3,$ $n_2 = 4,5,6,7,\dots$

Brackett series

For Brackett series $n_1 = 4,$ $n_2 = 5,6,7,8,\dots$

Pfund series

For Pfund series $n_1 = 5,$ $n_2 = 6,7,8,9,\dots$

Note :-

- (1) Lyman series falls in ultraviolet region , Balmer series appears in visible part, Paschen, Brackett and Pfund series found in infra-red region of the electromagnetic spectrum.
- (2) All the series are obtained in emission spectrum whereas only the Lyman series is obtained in absorption spectrum

Series Limit or last line or the limiting line

- (a) Series Limit or last line or the limiting line of Lyman Series is obtained when transition takes place from $n_2 = \infty$ to $n_1 = 1$.
- (b) Series Limit or last line or the limiting line of Balmer Series is obtained when transition takes place from $n_2 = \infty$ to $n_1 = 2$.
- (c) Series Limit or last line or the limiting line of Paschen Series is obtained when transition takes place from $n_2 = \infty$ to $n_1 = 3$.
- (d) Series Limit or last line or the limiting line of Brackett Series is obtained when transition takes place from $n_2 = \infty$ to $n_1 = 4$.
- (e) Series Limit or last line or the limiting line of Pfund Series is obtained when transition takes place from $n_2 = \infty$ to $n_1 = 5$.

6.6 H_α , H_β and H_γ line of a series

First line of any series is called H_α line of that series. For example:-

First line of any series is called H_α line of that series. For example:-

- (1) when transition takes place in the Lyman series from $n_2 = 2$ to $n_1 = 1$ then the line thus obtained is termed as H_α line of the Lyman series.
 - (2) when transition takes place in the Balmer series from $n_2 = 3$ to $n_1 = 2$ then the line thus obtained is termed as H_α line of the Balmer series.
 - (3) when transition takes place in the Lyman series from $n_2 = 4$ to $n_1 = 3$ then the line thus obtained is termed as H_α line of the Paschen series.
- And so on...

Second line of any series is called H_β line of that series. For example:-

- (1) when transition takes place in the Lyman series from $n_2 = 3$ to $n_1 = 1$ then the line thus obtained is termed as H_β line of the Lyman series.
- (2) when transition takes place in the Balmer series from $n_2 = 4$ to $n_1 = 2$ then the line thus obtained is termed as H_β line of the Balmer series.
- (3) when transition takes place in the Lyman series from $n_2 = 5$ to $n_1 = 3$ then the line thus obtained is termed as H_β line of the Paschen series.

And so on...

Third line of any series is called H_γ line of that series. For example:-

- (1) when transition takes place in the Lyman series from $n_2 = 4$ to $n_1 = 1$ then the line thus obtained is termed as H_γ line of the Lyman series.
- (2) when transition takes place in the Balmer series from $n_2 = 5$ to $n_1 = 2$ then the line thus obtained is termed as H_γ line of the Balmer series.
- (3) when transition takes place in the Lyman series from $n_2 = 6$ to $n_1 = 3$ then the line thus obtained is termed as H_γ line of the Paschen series.

And so on...

6.7 Limitations of Bohr's theory

- (1) Bohr's theory successfully explained the spectrum of hydrogen in terms of only one quantum number, but it could not explain many other aspects of spectra.
- (2) **Bohr's theory does not explain fine structure.** According to Bohr's theory each spectral line consists of a single wavelength but a careful study of spectral lines indicates that each line is not single but consists of several lines. These lines

are closed but separate and distinct. This is known as fine structure. Example: H_{α} line in Balmer series has been found to consist of 5 component lines.

- (3) Bohr applied the classical theory to find the radius of the orbit. Bohr applied quantum theory to explain existence of stationary orbit and for the calculation of emitted frequency. *Simultaneous application of classical and quantum theory is not justified.*
- (4) Bohr's theory does not give any information regarding **intensity of spectral line**.
- (5) Bohr's theory does not produce the selection rules which applied to transition of an electron from one energy level to another.
- (6) Bohr's theory **cannot be applied for many electron atoms**. However it can be applied to calculate the spectral information for hydrogen and hydrogen like atoms like He^+ , Li^{++} etc. Bohr's theory does not deal with **elliptical orbits**.

6.8 Ritz combination principle

By a combination of the terms that occur in the Rydberg or Balmer formula, other relations can be obtained holding good for new lines and new series.

By this principle Ritz predicted new series of lines in the hydrogen spectrum before they were actually discovered.

Example: we know that H_{α} and H_{β} lines of Balmer series can be represented as

$$\bar{\nu}_{\alpha} = R \left[\frac{1}{2^2} - \frac{1}{3^2} \right] \quad (1)$$

$$\bar{\nu}_{\beta} = R \left[\frac{1}{2^2} - \frac{1}{4^2} \right] \quad (2)$$

$$\bar{\nu}_{\gamma} = R \left[\frac{1}{2^2} - \frac{1}{4^2} \right] \quad (3)$$

Subtracting equation (1) from Equation (2), we get

$$\bar{\nu}_{\beta} - \bar{\nu}_{\alpha} = R \left[\frac{1}{3^2} - \frac{1}{4^2} \right] \quad (4)$$

Equation (4) represents a new line. It is the first line of a new series in the infrared part of the electromagnetic spectrum, discovered by the Paschen. Similarly, the

second line of The Paschen series can be obtained by Subtracting equation (1) from Equation (3).

Ritz combination principle can also be stated as following-

“ If lines at frequencies ν_{ij} and ν_{jk} exist in a spectrum with $j > i$ and $k > j$, then there will usually be a line at ν_{ik} , where $\nu_{ik} = \nu_{ij} + \nu_{jk}$. However not all combinations of frequencies are observed because of certain selection rules”.

If lines of frequency ν_{12} and ν_{23} are represented as

$$\nu_{12} = T_1 - T_2 \quad \text{and} \quad \nu_{23} = T_2 - T_3$$

then a line of frequency ν_{31} will exist, where

$$\nu_{31} = (T_1 - T_2) + (T_2 - T_3) = T_1 - T_3$$

6.9 Alkali Atomic Spectra

After hydrogen the simplest atoms to study with regard to their spectra are the alkali metals which are lithium, sodium, potassium, rubidium and caesium. The atoms of these elements have one electron in their outermost orbit. The spectra of all the elements consisting of atoms having one electron in their outermost orbit are similar and are called alkali spectra. The experimental study of alkali spectra was taken up by Liveig, Dewar, Rydberg and Bergmann. They observed that the spectral lines in the emission spectrum of an alkali atom formed four series:

- (1) **Principal series** of bright and most persistent lines.
- (2) **Sharp series** of fine line.
- (3) **Diffuse series** of comparatively broader lines.
- (4) **Fundamental or Bergmann series** in the infra-red region.

The following formula is used for the varies series related to alkali atomic spectra.

$$\bar{\nu} = R \left[\frac{1}{(2-\alpha)^2} - \frac{1}{(q-\beta)^2} \right]$$

Where $\bar{\nu}$ is wave number, α and β are characteristic Constants for the element. p and q are fixed term and running term respectively.

The details of various series of the alkali spectra are as following-

(1) Principal Series – For this Series

$$p = 1, q \geq 2$$

$$\bar{\nu} = R \left[\frac{1}{(1-\alpha)^2} - \frac{1}{(q-\beta_p)^2} \right]$$

Principal series consists of bright and most persistent lines.

(2) Sharp Series- For this Series

$$p = 2, q \geq 2$$

$$\bar{\nu} = R \left[\frac{1}{(2-\alpha)^2} - \frac{1}{(q-\beta_s)^2} \right]$$

Sharp series consists of fine spectral lines.

(3) Diffuse Series- For this Series

$$p = 2, q \geq 3$$

$$\bar{\nu} = R \left[\frac{1}{(2-\alpha)^2} - \frac{1}{(q-\beta_d)^2} \right]$$

Diffuse series has comparatively broader lines.

(4) Fundamental Series or Bergmann Series- For this Series

$$p = 3, q \geq 4$$

$$\bar{\nu} = R \left[\frac{1}{(3-\alpha)^2} - \frac{1}{(q-\beta_f)^2} \right]$$

Fundamental series lies in infra-red region.

Here β_p , β_s , β_d and β_f are the characteristic constants of principal, sharp, diffuse and fundamental series respectively. The other series can be written by using Ritz combination Principle.

6.10 Correspondence Principle

Statement:

“Quantum physics gives the same results as classical physics in the unit of large quantum number is called as Bohr’s corresponding principle”.

Proof :

According to electromagnetic theory-

$$\omega = 2\pi\nu \quad \text{where } \omega \text{ and } \nu \text{ are angular and linear}$$

frequency respectively

$$\therefore \frac{v}{r} = 2\pi\nu \quad \text{since } v = r\omega$$

$$\text{or } v = \frac{v}{2\pi r} \quad (1)$$

but the radius of hydrogen atom is given as

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

The velocity of an electron in nth orbit of a hydrogen atom is given as

$$v = \frac{1}{n} \left(\frac{e^2}{2\epsilon_0} \right) \quad (3)$$

Using equations (3) and (2) for equation (1), we have,

$$v = \frac{\frac{1}{n} \left(\frac{e^2}{2\epsilon_0} \right)}{2\pi \frac{n^2 h^2 \epsilon_0}{m \pi e^2}}$$

$$\therefore v = \left(\frac{2}{n^3} \right) \left(\frac{m e^4}{8 h^3 \epsilon_0^2} \right) \quad (4)$$

This is a Rutherford model, according to classical physics.

Now according to Bohr’s theory

The wavelength of radiation for the transition from n to (n-1) is given as

$$v = \frac{m e^4}{8 h^3 \epsilon_0^2} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

$$\begin{aligned}
&= \frac{me^4}{8h^3\epsilon_0^2} \left[\frac{1}{(n-1)^2} - \frac{1}{n^2} \right] \\
&= \frac{me^4}{8h^3\epsilon_0^2} \left[\frac{n^2 - (n-1)^2}{n^2(n-1)^2} \right] \\
&= \frac{me^4}{8h^3\epsilon_0^2} \left[\frac{n^2 - n^2 + 2n - 1}{n^2(n-1)^2} \right] \\
&= \frac{me^4}{8h^3\epsilon_0^2} \left[\frac{2n-1}{n^2(n-1)^2} \right] \tag{5}
\end{aligned}$$

If n is large then

$$n - 1 \approx n$$

$$2n - 1 \approx 2n$$

Then from (5), we have

$$v = \left(\frac{2}{n^3} \right) \left(\frac{me^4}{8h^3\epsilon_0^2} \right) \tag{6}$$

Equations (4) and (6) show that Quantum physics gives the same results as classical physics in the unit of large quantum number.

6.11 Sommerfield's Relativistic model of Atom

As we know that H_α , H_β , H_γ lines of Balmer Series are not single. Each Single line actually consists of very closed several lines packed together. Initial observation by Michelson through his interferometer shows a separation of 0.13\AA between the wave lengths of components of H_α line.

Bohr's theory could not explain fine structure of H_α line. In order to explain fine structure, Sommerfield introduces following modifications in Bohr's theory.

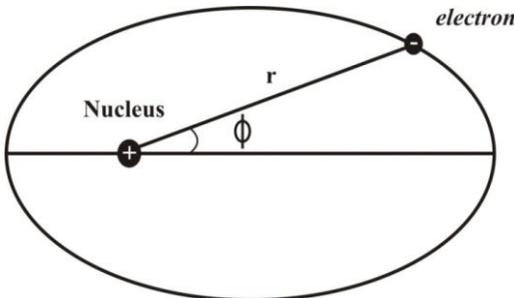


Fig. 6.4

1. Path of electron around nucleus is elliptical. Nucleus may be supposed as situated at any one of the foci of the elliptical orbit.
2. Velocity of electron varies considerably at different parts of the orbit which causes relativistic variation of mass of the electron.

Sommerfeld introduced two quantisation conditions which are as following.

$$\oint P_{\phi} d\phi = n_{\phi}h \quad (1)$$

$$\oint P_r dr = n_r h \quad (2)$$

Where P_{ϕ} is angular momentum

P_r is radial momentum

n_r is radial quantum number

n_{ϕ} is angular (Azimuthal) quantum number

n_r and n_{ϕ} are related to the following equation

$$n = n_r + n_{\phi} \quad (3)$$

Evaluation of Integral, given in eqⁿ (1) and (2)

From equation (1)

$$\oint P_{\phi} d\phi = n_{\phi}h$$

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

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

$$\therefore P_{\phi} \cdot 2\pi = n_{\phi}h$$

$$\therefore P_{\phi} = n_{\phi} \frac{h}{2\pi} \quad (4)$$

$$\text{and } P_{\phi} = mr^2 \frac{d\phi}{dt} \quad (5)$$

Now momentum along radius

$$\begin{aligned} P_r dr &= m \left(\frac{dr}{dt} \right) d\phi \\ &= m \left[\left(\frac{dr}{d\phi} \right) \left(\frac{d\phi}{dt} \right) \right] \left(\frac{dr}{d\phi} \right) d\phi \\ \therefore P_r dr &= m \left(\frac{dr}{d\phi} \right)^2 \left(\frac{dr}{d\phi} \right) d\phi \end{aligned} \quad (6)$$

From equation (5)

$$\begin{aligned} P_\phi &= mr^2 \frac{d\phi}{dt} \\ \therefore \frac{d\phi}{dt} &= \frac{P_\phi}{mr^2} \end{aligned} \quad (7)$$

Using equation (7) for equation (6), we have

$$\begin{aligned} P_r dr &= m \left(\frac{dr}{d\phi} \right)^2 \left(\frac{P_\phi}{mr^2} \right) d\phi \\ \therefore P_r dr &= \frac{1}{r^2} \left(\frac{dr}{d\phi} \right)^2 P_\phi d\phi \end{aligned} \quad (8)$$

The equation of an ellipse in Polar co-ordinates

$$\frac{1}{r} = \frac{(1 + \epsilon \cos \phi)}{a(1 - \epsilon^2)} \quad (9)$$

Taking log of the above equation

$$\log_e \frac{1}{r} = \log_e (1 + \epsilon \cos \phi) - \log_e a(1 - \epsilon^2)$$

Differentiating above equation with respect to ϕ , we have

$$\begin{aligned} r \left(-\frac{1}{r^2} \right) \left(\frac{dr}{d\phi} \right) &= \frac{(-\epsilon \sin \phi)}{(1 + \epsilon \cos \phi)} \\ \therefore \left(-\frac{1}{r} \right) \left(\frac{dr}{d\phi} \right)^2 &= \frac{(-\epsilon \sin \phi)^2}{(1 + \epsilon \cos \phi)^2} \\ \therefore \left(-\frac{1}{r} \right) \left(\frac{dr}{d\phi} \right)^2 &= \frac{(-\epsilon \sin \phi)^2}{(1 + \epsilon \cos \phi)^2} \end{aligned}$$

$$\therefore \frac{1}{r^2} \left(\frac{dr}{d\phi} \right)^2 = \frac{(\epsilon \sin \phi)^2}{(1 + \epsilon \cos \phi)^2} \quad (10)$$

Using equation (10) for equation (8), we have

$$P_r dr = \frac{(\epsilon \sin \phi)^2}{(1 + \epsilon \cos \phi)^2} P_\phi d\phi \quad (11)$$

Using equation (11) for equation (2), we have

$$P_\phi \int_0^{2\pi} \frac{(\epsilon \sin \phi)^2}{(1 + \epsilon \cos \phi)^2} d\phi = n_r h \quad (12)$$

The integral $I = \int_0^{2\pi} \frac{(\epsilon \sin \phi)^2}{(1 + \epsilon \cos \phi)^2} d\phi$ can be integrated by parts.

Now as

$$\int u dv = uv - \int v du$$

Let $u = \epsilon \sin \phi$ and $v = \frac{1}{1 + \epsilon \cos \phi}$

Now as $u = \epsilon \sin \phi$

Now as $v = \frac{1}{1 + \epsilon \cos \phi}$

$$\therefore \frac{dv}{d\phi} = \frac{\epsilon \sin \phi}{(1 + \epsilon \cos \phi)^2} \quad \text{or} \quad dv = \frac{\epsilon \sin \phi}{(1 + \epsilon \cos \phi)^2} d\phi$$

Then

$$\begin{aligned} I &= \left[\frac{\epsilon \sin \phi}{1 + \epsilon \cos \phi} \right]_0^{2\pi} - \int_0^{2\pi} \frac{\epsilon \cos \phi}{1 + \epsilon \cos \phi} d\phi \\ &= \left[\frac{\epsilon \sin 2\pi}{1 + \epsilon \cos 2\pi} - \frac{\epsilon \sin 0}{1 + \epsilon \cos 0} \right] - \int_0^{2\pi} \frac{\epsilon \cos \phi}{1 + \epsilon \cos \phi} d\phi \\ &= \left[\frac{\epsilon \times 0}{1 + \epsilon \times 1} - \frac{\epsilon \times 0}{1 + \epsilon \times 1} \right] - \int_0^{2\pi} \frac{\epsilon \cos \phi}{1 + \epsilon \cos \phi} d\phi \\ &= 0 - \int_0^{2\pi} \frac{\epsilon \cos \phi}{1 + \epsilon \cos \phi} d\phi \\ &= \int_0^{2\pi} \frac{-\epsilon \cos \phi}{1 + \epsilon \cos \phi} d\phi \end{aligned}$$

$$\begin{aligned}
&= \int_0^{2\pi} \left[\frac{1}{1 + \epsilon \cos \phi} - 1 \right] d\phi \\
&= \int_0^{2\pi} \frac{d\phi}{1 + \epsilon \cos \phi} - \int_0^{2\pi} d\phi \\
&= \int_0^{2\pi} \frac{d\phi}{1 + \epsilon \cos \phi} - 2\pi
\end{aligned}$$

Now $\int_0^{2\pi} \frac{d\phi}{1 + \epsilon \cos \phi}$ is a standard integral. It can be shown that

$$\int_0^{2\pi} \frac{d\phi}{1 + \epsilon \cos \phi} = \frac{2\pi}{(1 - \epsilon^2)^{1/2}}, \text{ therefore}$$

$$I = \frac{2\pi}{(1 - \epsilon^2)^{1/2}} - 2\pi \quad (13)$$

Using equation (13) for equation (12), we have

$$\frac{2\pi P_\phi}{(1 - \epsilon^2)^{1/2}} - 2\pi P_\phi = n_r h$$

$$\therefore \frac{n_\phi h}{(1 - \epsilon^2)^{1/2}} - n_\phi h = n_r h \quad \text{since } P_\phi = \frac{n_\phi h}{2\pi}$$

$$\therefore \frac{n_\phi}{(1 - \epsilon^2)^{1/2}} - n_\phi = n_r$$

$$\therefore n_r + n_\phi = \frac{n_\phi}{(1 - \epsilon^2)^{1/2}}$$

$$\therefore n = \frac{n_\phi}{(1 - \epsilon^2)^{1/2}}$$

$$\therefore 1 - \epsilon^2 = \frac{n_\phi^2}{n^2}$$

$$\therefore \frac{b^2}{a^2} = \frac{n_\phi^2}{n^2},$$

(Since for an ellipse $b^2 = a^2(1 - \epsilon^2)$, therefore $1 - \epsilon^2 = \frac{b^2}{a^2}$)

$$\therefore \frac{b}{a} = \frac{n_\phi}{n} \quad (14)$$

The above equation is the condition that determines the allowed elliptical orbits those for which the ratio of major and minor axis is that of two integers. (integer are 1, 2, 3,-----)

