Atomic physics course

Lectures in Atomic Physics
By
Dr. Khaled Salah

Faculty: Education

Level:4

Department: Physics

Course name: Atomic Physics

Publish date:2022

Page number:69

Author: Khaled Salaheldin

Content

1. ***Atomic physics conception***

Atomic physics is the field of physics that studies atoms as an isolated system of electrons and an atomic nucleus. It is primarily concerned with the arrangement of electrons around the nucleus and the processes by which these arrangements change. This comprises ions, neutral atoms and, unless otherwise stated, it can be assumed that the term ***atom*** includes ions.

The term ***atomic physics*** can be associated with nuclear power and nuclear weapons, due to the synonymous use of ***atomic*** and ***nuclear*** in Standard English. Physicists distinguish between atomic physics which deals with the atom as a system consisting of a nucleus and electrons and nuclear physics, which considers atomic nuclei alone.

As with many scientific fields, strict delineation can be highly contrived and atomic physics is often considered in the wider context of ***atomic***, ***molecular****, and* ***optical physics***. Physics research groups are usually so classified.

2. ***Models of the atomic structure***

In ancient Greece, there were two schools of thought regarding the structure of matter, namely ***Atomic theory*** conveying a particulate nature of matter and the ***continuous theory*** of matter proposed by Aristotle.

400 B.C- ***Democritus*** thought matter could not be divided indefinitely. This small particle he called “atomos” (***Atomic theory***).

350 B.C - ***Aristotle*** modified an earlier theory that matter was made of four "elements": earth, fire, water, air (***continuous theory***).

The continuous theory of matter having been proposed by such a prominent person at the time overshadowed the atomic theory of matter for some time.

2.1 Dalton's Model of the Atom

John Dalton, at the beginning of the 19th century, proposed an atomic model that allowed limited quantitative study of the atom.

Dalton's model was that the atoms were **tiny, indivisible, indestructible particles, like billiard balls,** and that each one had a **certain mass, size, and chemical behavior** that was determined by what kind of element it was. Dalton's model is silent about the composition and internal structure of the atom.

Discovery of Electron:

According to Dalton and scientists before him, the atom is the indivisible, and no scientist prior to the beginning of the 19th century considered that an atom might have a structure, in other words, that an atom is also constituted by smaller components.

The belief in the indivisibility of the atom began to waver because of the development of a deeper understanding of the relation between matter and electricity, not because scientists had become suspicious of its indivisibility.

In 1897, Sir William Crookes carried out a series of experiments to study the behavior of metals heated in a vacuum using cathode ray tubes. A cathode ray tube consists of two metal electrodes in a partially evacuated glass tube. An evacuated tube is a glass tube from which most of the air has been removed. The negatively charged electrode is called cathode whereas the positively charged electrode is called anode. These electrodes are connected to a high voltage source. Such a cathode ray tube has been shown in Fig. 1.

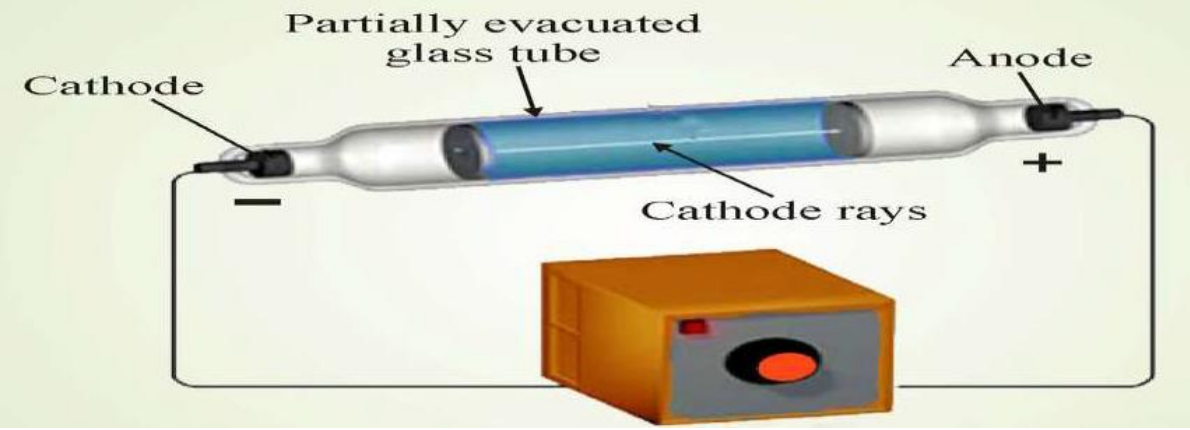


Fig.1 A cathode ray tube

Observation

It was observed that when very high voltage was passed across the electrodes in evacuated tube at 0.0001 atm. pressure, the cathode produced a stream of particles with greenish glow at anode. These particles were shown to travel from cathode to anode and were called **cathode rays**. In the absence of external magnetic or electric field these rays travel in straight line. Rays are called **cathode rays** because they are emitted by the negative electrode, or cathode, in a vacuum tube.

In 1897, an English physicist Sir J.J. Thomson showed that the rays were made up of a stream of ***negatively charged particles***. This conclusion was drawn from the experimental observations when the experiment was done in the presence of an external electric field.