Shape of the Orbits

Case I if $n = 2$

If $n = 1$, then $n_s = 1$

Now from the condition given in equation (14)

$$\frac{b}{a} = \frac{n_\phi}{n} = \frac{1}{1}$$

$$\Rightarrow b = a$$

\Rightarrow Circular Orbit

$$n=1, n_\phi = 1 \\ \Rightarrow 1_1 \Rightarrow 1s$$

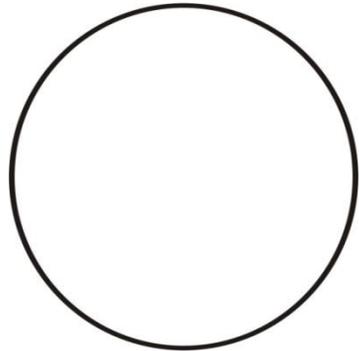


Fig. 6.5

(2) Case II $n = 2$

If $n = 2$, then $n_s = 1, 2$

(a) for $n = 2$ and $n_s = 1$

Now from the condition given in equation (14)

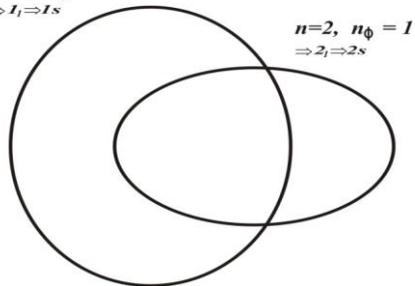
$$\frac{b}{a} = \frac{n_\phi}{n} = \frac{1}{2}$$

$$\Rightarrow a = 2b$$

\Rightarrow Elliptical orbit

$$\Rightarrow 2_1 \Rightarrow 2s$$

$$n=1, n_\phi = 1 \\ \Rightarrow 1_1 \Rightarrow 1s$$



$$n=2, n_\phi = 1 \\ \Rightarrow 2_1 \Rightarrow 2s$$

(b) for $n = 2$ and $n_s = 2$

from the condition given in equation (14)

$$\frac{b}{a} = \frac{n_\phi}{n} = \frac{2}{2}$$

$$\Rightarrow a = b$$

Fig.6.6

\Rightarrow **Circular Orbit**

$\Rightarrow 2_2 \Rightarrow 2p$

(3) Case II $n = 3$

If $n = 3$, then $n_\phi = 1, 2, 3$

(a) for $n = 3$ and $n_\phi = 1$

Now from the condition given in equation (14)

$$\frac{b}{a} = \frac{n_\phi}{n} = \frac{1}{3}$$

$$\Rightarrow a = 3b$$

\Rightarrow **Elliptical orbit**

$$\Rightarrow 3_1 \Rightarrow 3s$$

(c) for $n = 3$ and $n_\phi = 2$

Now from the condition given in equation (14)

$$\frac{b}{a} = \frac{n_\phi}{n} = \frac{2}{3}$$

$$\Rightarrow 2a = 3b$$

\Rightarrow **Elliptical orbit**

$$\Rightarrow 3_2 \Rightarrow 2p$$

(c) for $n = 3$ and $n_\phi = 3$

Now from the condition given in equation (14)

$$\frac{b}{a} = \frac{n_\phi}{n} = \frac{3}{3}$$

$n=3, n_\phi = 3$
 $\Rightarrow 3_3 \Rightarrow 3d$

$n=3, n_\phi = 2$
 $\Rightarrow 3_2 \Rightarrow 3p$

$n=3, n_\phi = 1$
 $\Rightarrow 3_1 \Rightarrow 3s$

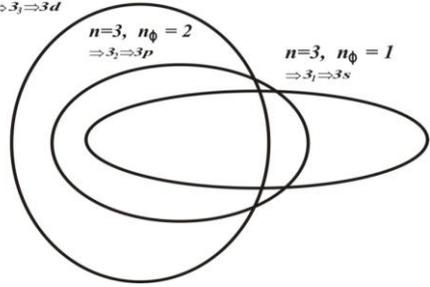


Fig. 6.7

$$\Rightarrow a = b$$

\Rightarrow **Circular Orbit**

$$\Rightarrow 3_3 \Rightarrow 3d$$

Total Energy of the atom

The total energy of an electron in elliptical orbit will be the sum of kinetic energy and potential energy of the electron i.e.

$$E_n = K.E. + P.E. \quad (15)$$

but
$$K.E. = \frac{1}{2}mv^2 + \frac{1}{2}I\omega^2$$

$$\therefore K.E. = \frac{1}{2}m\left(\frac{dr}{dt}\right)^2 + \frac{1}{2}mr^2\left(\frac{d\phi}{dt}\right)^2$$

$$\therefore K.E. = \frac{1}{2}m\left[\left(\frac{dr}{dt}\right)^2 + \left(r\frac{d\phi}{dt}\right)^2\right] \quad (16)$$

where $\frac{dr}{dt}$ is the radial component of the velocity and $r\frac{d\phi}{dt}$ is the transverse component of velocity.

and
$$P.E. = \frac{-Ze^2}{4\pi\epsilon_0 r} \quad (17)$$

Using equation (16) and (17) for equation (15), we have

$$E_n = \frac{1}{2}m\left[\left(\frac{dr}{dt}\right)^2 + \left(r\frac{d\phi}{dt}\right)^2\right] + \frac{-Ze^2}{4\pi\epsilon_0 r} \quad (18)$$

It can be shown that

$$E_n = -\left[\frac{mZ^2e^4}{8\epsilon_0^2h^2}\right]\frac{1}{n^2} \quad (19)$$

The expression of total energy is the same by Bohr energy expression. This means that the theory of elliptical orbit introduces no new energy levels. No new spectral lines, which would explain the fine structure are to be expected because of this multiples of orbit. Hence Sommerfeld proceeded further to find the two problem

of fine structure of spectral lines on the basis of variation of mass of the electron with velocity.

6.12 Sommerfield Relativistic theory

In elliptical orbit the velocity of electron varies (since angular momentum = constant, i.e., $mvr = \text{constan}r$, i.e., $vr = \text{constant}$, which means $v \propto \frac{1}{r}$). It will be maximum at perihelion (i.e. the point when electron is closest to nucleus) and minimum at aphelion (i.e. the point, farthest from nucleus). Sommerfield showed that the relativistic equation which describes the path of electron is given by:

$$\frac{1}{r} = \frac{1+\epsilon \cos \psi\phi}{a(1-\epsilon^2)} \tag{20}$$

Where
$$\psi^2 = 1 - \frac{Z^2 e^4}{16\pi^2 \epsilon_0^2 p^2 c^2} \tag{21}$$

The Path of electron is given by the equation (20) is a rosette.

Rosette : Rosette is a Precessing ellipse i.e. an ellipse whose major axis processes slowly in the plane of the ellipse about an axis through the nucleus.

It can be shown that the total energy E_n in the relativistic theory is given as-

$$E_n = -\frac{mZ^2 e^4}{8\epsilon_0^2 h^2 n^2} - \frac{mZ^2 e^4 \alpha^2}{8\epsilon_0^2 h^2} \left[\frac{n}{n_\phi} - \frac{3}{4} \right] \frac{1}{n^4} \tag{22}$$

Where
$$\alpha = \frac{e^2}{2\epsilon_0 ch} = \frac{1}{137} \tag{23}$$

α is a dimensionless quantity and is called as fine structure constant Fine structure of $H\alpha$ line with the help of Bohr.

In equation (22), first term is the energy of the electron in the orbit with the principal quantum number n . The second term is the Sommerfield relativity correction. This term shows that the energy does depend on the azimuthal quantum number n_ϕ . This result in a splitting of the energy levels of

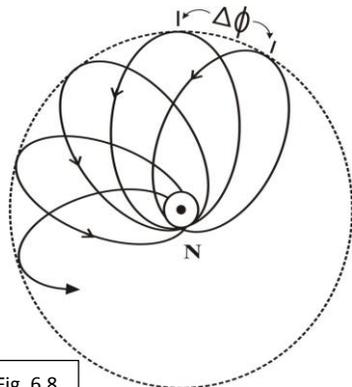


Fig. 6.8

the atom, for a given value of n , into n components, corresponding to the n permitted values of n_ϕ .

6.13 Vector Atom Model

Introduction

(1) Bohr's was able to explain only the line spectra of the hydrogen type of atoms. It could not explain the fine structure of the spectral lines. Although Sommerfield theory was able to give an explanation of the fine structure of the spectral line of hydrogen, but it could not predict the correct number of the fine structure lines. The above theory neither could explain the complex spectra of alkali metals like sodium nor could give information about the relative intensities of the lines.

(2) These older theories were inadequate to explain new discoveries like Zeeman effect and Stark effect.

(3) Another drawback of the Bohr model was that it could not explain how the orbital electrons in an atom were distributed around the nucleus. Therefore, in order to explain the complex spectra of atoms and their relation to atomic structure, the vector atom model was introduced.

The two distinguish features of the vector atom model are:-

(a) Spatial quantisation.

(b) Spinning electron hypothesis

(a) Space quantisation- According to this concept magnitude as well as direction or orientation of orbits are quantised. To specify the orientation of the orbits in space, there is a requirement of a fixed reference axis. This reference axis is chosen along the direction of external magnetic field that is applied to the atom. The different permitted orientations of an electron orbit are determined by the fact that the projections of the quantised orbits on the field direction must themselves be quantised.

Importance The idea of space quantisation leads to an application of Zeeman effect.

Experimental proof of space quantisation

The Stern-Gerlach experiment provided an excellent proof of the space quantisation of atom.

(b) Spinning Electron

To account for the observed fine structure of spectral lines and to explain the anomalous Zeeman Effect. The concept of spinning electron was introduced by unlenbeck of Goudsmith in 1926.

According to their Hypothesis the electron spins about an axis of own, while it also moves around the nucleus of the atom in its orbit. According to the quantum theory, the spin of the electron should also be quantised. Hence a new quantum number called the spin quantum number (s) is introduced. Since the orbital motion and spin motion are quantised in magnitude and direction, they are considered as quantised vectors. Hence the atom model, based on these quantised vectors is called **vector atom model**.

6.14 Quantum numbers related to the vector atom model

The quantum numbers related to the vector atom model are as following.

1. Principal quantum number (n)
2. Orbital quantum number (l)
3. Spin quantum number (s)
4. Total angular momentum quantum number (j)
5. Magnetic orbital quantum number (m_l)
6. Magnetic spin quantum number (m_s)
7. Magnetic total angular momentum quantum number (m_j)

(1) Principal quantum number (n)

- It represents the serial of shell.
- Identical with that used in Bohr and Sommerfield theory.

- Principal quantum number (n) can take any positive integral value (excluding zero). i.e. $n = 1, 2, 3, \dots$
- $n = 1 \Rightarrow$ K Shell
- $n = 2 \Rightarrow$ L Shell
- $n = 3 \Rightarrow$ M Shell
- $n = 4 \Rightarrow$ N Shell
- -----
- -----
- This quantum number governs the energy and major axis of the ellipse.

(2) Orbital quantum Number (l)

- It represents subshell
- Its value is from 0 to $(n-1)$
- By convention the electrons for which:-
- $l = 0$ is called s electron
- $l = 1$ is called p electron
- $l = 2$ is called d electron
- $l = 3$ is called f electron
- The orbital angular momentum, associated to the orbital motion of the electron is given as-

- $$P_l = \frac{lh}{2\pi}$$

But according to the quantum mechanics

$$P_l = \sqrt{l(l+1)} \frac{h}{2\pi}$$

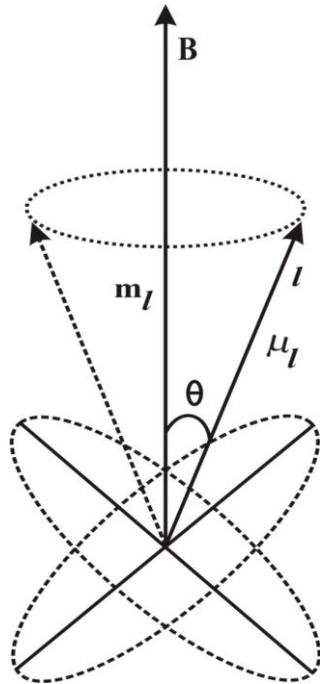


Fig. 6.9

- It governs the degree with which the electron is attached to nucleus. Larger is the value of l weaker is the bond with which it is maintained with the nucleus.

Example (a) if $n = 1$

Then $l = 0$

Example (b) if $n = 2$

then $l = 0, 1$

Example (c) if $n = 1$

then $l = 0, 1, 2$

Note: Maximum number of electrons in a subshell

s	2 electron
p	6 electron
d	10 electron
f	14 electron

(3) Spin Quantum Number (s)

- The magnitude of spin quantum number is always $\frac{1}{2}$.
- At first sight, $s = \frac{1}{2}$ contradicts the integral multiple rule of quantisation of angular momenta. But the use of half integer for 's' consistently leads to results which are in completely agreement with the experimental facts. Moreover the wave mechanical treatment of the spinning electron, given by Dirac leads to the aforesaid half integral property.
- The spin angular momentum, associated to the spin motion of the electron is given as-

$$P_s = \frac{sh}{2\pi}$$

But according to the quantum mechanics

$$P_s = \sqrt{l(l+1)} \frac{h}{2\pi}$$

(5) **Total Angular momentum quantum Number (j)**

- It represents the total angular momentum of the electron which is the

of the orbital angular momentum and spin angular momentum. The vector \vec{j} is defined by the following equation.

$$\vec{j} = \vec{l} + \vec{s}, \text{ with the restriction that } \vec{j} \text{ is positive.}$$

Since $S = \frac{1}{2}$ (always), therefore $j = l \pm \frac{1}{2}$, plus sign is applied when s is parallel to l and minus sign is applied when s is antiparallel to s.

The spin angular momentum μ of the electron is given as-

$$P_j = \frac{j\hbar}{2\pi}$$

But according to the quantum mechanics

$$P_s = \sqrt{j(j+1)} \frac{h}{2\pi}$$

If the atom is placed in a magnetic field so that some preferential axis in space is determined, then the magnetic field exerts its direct influence on both the orbital and spin motions which constitute elementary magnets. Therefore to explain the splitting of spectral lines in a magnetic field, The following three more magnetic quantum numbers are introduced.

(6) **Magnetic Orbital Quantum Number (m_l)**

- This is the numerical value of projection of orbital angular momentum vector \vec{l} on the magnetic field direction.
- Its value is from $-l$ to $+l$

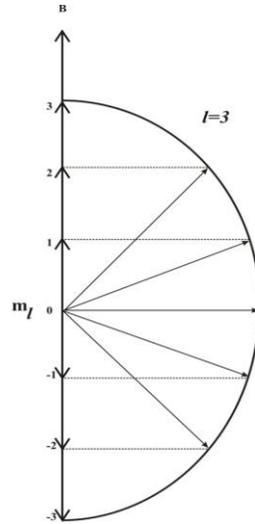


Fig. 6.11

- Total values of m_l are $(2l + 1)$

Examples

(a) If $l = 1$ then $m_l = -1, 0, +1$ (since total values of $m_l = 2 \times 1 + 1 = 3$)

(b) If $l = 2$ then $m_l = -2, -1, 0, +1, +2$ (since total values of $m_l = 2 \times 2 + 1 = 5$)

(7) Magnetic Spin Quantum Number (m_s)

- This is the numerical value of projection of spin angular momentum vector \vec{S} on the magnetic field direction.
- Its value is from $-S$ to $+S$ excluding zero
- Total values of m_s are $(2l + 1)$
- Since S can never equal to zero, therefore m_s can have two quantised values $+\frac{1}{2}$ and $-\frac{1}{2}$, i.e, Its value is $m_s = +\frac{1}{2}$ or $m_s = -\frac{1}{2}$

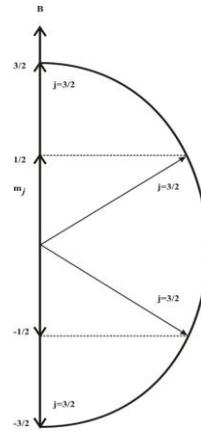


Fig. 6.12

(8) Magnetic total angular momentum quantum Number (m_j)

This is the numerical value of projection of total angular momentum vector \vec{J} on the magnetic field direction.

- Its value is from $-j$ to $+j$ excluding zero
- Total values of m_j are $(2j + 1)$

Example-

if $j = 3/2$ then $m_j = -3/2, -1/2, +1/2, +3/2$

since total values of $m_j = 2 \times 3/2 + 1 = 3 + 1 = 4$

if $j = 5/2$ then $m_j = -5/2, -3/2, -1/2, +1/2, +3/2, +5/2$

since total values of $m_j = 2 \times 5/2 + 1 = 5 + 1 = 6$

Note:-

- (a) The quantum numbers m_l and m_s are significant only in very strong magnetic field where the coupling between l and s is broken while m_j is effective in ordinary fields.
- (b) Small letters as l, s, p, d, f , etc. are used to designate the state of an electron.
- (c) Capital letters as L, S, P, D, F , etc. are used to DESCRIBE the state of the atom as a whole.

6.15 Selection Rules

- (a) Selection rule for L**

$$\Delta L = \pm 1$$

- (b) Selection rule for J**

$$\Delta J = \pm 1, 0 \text{ but } 0 \rightarrow 0 \text{ is excluded}$$

- (c) Selection rule for S**

$$\Delta S = 0$$

- (d) Selection rule for m_L**

$$\Delta m_L = \pm 1, 0$$

- (e) Selection rule for m_S**

$$\Delta m_S = 0$$

- (f) Selection rule for m_j**

$$\Delta m_j = \pm 1, 0$$

6.16 Intensity Rules

$\Delta L = -1, \Delta J = -1$	<i>Most intense line</i>
$\Delta L = -1, \Delta J = 0$	<i>Less intense</i>
$\Delta L = +1, \Delta J = +1$	<i>Weaker</i>

$\Delta L = +1, \Delta J = 1$	<i>Weakest</i>
$\Delta L = -1, \Delta J = +1$	<i>No line (forbidden)</i>
$\Delta L = +1, \Delta J = -1$	<i>No line (forbidden)</i>

6.17 The Interval Rule

Lande discovered a rule regarding the interval in frequency between the different levels constituting a multiplet. It states that “ *The frequency interval between two levels with total angular momentum $J + 1$ and J respectively is proportional to $(J+1)$* ”.

6.18 L S Coupling or Russel-Saunders Coupling

This type of coupling holds for most atoms and for weak magnetic field

The type of coupling which occurs most frequently is the LS coupling. In this type, the angular

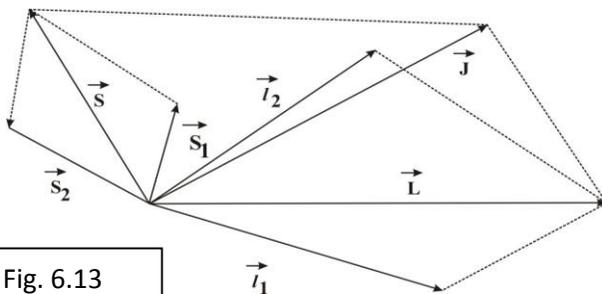


Fig. 6.13

momentum of various electrons combine to give total orbital angular of electrons combine to give total spin momentum together to give total angular momentum \vec{J} of whole atom

Mathematically,

$$\vec{L} = \vec{l}_1 + \vec{l}_1 + \vec{l}_1 + \dots \quad (1A)$$

$$\therefore \vec{L} = \sum \vec{l}_i \quad (1B)$$

Similarly

$$\vec{S} = \vec{s}_1 + \vec{s}_2 + \vec{s}_3 + \dots \quad (2A)$$

$$\therefore \vec{S} = \sum \vec{s}_i \quad (2B)$$

Now total angular momentum \vec{J} of the atom will be obtained by adding equations

(1A) and (2A)

$$\vec{J} = \vec{L} + \vec{S}$$

$$\text{or } \vec{J} = \sum \vec{l}_i + \sum \vec{s}_i$$

This type coupling is also known as *Russel-Saunders Coupling (or RS coupling)*

6.19 J J coupling

This type of coupling holds for the heaviert atoms and for strong magnetic fields.

When interaction between spin-spin and orbital-orbital vectors is weaker than the interaction between spin-orbital vectors then such coupling is used.