Properties of cathode rays:

- Cathode rays travel in straight line.
- The particles constituting cathode rays carry mass and possess kinetic energy.
- The particles constituting cathode rays have negligible mass but travel very fast.
- Cathode ray particles carry negative charge and are attracted towards positively charged plate when an external electric field is applied.
- The nature of cathode rays generated was independent of the nature of the gas filled in the cathode ray tube as well as the nature of metal used for making cathode and anode. In all the cases the charge to mass ratio (e/m) was found to be the same.

These particles constituting the cathode rays were later called electrons. Since it was observed that the nature of cathode rays was the same irrespective of the metal used for the cathode or the gas filled in the cathode ray tube. This led Thomson to conclude that all atoms must contain electrons. This meant that the atom is not

indivisible as was believed by Dalton and others. In other words, we can say that the Dalton's theory of atomic structure failed partially.

2.2 Thomson's Model

On the basis of his experiments on discharge tubes, Thomson proposed that atoms can be considered as a large positively charged body with a number of small negatively charged electrons scattered throughout it. This model (Fig.2) was called as ***plum pudding model*** of the atom.

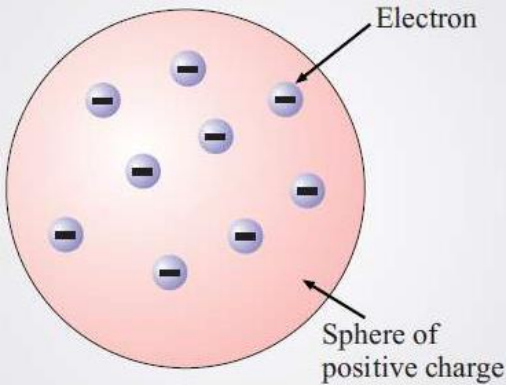


Fig. 2 : Thomson‟s plum-pudding model

Fig.3 **J.J.Thomson (1856-1940)**
Won Nobel prize in Physics in 1906

The electrons represent the plums in the pudding made of positive charge. It is sometimes also called as **watermelon model**. In this, the juicy pulp of the watermelon represents the positive charge and the seeds represent the electrons.

2.3 Rutherford's Model of the Atom

Ernest Rutherford and his co-workers were working in the area of radioactivity. They were studying the effect of alpha (α) particles on matter. The alpha particles

are helium nuclei, which can be obtained by the removal of two electrons from the helium atom.

In 1910, Hans Geiger (Rutherford's technician) and Ernest Marsden (Rutherford's student) performed the famous α- ray scattering experiment. This led to the failure of Thomson's model of atom. Let us learn about this experiment

α-Ray scattering experiment

In this experiment a stream of αparticle from a radioactive source was directed on a thin (about 0.00004 cm thick) piece of gold foil. On the basis of Thomson's model it was expected that the alpha particles would just pass straight through the gold foil and could be detected by a photographic plate placed behind the foil. However, the actual results of the experiment, Fig. 4, were quite surprising.

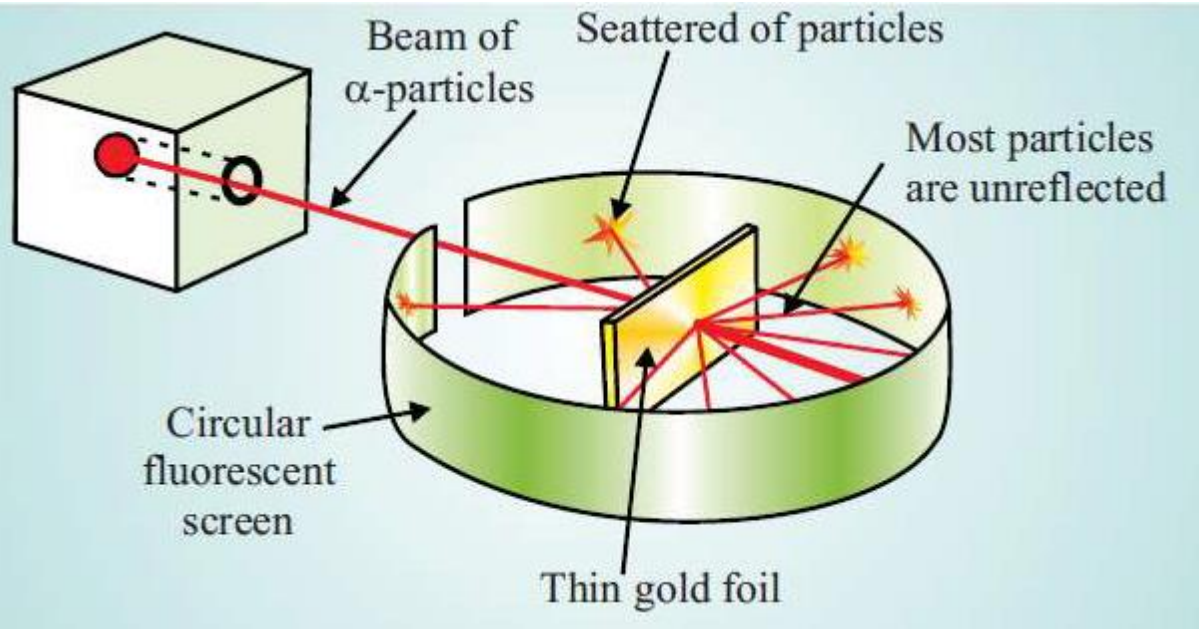


Fig. 4 : The experimental set-up of α- ray scattering experiment performed by Geiger and Marsden

It was observed in α Ray scattering experiment that:

(i) Most of the α-particles passed straight through the gold foil.

(ii) Some of the α-particles were deflected by small angles.

(iii) A few particles were deflected by large angles.

(iv) About 1 in every 12000 particles experienced a rebound

These results led Rutherford to conclude that:

- The atom contained some dense and positively charged region located at the center of the atom that he called as **nucleus**.
- All the ***positive charge*** of the atom and ***most of its mass*** was contained in the ***nucleus***.
- The rest of the atom must be empty space which contains the much smaller and negatively charged electrons (Fig. 5).

The model proposed by Rutherford explained the observation in the α-ray scattering experiments as shown below in Fig 6.

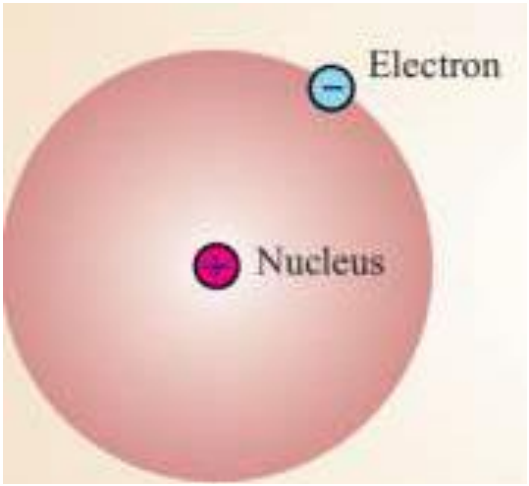


Fig.5 Rutherford's model of atom

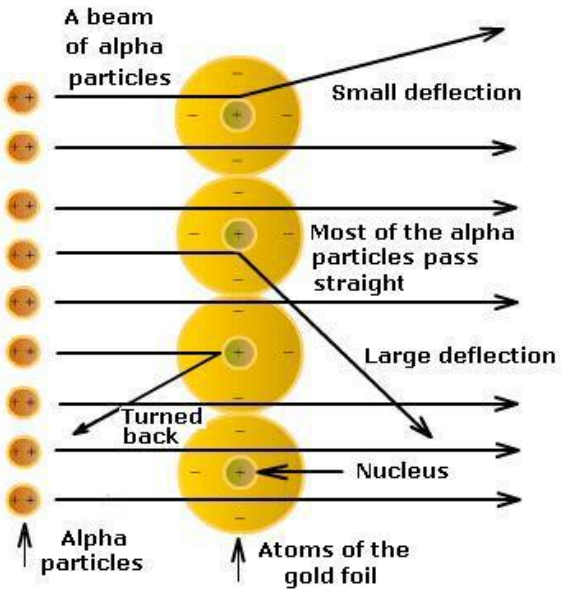


Fig. 6 Explanation of the results of scattering experiment

The αparticles passing through the atom in the region of the electrons would pass straight without any deflection. Only those particles that come in close vicinity of the positively charged nucleus get deviated from their path. Very few α-particles, those that collide with the nucleus, would face a rebound.

On the basis of his model, Rutherford was able to predict the size of the nucleus. He estimated that the radius of the nucleus was at least 1/10000 times smaller than that of the radius of the atom.

Theoretical Description

Assumptions

1. The scatterer is so massive that it does not recoil significantly; therefore **the initial and final kinetic energies of the αparticle are practically equal.**
2. The target is so thin that **only a single scattering occurs.**

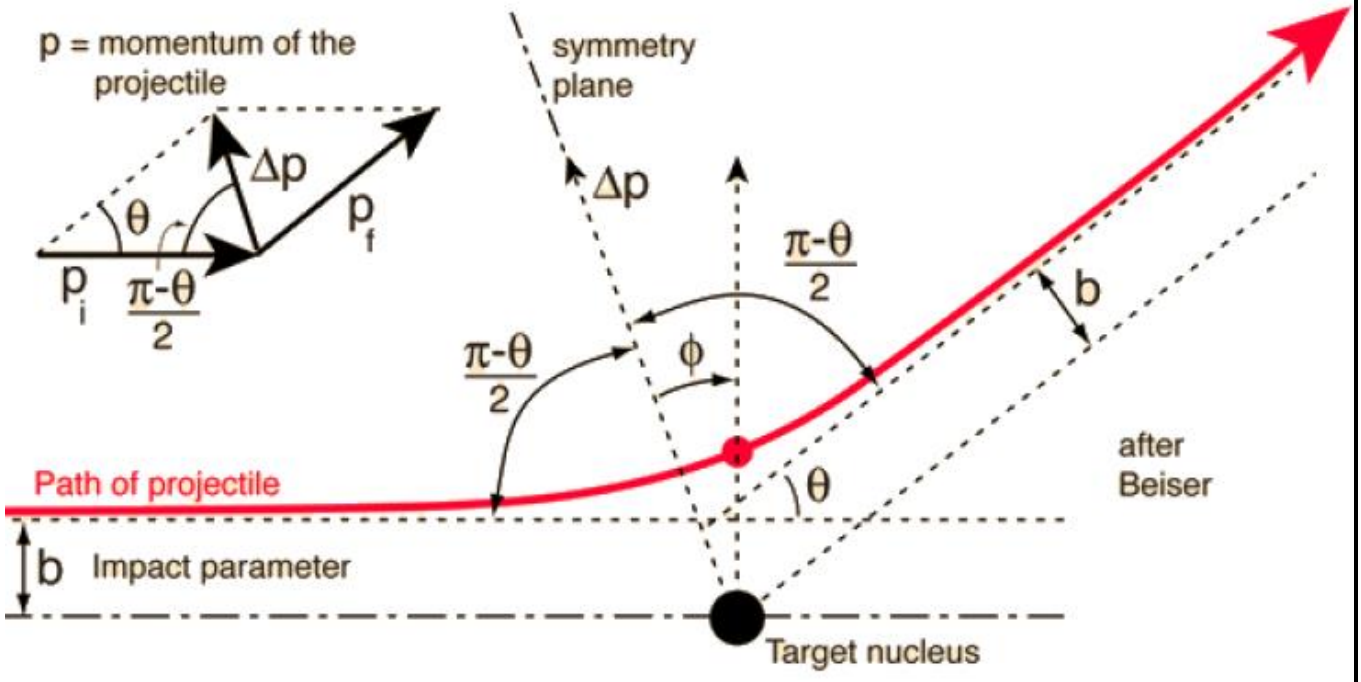
3. The bombarding particle and target scatterer are so small that they may **be treated as point masses and charges**.