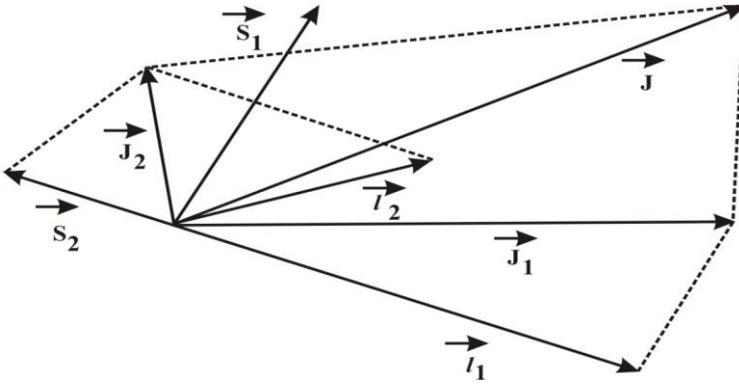


Fig. 6.14

combine to give total angular momentum vector (\vec{J}) of the electron. Now total angular momentum vectors of all the electrons can be added together. We get total angular momentum J of whole atom. In this type of coupling, the interaction between the spin and orbital vectors of each electron is stronger than the interaction between either spin vector or orbital vector of the different electron.

This type of coupling is found in heavy atom.

$$\vec{l}_1 + \vec{s}_1 = \vec{J}_1$$

$$\vec{l}_2 + \vec{s}_2 = \vec{J}_2$$

$$\vec{l}_3 + \vec{s}_3 = \vec{J}_3$$

.....

$$\vec{J} = \vec{J}_1 + \vec{J}_2 + \vec{J}_3 + \dots \quad (3)$$

$$\therefore \vec{J} = \sum \vec{J}_i \quad (4)$$

6.20 Bohr magneton

Orbital magnetic moment- We know that due to the orbital motion of the electron, orbital current flows, which is responsible for generated magnetic field. This magnetic field is characterised by orbital magnetic moment μ_β .

The orbital magnetic moment is quantised. The smallest unit of the orbital moment is called 'Bohr magneton' (μ_β). All other values of orbital magnetic moment are the integral multiple of μ_β .

$$\mu_\beta = \frac{eh}{4\pi m}$$

Proof- Let an electron of charge e moves around the nucleus N in an elliptical orbit from P_1 to P_2 in a very short interval of time dt . Let the radius vector joining the nucleus and electron sweeps an area dA in time dt . If A is the total area which has been swept by the radius vector in T time which is the time period of revolution of the electron, then electric current in the orbit will be given as

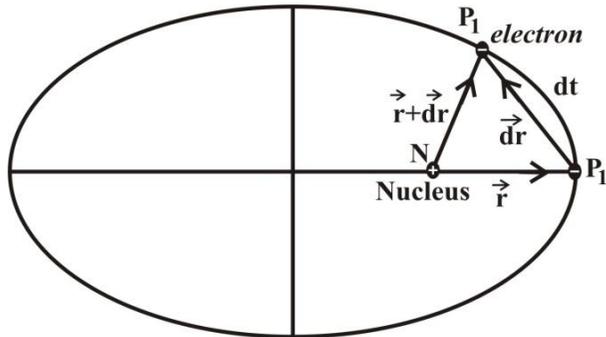


Fig. 6.15

$$i = \frac{e}{T} \quad (1)$$

Magnetic moment due to orbital motion is defined as

$$\mu_l = i \times A \quad (2)$$

and

$$A = \int_0^A dA \quad (3)$$

$$\therefore \vec{dA} = \frac{1}{2} (\vec{r} \times \vec{dr})$$

$$\begin{aligned} \therefore \quad \frac{d\vec{A}}{dt} &= \frac{1}{2} \left(\vec{r} \times \frac{d\vec{r}}{dt} \right) \\ \therefore \quad \frac{d\vec{A}}{dt} &= \frac{1}{2} (\vec{r} \times \vec{v}) \\ \therefore \quad \frac{d\vec{A}}{dt} &= \frac{1}{2m} (\vec{r} \times m\vec{v}) \\ \therefore \quad \frac{d\vec{A}}{dt} &= \frac{1}{2m} (\vec{r} \times \vec{P}) \\ \therefore \quad \frac{d\vec{A}}{dt} &= \frac{\vec{P}_l}{2m} \quad \text{where } \vec{P}_l = \vec{r} \times \vec{P}, \end{aligned}$$

\vec{P}_l is called orbital angular momentum

now we know that in motion under central force, the external torque is zero, consequently angular momentum will remain constant. i.e, $\vec{P}_l = \text{constant}$, hence,

$$\begin{aligned} \frac{d\vec{A}}{dt} &= \frac{\vec{L}}{2m} = \text{constant} \\ \therefore \quad \frac{dA}{dt} &= \frac{P_l}{2m} \\ \therefore \quad dA &= \frac{L}{2m} dt \end{aligned} \quad (4)$$

Using equation (4) for equation (3), we get

$$\begin{aligned} A &= \int_0^T \frac{L}{2m} dt \\ \text{or} \quad A &= \frac{L}{2m} \int_0^T dt \\ \text{or} \quad A &= \frac{L}{2m} T \end{aligned} \quad (5)$$

Using equation (1) and (5) for equation (4), we get

$$\begin{aligned} \mu &= \frac{e}{T} \times \frac{L}{2m} T \\ \text{or} \quad \mu &= \frac{eL}{2m} \end{aligned} \quad (6)$$

but $L = \frac{lh}{2\pi}$, where h is Planck's constant and l is orbital quantum number.

Substituting the value of L in equation (6), we get

$$\mu_l = \frac{eh}{4\pi m} l \quad (7)$$

From the above equation, this is obvious that orbital angular momentum (μ_l) is quantised.

When we put $l = 1$, in the above equation, then minimum value of orbital magnetic moment, which is known as Bohr Magnetron (μ_β) is obtained, i.e.,

$$\mu_\beta = \frac{eh}{4\pi m} \quad (8)$$

Important points regarding orbital magnetic moment

(i) $\mu_\beta = 9.274 \times 10^{-24}$ Joule/Tesla

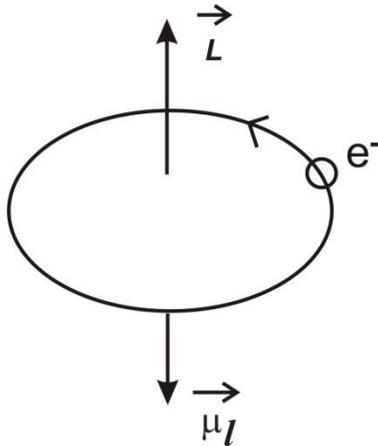


Fig. 6.16

(iii) $\vec{\mu}_l$ is directed opposite to \vec{L} , since charge on the electron is negative.

$$\mu_l = \frac{eh}{4\pi m} l$$

$$\text{or} \quad \mu_l = \frac{e}{2m} \left(\frac{lh}{2\pi} \right)$$

$$\therefore \quad \mu_l = \frac{e}{2m} L \quad \text{Since} \quad L = \frac{lh}{2\pi}$$

$$\therefore \quad \frac{\mu_l}{L} = \frac{e}{2m}$$

But $g = \frac{\mu_l}{L}$, g is called gyromagnetic ratio.

$$\therefore \quad g = \frac{e}{2m}$$

$$g = \frac{\mu_l}{L} = \frac{e}{2m}$$

The value of g can be calculated from the above equation, which comes out as

$$g = 8.8 \times 10^9 \text{ C/kg}$$

6.21 Magnetic Dipole moment due to spin (spin magnetic moment)

An electron spinning about its axis should also behave as a tiny magnet possesses a magnetic dipole movement due to this spin.

However nothing is known about the shape of an electron or manner in which its charge is distributed. Hence it is impossible to calculate its spin magnetic dipole moment in similar way to that used for the orbital motion. In order to obtain agreement with experimental results. The spin magnetic dipole moment is

$$\vec{\mu}_s = 2 \left(\frac{e}{2m} \right) \vec{S} \quad (\text{vector form}) \quad (1A)$$

$$\mu_s = 2 \left(\frac{e}{2m} \right) S \quad (\text{scalar form}) \quad (1B)$$

Where $\vec{\mu}_s$ is the spin magnetic moment and \vec{S} is the spin magnetic moment quantum number with

$$S = \frac{sh}{2\pi} \quad (2)$$

Using equation (2) for equation (1B), we get

$$\mu_s = \frac{eh}{4\pi m} s \quad (3)$$

6.22 Stern and Gerlach Experiment

The experiment performed by Stern and Gerlach in 1921 is based on the behaviour of a magnetic dipole (atomic magnet) in a non-uniform magnetic field which demonstrated directly that an atom placed in a magnetic field can take only certain discrete orientations with respect to the field. This experiment thus gives the very direct and most convincing proof of the essential features like space quantisation, electron spin and quantised magnetic dipole moment of atom of the ‘vector atom model’.

Principle- We know that the orbital and spin motions of the electrons in the atoms provide the atoms with magnetic moments, i.e., an atom is regarded as an elementary magnet or a magnetic dipole.

If this atomic magnet be placed in an external magnetic field. It will be acted upon by the magnetic field in the following two ways-

(1) ***When the external magnetic field is uniform***

In a uniform magnetic field, the two poles of the atomic magnet which is a magnetic dipole will experience equal and opposite forces in different lines of action (which will constitute a torque).

(2) ***When the external magnetic field is non-uniform***

In this case the opposite forces (which are not in the same line of action) on the two poles of the atomic magnet will not be equal.

In a uniform magnetic field, the atomic magnet which is a magnetic dipole will experience a torque. If the dipole moves in such a field in a direction normal to the field, then over and above of the rotation of its axis into the direction of the field, it will be deviated from its straight line path.

Expression for the deviation

Let the magnetic field is non homogeneous along the x axis, so that the magnetic field gradient $\frac{dB}{dx}$ is positive.

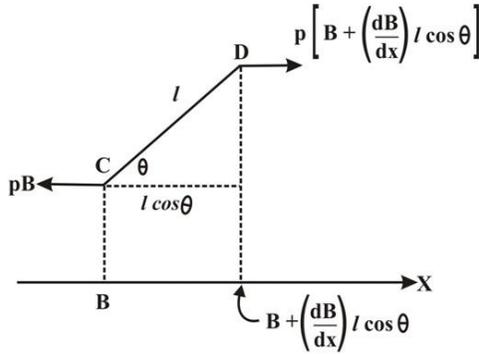


Fig. 6.17

Let p is the Pole strength of the atomic magnet, l is the length of the atomic magnet, μ is the magnetic moment of the magnetic moment and θ is the angle between the axis of the atomic magnet and direction of the magnetic field. If field strength at one of the poles be B , then at the other pole it will be $B + \frac{dB}{dx} l \cos \theta$. Hence the forces on the two poles are pB and $p \left(B + \frac{dB}{dx} l \cos \theta \right)$. Therefore two equal and opposite forces pB will form a the rotating couple while the extra force $p \frac{dB}{dx} l \cos \theta$ acting on one of the pole will displace the atom as a whole.

Therefore the translatory force (F_x) will be given as

$$\begin{aligned} \therefore F_x &= p \left(\frac{dB}{dx} \right) l \cos \theta \\ \therefore F_x &= \frac{dB}{dx} (pl) \cos \theta \\ \therefore F_x &= \frac{dB}{dx} (\mu) \cos \theta \quad (1) \end{aligned}$$

And acceleration 'a' will be given as

$$a = \frac{F_x}{m} \quad (\text{m is the mass of the atomic magnet})$$

therefore from equation (1),

$$a = \frac{1}{m} \left[\frac{dB}{dx} (\mu) \cos\theta \right] \quad (2)$$

Now displacement ' d_x ' can be calculated by the following equation

$$d_x = ut + \frac{1}{2} at^2$$

As before the application of external magnetic field, $u = 0$, therefore

$$d_x = \frac{1}{2} at^2 \quad (3)$$

Using equation (2) for equation (3), we have

$$d_x = \frac{1}{2m} \left[\frac{dB}{dx} (\mu) \cos\theta \right] t^2 \quad (4)$$

Now as $t = \frac{L}{v}$, where t , is the time of flight through the field and L is the length of the path in the field (Note: the velocity of the atom perpendicular to the field remains unaffected by the force in the field direction, since there is no force hence no acceleration in the direction which is perpendicular the direction of the magnetic field), therefore from equation (4),

$$d_x = \frac{1}{2m} \left[\frac{dB}{dx} (\mu) \cos\theta \right] \left(\frac{L}{v} \right)^2 \quad (5)$$

From equation (5), if d_x , m , $\frac{dB}{dx}$, L and v are known then μ can be calculated.

If $\frac{dB}{dx} = 0$, then $d_x = 0$, i.e, there is no deviation.

Experimental arrangement

The sketch diagram of the Stern And Gerlach experiment has been shown in the figure 6.18. S_1 and S_2 are the slits, P is the photographic Plate, M and M are the pole pieces which produce non-magnetic field due to the shape of the pole Pieces.

Silver is boiled in an oven. Atoms of silver stream out from the opening in the oven. This stream is passed through a non-uniform magnetic field and finally

the atoms fall on a photographic plate P. The whole arrangement is enclosed in evacuated chamber in order to avoid collision of silver atom with gas molecules.

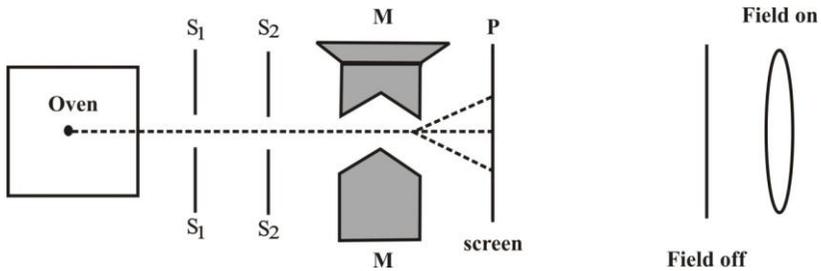


Fig. 6.18

On applying the non-homogenous magnetic field. It was found the stream of silver atoms splits in two separated lines. By knowing $\frac{dB}{dx}$, L , V and d_x , μ can be calculated from equation (5). It was found that each silver atom had a magnetic moment of one Bohr magneton in the direction of the field.

Need of inhomogeneous magnetic field

If the field were homogeneous, then the atoms (tiny magnets) would have experienced only a turning moment, and no deflecting force. As such, we could not obtain the deflected components inspite of the orientation of the atoms relative to the field.

Atoms not ions

In the Stern-Gerlach experiment, a beam of neutral atoms is passed through an inhomogeneous magnetic field, and each atom experiences a transverse force depending upon its orientation with respect to the field, If ions were used, they would be subjected to Lorentz force also due to their charge and their deflection would no longer be transverse so that no traces would be obtained on the photographic plate.

6.23 Pauli's exclusion Principle

Pauli's exclusion Principle is also referred as equivalence principle.

Statement

“Every completely defined quantum state in an atom can be occupied by only one electron”.

or

“No two electrons in an atom exist in the same quantum state”.

or

“No two electrons in an isolated atom may have same four quantum Number”. As the four quantum numbers n, l, m_l, m_s determine the state of an electron completely.

Explanation

The principle implies that each electron in an atom must have a different set of quantum numbers n, l, m_l and m_s . If two electrons have all their quantum numbers identical, then one of those two electrons would be excluded from entering into the constitution of the atom. Therefore the above principle is called exclusion principle.

Application

- (1) **The Pauli exclusion principle enables us to calculate the number of electrons that can occupy a given subshell.**

Case 1 If $n = 1$, then $l = 0, m_l = 0, m_s = +\frac{1}{2}, -\frac{1}{2}$

then according to Pauli's exclusion principle, the following combination of n, l, m_l and m_s would be possible only-

n	l	m_l	m_s
1	0	0	+1/2
1	0	0	-1/2

It is obvious from above table that maximum number of electrons which can be accommodated in K shell ($n=1$) is 2.

Case 2 If $n = 2$, then $l = 0, 1$,

for $l = 0, m_l = 0$,

and for $l = 1, m_l = -1, 0, +1$,

$$\text{and } m_s = +\frac{1}{2}, -\frac{1}{2}$$

then according to Pauli's exclusion principle, the following combination of n, l, m_l and m_s corresponding to $n = 2$ would be possible only-

n	l	m_l	m_s
2	0	0	+1/2
2	0	0	-1/2
2	1	-1	+1/2
2	1	-1	-1/2
2	1	0	+1/2
2	1	0	-1/2
2	1	1	+1/2
2	1	1	-1/2

It is obvious from above table that maximum number of electrons which can be accommodated in L shell ($n=2$) is 8.

Similarly it can be shown that maximum number of electrons which can be accommodated in M shell ($n=3$) and N shell ($n=4$) is 18 and 32 respectively.

(1) It can be shown mathematically also that maximum number of electrons which can be accommodated in a shell with principal quantum number n is $2n^2$.

The no. of electrons that can be accommodated in a shell with principal quantum number (n) is equal to sum of the electrons in the constituent n sub shells

$$\begin{aligned}
 &= \sum_{l=0}^{n-1} 2(2l + 1) \\
 &= 2[1 + 3 + 5 + 7 + \dots + [2(n - 1) + 1]] \\
 &= 2[1 + 3 + 5 + 7 + \dots + (2n - 1)] \\
 &= 2 \cdot \frac{n}{2} [2 \times 1 + (n - 1) \times 2]
 \end{aligned}$$

(Since sum of Arithmathical Progression (A.P.) = $\frac{n}{2} [2a + (n - 1)d]$, where a is first term, d is the common difference and n is the number of total terms.)

$$= n[2 + 2n - 2]$$

$$= n(2n)$$

$$= 2n^2$$

Note: *A direct consequence of the Pauli's Principle is that every closed shell opr sub-shell is balanced with respect to angular momenta both as regards orbital and spin motions and hence contributes nothing to the total angular momentum of the atom as a whole.*

Solved Problems

Problem: Among LS and JJ coupling schemes, which one holds for the light atoms.

Solution: LS coupling generally takes place in the case light atoms because the interaction between orbital angular momentum vectors $\vec{l}_1, \vec{l}_2, \vec{l}_3, \dots$ etc. among different electrons in the atom is much greater than spin orbit interaction of the same electron i.e, between \vec{l}_1 and \vec{s}_1 of electron 1 and \vec{l}_2 and \vec{s}_2 of the electron 2.

However in heavy atoms, the nuclear charge is very large and produces a spin orbit interaction comparable in magnitude to the coulomb interaction between various \vec{l} vectors and between \vec{s} vectors so that LS coupling breaks down, the resultant angular momentum vectors $\vec{l}_1, \vec{l}_2, \vec{l}_3, \dots$ etc of individual electrons add directly to form the total angular momentum vector \vec{J} of the whole atom.

Thus LS coupling holds for light atoms.

Exercise

Theoretical

- (1) Derive the formula for the radius, speed and energy of an electron in n^{th} orbit of a hydrogen atom according to the Bohr model.
(L.U. 2014)
- (2) Write down Bohr's postulates of Hydrogen atom. Hence obtain an expression for energy of n^{th} orbit.
(L.U. 2010)
- (3) Find the velocity of an electron in the n^{th} Bohr Orbit. Prove that for an electron : .
(LU 2015)
- (4) Show that wavelength of electron revolving in first Bohr orbit is equal to the circumference of orbit.
(L.U. 2010)
- (5) Give an account of Bohr's atomic model and explain the various spectral series of hydrogen. Why does this theory fail to explain the atomic spectra of more complex atoms?
(L.U. 2007)
- (6) Bohr-Sommerfeld theory of hydrogen atom.
(L.U. 2013)
- (7) Discuss analytically the Bohr-Sommerfeld theory of elliptical orbits of hydrogen atom and compare its results with those of Bohr's theory of circular orbits. .
(L.U. 2009)
- (8) What is meant by space quantization? Explain with suitable examples. Discuss various quantum numbers used in vector model of atom.
(L.U. 2011)
- (9) Describe the main features of vector atom model and mention various quantum numbers associated with this model.
(LU 2016)
- (10) Give an account of LS coupling and jj coupling with suitable examples.

- (L.U. 2012)**
- (11) Give a brief account of LS and JJ coupling.
- (L.U. 2008)**
- (12) Explain, what is meant by L-S and J-J coupling in atoms having more than one electrons.
- (L.U. 2014)**
- (13) Explain why do spin-orbit coupling splits all states except S states into two substates.
- (L.U. 2014)**
- (14) Describe Stern-Gerlach experiment with necessary theory. Explain, how this experiment confirms space quantization and electron spin.
- (L.U. 2011)**
- (15) In Stern Gerlach experiment, state clearly :
- (i) What was the aim of the experiment? (ii) Why Ag atoms were chosen. (iii) What was the need of magnetic field was chosen (iv) What are the important conclusions of the experiment. (v) Can the experiment be performed with ions rather with neutral atoms? (vi) How does experiment support the concept of electron spin. .
- (L.U. 2009)**
- (16) How does Stern-Gerlach experiment support the concept of electron spin?
- (L.U. 2012)**
- (17) Explain what is the magnetic moment of an electron in an atom and derive an expression for it. Hence show that the ratio of the orbital magnetic moment and angular momentum of electron in the atom is $e/2m$.
- (L.U. 2012)**
- (18) What do you understand by Bohr-magneton? Deduce an expression for it in terms of universal constants.
- (L.U. 2016)**
- (19) Describe Stern-Gerlach experiment with necessary theory. Explain how this experiment confirms space quantization and electron spin.
- (L.U. 2010)**
- (20) Prove that maximum number of electrons which can be accommodated by nth orbit is $2n^2$

- (21) Radius of orbit. (L.U. 2012)
(L.U. 2008)

Short answer type

- (1) An electron revolves round the nucleus in the first Bohr circular orbit of hydrogen atom. Calculate: (L.U. 2008)
- (2) What are the defects of Bohr's theory of hydrogen atom? . (L.U. 2015)
- (3) State which features of Bohr-Sommerfield theories are still valid. (L.U. 2007)
- (4) Calculate the radius of first Bohr orbit. (L.U. 2012)
- (5) Calculate the value of Rydberg constant, assuming that wavelength of H_{α} line is 6563\AA . (L.U. 2014)
- (6) Calculate the value of longest wavelength in Paschen series. (L.U. 2009)
- (7) Differentiate between Balmer and Paschen series with reference to Hydrogen spectra. (L.U. 2011)
- (8) If a_0 is the radius of the Bohr orbit. Calculate the radius of the fourth Bohr orbit in a hydrogen atom. (L.U. 2013)
- (9) Explain, why electrons are not effective in scattering α – particles and protons. (L.U.2013)
- (10) Mention different Quantum numbers associated with vector atom model. (L.U. 2013)
- (11) Explain 'space quantisation' giving suitable examples. (L.U. 2009)
- (12) Mention different quantum numbers associated with vector atom model. (L.U. 2014)
- (13) What are spin and screening doublets? (L.U. 2007)
- (14) What are spin and screening doublets? (L.U. 2008)
- (15) What do you mean by parallel spin of electron? (L.U. 2008)
- (16) Find Lande g factor for $3P_{\frac{1}{2}}$ energy level. (L.U. 2008)
- (17) Explain the L-S coupling scheme for a two electron system. (L.U. 2013)

- (18) The quantum numbers of two electrons in a two-valence electron atom are : **(L.U. 2013)**
 $n_1 = 6, l_1 = 3, s_1 = \frac{1}{2}$; and $n_2 = 5, l_2 = 3, s_2 = \frac{1}{2}$.
 Assuming J-J coupling, find possible values of J.
- (19) Find the number of quantum states of 2P subshell. • **(L.U. 2015)**
- (20) What is meant by L-S coupling? • **(L.U. 2015)**
- (21) In the study of space quantization, draw possible orientation for $J=2$. • **(L.U. 2015)**
- (22) Explain the 'principle of superposition'. **(L.U. 2012)**
- (23) Moment of inertia of electron. **(L.U. 2008)**
- (24) moment of momentum of electron and (L.U. 2008)
- (25) current set-up in the orbit. (L.U. 2008)
- (26) Discuss the principle of superposition. **(L.U. 2014)**
- (27) Which quantum numbers you use to distinguish between two electrons in an atom?
- (28) Find, n, L, s, and j for ground state $3^2S_{1/2}$ of Sodium. **(L.U. 2016)**
- (29) Find Lande g factor for $^2S_{1/2}$ energy level. • **(L.U. 2015)**
- (30) Find the value of l and s for the state $^2D_{3/2}$ of an atom. **(L.U. 2010)**

(C) Numerical Problems

- (1) The quantum number of the two optical electrons in an atom are :

$$n_1 = 5, l_1 = 0, S_1 = \frac{1}{2}$$

$$n_2 = 4, l_2 = 1, S_2 = \frac{1}{2}$$

- (i) Assuming L-S coupling, find the possible values of L and hence J.
- (ii) Assuming J-J coupling, find the possible values of J

- (2) Find the orbital radius and velocity of the electron in hydrogen atom.
Binding energy of hydrogen atom : $E = -13.6 \text{ eV}$. **(L.U. 2014)**
- (3) An electron in ground state of Hydrogen atom is excited by absorbing photon of energy 10.2 eV . Calculate its angular momentum. **(L.U. 2016)**
- (4) The energy of an electron in an excited hydrogen atom is -3.4 eV .
Calculate angular momentum of electron. **(L.U. 2010)**

Chapter 7

Applications of vector atom model

7.1 Optical spectra

The valence electron of an atom determine the chemical and optical properties of their atoms. The valence electron thus, also called as optical electron. The electrons in the closed inner orbits do not take part in the emission of spectral lines.

Spectral terms

Atoms are divided into following two main categories:-

One electron system (b) many electron system

(a) **One electron system:** The alkali metals such as Na and K have a single valence electron outside completely filled subshells. Therefore alkali metals have hydrogen like or one electron spectra.

Many electron system: In the many electron system, the atoms have more one valence electron outside completely filled subshells. For example, the alkaline earths which are two electron system have similar spectra.

Spectral Notation

(1) The states of the atom, in which the values of its L vector are 0,1,2,3,4,..... are represented by S,P,D,F,G,..... respectively.

(2) A spectral term is represented by ${}^r X_l$,

where $X \Rightarrow$ S or P or D or F or G.....(e.g. when $L=0$, then $X = S$; when $L = 1$, then $X = P$; when $L = 2$, then $X = D$.)

and J is total angular momentum, defined as

$$\vec{J} = \vec{L} + \vec{S} \quad \Rightarrow \quad J = L \pm S \quad \text{with} \quad S = \frac{1}{2}$$

And r is multiplicity, defined by $r = 2S + 1$,

Note:

$r = 1 \Rightarrow$ Singlet State

$r = 2 \Rightarrow$ Doublet State

$r = 3 \Rightarrow$ Triplet State

$r = 4 \Rightarrow$ multiplet State

7.2 Fine Structure of D line of Sodium

We know that ten out of the eleven electron of the normal sodium atom are interlocked in closed shells, so that the eleventh free free electron alone is responsible for the spectrum. From Bohr's theory, it has been shown that the D line belongs to the principal series which are due to transitions from P states to the S states.

Now for the upper P state

$$L = 1$$

$$\therefore J = L + S \text{ or } L - S$$

$$= 1 + \frac{1}{2} \text{ or } 1 - \frac{1}{2}$$

$$= \frac{3}{2} \text{ or } \frac{1}{2}$$

$$r = 2S + 1 = 2 \times \frac{1}{2} + 1 = 2$$

\therefore for the upper P- state, spectral terms are ${}^2P_{3/2}, {}^2P_{1/2}$

Now for the Lower S- state

$$L = 0$$

$$\therefore J = L + S \text{ or } L - S$$

$$= 0 + \frac{1}{2} \text{ or } 0 - \frac{1}{2}$$

$$J = \frac{1}{2}$$

$$r = 2S + 1 = 2 \times \frac{1}{2} + 1 = 2$$

for the Lower S state, spectral terms is ${}^2S_{1/2}$

By using the following Selection Rules

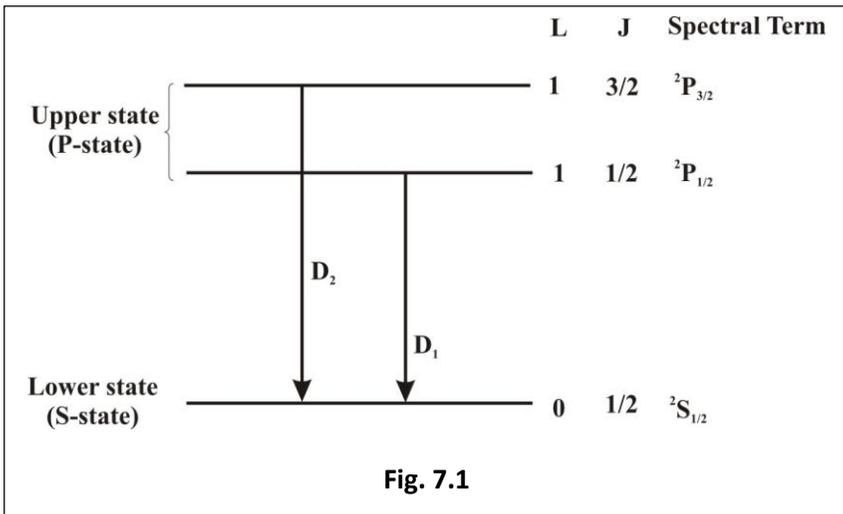
$$\Delta L = \pm 1$$

$$\Delta J = \pm 1, 0 \text{ but } 0 \rightarrow 0 \text{ is excluded}$$

$$\Delta S = 0, \text{ etc.}$$

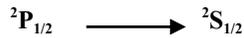
We find that all transitions are possible.

Energy level diagram

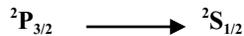


Using intensity Rule

⇒ **D₁ line**, is originated due to transition from



⇒ **D₂ line**, is originated due to transition from



⇒ D₂ line will be most intense since for this line

$$\Delta L = 0 - 1$$

$$= -1$$

and $\Delta J = 1/2 - 3/2$

$$= -1$$

(Since for the Most intense line $\Delta L = -1$, $\Delta J = -1$)

$$\Delta L = -1, \quad \Delta J = -1$$

\Rightarrow D_1 line will be less intense since for this line

$$\begin{aligned} \Delta L &= 0 - 1 \\ &= -1 \end{aligned}$$

$$\begin{aligned} \text{and} \quad \Delta J &= 1/2 - 1/2 \\ &= 0 \end{aligned}$$

(Since for the less intense line $\Delta L = -1$, $\Delta J = -1$)

7.3 Fine Structure of H_α line (of Balmer Series)

We know that for Balmer Series

$$\frac{1}{\lambda} = R \left[\frac{1}{2^2} - \frac{1}{n^2} \right] \quad (1)$$

H_α line of Balmer Series is the first line of Balmer series, i.e., H_α line is obtained when transition from upper state $n = 3$ to lower state $n = 2$ takes place.

For upper State $n = 3$

$$L = 0, 1, 2$$

When $L = 0$

Then from $J = L \pm S$

$$\Rightarrow J = 0 + \frac{1}{2}, 0 - \frac{1}{2}$$

$$\Rightarrow J = \frac{1}{2}$$

$$\text{And } r = 2 \times 1/2 + 1 = 2$$

$$\Rightarrow {}^2S_{1/2} \quad (\text{Note : } L = 0 \Rightarrow S)$$

When $L = 1$

Then from $J = L \pm S$

$$\Rightarrow J = 1 + \frac{1}{2}, 1 - \frac{1}{2}$$

$$\Rightarrow J = \frac{3}{2}, \frac{1}{2}$$

$$\text{And } r = 2 \times 1/2 + 1 = 2$$

$$\Rightarrow {}^2P_{3/2}, {}^2P_{1/2} \quad (\text{Note : } L = 1 \Rightarrow P)$$

When L = 2

Then from $J = L \pm S$

$$\Rightarrow J = 2 + \frac{1}{2}, 2 - \frac{1}{2}$$

$$\Rightarrow J = \frac{5}{2}, \frac{3}{2}$$

$$\text{And } r = 2 \times 1/2 + 1 = 2$$

$$\Rightarrow {}^2D_{5/2}, {}^2D_{3/2} \quad (\text{Note : } L = 2 \Rightarrow D)$$

Therefore spectral terms corresponding to upper state $n = 3$ are

$${}^2S_{1/2}, {}^2P_{3/2}, {}^2P_{1/2}, {}^2D_{5/2}, {}^2D_{3/2}$$

For lower State n = 2

$$L = 0, 1$$

When L = 0

Then from $J = L \pm S$

$$\Rightarrow J = 0 + \frac{1}{2}, 0 - \frac{1}{2}$$

$$\Rightarrow J = \frac{1}{2}$$

$$\text{And } r = 2 \times 1/2 + 1 = 2$$

$$\Rightarrow {}^2S_{1/2} \quad (\text{Note : } L = 0 \Rightarrow S)$$

When L = 1

Then from $J = L \pm S$

$$\Rightarrow J = 1 + \frac{1}{2}, 1 - \frac{1}{2}$$

$$\Rightarrow J = \frac{3}{2}, \frac{1}{2}$$

$$\text{And } r = 2 \times 1/2 + 1 = 2$$

$$\Rightarrow {}^2P_{3/2}, {}^2P_{1/2} \quad (\text{Note : } L = 1 \Rightarrow P)$$

Therefore spectral terms corresponding to lower state $n = 2$ are

$${}^2S_{1/2}, {}^2P_{3/2}, {}^2P_{1/2}$$

i.e. from $n = 3$ which corresponds to ${}^2D_{5/2}, {}^2D_{3/2}, {}^2P_{3/2}, {}^2P_{1/2}, {}^2S_{1/2}$ to $n=2$ which corresponds to ${}^2P_{3/2}, {}^2P_{1/2}, {}^2S_{1/2}$. It is obvious that mathematically, following 15 transitions are possible.

$$D_{5/2} \rightarrow P_{3/2}$$

$$D_{5/2} \rightarrow P_{1/2}$$

$$D_{5/2} \rightarrow S_{1/2}$$

$$D_{3/2} \rightarrow P_{3/2}$$

$$D_{3/2} \rightarrow P_{1/2}$$

$$D_{3/2} \rightarrow S_{1/2}$$

$$P_{3/2} \rightarrow P_{3/2}$$

$$P_{3/2} \rightarrow P_{1/2}$$

$$P_{3/2} \rightarrow S_{1/2}$$

$$P_{1/2} \rightarrow P_{3/2}$$

$$P_{1/2} \rightarrow P_{1/2}$$

$$P_{1/2} \rightarrow S_{1/2}$$

$$S_{1/2} \rightarrow P_{3/2}$$

$$S_{1/2} \rightarrow P_{1/2}$$

$$S_{1/2} \rightarrow S_{1/2}$$

But possibility of the above transitions will be ascertained by the selection rules, as shown in the following table.

Transition	L ₁	L ₂	ΔL	J ₁	J ₂	ΔJ	$\Delta L, \Delta J$	Possibility of transition
	1							

$D_{5/2} \rightarrow P_{3/2}$	2	1	-1	5/2	3/2	-1	$\Delta L = -1, \Delta J = -1$	Possible
$D_{5/2} \rightarrow P_{1/2}$	2	1	-1	5/2	1/2	-2	$\Delta L = -1, \Delta J = -2$	<i>Impossible</i>
$D_{5/2} \rightarrow S_{1/2}$	2	0	-2	5/2	1/2	-2	$\Delta L = -1, \Delta J = -1$	Possible
$D_{3/2} \rightarrow P_{3/2}$	2	1	-1	3/2	3/2	0	$\Delta L = -1, \Delta J = 0$	Possible
$D_{3/2} \rightarrow P_{1/2}$	2	1	-1	3/2	1/2	-1	$\Delta L = -1, \Delta J = -1$	Possible
$D_{3/2} \rightarrow S_{1/2}$	2	0	-2	3/2	1/2	-1	$\Delta L = -2, \Delta J = -1$	<i>Impossible</i>
$P_{3/2} \rightarrow P_{3/2}$	1	1	0	3/2	3/2	0	$\Delta L = 0, \Delta J = 0$	<i>Impossible</i>
$P_{3/2} \rightarrow P_{1/2}$	1	1	0	3/2	1/2	-1	$\Delta L = 0, \Delta J = -1$	<i>Impossible</i>
$P_{3/2} \rightarrow S_{1/2}$	1	0	-1	3/2	1/2	-1	$\Delta L = -1, \Delta J = -1$	Possible
$P_{1/2} \rightarrow P_{3/2}$	1	1	0	1/2	3/2	+1	$\Delta L = 0, \Delta J = +1$	<i>Impossible</i>
$P_{1/2} \rightarrow P_{1/2}$	1	1	0	1/2	1/2	0	$\Delta L = 0, \Delta J = 0$	<i>Impossible</i>
$P_{1/2} \rightarrow S_{1/2}$	1	0	0	1/2	1/2	0	$\Delta L = 0, \Delta J = 0$	<i>Impossible</i>
$S_{1/2} \rightarrow P_{3/2}$	0	1	+1	1/2	3/2	+1	$\Delta L = +1, \Delta J = +1$	Possible
$S_{1/2} \rightarrow P_{1/2}$	0	1	+1	1/2	1/2	0	$\Delta L = +1, \Delta J = 0$	Possible
$S_{1/2} \rightarrow S_{1/2}$	0	0	0	1/2	1/2	0	$\Delta L = 0, \Delta J = 0$	<i>Impossible</i>

It is obvious from the above table, that after applying selection rules, the allowed transitions reduces to 7 in Number, which are as following-

$$\mathbf{D_{5/2} \rightarrow P_{3/2}}$$

$$\mathbf{D_{3/2} \rightarrow P_{3/2}}$$

$$\mathbf{D_{3/2} \rightarrow P_{1/2}}$$

$$\mathbf{P_{3/2} \rightarrow S_{1/2}}$$

$$\mathbf{P_{1/2} \rightarrow S_{1/2}}$$

$$\mathbf{S_{1/2} \rightarrow P_{3/2}}$$

$$\mathbf{S_{1/2} \rightarrow P_{1/2}}$$

Two pairs in separate cases of these and allowed transitions are identical i.e.

(a) The lines, obtained by the transitions between coincident levels, which are $P_{3/2} \rightarrow S_{1/2}$ and $S_{1/2} \rightarrow P_{3/2}$ are identical.

(b) The lines, obtained by the transitions between coincident levels, which are $P_{1/2}$
 $\rightarrow S_{1/2}$ and $S_{1/2} \rightarrow P_{1/2}$.

Note: The above pairs represent coincident levels as for these pairs :

$$\Delta L = \pm 1, \quad \Delta J = 0.$$

Energy Level Diagram-

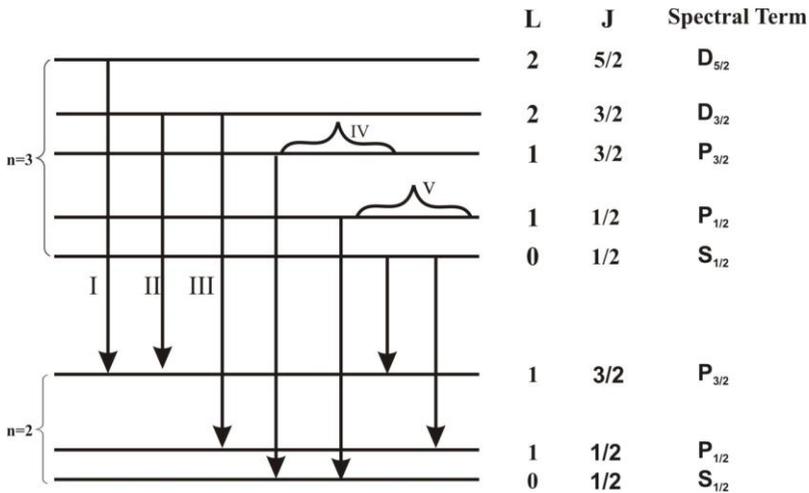


Fig. 7.2

Intensity of the lines

By applying rules of intensity, we can predict the relative intensity of the lines.