4. Only the **Coulomb force is effective**.

The Relationship between the Impact Parameter b and the Scattering Angle θ:

The minimum distance for an α-particle to approach the target nucleus known as ***impact parameter*** denoted by 'b' and the scattering angle 'θ' were studied by Rutherford. For head on collision obviously b=0, and as the distance of closest approach 'D', the repulsive force of the nucleus would stop the approaching α-particles and all the K.E. of it is transferred to P.E, given by the relation,

$$\mathbf{D = (1/4\pi\varepsilon)\,(2Ze^2/K.E)}$$



The relationship between the impact parameter *b* and the scattering angle *θ*:-

When *b* is small,

- ***r gets small***.
- ***Coulomb force gets large.***
- ***θ can be large and the particle can be repelled backward.***

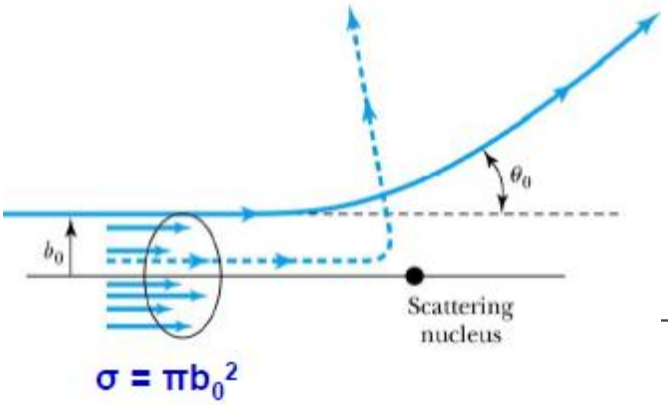
$$b = \frac{Z_1 Z_2 e^2}{8\pi\varepsilon_0 K}\cot\frac{\theta}{2} \quad where\ K = \tfrac{1}{2}mv_0^2$$

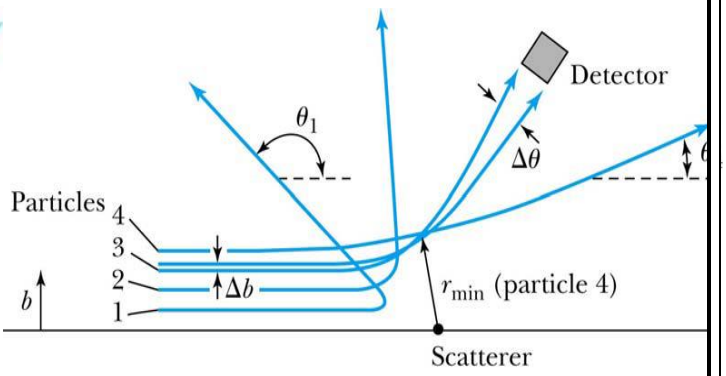
• Particles are incident at varied impact parameters all around the scatterer.

• Any particle inside a circle of area πb_0^2 will be scattered at angles greater than θ_0.

• Define cross section $\sigma = \pi b_0^2$ for scattering at an angle greater than θ_0.

• σ related to the probability for a particle being scattered by the nucleus





Rutherford scattering equation

- By considering all the scatters in the foil, the fraction of incident particles scattered at an angle greater than θ is:

$$f = \frac{\text{target area exposed by scatterers}}{\text{total target area}} = \pi nt\left(\frac{Z_1 Z_2 e^2}{8\pi\varepsilon_0 K}\right)^2 \cot^2\frac{\theta}{2}$$

- In actual experiment a detector is positioned from θ to θ + $d\theta$ that corresponds to incident particles between b and $b + db$.

The number of particles scattered per unit area is

$$N(\theta) = \frac{N_i nt}{16}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2 \frac{Z_1^2 Z_2^2}{r^2 K^2 \sin^4(\theta/2)}$$

The Important Points

The scattering is **proportional to the square of the atomic number** of ***both*** the incident particle (***Z1***) and the target scatterer (***Z2***).

2. The number of scattered particles is **inversely proportional to the square of the kinetic energy** of the incident particle.

3. For the scattering angle θ, **the scattering is proportional to 4th power of sin (θ /2)**.

4. The Scattering is **proportional to the target thickness** for thin targets.

DRAWBACKS OF RUTHERFORD'S MODEL

- Rutherford's model is ***unable to explain the stability of the atom.***

According to Rutherford's model the negatively charged electrons revolve in circular orbits around the positively charged nucleus. However, according to Maxwell's electromagnetic theory, if a charged particle accelerates around another

charged particle then it would continuously lose energy in the form of radiation. The loss of energy would slow down the speed of the electron. Therefore, the electron is expected to move in ***a spiral fashion*** around the nucleus and eventually fall into it as shown in Fig. 7.

In other words According to Rutherford's model, the atom will not be stable. However, we know that the atom is stable and such a collapse does not occur. Thus, ***Rutherford's model is unable to explain the stability of the atom***.

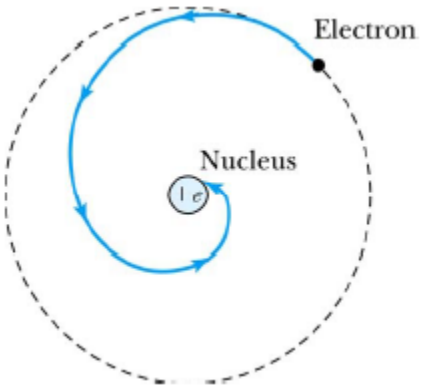


Fig. 7: The electron in the Rutherford's model is expected to spiral into the nucleus

- The Rutherford's model also ***does not say anything about the way the electrons are distributed around the nucleus.***
- The Rutherford's models also ***fail to explain the relationship between the atomic mass and atomic number*** (the number of protons).This problem was solved later by Chadwick by discovering neutron.

Difference Between Thomson and Rutherford Model of Atom

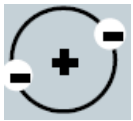
Thomson vs. Rutherford Model of Atom	
Thomson model of atom is the model which states that electrons are embedded in a positively charged solid material which is spherical in shape.	Rutherford model of atom is the model which explains that there is a nucleus in the center of the atom and electrons are located around the nucleus.
Nucleus	
Thomson model of atom does not give any detail about the nucleus.	Rutherford model of atom provides details about the nucleus of an atom and its location inside the atom.
Location of Electrons	
According to Thomson model of atom, electrons are embedded in a solid material.	Rutherford model says electrons are located around the nucleus.
Orbitals	
Thomson model of atom does not give details about orbitals.	Rutherford model of atom explains about orbitals and that electrons are located in these orbitals.
Mass	
Thomson model of atom explains that the mass of an atom is the mass of positively charged solid where electrons are embedded.	According to the Rutherford model of atom, the mass of an atom is concentrated in the nucleus of the atom.

Evolving Electrons Model

- Dalton's "Billiard ball" model (1808) Atoms are solid and indivisible.

- Thomson "Plum pudding" model (1904) Negative electrons in a positive framework.

- Rutherford model (around 1911) Atoms are mostly empty space. Negative electrons orbit a positive nucleus.



Chapter 2

Electromagnetic Radiations

2.1 Electromagnetic radiation

Electromagnetic radiation is a kind of energy, which is transmitted through space in the form of electric and magnetic fields. These do not require any medium to propagate. Visible light, radiant heat, radio waves, X-rays and gamma radiation are some of the examples of electromagnetic radiations. According to the Maxwell's theory, an electromagnetic radiation can be visualized as oscillating electric and magnetic fields. These travel as waves in the planes perpendicular to each other and also to the direction of propagation as shown in the following figure 8.

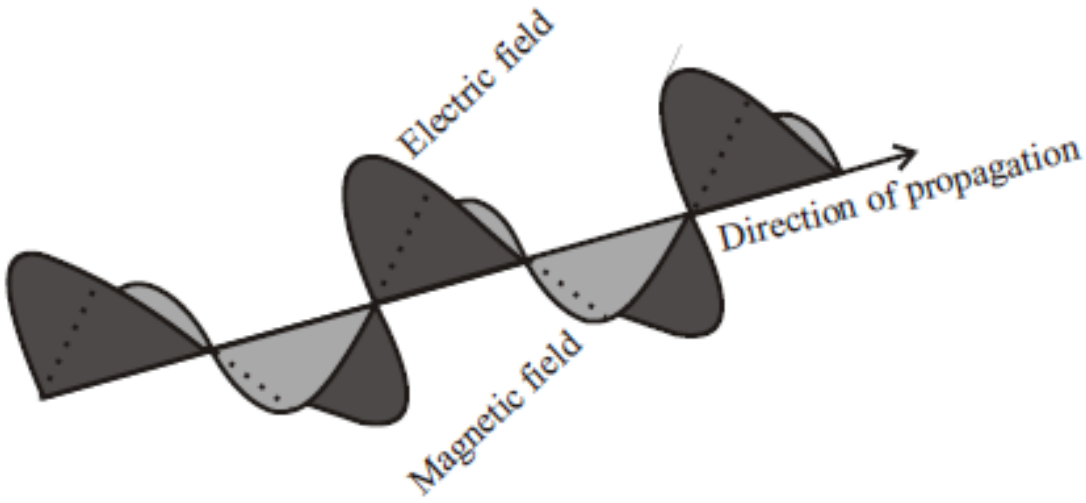


Figure 8 Electromagnetic waves

Electromagnetic waves can transfer energy **without** a medium. Electromagnetic waves are transverse waves that transfer electrical and magnetic energy. An electromagnetic wave consists of vibrating electric and magnetic fields that move through space at the speed of light.