- ⇒ First line ($D_{5/2} \rightarrow P_{3/2}$) is most intense, Since for this transition, $\Delta L = -1$, $\Delta J = -1$.
- ⇒ Second line ($D_{3/2} \rightarrow P_{3/2}$) is Less intense, Since for this transition, $\Delta L = -1$, $\Delta J = 0$.
- ⇒ Third line ($D_{3/2} \rightarrow P_{1/2}$) is most intense, Since for this transition, $\Delta L = -1$, $\Delta J = -1$.

- ⇒ Fourth line (I) ($P_{3/2} \rightarrow S_{1/2}$) is **most intense**, Since for this transition, $\Delta L = -1$, $\Delta J = -1$.
- ⇒ Fourth line (II) ($S_{1/2} \rightarrow P_{3/2}$) is **weak**, Since for this transition, $\Delta L = +1$, $\Delta J = +1$.
- ⇒ Fifth line (I) ($P_{1/2} \rightarrow S_{1/2}$) is **less intense**, Since for this transition, $\Delta L = -1$, $\Delta J = 0$.
- ⇒ Fifth line (II) ($S_{1/2} \rightarrow P_{1/2}$) is **weakest** Since for this transition, $\Delta L = +1$, $\Delta J = 0$.

Note: (1) Fourth line (I) and Fourth line (II) are merged into a single line as these lines are obtained by the transitions between coincident levels ; $P_{3/2} \rightarrow S_{1/2}$ and $S_{1/2} \rightarrow P_{3/2}$.

(2) Fifth line (I) and Fifth line (II) are merged into a single line as these lines are obtained by the transitions between coincident levels ; $P_{1/2} \rightarrow S_{1/2}$ and $S_{1/2} \rightarrow P_{1/2}$

7.4 Introduction of Zeeman Effect

It is a magneto optical phenomenon in which spectral lines of the spectrum of a light source are affected by an applied magnetic field. This was first observed by Zeeman in 1896 and therefore known as Zeeman effect.

Among the various magneto optical phenomena, The Zeeman effect is one of very great importance, as it provides a link between the spectroscopic and magnetic properties of element and throws much light on atomic magnetism.

Zeeman effect can be studied into two following categories-

- (i) Normal Zeeman effect
- (ii) Anomalous Zeeman effect

(i) Normal Zeeman Effect

It is observed that if a source of light producing the line spectrum is placed in a strong magnetic field then spectral lines are splitted in the following way-

- (1) three lines (triplet), when viewed in the transverse direction i.e., in a direction which is perpendicular to the direction of the applied magnetic field
- (2) two lines (doublet), when viewed in the transverse direction i.e., in a direction which is perpendicular to the direction of the applied magnetic field.

(ii) Anomalous Zeeman Effect – When the light source producing line spectrum is placed in a very weak magnetic field then the spectral lines are splitted comparatively into more number of lines with respect to strong magnetic field. This is called anomalous Zeeman effects.

7.5 Normal Zeeman Effect

It is observed that if a source of light producing the line spectrum is placed in a strong magnetic field then spectral lines are splitted in the following way-

- (1) three lines (triplet), when viewed in the transverse direction i.e., in a direction which is perpendicular to the direction of the applied magnetic field

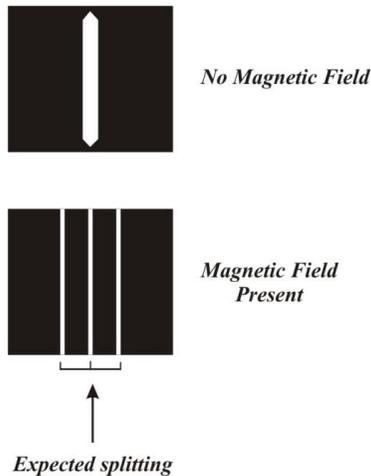


Fig. 7.3

- (2) two lines (doublet), when viewed in the transverse direction i.e., in a direction which is perpendicular to the direction of the applied magnetic field. The experimental arrangement for observing Normal Zeeman Effect is shown as:

Experimental Arrangement

An electromagnet of capable of producing a very strong magnetic field and having conical pole pieces, through which holes have been drilled lengthwise, is set up. A sodium light source, emitting spectral lines is between the pole pieces. The spectral lines are observed with a high resolving power instrument such as Lummer Gehrcke plate in conjunction with constant deviation spectrometer.

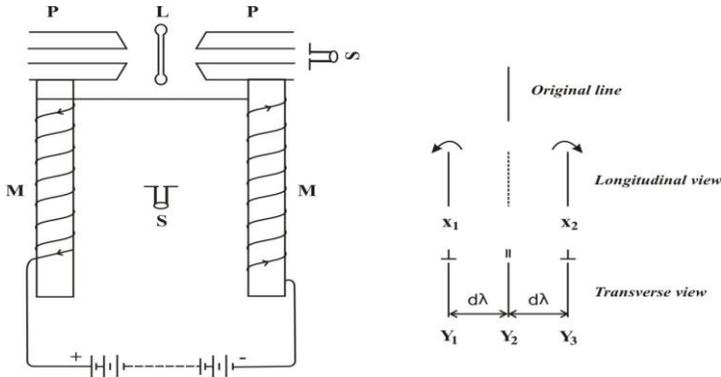


Fig. 7.4

X_1 and $X_2 \Rightarrow$ Circularly Polarised spectral lines in the opposite manner i.e. the first is left handed circularly Polarised and the second one is Right handed circularly polarised.

$Y_1 \Rightarrow$ Plane Polarised having vibration perpendicular to the plane of paper.

$Y_2 \Rightarrow$ Plane Polarised having vibration Parallel to the plane of paper.

$Y_3 \Rightarrow$ Plane Polarised having vibration perpendicular to the plane of paper.

7.6 Theory of Normal Zeeman effect

(Lorentz classical theory of Normal Zeeman Effect)

The emission of light by glowing gas is due to the vibratory motion of the electrons. The electrons in the atom execute simple harmonic vibrations about the

centre of the atom. The frequency of the spectral line is given by the frequency of vibration of the electron.

Any linear motion of the electron can be resolved in to three components, a linear motion along the magnetic field and two opposite circular motions to the field.

It is known that No force acts upon a charge when it moves in the direction of the field. So the linear motion along the field is not affected by the field and hence the frequency of this component is unchanged by the magnetic field. The other two circular components are affected by the magnetic field, one being retarded and other being accelerated hence the frequency of one of these circular components is increased and that of the other is decreased by the same amount.

Expression for the Zeeman of Shift-

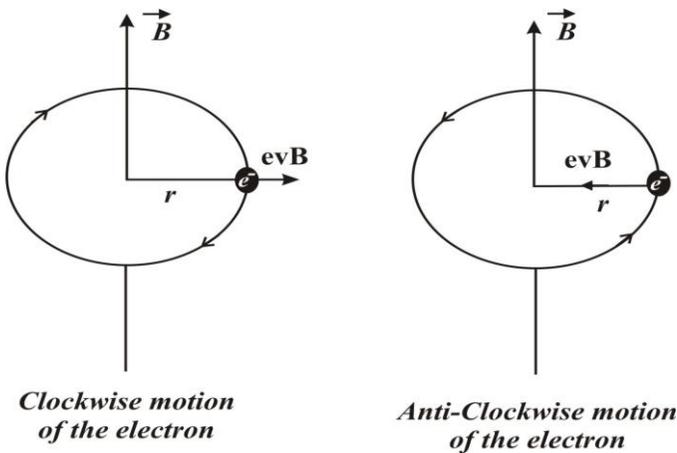


Fig. 7.5

For the clockwise motion of electron

$$F - evB = m (\omega + \delta\omega)^2 r$$

$$\text{or} \quad m\omega^2 r - evB = m (\omega + \delta\omega)^2 r$$

$$\text{or} \quad m\omega^2 r - evB = m\omega^2 r + m (\delta\omega)^2 r + 2\omega(\delta\omega)mr$$

Neglecting $(\delta\omega)^2$ term, as it is very small, we have

$$\begin{aligned}
 -evB &= +2 \omega (\delta\omega)mr \\
 \therefore \delta\omega &= -\frac{evB}{2mr\omega} \\
 \therefore \delta\omega &= -\frac{er\omega B}{2mr\omega} && \text{(Since } v = r\omega) \\
 \therefore \omega &= -\frac{Be}{2m} && (1)
 \end{aligned}$$

For the anticlockwise motion of electron

$$\begin{aligned}
 F + evB &= m (\omega + \delta\omega)^2 r \\
 \therefore m\omega^2 r - evB &= m (\omega + \delta\omega)^2 r \\
 \therefore m\omega^2 r + evB &= m\omega^2 r + m (\delta\omega)^2 r + 2 \omega (\delta\omega)mr
 \end{aligned}$$

Neglecting $(\delta\omega)^2$ term, as it is very small, we have

$$\begin{aligned}
 evB &= +2 \omega (\delta\omega)mr \\
 \therefore \delta\omega &= \frac{evB}{2mr\omega} \\
 \therefore \delta\omega &= \frac{er\omega B}{2mr\omega} && \text{(Since } v = r\omega) \\
 \text{or } \omega &= +\frac{Be}{2m} && (2)
 \end{aligned}$$

From equation (1) and (2), we have

$$\delta\omega = \pm \frac{Be}{2m} \quad (3)$$

$$\text{Now } \omega = 2\pi\nu \quad (4)$$

Using equation (4) for equation (3), we have

$$\begin{aligned}
 2\pi\delta\nu &= \pm \frac{Be}{2m} \\
 \therefore \delta\nu &= \pm \frac{Be}{4\pi m} && (5) \\
 \therefore \delta\left(\frac{c}{\lambda}\right) &= \pm \frac{Be}{4\pi m}
 \end{aligned}$$

$$\therefore -\frac{c}{\lambda^2} \delta\lambda = \pm \frac{Be}{4\pi m}$$

$$\therefore \delta\lambda = \mp \frac{Be\lambda^2}{4\pi mc} \quad (6)$$

7.7 Anomalous Zeeman Effect

We know that In the case of Normal Zeeman effect (when the magnetic field is strong) the sodium D line is splitted into three (transverse view) or two (longitudinal view) components.

But this has been observed that when sodium light source is placed in a very weak magnetic field then the D_1 , D_2 spectral lines of sodium are splitted into more components in comparison to strong magnetic field. **This is called anomalous Zeeman effect.** The splitting of D_1 and D_2 lines of sodium light source is observed as

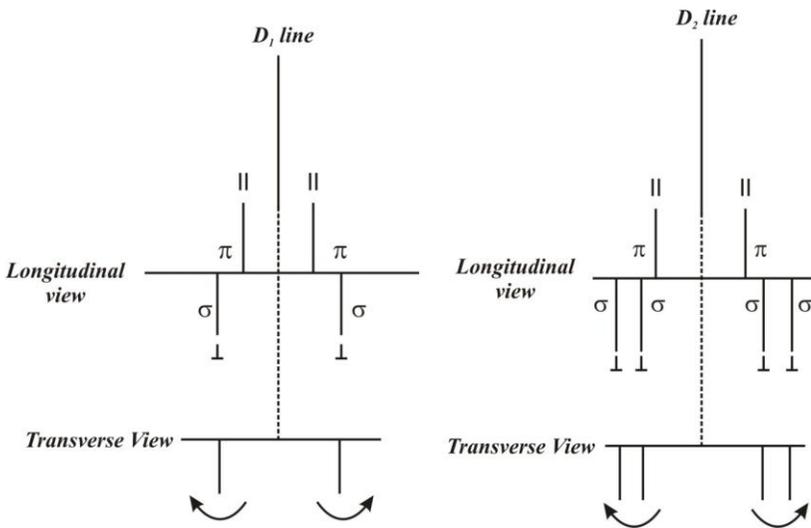


Fig. 7.6

Parallel or π component \Rightarrow Plane Polarised component having vibration Parallel to the plane of paper.

Perpendicular or σ component \Rightarrow Plane Polarised component having vibrations perpendicular to the plane of paper.

 \Rightarrow Circularly Polarised in the opposite manner.

Theory

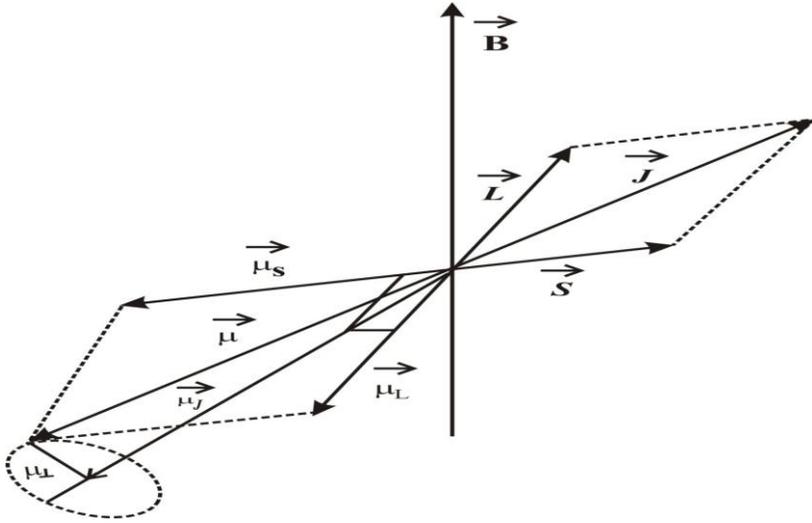


Fig. 7.7

It can only be explained by the introduction of spin of the electron.

We know that

$$\vec{\mu}_L = \left(\frac{eh}{4\pi m} \right) \vec{L} \quad (1)$$

$$\vec{\mu}_S = 2 \left(\frac{eh}{4\pi m} \right) \vec{S} \quad (2)$$

Where

$\vec{L} \Rightarrow$ Orbital angular momentum vector

$\vec{S} \Rightarrow$ Spin angular momentum vector

$\vec{J} \Rightarrow$ Total angular momentum vector

$\vec{\mu}_L \Rightarrow$ Orbital magnetic moment vector

$\vec{\mu}_S \Rightarrow$ Spin magnetic moment vector

$\vec{\mu}_J \Rightarrow$ Total magnetic momentum vector

$\vec{\mu}$ vector Precesses about $\vec{\mu}_J$ vector

From equation (1) and (2) it is clear that the ratios $\frac{\mu_L}{L}$ and $\frac{\mu_S}{S}$ are not equal.

Resolving the vector $\vec{\mu}$ in to two components, which are parallel to \vec{J} $\vec{\mu}_J$ and the other perpendicular to it $\vec{\mu}_\perp$ such that $\vec{\mu} + \vec{\mu}_\perp = \vec{\mu}_J$. If the precession of $\vec{\mu}$ and \vec{J} occurs sufficiently rapidly, the value of the Perpendicular component $\vec{\mu}_\perp$ will be constant by changing in direction, such that its time average over a period will be zero under these conditions

$$\vec{\mu}_J = \vec{\mu}_L \cos(\vec{L}, \vec{J}) + \vec{\mu}_S \cos(\vec{S}, \vec{J}) \quad (\text{vector form}) \quad (4)$$

$$\mu_J = \mu_L \cos(L, J) + \mu_S \cos(S, J) \quad (\text{scalar form}) \quad (5)$$

$$\begin{aligned} &= \left(\frac{eh}{4\pi m} \right) L \left[\frac{L^2 + J^2 - S^2}{2LJ} \right] + 2 \left(\frac{eh}{4\pi m} \right) S \left[\frac{S^2 + J^2 - L^2}{2SJ} \right] \\ &= \left(\frac{eh}{4\pi m} \right) \left[\frac{L^2 + J^2 - S^2}{2J} \right] + 2 \left(\frac{eh}{4\pi m} \right) \left[\frac{S^2 + J^2 - L^2}{2J} \right] \\ &= \left(\frac{eh}{4\pi m} \right) \left[\frac{L^2 + J^2 - S^2 + 2S^2 + 2J^2 - 2L^2}{2J} \right] \\ &= \left(\frac{eh}{4\pi m} \right) \left[\frac{3J^2 + S^2 - L^2}{2J} \right] \\ &= \left(\frac{eh}{4\pi m} \right) J \left[1 + \frac{J^2 + S^2 - L^2}{2J^2} \right] \\ &= \left(\frac{eh}{4\pi m} \right) J \left[1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \right] \end{aligned}$$

Therefore
$$\mu_J = \left(\frac{eh}{4\pi m} \right) g J \quad (6)$$

Where
$$g = 1 + \frac{J(J+1)+S(S+1)-L(L+1)}{2J(J+1)} \quad (7)$$

g is called Lande's splitting factor

if the atom is placed in a weak magnetic field, the total angular momentum vector \vec{J} precesses about the direction of the magnetic field.

The additional energy ΔE due to the action of the magnetic field on this atomic magnet is given as

$$\Delta E = \mu_J B \cos(J, B) \quad (8)$$

Using equation (6) for (8)

$$\begin{aligned} \Delta E &= \left(\frac{eh}{4\pi m} \right) g J B \cos(J, B) \\ E &= \left[\left(\frac{eh}{4\pi m} \right) g B \right] J \cos(J, B) \quad (9) \end{aligned}$$

but $J \cos(J, B)$ is the Projection of J in the direction of \vec{B} , which is equal to magnetic total angular momentum quantum number,

i.e.,
$$m_J = J \cos(J, B) \quad (10)$$

using equation (9) for (10)

$$\Delta E = \left[\left(\frac{eh}{4\pi m} \right) g B \right] m_J \quad (11)$$

⇒ The quantity $\left(\frac{eh}{4\pi m} \right) B$ is called Lorentz unit.

⇒ It is unit of energy.

⇒ It is used for measuring the energy of the splitted energy levels in a magnetic field

State	L	S	J	g	m_J	gm_J
$^2S_{1/2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	2	$\frac{1}{2}, \frac{1}{2}$	1, -1
$^2P_{1/2}$	1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{2}{3}$	$\frac{1}{2}, -\frac{1}{2}$	$\frac{1}{3}, -\frac{1}{3}$

${}^2P_{3/2}$	1	$\frac{1}{2}$	$\frac{3}{2}$	$\frac{4}{3}$	$\frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$	2, $\frac{2}{3}, -\frac{2}{3}, -2$
---------------	---	---------------	---------------	---------------	--------------------------------------------------------	------------------------------------

$$g = \frac{1+J(J+1)+S(S+1)-L(L+1)}{2J(J+1)}$$

$$= 1 + \frac{\left(\frac{1 \cdot 3}{2 \cdot 2} + \frac{1 \cdot 3}{2 \cdot 2} - 1\right)}{\frac{2 \cdot 3}{2 \cdot 2}}$$

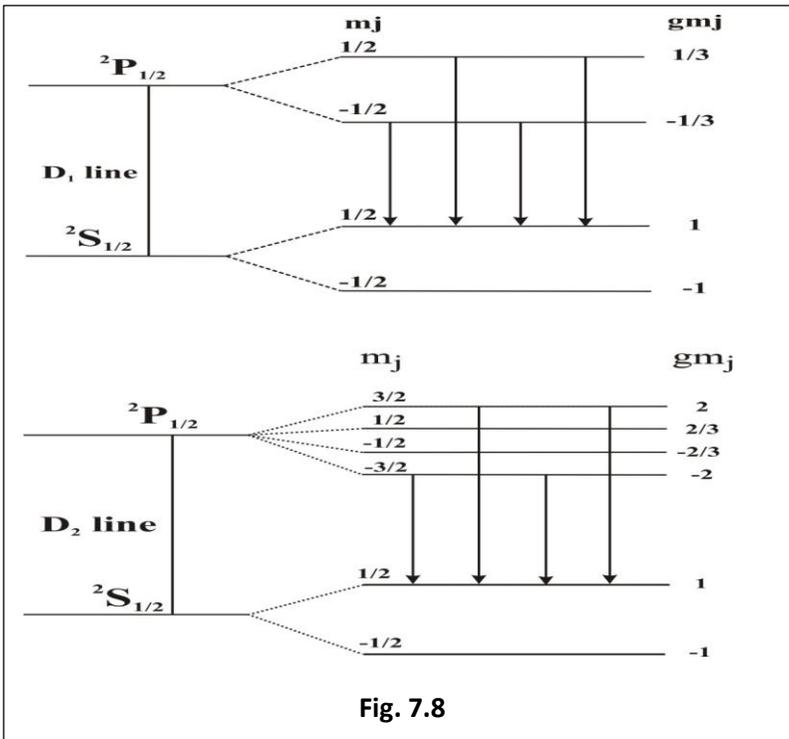
$$= 1 + \frac{3}{2} \times \frac{2}{3}$$

$$= 1 + 1 = 2$$

The values of m_j are from $-J$ to $+J$

Total values of $m_j = (2J + 1)$

S = Spin quantum Number. It has only one value ($s = \frac{1}{2}$)



7.8 Stark Effect- It is an electro optical Phenomenon. In this effect splitting of spectral lines takes place due to the action of an external electric field on a radiating substance.