2.2 Producing Electromagnetic (EM) Waves

Electromagnetic waves are produced by charged particles. Every charged particle has an electric field surrounding it. The electric field produces electric forces that can push or pull on other charge particles. When a charged particle moves it produces a Magnetic field .A **magnetic field** can exert magnetic forces that can act on certain materials. When a charged particle changes its motion, its magnetic field changes. The changing magnetic field causes the electric field to change. When one field vibrates, so does the other. The two fields constantly cause each other to change and this produces an **Electromagnetic wave.** For electromagnetic waves, the electric field and magnetic field are always in phase. Their magnitudes are related by E= c B at all times.

Q1: Suppose that the electric field of an electromagnetic wave decreases in magnitude. The magnetic field:

1) decrease 2) increase 3) remains constant

2.2 Characteristic Parameters of Electromagnetic (EM) waves

The electromagnetic waves are characterized by a number of parameters. These are:

Amplitude: This refers to the **maximum height to which the wave oscillates**. It equals the height of the crests or depth of the troughs.

Wavelength: It is the linear **distance between two consecutive wave-crests or**

wave- troughs as shown in Fig 9 . It is represented by a Greek letter lambda λ and is expressed in terms of m, cm, nm or Angstrom (1Å = 10^{-10} m).

Frequency: It is defined as the **number of wave crests or wave troughs that pass through a given point per second**. It is represented by a Greek letter nu (ν) and is expressed in terms of s^{-1}(second inverse or per second). It is also called as Hz (Hertz).

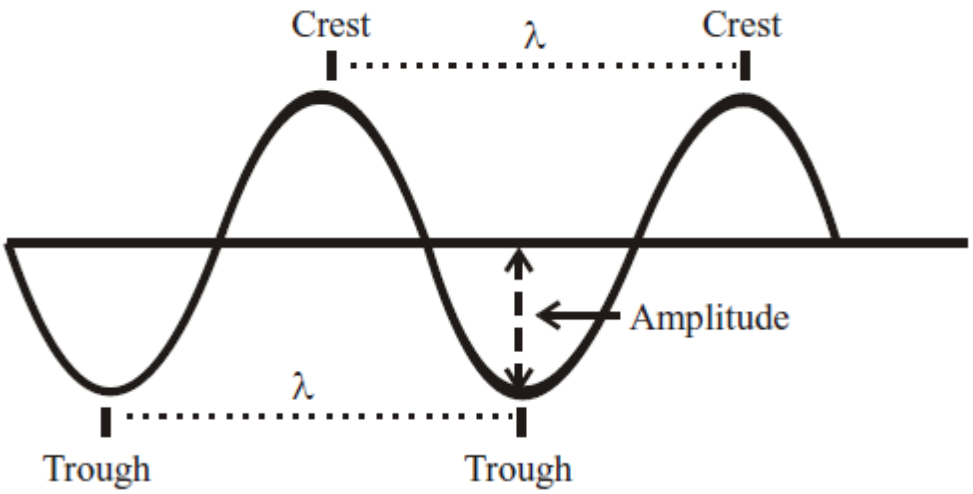


Figure 9. *Characteristics of electromagnetic wave*

Wave number: It equals **the number of waves per unit length**. It is denoted as $\overline{\nu}$ (nu bar) and is equal to the reciprocal of the wavelength. The SI unit of $\overline{\nu}$ is m^{-1} (meter inverse). However, sometimes it is also expressed as cm^{-1} (centimeter inverse).

$$\overline{v} = \frac{1}{\lambda}$$

Velocity: it is defined as the linear **distance travelled by the wave in one second**.

The velocity in meters per second can be obtained by multiplying frequency in Hertz (s^{-1}) with wavelength in meters.

$$c = \nu\lambda \qquad \text{or} \qquad \nu = \frac{c}{\lambda}$$

- Maxwell determined theoretically that EM waves propagate through a vacuum at a speed given by

$$c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}}$$

e_0: electric permittivity of free space

m_0: magnetic permeability of free space

$$c = \frac{1}{\sqrt{\varepsilon_0 \mu_0}} = \frac{1}{\sqrt{\left(8.85\times10^{-12}\ \mathrm{C^2/Nm^2}\right)\left(4\pi\times10^{-7}\ \mathrm{Ns^2/C^2}\right)}} = 3.00\times10^{8}\ \mathrm{m/s}$$

This value is essentially identical to the speed of light measured by Foucault in 1860!

The velocity of a radiation depends on the medium. In vacuum the velocity is equal to 3.00 x 10^8 m s^{-1}. This speed is called the **speed of light.** At this speed, light from the sun takes about 8 minutes to travel to the Earth (150 million km).

2.3 Propagation of EM waves

As shown in figure 8 the following points should be recognized during propagation of EM waves:

- E and B fields are perpendicular to each other.

- Both fields are perpendicular to the direction of propagation.
- EM waves are transverse wave.
- Electric field and magnetic field are always in phase.
- E &B increase and decrease at same times.
- Changing B field creates E field. $E=cB$
- Changing E field creates B field
- B field is always much smaller than E field in EM waves.