Even very strong electric fields are weak compared to the interatomic fields. Hence the action of electric field on the motion of the atomic electron can be regarded as small perturbation. Consequently the Stark line splitting is very minute and can be observed only with instrument having a high resolving power.

7.9 Paschen-Back Effect- Paschen and Back found that whatever the anomalous Zeeman effect pattern of a given line in a weak magnetic field, the pattern always approximates the normal Zeeman triplet when the field is progressively increased. This reduction may occur either through the coalescence of lines through the displacement of certain lines. This phenomenon is called Paschen-Back effect.

Solved Problems

Problem 1. Write the spectral terms corresponding to $n = 1$

Solution- since $n = 1$

then $l = 0$

when $L = 0$

then $X = S$

$$r = 2s + 1$$

$$r = 2 \times \frac{1}{2} + 1$$

$$r = 2$$

$$J = L + S \quad \text{or} \quad L - S$$

$$= 0 + \frac{1}{2} \quad \text{or} \quad 0 - \frac{1}{2}$$

$$\boxed{J = \pm \frac{1}{2}}$$

\Rightarrow Spectral term corresponding to $n = 1$ is ${}^2S_{\frac{1}{2}}$

Problem 2 Write the spectral terms corresponding to $n = 2$

Solution- since $n = 2$

then $L = 0, 1$

when $L = 0$ then $X = S$

$$J = L + S \quad \text{or} \quad L - S$$

$$= 0 + \frac{1}{2} \quad \text{or} \quad 0 - \frac{1}{2}$$

$$J = +\frac{1}{2}$$

$$r = 2s + 1$$

$$= 2 \times \frac{1}{2} + 1$$

$$= 2$$

when $L = 1$ then $X = P$

$$\begin{aligned}
 J &= L+S \text{ or } L-S \\
 &= 1+1/2 \text{ or } 1-1/2 \\
 &= 3/2 \text{ or } 1/2 \\
 r &= 2s + 1 \\
 &= 2 \times 1/2 + 1 \\
 &= 2
 \end{aligned}$$

Spectral terms corresponding to $n = 2$ is ${}^2S_{1/2}, {}^2S_{3/2}, {}^2S_{1/2}$

Problem 3 Write the spectral terms corresponding to $n = 3$

Solution

since $n = 3$

then $L = 0, 1, 2$

when $L = 0$ then $X = S$

$$\begin{aligned}
 J &= L+S \text{ or } L-S \\
 &= 0+1/2 \text{ or } 0-1/2 \\
 J &= +1/2 \\
 r &= 2s + 1 \\
 &= 2 \times 1/2 + 1 \\
 &= 2 \\
 &\Rightarrow {}^2S_{1/2}
 \end{aligned}$$

when $L = 1$ then $X = P$

$$\begin{aligned}
 J &= L+S \text{ or } L-S \\
 &= 1+1/2 \text{ or } 1-1/2 \\
 &= 3/2 \text{ or } 1/2
 \end{aligned}$$

$$r = 2s + 1$$

$$= 2 \times \frac{1}{2} + 1$$

$$= 2$$

$$\Rightarrow {}^2P_{3/2}, {}^2P_{1/2}$$

when $L = 2$ then $X = D$

$$J = L+S \text{ or } L-S$$

$$= 2+1/2 \text{ or } 2-1/2$$

$$J = 5/2 \text{ or } 3/2$$

$$r = 2s + 1$$

$$= 2 \times \frac{1}{2} + 1$$

$$= 2$$

$$\Rightarrow {}^2D_{5/2}, {}^2D_{3/2}$$

Total Spectral terms corresponding to $n = 3$ are ${}^2S_{1/2}, {}^2P_{3/2}, {}^2P_{1/2}, {}^2D_{5/2}, {}^2D_{3/2}$

Exercise

(A) Descriptive type

- (1) Draw energy level diagram for sodium and explain the Fine structure of spectral lines. **(L.U. 2013)**
- (2) Give an account of Normal Zeeman effect. Does sodium give normal Zeeman effect? Give reasons for your answer. **(L.U. 2012)**
- (3) Explain splitting of D_1 and D_2 lines when. Na source of light is put in magnetic field. **(LU 2015)**
- (4) Give an account of Normal Zeeman Effect. **(L.U. 2009)**
- (5) Distinguish between normal and anomalous Zeeman Effect. Discuss with necessary theory the Zeeman pattern for the D_1 and D_2 lines of sodium. **(L.U. 2008)**
- (6) Distinguish between normal and anomalous Zeeman effect. **(L.U. 2010)**
- (7) Give an account of normal Zeeman effect, Does sodium give normal Zeeman effect? Give reason for your answer. **(L.U. 2007)**
- (8) Distinguish between normal and anomalous Zeeman Effect.
Explain Paschen-Back effect. **(L.U. 2012)**
- (9) What is Paschen-Back effect? Explain. **(LU 2015)**
- (10) Discuss with necessary theory the Zeeman pattern for the D_1 and D_2 lines of sodium. **(L.U. 2011)**
- (11) Give the spectral features of alkali spectra. Draw an energy level diagram for sodium and illustrate the transitions which give rise to the D_1 and D_2 lines. **(L.U. 2007)**
- (12) What are main features of Alkali spectra . Explain fine structure of spectra. Explain fine structure of spectral lines. Discuss the effect of magnetic field on emission sepectru of sodium. **(LU 2016)**

- (13) Describe main features of alkali spectra. Show transitions corresponding to sodium D_1 and D_2 lines. **(L.U. 2010)**
- (14) What is meant by “fine structure” of spectral lines? Describe, how electron spin, coupled with orbital motion explains the fine structure of alkali spectra. **(L.U. 2008)**
- (15) Write notes on any two of the following :
- (a) Paschen-Back effect **(L.U. 2013)**
 - (b) Anomalous Zeeman Effect. **(L.U. 2013)**
 - (c) Screening doublets. **(L.U. 2013)**
- (16) Write short notes on any two of the following :
- (a) Screening doublets. **(L.U. 2014)**
 - (b) Paschen-Back effect. **(L.U. 2014)**
 - (c) Anomalous Zeeman effect. **(L.U. 2014)**

(B) Short answer type

- (1) Why Normal Zeeman effects occurs only in atoms with are even number of electrons? Expalin. **(L.U. 2008)**
- (2) Sodium give D_1 and d_2 lines. Names any other element giving the same lines. **(L.U. 2007)**
- (3) Explain in short spin and screening doublets. **(L.U. 2012)**
- (4) Why normal Zeeman-effect occurs only in atoms with an even number of electrons? Expalin. **(L.U. 2009)**
- (5) Normal Zeeman effect is observed only in atoms with even number of electrons. Why? **(LU 2016)**
- (6) Give a short account of doublet fine structure of alkali metals. **(L.U. 2009)**

(C) Numericals

Calculate normal zeeman shift of the Line (6438\AA) in a magnetic field of $0.5T$. . **(LU 2015)**

Chapter 8

X-Ray Spectra

8.1 Introduction

X-rays were discovered by William Roentgen in 1895. These are high energy photons of energy ranging from 1 KeV to 100 KeV. They are electromagnetic radiation, having a very short wavelength of the order of 1Å. The wavelength range of X-rays is from 0.1 to 100 Å, while the range of frequency is from 3×10^{16} Hz to 3×10^{19} Hz.

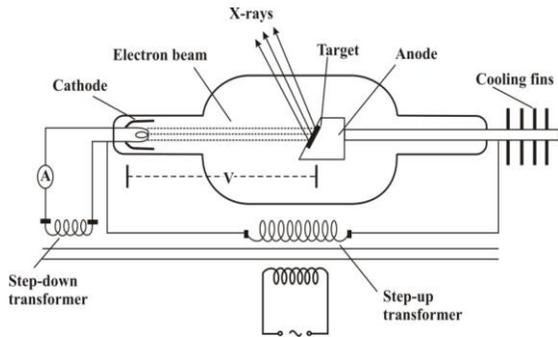


Fig. 8.1

8.2 Production of X-rays

The modern X-ray tube was designed by Dr. Coolidge and is known after his name as Coolidge tube. It is widely used for commercial and medical purposes and is shown in Fig.8.1.

The Cathode C consists of a tungsten filament, heated by passing a current through it. It then emits a large number of electrons called thermions which travel towards the anti-cathode A also called the target with a velocity depending upon the potential difference applied between A and C. By surrounding the cathode with a molybdenum shield M, maintained at a negative potential with respect to the filament circuit, the rays can be focused to a fine spot on A, as without the shield the electrons would fly away in all directions. The tube is completely evacuated to the no-discharge stage, so that no ionization can take place.

A current of 30 mA at a voltage of 100,000 volts is used; the high voltage is obtained from a step-up transformer. The tube acts as its own rectifier, unless the anode attains such a high temperature that it begins to emit electrons.

The anti-cathode in a Coolidge tube must have the following characteristics:

- (i) High atomic weight, to produce hard X-rays.
- (ii) High melting point to withstand the high temperature developed, as most of the energy of the impinging electron is converted into heat.
- (iii) High thermal conductivity, to get rid of the heat produced.
- (iv) Low vapour pressure at high temperatures.

The Tantalum, platinum and tungsten fulfil these requirements, but tungsten is the best and is widely used, In actual practice, a heavy block of this metal is mounted on a thick copper rod and the face is sloped at about 45° to the electron beam, The heat generated by the impact of electrons is removed by special devices. In some cases, the anode is water-cooled.

8.3 Control of intensity and quality and penetrating power

Control of intensity

The higher the potential difference between the cathode and the anti-cathode, the greater is the velocity of electrons emitted. The electrons possessing greater energy produce more penetrating X-rays, The quality of X-rays, therefore, varies with the difference of potential between the cathode and the anti-cathode.

Control of quality

The number of electrons given out by the filament is proportional to its temperature, which can be adjusted by varying the current in the filament circuit. The intensity of X-rays, therefore, varies with the filament current. Thus, separate control of quality and intensity can be achieved.

Control of penetrating power

The penetrating power of X-Rays depending upon

- (a) The applied potential difference.
- (b) The atomic weight of the material of the anti-cathode.

The greater the potential difference and higher the atomic weight, the more penetrating are the X-rays produced. The X-rays having a high penetrating power are known as hard X-rays and those with low penetrating power are known as soft X-rays in matter.

8.4 X-ray spectrum

The dependence of intensity of X-rays emitted by a source on wavelength (or frequency) is known as its X-ray spectrum.

It has been observed that the X-ray spectrum emitted by all the target materials consists of a continuous spectrum, having radiations of all possible wavelength, within a certain range and superimposed upon it a sharp line spectrum of definite wavelength known as characteristic spectrum, the lines being characteristic of the material used as target.

8.5 Continuous spectrum

The X-rays emitted by all the target materials have a continuous distribution of intensity above a certain minimum wavelength λ_m given by

$$\lambda_m = \frac{1.242 \times 10^{-2}}{V} \text{ m} = \frac{12420 \times 10^{-10}}{V} \text{ m} = \frac{12420}{V} \text{ \AA}$$

Where V is the applied voltage. This relation is known as Duana-Hunt law. The minimum wavelength as continuous spectrum boundary or Duana-Hunt limit is independent of the nature of the target.

Origin and mechanism of production

Continuous X-rays are produced by the phenomenon of Bremsstrahlung, which is a German word meaning 'braking' or 'slowing down' radiation. Electrons emitted from the cathode in the X-rays tube are accelerated towards the target, strike it, penetrate deep into the interior of its atoms and are attracted by the nuclei due to strong electrostatic interaction. The electron therefore, deviates from its original path. The deviation of the electron from its straight line path is equivalent to its collision with the nucleus. So the electron loses some of its energy due to the

collision. This energy appears as an X-ray photon. If E_i is the initial kinetic energy of the electron and E_f is the final kinetic energy, then the energy of the X-ray photon = $E_i - E_f$. If ν is the frequency of the X-ray photon emitted, then

$$h\nu = E_i - E_f$$

The electron may suffer several collisions with various nuclei before coming to rest. Each collision is accompanied by the emission of an X-ray photon. Hence, a number of photons of different frequencies are emitted. As there are a large number of electrons in the beam and each electron suffers collision in a different way, we get photons of almost all frequencies or wavelength, thus producing a continuous X-ray spectrum.

The production of continuous spectrum is the result of inverse photoelectric effect with electron kinetic energy $E_i - E_f$ being transformed into a photon of energy $h\nu$

Lowest wavelength limit of continuous spectrum

According to classical theory, the continuous X-ray spectrum should consist of all frequencies between zero and infinity. But according to quantum theory, there is a minimum wavelength only, upto which the continuous X-ray spectrum extends. To find the value of λ_{\min} , let the velocity of the incident electron decrease from v_i to v_f due to interaction with the nucleus. Then frequency of X-ray photon is given by

$$h\nu = \frac{1}{2} m v_i^2 - \frac{1}{2} m v_f^2$$

When the electron is completely brought to rest by electrostatic interaction i.e. $v_f = 0$, the entire kinetic energy of the electron is radiated as an X-ray photon and the photon has maximum frequency or minimum wavelength given by

$$h\nu_{\max} = \frac{1}{2} m v_i^2$$

or

$$\nu_{\max} = \frac{m v_i^2}{2h}$$

$$\therefore \lambda_{\min} = \frac{c}{v_{\max}} = \frac{2ch}{mv_i^2}$$

λ_{\min} **IS Inversely proportional to accelerating velocity :**

If V is the potential difference between the cathode and the target to accelerate the electron, then

$$\therefore \frac{1}{2} mv_i^2 = V_e$$

$$hv_{\max} = V_e$$

$$\text{Now } \lambda_{\min} = \frac{c}{v_{\max}} = \frac{ch}{eV} = \frac{1.242 \times 10^{-6}}{V} \text{ m}$$

According to relation (ii) 'the lowest wavelength limit of continuous spectra is inversely proportional to the accelerating potential of *X-ray tube*' or

$$\lambda_{\min} \propto \frac{1}{V}$$

Graph between relative intensity and wavelength

The plot of relative intensity of X-ray spectra versus wavelength at four different potential differences applied to an X-ray tube between the cathode and the target (Tungsten) is shown in Fig.8.2. It is clear from the graph that as the potential difference V applied to the X-ray tube increases from 30 kV to 40 kV to 50 kV and then to 70 kV the minimum wavelength limit decrease from 0.4 \AA to 0.3 \AA to 0.24 \AA and then to 0.17 \AA showing thereby that $\lambda_{\min} \propto \frac{1}{V}$ or $\lambda_{\min} \times V = \text{a constant}$.

Other special features of the continuous X-ray spectrum are :-

(1) Change of target material

As $\lambda_{\min} = \frac{ch}{eV}$ and c , h , and e are constants, the cut-off wavelength

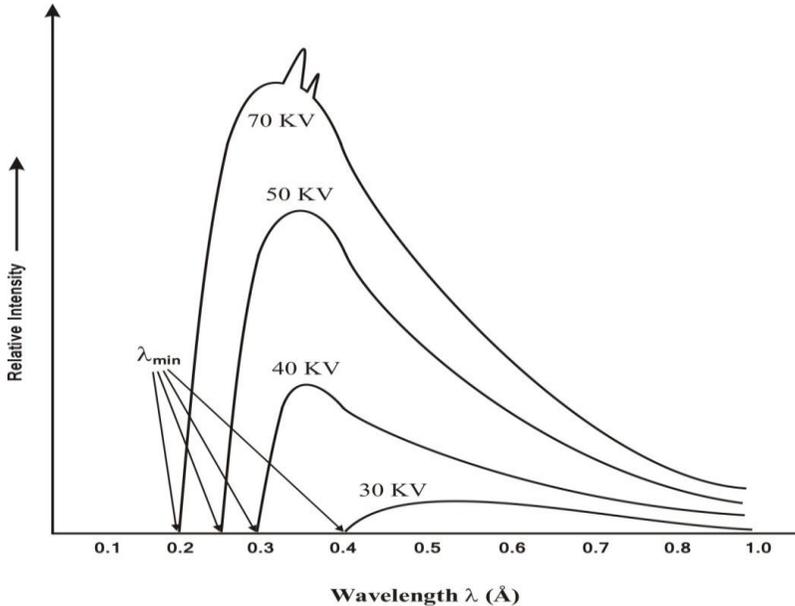


Fig. 8.2

says therefore same for all target materials. In other words, the range of the continuous spectrum does not depend upon the nature of the target material. Hence, the plots will remain unchanged with change in target material.

(2) Change in accelerating voltage

- (i) (i) The continuous spectrum ends abruptly at a minimum wavelength λ_{\min} . The value of λ_{\min} decreases with increasing accelerating potential.
- (ii) The intensity rises to a maximum at a certain wavelength, after which it gradually falls off. The intensity never reaches zero, showing that the radiation contains all possible wavelengths, above a certain minimum.

- (iii) The wavelength corresponding to maximum intensity λ_{\min} shifts gradually to lower wavelength side as the accelerating potential is increased, in such a way that $(\lambda_m V^{1/2})$ is almost a constant.
- (iv) For a particular target material, the intensity of continuous X-ray spectrum, corresponding to all wavelength as well as the maximum intensity, increase with accelerating potential.
- (v) **For applied potential difference 70 kV, two sharp peaks are seen. The sharp peaks are due to characteristic radiation.** The line spectra is absent till the potential difference is greater than a particular value. The smoothly varying curves represent the continuous spectrum and the superimposed lines on the continuous background constitute the characteristic spectrum

8.6 Characteristic X-ray Spectrum

The characteristic of X-ray spectrum consists of sharp peaks super-imposed on the continuous spectrum. Their wavelength is characteristic of the target element. It is highly monochromatic and independent of the applied voltage. The intensity of the characteristic spectrum lines is very large-sometimes 10^4 times that of the continuous spectrum in that region.

The characteristic X-rays from substances of higher atomic number are of shorter wavelength than those from substances of lower atomic number and hence are more penetrating. The characteristic wavelength is given by Moseley's law

$$\lambda ((Z-b)^2 = a \text{ (constant)})$$

Where the value of b is different for different groups.

Every substance gives rise to a particular set of characteristic X-rays, consisting of one or more series, known as K,L,M, N, etc. series. The X-rays in K series of a particular element have smaller wavelength than in the L or M series, whereas the wavelength of the X-rays in the same series say K, produced from an element of higher atomic weight is less than that produced from an element of lower atomic weight.

The characteristic X-ray spectrum consists of sharp lines the wavelength of which only depends upon the target element. The characteristic wavelength is given by Moseley's law; $\lambda (Z-b)^2 = a$ (**constant**) where Z is the atomic number of the target element.

As the wavelength is characteristic of the target element it is known as characteristic spectrum. Characteristic X-ray spectrum is independent of applied voltage.

Production of characteristic X- rays

An atom consists of a central nucleus having a positive charge and revolving round it, in more or less circular orbits, a suitable number of electrons. The electron in the inner-most orbit is attracted by the nucleus with greatest force and to detach it from the atom maximum energy is required. The innermost orbit is given the name K level or shell and the outer-orbits L,M, etc. levels respectively. Thus more energy is required to detach an electron from an inner level than from an outer level.