2.4 Energy in electromagnetic (EM) waves

- EM waves carry energy as the electric and magnetic fields have energy stored with them
- Energy densities:

$$u_E = \frac{1}{2}\varepsilon_0 E^2 \qquad u_B = \frac{1}{2}\frac{B^2}{\mu_0}$$

- For EM wave:

$$u_B = \frac{1}{2}\frac{B^2}{\mu_0} = \frac{1}{2}\frac{(E/c)^2}{\mu_0} = \frac{1}{2}\frac{E^2}{c^2\mu_0} = \frac{E^2}{2\mu_0}\left(\sqrt{\varepsilon_0\mu_0}\right)^2 = \frac{1}{2}\varepsilon_0 E^2 = u_E$$

- Total energy density in EM wave:

$$u = u_E + u_B = \varepsilon_0 E^2 = \frac{B^2}{\mu_0}$$

The energy is equally shared by the two fields in a given volume.

The energy transported through a unit area per unit time is called the ***intensity***.

2.5 Models of Electromagnetic radiation

Two models are used to explain the properties of electromagnetic radiation, ***wave model and particle model***. Many properties of electromagnetic radiation can be explained by a wave model. Some properties are best explained by a particle model as described below. Both a wave model and a particle model are needed to explain all of the properties light. The electromagnetic radiations show the characteristics of particles. These are called as ***quanta***. These quanta are actually ***bundles of energy***. A quantum of visible light is called a ***photon***. The energy of the quantum (or photon) is proportional to the frequency of the radiation. The two are related as

$$\mathbf{E = } \boldsymbol{h\nu}$$

The energy of the quantum can also be related to the wavelength or wave number as

$$E = h\frac{c}{\lambda} \text{ or } E = hc\overline{\nu}$$

the energy of photon can be readily calculated from these equations if we know the frequency, wavelength or wave number.

Q_2. A microwave radiation has a frequency of 12 gigahertz. Calculate the energy of the photon corresponding to this radiation. (h = 6.626 $\times 10^{-34}$ J s and 1 gigahertz = 10^9 Hz.).

Q_3. The green light has a wavelength of 535 nm. Calculate the energy of a photon of green light.

Photoelectric effect - electrons and light.

At the end of the 19th century scientist noted that when some ***metals*** are ***illuminated*** by a strong source of ***light***, ***electrons*** are ***emitted*** from the surface of the metal. This is called the ***photoelectric effect*** and the ***electrons*** are called ***photoelectrons*** to show how were created (although they are no different from normal electrons). But the scientists were confused. The ***kinetic energy*** of the ejected ***photoelectrons*** was found to depend on the ***frequency*** of ***light*** and the ***type*** of ***metal*** used and not, as expected, on the ***brightness*** of the ***light*** source. Intuitively we imagine that ***increasing*** the ***amplitude*** of the ***incident waves*** would cause the ***kinetic energy*** of the ejected ***photoelectrons*** to ***increase***, in the same way that a large amplitude water wave would impart more kinetic energy to pebbles on a beach. However although the ***amplitude*** of the ***incident light*** had ***no effect*** on the ***kinetic energy*** of the ejected ***photoelectrons***, ***greater kinetic energy*** could be imparted to the ejected ***photoelectrons*** by ***increasing the frequency*** of the ***incident light***!!! This initially made no sense. The figure (10) below shows the results observed.