When an atom is bombarded by fast moving electrons, an electron coming with a high velocity penetrates through the outer shell containing electrons and removes an electrons from one of the inner shells. An incoming electron out an electron from K shell of an atom is shown in Fig. 8.3 (b). The incident and the dislodged electrons both rush out of the atom, causing a vacancy in the K shell or level.

Transitions for K -series. As soon as a vacancy in the K -shell is caused as explained above, Immediately one of the electrons from the higher levels (e.g. L level) jumps into the K level. A radiation of frequency ν is emitted at the same time. The frequency of the radiation, on the quantum theory, is given by the relation

$$E_K - E_L = h\nu$$

OR

$$\nu = \frac{E_K - E_L}{h}$$

Where E_k is the energy required to extract an electron from the K level and E_L is

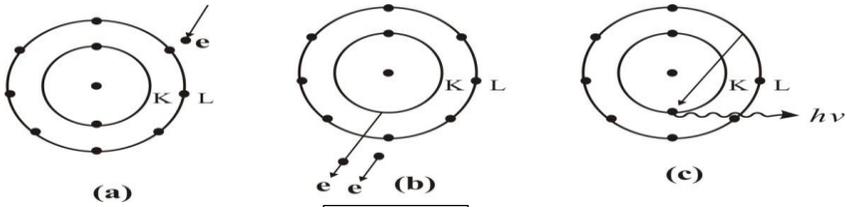


Fig. 8.3

energy required to extract an electron from the L level and h is Planck's constant having a value equal to 6.62×10^{-34} Joule-sec. The frequency of the radiation is very high and is of the order of 10^{18} per second.

The wavelength of the corresponding X-ray is given by

$$\lambda = \frac{c}{\nu} = \frac{hc}{E_K - E_L}$$

If an electron from the M level falls into the K level, X-rays of still higher frequency (shorter wave-length) will be produced. The frequencies of X-rays produced by the fall of an electron from an outer level to the K level can be arranged into a series, called K series, consisting of K_α , K_β , K_γ etc. lines, as shown in Fig. 8.4.

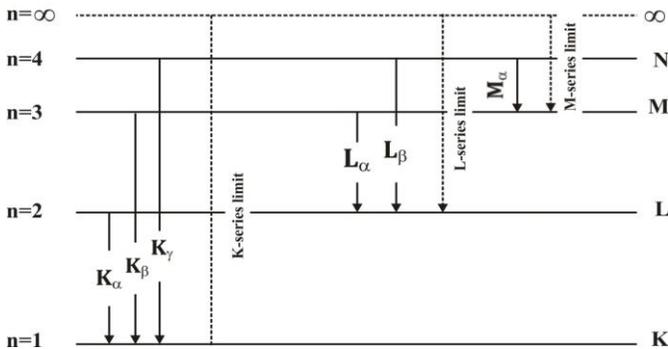


Fig. 8.4

level to K level gives rise to K_α line and from M level to K level K_β line and so on, till we get the limiting line, known as K -series limit.

Transition for L series : Similarly, when the incident electrons carry a lesser amount of energy, an electron is displaced from the L level and an electron from M or other outer level takes its place, so that a radiation of a lower frequency than that of K series is emitted. This corresponds to the L series of the X-ray spectrum. It is evident that from the same element, the L lines of the X-ray spectrum have smaller frequency (larger wavelength) than the K lines. A jump from M shell to L shell gives rise to L_{α} line and from N shell to L shell gives rise to L_{β} line and so on, till we get the limiting line, known as L-series limit.

The wavelength of these lines in the K, L, or M series depend upon the atomic weight of the anti-cathode and these wavelengths are known as **characteristic X-rays** for the material of the given anticathode or target.

Line spectrum

Line spectrum is the characteristic X-ray spectrum emitted when the incident electron knocks out an electron of the target atom from the K, L, M etc. level thereby causing a vacancy in the particular orbit, say K -level. At this stage an electron from a higher level say L level jumps into the K -level thereby giving out an X-ray spectral line of frequency ν given by

$$\nu = \frac{E_k - E_L}{h}$$

Where E_K is the energy required to extract the electron from the K -level and E_L the energy required to extract the electron from L -level. This frequency is known as K_{α} line.

Similarly if a vacancy is caused in the L -level and an electron jumps in to it from the m -level we get the L_{α} line. Thus the line spectrum is characteristic of the target atom.

8.7 Bremsstrahlung

In an X-ray tube, electrons emitted from the anode and accelerated towards the anticathode or target are '**slowed down**' or undergo '**braking**' due to the strong electrostatic interaction of the nucleus. In the process, the electron loses some of its energy. This energy appears as an X-ray photon. As we get photons of almost

all energies upto a certain maximum, it gives rise to a continuous X-ray spectrum having a maximum frequency or minimum wavelength.

Since these continuous X-rays are produced due to ‘**slowing down**’ or ‘**braking**’ of the fast moving electron, these are known as ‘**Bremsstrahlung**’ which is the German word for ‘slowing down’ or ‘braking’.

Difference in origin of X-rays and visible light : When an atom is excited, the outermost valence electron moves to one of the higher energy excited states (or virtual orbits). The life of the electron in these orbits or excited states is very small. The electron, therefore, jumps back to its ground state or a lower energy state (orbit); the difference in the energy of the two states is radiated as electromagnetic radiation (light).

The transitions of the outer electron of an atom usually involve only a few electron volts of energy. Even removing an electron requires 13.6 eV for hydrogen and 24.6 eV for helium. These transitions accordingly are associated with photons whose wavelengths lie in the near visible part of the electromagnetic spectrum.

X-rays, on the other hand, are produced by transitions among inner electron orbits. **For example**, if a high energy fast moving electron a *K* electron from an atom, the vacancy in the *K*-shell is filled by an electron jumping into *K*-orbit from *L, M, N* etc orbit. In the process, the difference in energy is radiated as an X-ray photon.

The inner electrons of an atom, particularly the heavier one’s, are not well shielded from the full nuclear charge by intervening electron shells and are, therefore very tightly bound. In Sodium, for example, only 5.13 eV energy is required to remove the outermost 3 *s* (M_I of *M* shell) electron, while the corresponding figures for the inner electrons are 31 eV for each 2 *p* (L_{II} L_{III} of *M* shell), 63 eV for each 2 *s* (L_I of *L* shell) and 104.1 eV for each 1 *s* (*K* shell) electron. Transitions involving inner electrons of the atom give rise to high energy photons, lying in the X-ray region of the electro-magnetic spectrum, having wavelength much smaller than those of visible light.

Hence production of visible light is due to transitions between the virtual or excited states of the valence electron whereas X-ray are due to the transitions of the inner electrons in *K, L, M* etc shells.

Difference between and X-ray production inverse of photo-electric effect :

In photo-electric effect the energy of the incident photon is absorbed by an electron in the metal and it is knocked out carrying the energy of the incident photon. If v is the velocity of the electron ejected, E its kinetic energy and ν the frequency of the incident photon, then

$$h\nu = \frac{1}{2} mv^2 = E$$

The production of continuous X-rays spectra is the result of inverse photo-electric effect, in which the kinetic energy of the incident fast moving electron is carried by the emitted X-ray photon. If E_i is the initial kinetic energy of the electron, E_f the final kinetic energy, then the energy of the X-ray photon emitted = $E_i - E_f = E$. If ν is the frequency of the photon, then

$$h\nu = E_i - E_f = E$$

Therefore, it is quite appropriate to regards X-ray production as inverse of photo-electric effect.

8.8 Moseley's law

The frequency of the K lines produced from an element of higher atomic number is greater than that produced from element of lower atomic number.

The higher the atomic number, higher is the frequency of X-ray produced and more penetrating are the rays. It can be shown by the application of Bohr's theory of the atom that if ν is the frequency of the characteristic X-radiation, then

$$\sqrt{\nu} \propto (Z - b)$$

Or $\nu^{1/2} = k (Z - b)$

Where Z is the atomic number of the which the value for K series, L series screening constant. This is known as 1

The frequency of spectral lin the atomic number of the element emi

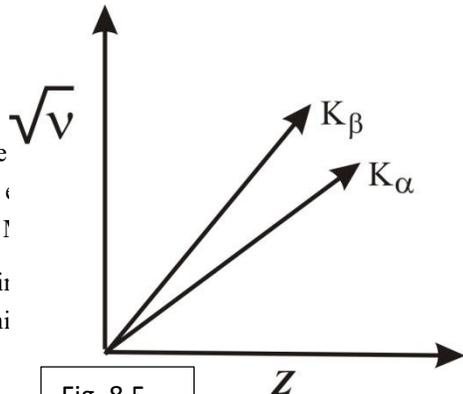


Fig. 8.5

It is very good rule to take the screening constant b as the number of extra nuclear electrons inside the orbit to which the electron falls in radiating together with $\frac{1}{2}(n-1)$, where n is the number of electrons in the orbit, For hydrogen $b=0$, for helium $b=\frac{1}{2}$

Taking the case of copper for K -lines, $b=\frac{1}{2}$, as there are two electrons in the innermost orbit, in the second orbit there are 8 electrons, so that in falling into this orbit, a L line would be produced and

$$b = 2 + \frac{1}{2}(8-1) = 5.5$$

(b) Derivation of Moseley's law according to Bohr's theory :

According to Bohr's theory the energy of an electron in the n th orbit of a hydrogen like atom of atomic number Z is given by

$$E_n = -\frac{mZ^2e^4}{8\varepsilon_0^2h^2} \cdot \frac{1}{n^2}$$

For states with principal quantum number n_1 and n_2 , the corresponding energy of the electron is given by

$$E_{n_1} = -\frac{mZ^2e^4}{8\varepsilon_0^2h^2} \cdot \frac{1}{n_1^2}$$

and

$$E_{n_2} = -\frac{mZ^2e^4}{8\varepsilon_0^2h^2} \cdot \frac{1}{n_2^2}$$

$$\therefore \text{Energy difference } E_{n_1} - E_{n_2} = \frac{me^4}{8\varepsilon_0^2h^2} \left[\frac{(Z-b_2)^2}{n_2^2} - \frac{(Z-b_1)^2}{n_1^2} \right]$$

When Z has a very high value $b_1 = b_2 = b$, then

$$E_{n_1} - E_{n_2} = \Delta E = \frac{me^4(Z-b)^2}{8\varepsilon_0^2h^2} \left[\frac{1}{n_2^2} - \frac{1}{n_1^2} \right]$$

$$\therefore \nu = \frac{\Delta E}{h} = \frac{me^4(Z-b)^2}{8\varepsilon_0^2h^2} \left[\frac{1}{n_2^2} - \frac{1}{n_1^2} \right]$$

According to Bohr's theory of spectrum of hydrogen like atoms

$$\frac{1}{\lambda} = RZ^2 \left[\frac{1}{n_2^2} - \frac{1}{n_1^2} \right]$$

Where $R = \frac{me^4}{8\epsilon_0^2ch^3}$ is Rydberg's constant, the value of which is $1.097 \times 10^7 \text{ m}^{-1}$.

1. From relation

(ii) we have

$$v = \frac{c}{\lambda} = c RZ^2 \left[\frac{1}{n_2^2} - \frac{1}{n_1^2} \right]$$

Where $cR = \frac{me^4}{8\epsilon_0^2h^3}$

Substituting $\frac{me^4}{8\epsilon_0^2h^3} = cR$ in equation (i), we get

$$v = \frac{c}{\lambda} = cR (Z - b)^2 \left[\frac{1}{n_2^2} - \frac{1}{n_1^2} \right]$$

Frequency of K_α line. The frequency v of the k_α line in Moseley's work is obtained by putting $n_1 = 2$ and $n_2 = 1$ so that the above equation becomes

$$v = \frac{c}{\lambda} = cR (Z - b)^2 \left[\frac{1}{1^2} - \frac{1}{2^2} \right]$$

For k_α line, $b = 1$ as explained below.

$$\therefore v = R c (Z - 1)^2 \left[\frac{1}{1^2} - \frac{1}{2^2} \right] = \frac{3}{4} cR (Z - 1)^2$$

In other words, the k_α line in the X-ray spectrum is emitted when the electron jumps from the orbit $n=2$ to the $n=1$. In the case of hydrogen, this gives a line in the Lyman series in the ultraviolet region. The factor $(Z-1)$ in place of Z is due to the fact that when one of the two electrons in the K shell is knocked out, the remaining one electron lowers the positive charge on the nucleus from Z to $(Z-1)$ and the electron jumping from the L level to fill the vacancy in the K level moves in an electric field of magnitude $(Z-1)e$.

Thus with $b=1$, we have

$$\nu = \frac{3}{4} cR (Z - 1)^2$$

$$\text{or} \quad \nu^{1/2} = \left(\frac{3}{4} cR\right)^{1/2} (Z-1)$$

$$= k (Z-1)$$

Thus the value of the constant k for K_α line is given by

$$K \text{ (for } K_\alpha \text{ line)} = \left(\frac{3}{4} cR\right)^{1/2}$$

$$= \left[\frac{3}{4} (3 \times 10^8 \text{ ms}^{-1}) \times 1.097(10^7 \text{ m}^{-1})\right]^{1/2}$$

$$= 4.97 \times 10^7$$

Relation (iii) may also be put as

$$\nu = k^2 (Z-1)^2 = a (Z-1)^2$$

$$= a (Z - b)^2$$

Where $a = 0.247 \times 10^{16} \text{ s}^{-1}$ and $b = 1$

Thus Eq. (iv) gives the approximate relation for K_α – line of an element.

(c) Importance and conclusions : According to this law, it is the atomic number and not the atomic weight of the element which determines its characteristic properties, both physical and chemical. According to Moseley's law, the atomic number is the number of positive units of electric charge on the nucleus of an atom. The atoms must be arranged in the periodic table according to their atomic numbers and not according to their atomic weights. Moseley thus corrected the positions of argon, cobalt and tellurium in the periodic table and he found that in the new positions the elements were in places corresponding to their chemical properties. The atomic weight of tellurium ($Z=52$) is 127.61 and that of iodine ($Z=53$) is 126.92. Hence in the periodic table, tellurium should precede iodine, though its atomic weight is greater.

Similarly $Z = 27$ for cobalt and $Z = 28$ for nickel, but their respective atomic masses are 58.93 and 58.71. The order, on the basis of atomic mass, does not explain the chemical properties of cobalt and nickel, but when these are placed in the periodic table according to the atomic numbers, they are in the right place.

Moseley also pointed out the existence of gaps in the group of rare earth elements at values $Z = 43, 61, 72$ and 75 . These elements have been subsequently discovered. The first two, technetium and promethium, have no stable isotope and were first produced in the laboratory many years later. The last two hafnium and rhenium, were isolated in 1920's.

Need of high atomic weight material as target

For most of the purposes we need hard X-rays which have a high penetrating power. The penetrating power depends upon the energy of X-rays and hence on the frequency. According to Mosley' law the frequency of X-rays is given by

$$\nu = Rc (Z - b)^2 \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

Where R is Rydberg's constant, c the velocity of light, Z the atomic weight of the material of the target and b the screening constant. Thus frequency is proportional to the square of the atomic number. Materials of high atomic number have high atomic weight and hence are more useful for producing highly penetrating X-rays.

8.9 Bragg's Law-

The wavelength of X-rays is very small, hence an ordinary diffraction grating cannot be used to measure it. W.L. Bragg discovered that X-rays can be regularly reflected by the cleavage planes of the crystals when the rays are incident on their surface nearly at glancing angle. The cleavage planes are successive atomic planes in the crystal. X-rays that penetrate more deeply into the crystal are reflected from the lower planes and thus several beams of X-rays reflected from various planes are obtained. The intensity of the reflected beam at certain angles will be maximum, where the two reflected waves from two different planes have a path-difference equal to an integral multiple of the wavelength of X-rays, while at some other angles, the intensity will be minimum.

Consider parallel lattice planes equidistant from one another in a crystal structure, separated by a distance d . Suppose a beam of X-rays AB of wavelength λ is incident on a layer of atoms in one cleavage plane P of a crystal at a glancing angle

θ at B and after reflection goes along BC. The ray DE incident on cleavage plane Q after reflection goes along EF. Draw BG perpendicular on DE and BH perpendicular on EF, then BG is the incident wave front and BH the reflected wave front.

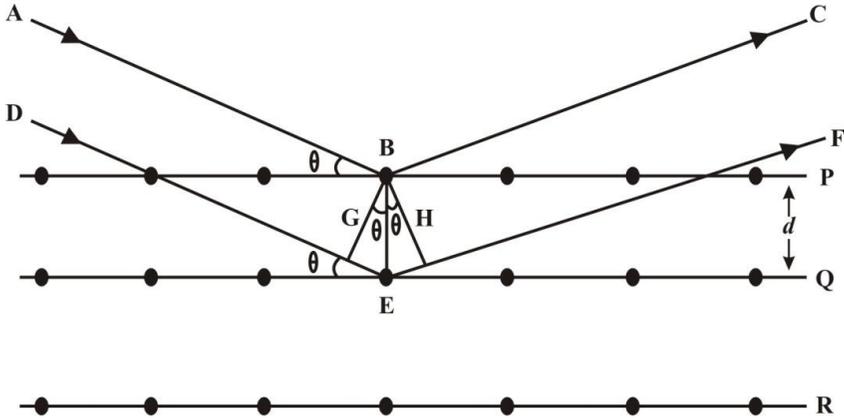


Fig. 8.6

Path difference between the two wave fronts

$$= GE + EH$$

Now in ΔBGE

$$GE = BE \sin\theta = d \sin\theta$$

And in ΔBEH

$$EH = BE \sin\theta = d \sin\theta$$

\therefore Path - difference

$$GE + EH = 2 d \sin\theta$$

If this path-difference is an integral multiple of wavelength λ , constructive interference will take place between the reflected beams. Thus the intensity will be maximum if

$$2 d \sin\theta = n \lambda \quad \text{where } n = 1, 2, 3 \dots$$

For $n = 1$ we get the first order spectrum and for $n = 2$ we get the second order spectrum and so on. This phenomenon is similar to that of the optical diffraction

with diffraction grating with only this difference that here various parallel planes of the crystal act as lines in the grating.

The above equation $2d \sin\theta = n\lambda$ is Bragg's equation and represents Bragg's law.

Failure of diffraction of X-rays from transparent grating. The phenomenon of diffraction of waves takes place only when the size of the object from which diffraction takes place is of the order of wavelength of the waves. For example, sound waves which have a wavelength of a few metres, can bend round walls and objects of large size.

The wavelength of visible light is of the order of 4000Å to 8000Å . To study the diffraction of light we use transparent diffraction gratings having about 6000 lines per cm. Thus a slit is formed between two consecutive lines, giving rise to transparencies and opacities. The size of each opacity or transparency is about $1.6 \times 10^4 \text{Å}$. This size is comparable to the wavelength of yellow light which = 6000Å = $0.6 \times 10^4 \text{Å}$.

In order to study the diffraction of X-rays it is necessary to have grating whose slit width ranges from 0.1Å to 100Å . Such a fine grating is not available. On the other hand, it has been observed that crystals have a regular arrangement of atoms in the crystal structure and the spacing between adjacent lattice planes is comparable to wavelength of X-rays.

It is for this reason that crystals are used to study the diffraction of X-rays as transparent gratings cannot be used for the purpose.

8.10 Properties of X-rays

- (i) They are not deflected by electric and magnetic fields. This property distinguishes them from cathode rays and indicates that the X-rays do not consist of charged particles.
- (ii) They are highly penetrating and can pass through many solids, which are opaque to ordinary light.

The penetrating power of X-rays depends upon

- (a) The applied potential difference,
- (b) The atomic weight of the material of the target or anti cathode,

The greater the potential difference and higher the atomic weight, the more penetrating are the X-rays produced.

(iii) They cause fluorescence in many substances, e.g., barium platino-cyanide, cadmium tungstate, zinc sulphate, etc.

(iv) They produce a photo-chemical action and effect a photographic plate and they are even more effective than light.

(v) They ionize a gas and eject electrons from certain metals on which they fall (photo-electric effect).

(vi) They are propagated in straight lines with the velocity of light i.e., 3×10^8 metres/sec.

(vii) Like light, X-rays consist of electromagnetic waves of very short wavelength and show reflection, refraction, interference, diffraction and polarization in a similar way. These effects can be demonstrated by suitable arrangements.

(viii) When X-rays are incident on matter, they give rise to a complex phenomenon known as secondary radiations, which consist of three different types of rays:

(a) Scattered X-rays. They are practically of the same nature and wavelength as the original or the primary rays. Their properties do not depend upon the nature of the scattering substance.

(b) Corpuscular rays. They consist of fast moving electrons produced by the photoelectric process. Their properties are independent of nature of the scattering substance, but depend upon the quality of primary X-rays.

(c) Characteristic X-rays. The wavelength of the characteristic X-rays is equal to or less than the primary X-rays, but it is characteristic of the substance upon which the primary X-rays are incident and is independent of the wavelength of the primary X-rays.

(ix) They have a destructive effect on living tissues. Exposure of human body to X-rays causes reddening of the skin and surface sores.

(i) Surgery. X-rays can pass through flesh and not through bones. They are of extensive use in surgery to detect fractures, foreign bodies, diseased organs etc. The patient is made to stand between an X-ray source and a fluorescent screen. The luminosity of the screen depends upon the stopping power of different parts of the body. Thus a deep shadow of the bones and a light shadow of the flesh will be obtained. A photograph may also be obtained. It is called a radiograph. If the various parts do not show sufficient contrast, artificial means are adopted, e.g., in radio-graphing the portions of the alimentary tract, the patient is fed with meal of barium sulphate.

(ii) Radiotherapy, X-rays kill the diseased tissues of the body. Hence they are used to cure intractable skin disease, malignant tumours etc. If the affected part is superficial soft rays are applied and for deep-seated organs hard rays are used.

(iv) Industry. X-rays are employed in industry to detect defects in motor tyres, golf and tennis balls, wood and wireless valves. They are used in testing the uniformity of insulating material and for detecting the presence of pearls in oysters.

(v) Detective departments. X-rays are used at custom posts for detection of contraband goods like explosive, opium, etc. concealed in leather or wooden cases, in examining of parcels without opening them and in the detection of distinguishing real diamonds, gems and pearls from artificial ones, pure ghee from vegetable ghee and real documents from forged ones.

(vi) Scientific research. X-rays have been employed to investigate the structure of crystals, structure and properties of atoms and arrangement of atoms and molecules

Solved Problems

Problem 1. Why high atomic weight material is used as target?

Solution: According to Mosley' law the frequency of X-rays is given by

$$\nu = Rc (Z - b)^2 \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

Where R is Rydberg's constant, c the velocity of light, Z the atomic weight of the material of the target and b the screening constant. Thus frequency is proportional to the square of the atomic number. Materials of high atomic number have high atomic weight and hence are more useful for producing highly penetrating X-rays.

Problem 2. Determine wavelength of K_α X-rays emitted by an element having $Z = 79$, $a = 2.468 \times 10^{15} \text{ s}^{-1}$ and $b = 1$. Using the data find the wavelength of K_β line.

Solution: Wavelength of K_α line,

$$\lambda_1 = \frac{hc}{E_K - E_L} = 0.2 \text{ \AA} = 0.2 \times 10^{-10} \text{ m}$$

$$\therefore E_K - E_L = \frac{hc}{\lambda_1} = \frac{6.62 \times 10^{-34} \times 3 \times 10^8}{0.2 \times 10^{-10}} = 99.3 \times 10^{-16} \text{ J}$$

$$\text{Wavelength of } L_\alpha \text{ line, } \lambda_2 = \frac{hc}{E_L - E_M} = 1.6 \text{ \AA} = 1.6 \times 10^{-10} \text{ m}$$

$$\therefore E_L - E_M = \frac{hc}{\lambda_2} = \frac{6.62 \times 10^{-34} \times 3 \times 10^8}{1.6 \times 10^{-10}} = 12.4 \times 10^{-16} \text{ J}$$

$$\text{Wavelength of } K_\beta \text{ line, } \lambda = \frac{hc}{E_K - E_M}$$

$$\begin{aligned} \text{Now } E_K - E_M &= E_K - E_L + E_L - E_M = 99.3 \times 10^{-16} + 12.4 \times 10^{-16} \text{ J} \\ &= 111.7 \times 10^{-16} \text{ J} \end{aligned}$$

$$\therefore \lambda = \frac{hc}{E_K - E_M} = \frac{6.62 \times 10^{-34} \times 3 \times 10^8}{111.7 \times 10^{-10}} = 0.18 \times 10^{-16} \text{M} = 0.18 \text{ \AA}$$

Problem 3: An X-ray tube operates at the voltage given below, Find the maximum speed of electrons striking the anticathode and shortest wavelength of X-rays produced.

- (i) 10 KV
- (ii) 20 KV
- (iii) 100 KV
- (iv) 50 KV

Solution:

Let V be the difference of potential applied to the X-ray tube, then the work done on the electron in moving from the cathode to the anticathode is V_e , where e is the charge on the electron.

If v is the maximum velocity acquired by the electron, then

$$\text{Maximum kinetic energy} = \frac{1}{2}mv^2$$

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

$$\text{or } v = \sqrt{\frac{2Ve}{m}} = \sqrt{v} = \sqrt{\frac{2e}{m}}$$

$$= \sqrt{V} \sqrt{\frac{2 \times 1.6 \times 10^{-19}}{9 \times 10^{-31}}} =$$

$$\sqrt{V} \times 0.596 \times 10^6$$

$$(i) \quad v = 40 \text{ kV} = 40,000 \text{V}$$

$$\therefore v = \sqrt{40,000} \times 0.596 \times 10^6 =$$

$$200 \times 0.596 \times 10^6 = 119.2 \times 10^6 \text{ms}^{-1}$$

$$(ii) \quad v = 20 \text{ kV} = 20,000\text{V}$$

$$\therefore v = \sqrt{20,000} \times 0.596 \times 10^6 = 84.27 \times 10^6 = 84.27 \times 10^6 \text{ms}^{-1}$$

$$(iii) \quad v = 100 \text{ kV} = 100,000\text{V}$$

$$\therefore v = \sqrt{100,000} \times 0.596 \times 10^6 = 188.45 \times 10^6 \text{ms}^{-1}$$

$$(iv) \quad v = 50 \text{ kV} = 50,000\text{V}$$

$$\therefore v = \sqrt{50,000} \times 0.596 \times 10^6 = 133.27 \times 10^6 \text{ms}^{-1}$$

$$\text{Shortest wavelength } \lambda_m = \frac{ch}{eV} = \frac{12420 \times 10^{-10}}{v} \text{ m} = \frac{12420}{V} \text{ \AA}$$

$$(i) \quad v = 40 \text{ kV} = 40,000\text{V}$$

$$\therefore \lambda_m = \frac{12420}{40,000} = 0.31 \text{ \AA}$$

$$(ii) \quad v = 20 \text{ kV} = 20,000\text{V}$$

$$\therefore \lambda_m = \frac{12420}{20,000} = 0.62 \text{ \AA}$$

$$(iii) \quad v = 100 \text{ kV} = 100,000\text{V}$$

$$\therefore \lambda_m = \frac{12420}{100,000} = 0.124 \text{ \AA}$$

$$(iv) \quad v = 50 \text{ kV} = 50,000\text{V}$$

$$\therefore \lambda_m = \frac{12420}{50,000} = 0.248 \text{ \AA}$$

Problem 4: Electrons are accelerated in a television tube through a potential difference of 9.8 kV. Find the highest frequency and minimum wavelength of the electromagnetic

waves emitted, when these strike the screen of the tube. In which region of the spectrum will these waves lie?

Solution:

Minimum wavelength is given by

$$\lambda_{\min} = \frac{hc}{eV} = \frac{12420 \times 10^{-10}}{V} \text{ m} = \frac{12420}{V} \text{ \AA}$$

Here $V = 9.8 \text{ kV}$

$$\therefore \lambda_m = \frac{12420}{9.8 \times 10^3} = 12.6 \text{ \AA}$$

$$V_{\max} = \frac{c}{V_{\min}} = \frac{3 \times 10^8}{1.26 \times 10^{-10}} = 2.38 \times 10^{18} \text{ Hz}$$

The waves lie in the X-ray region of the electro-magnetic spectrum.

Problem 5 : If the K , L and M energy levels of Pt are 78000, 12000 and 3000 eV respectively, calculate the wavelength of K_α and K_β lines from Pt. $1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$ and $h = 6.55 \times 10^{-34} \text{ Joule - sec}$.

Solution:

$$\text{Energy of } K \text{ level, } E_K = 78000 \text{ eV}$$

$$= 78000 \times 1.6 \times 10^{-19} \text{ Joule}$$

$$\text{Energy of } L \text{ level, } E_L = 12000 \times 1.6 \times 10^{-19} \text{ Joule}$$

$$\text{Energy of } M \text{ level, } E_M = 3000 \times 1.6 \times 10^{-19} \text{ Joule}$$

$$\begin{aligned} \text{Wavelength of } K_\alpha \text{ line, } \lambda_1 &= \frac{hc}{E_K - E_L} \\ &= \frac{6.55 \times 10^{-34} \times 3 \times 10^8}{(78000 - 12000) \times 1.6 \times 10^{-19}} \\ &= 0.1886 \times 10^{-10} \text{ m} = 0.186 \text{ \AA} \end{aligned}$$

$$\text{Wavelength of } K_\beta \text{ line, } \lambda_2 = \frac{hc}{E_M - E_K}$$

$$= \frac{6.55 \times 10^{-34} \times 3 \times 10^8}{(78000-3000) \times 1.6 \times 10^{-19}}$$

$$= 0.163 \times 10^{-10} \text{ m} = 0.163 \text{ \AA}$$

Problem 6 : An X-ray tube operating at (i) 30 kV, (ii) 44 kV (iii) 50 kV and (iv) 200 kV emits a continuous spectrum with shortest wavelength (i) 0.414 Å, (ii) 0.284 Å, (iii) $0.248 \times 10^{-10} \text{ m}$ and (iv) $6.2 \times 10^{-12} \text{ m}$; calculate Planck's constant. Given $e = 1.6 \times 10^{-19} \text{ C}$ and $c = 3 \times 10^8 \text{ ms}^{-1}$.

(LU. 1995, 1992; P.U. 1992, 1990)

Solution:

Minimum wavelength is given by

$$\lambda_{\min} = \frac{ch}{eV}$$

$$\therefore h = \frac{eV}{c} \lambda_{\min}$$

Now $e = 1.6 \times 10^{-19} \text{ C}$ and $c = 3 \times 10^8 \text{ ms}^{-1}$

$$\therefore \frac{e}{c} = \frac{1.6 \times 10^{-19}}{3 \times 10^8} = 0.5333 \times 10^{-27} \text{ C ms}^{-1}$$

$$\therefore h = 0.5333 \times 10^{-27} \text{ V } \lambda_{\min}$$

(i) $V = 30 \text{ kV} = 30,000 \text{ V}$; $\lambda_{\min} = 0.414 \text{ \AA} = 0.414 \times 10^{-10} \text{ m}$

$$\therefore h = 0.5333 \times 10^{-27} \times 3 \times 10^4 \times 0.414 \times 10^{-10} = 0662 \times 10^{-33}$$

$$= 662 \times 10^{-34} \text{ Js}$$

(ii) $V = 44 \text{ kV} = 44,000 \text{ V}$; $\lambda_{\min} = 0.284 \text{ \AA} = 0.284 \times 10^{-10} \text{ m}$

$$\therefore h = 0.5333 \times 10^{-27} \times 44 \times 10^3 \times 0.284 \times 10^{-10} = 6.66 \times 10^{-34} \text{ Js}$$

(iii) $V = 50 \text{ kV} = 50 \times 10^3 \text{ V}$; $\lambda_{\min} = 0.248 \times 10^{-10} \text{ m}$

$$\therefore h = 0.5333 \times 10^{-27} \times 50 \times 10^3 \times 0.248 \times 10^{-10} = 6.61 \times 10^{-34} \text{ Js}$$

(iv) $V = 200 \text{ kV} = 2 \times 10^5 \text{ V}$; $\lambda_{\min} = 6.2 \times 10^{-10} \text{ m}$

$$\therefore h = 0.5333 \times 10^{-27} \times 2 \times 10^5 \times 6.2 \times 10^{-12} = 6.61 \times 10^{-34} \text{ Js}$$

Problem 7: What voltage must be applied to an X-ray tube for it to emit X-rays with minimum wavelength of (i) 40 pm (ii) 0.5 Å (iii) 0.1 Å. (LU. 1991)

Solution: Minimum wavelength is given by

$$\lambda_{\min} = \frac{ch}{eV}$$

$$\therefore \text{Voltage that must be applied } V = \frac{ch}{e \lambda_{\min}} = \frac{ch}{e} \frac{1}{\lambda_{\min}}$$

Here $c = 3 \times 10^8 \text{ ms}^{-1}$; $h = 6.626 \times 10^{-34} \text{ Js}$; $e = 1.6 \times 10^{-19} \text{ C}$

$$\therefore \frac{ch}{e} = \frac{3 \times 10^8 \times 6.626 \times 10^{-34}}{1.6 \times 10^{-19}} = 12.42 \times 10^{-7}$$

$$(i) \lambda_{\min} = 40 \text{ pm} = 40 \times 10^{-12} \text{ m}$$

$$\therefore V = \frac{ch}{e} \cdot \frac{1}{\lambda_{\min}} = \frac{12.42 \times 10^{-7}}{40 \times 10^{-12}} = 31 \times 10^3 \text{ V} = 31 \text{ kV}$$

$$(ii) \lambda_{\min} = 0.5 \text{ Å} = 0.5 \times 10^{-10} \text{ m}$$

$$\therefore V = \frac{12.42 \times 10^{-7}}{0.5 \times 10^{-10}} = 24.84 \times 10^3 \text{ V} = 24.84 \text{ kV}$$

$$(iii) \lambda_{\min} = 0.1 \text{ Å} = 0.1 \times 10^{-10} \text{ m}$$

$$\therefore V = \frac{12.42 \times 10^{-7}}{0.1 \times 10^{-10}} = 124.1 \times 10^3 \text{ V} = 124.1 \text{ kV}$$

Problem 8: An X-ray tube is operated at an anode potential of 10 kV and anode current of 15 mA. Calculate (i) number of electrons hitting the anode per second and (ii) the minimum wavelength produced by the X-ray tube.

(LU. 1993, 1990)

Solution:

$$\text{Current} = 15 \text{ mA} = 15 \times 10^{-3} \text{ A}$$

∴ Charge conveyed to the anode per second = $15 \times 10^{-3} \text{ C}$

Charge on the electron = $1.6 \times 10^{-19} \text{ C}$

∴ Number of electrons hitting the anode per second

$$= \frac{15 \times 10^{-3}}{1.6 \times 10^{-19}} = 9.4 \times 10^{16} \text{ electrons per second.}$$

$$\text{Now } \lambda_{\min} = \frac{ch}{eV} = \frac{3 \times 10^{-8} \times 6.62 \times 10^{-34}}{1.6 \times 10^{-19} \times 10 \times 10^{-3}} = 1.24 \times 10^{-10} \text{ m} = 1.24 \text{ \AA}$$

Problem 9. Calculate the frequency of ka line when atomic number of the anticathode is 79. Given $R = 1.097 \times 10^7 \text{ m}^{-1}$

Solution:

The Frequency of the K_{α} line is given by

$$\nu = Rc (Z-1)^2 \left[\frac{1}{1^2} - \frac{1}{2^2} \right] = \frac{3}{4} cR (Z-1)^2$$

Substituting the values, we have

$$\nu = \frac{3 \times 3 \times 10^8 \times 1.097 \times 10^7 (79 - 1)^2}{4} = 1.502 \times 10^{19} \text{ s}^{-1}$$

Exercise

Theoretical

- (1) Explain the origin of continuous and characteristic X-ray. Give difference between them. **(L.U. 2010)**
- (2) What are continuous X-rays? Explain their origin and derive Duane-Hunt rule. **(L.U. 2008)**
- (3) Explain the origin of continuous X-rays and discuss the significance of short wavelength limit. **(L.U. 2013)**
- (4) Describe 'Duane-Hunt Law, and 'Mosley Law' related to x-ray spectrum and give their importance. **(LU 2016)**
- (5) Distinguish between characteristic and continuous X-rays. **(L.U. 2011)**
- (6) Differentiate between continuous and characteristics X-ray. **(L.U. 2014)**
- (7) Distinguish between characteristic and continuous X-rays. . **(L.U. 2009)**
- (8) State and discuss Mosley's law. **(L.U. 2014)**
- (9) Derive Moseley's law on the basis of Bohr's theory discuss the significance of this law. **(L.U. 2012)**
- (10) State Moseley's law and explain its significance. **(L.U. 2011)**
- (11) State Mosley's law and explain its significance. . **(L.U. 2009)**
- (12) Explain the importance of Mosely's law. **(L.U. 2007)**
- (13) State and discuss Mosley's law. **(L.U. 2013)**
- (14) What are characteristic X-rays? Explain their origin, derive Meseley law. **(LU 2015)**
- (15) Different between continuous and characteristics X-rays. **(LU 2015)**

Short answer type

- (1) Explain the process by which X-ray are produced from the impact of electrons on the atoms of the target element. Can X-rays be produced from hydrogen? Give reasons for your answer. **(L.U. 2007)**
- (2) Discuss the construction and working of an X-ray tube. **(L.U. 2013)**
- (3) What are spin doublets in X-ray spectra? **(L.U. 2014)**
- (4) How the wavelength of characteristic X-rays emitted, is related to atomic number of target element? **(LU 2016)**
- (5) What is Bragg's law **(L.U. 2009)**
- (6) What are spin doublets in X-ray spectra? **(L.U. 2013)**
- (7) What is Bragg's law? **(L.U. 2008)**
- (8) Show K_{α} and k_{β} lines superposed on continuous X-ray spectrum of a metal. **(L.U. 2010)**
- (9) The minimum wavelength of X-rays generated. **(L.U. 2010)**

Numerical problems

- (1) P.D. across an X-ray tube is 10^5 volt. Find the maximum frequency of the X-ray emitted. **(L.U. 2007)**
- (2) A neutron beam of energy of energy 0.04 strikes a crystal surface at glancing angle $13^{\circ} 10^0$. Calculate Bragg spacing for the first order reflection maxima. **(L.U. 2008)**
- (3) The minimum wavelength recorded in an X-ray continuous spectrum of a 50 kV tube is 24.7×10^{-12} m. Calculate the value of Planck's constant. **(L.U. 2009)**
- (4) An X-ray tube operates at 20 kV and carries current 2mA. Find :-
(L.U. 2010)
 - (I) Number of electrons striking the target per second. **(L.U. 2010)**
 - (II) Maximum speed with which electrons strike the target. **(L.U. 2010)**
- (5) If the minimum wavelength recorded in the continuous X-rays spectrum of 50 kV tube is 24.7×10^{-12} meter. Calculate the value of Planck's constant. **(L.U. 2012)**

- (6) Potential difference across an X-ray tube is 10^5 volt. Find the maximum frequency of the X-ray emitted. **(L.U. 2011)**
- (7) Calculate the wavelength of the K_{α} line, from a copper target assuming Moseley's law. Rydberg constant for hydrogen = 10967800m^{-1} and screening constant = 1. **(L.U. 2014)**
- (8)** If the K_{α} radiation of Mo ($z = 42$) has a wavelength of 0.71 \AA , calculate the wavelength of the corresponding radiation of Cu ($z = 29$). **(LU 2015)**
- (9) X-rays of wavelength 0.5 \AA and intensity 10W are produced by a Coolidge Tube. Calculate **(LU 2015)**