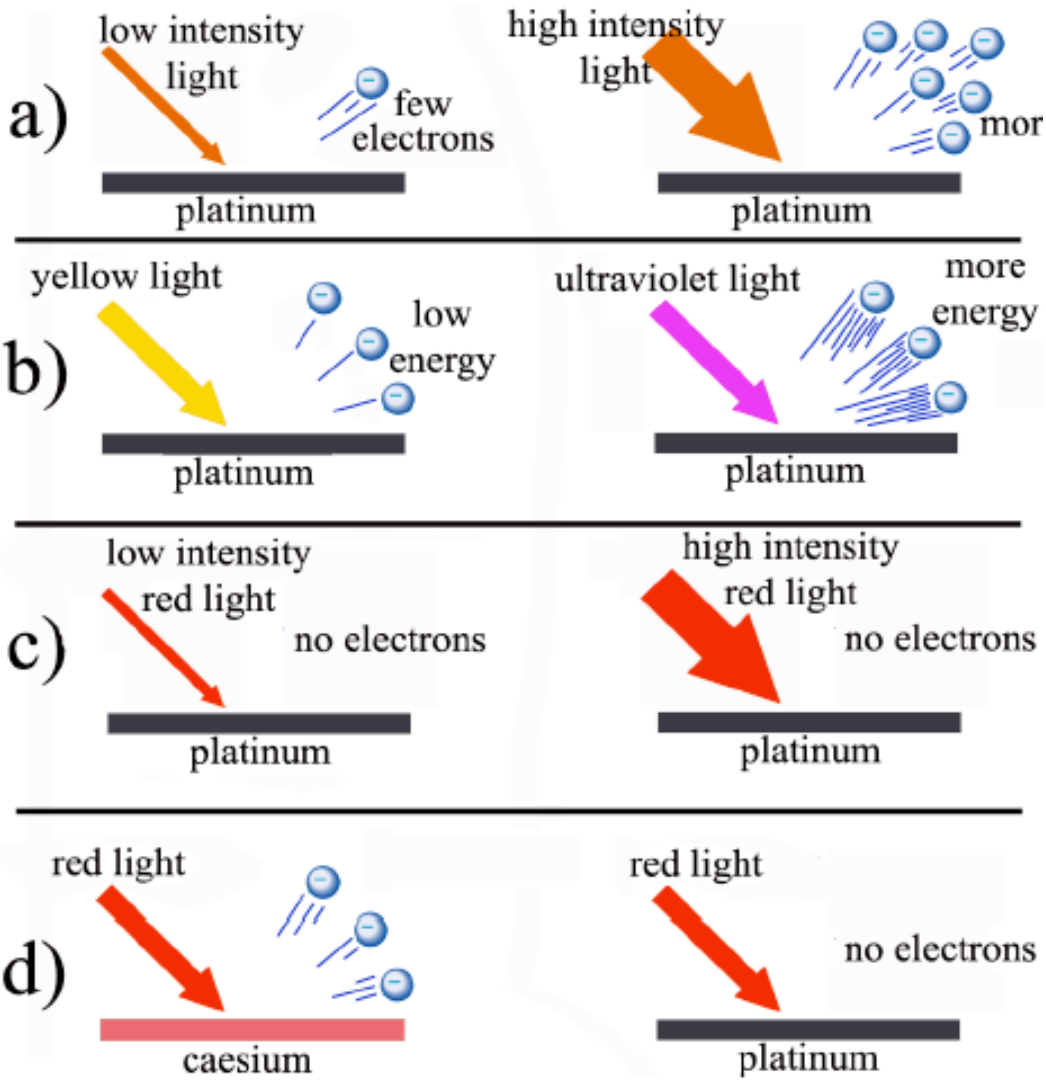


Fig.10 ***Photoelectric effect***

Einstein offered an explanation in 1905 by ***proposing that light was not simply a wave but rather made up of tiny quanta or packets of energy***, the ***energy of a single photon proportional to the frequency of light.***

$$E_{photon} = h\nu$$

where *h* is known as Plank's constant (6.626×10-34Js) and $\nu$is the frequency of the light in Hz.

Einstein proposed that there was a minimum energy E_0 required to release a photoelectron from a metal. He called E_0 the work function and suggested that this value was a constant for a particular metal, but was different for different metals. When a photon is absorbed within a metal, some of the photon's energy will be used up in freeing the photoelectron from the metal, and if there is any energy remaining, then this will appear as kinetic energy of the ejected photoelectron.

$$E_{\text{Kinetic energy}} = h\nu - E_0$$

Key points of the photoelectric effect:-

a) The fact that the number of photoelectrons increases with the intensity of the light is explained by each photon liberating exactly one photoelectron. A higher intensity of light implies that more photons are present and so more photoelectrons are ejected.

b) The fact that the maximum kinetic energy of the photoelectrons depends on the frequency of light is explained because photons corresponding to light of a higher frequency carry more energy. So after E_0 has been used up, there is more energy left over to appear as kinetic energy of the photoelectron.

c) The fact that there is a lower limit for the frequency of light, below which no photoelectrons are emitted is due to the fact that since the minimum energy required to eject an electron is E_0, then the minimum frequency of light needed to do this is $E_0 = h\nu$

d) The fact that for the same light source some metals eject photoelectrons and other do not is due to the different work function E_0 of different metals. Metals, such as caesium, with a lower work function need less of the photon's energy to release a photoelectron and so are more likely to exhibit photoelectron emission.

Example

Imagine a ray of green light of wavelength λ = 530 nm incident on a metal with a work function of 1.1eV. What is the kinetic energy given to a photoelectron ejected from this metal? What is the lowest wavelength of light that can release an electron from this metal?

The frequency of green light is found by

$$c = \lambda \nu$$

where c is the velocity of light, so

$$\nu_{\text{green light}} = \frac{3\times10^{8}}{530\times10^{-9}} = 5.66\times 10^{14}\ \text{HZ}$$

$$E_{\text{green photon}} = h\nu = 6.626\times10^{-34}\times 5.66\times 10^{14} = 3.54\times 10^{-19}\ \text{J}$$

$$E_{\text{green photon}} = \frac{3.54\times10^{-19}}{1.6\times10^{-19}} = 2.3\ \text{eV}$$

The energy required to release an electron from the metal is 1.1 eV. The remaining energy of 2.3 - 1.1 =1.2 eV is given to the ejected photoelectron in the form of kinetic energy.

The energy requiredto release an electron is 1.1 eV and so the minimum energy is

$E_{photon} = 1.1$ eV

Therefore the lowest frequency is

$$\nu_{lowest} = \frac{E}{h} = \frac{1.1\times1.6\times10^{-19}}{6.626\times10^{-34}} = 2.81\times 10^{-14}\ \text{HZ}$$

$$\lambda_{lowest} = \frac{3\times10^{8}}{2.81\times10^{-14}} = 1.067\ \mu\text{m}$$

The Compton Effect – particle nature of light:-

Compton Effect was discovered by Arthur Holly Compton in 1923 and for this discovery he was awarded by the Nobel Prize in Physics in 1927. He studied the scattering of x-rays of known frequency from graphite and looked at the recoil electrons and the scattered x-rays (Fig.11). When a scattering of a ***high energy photon*** by a free charged particle (usually a loosely bound outer-shell electron in target material) an increase in wavelength between scattered and initial photon was observed, this is called Compton Effect. It is also known as **Compton Scattering.**

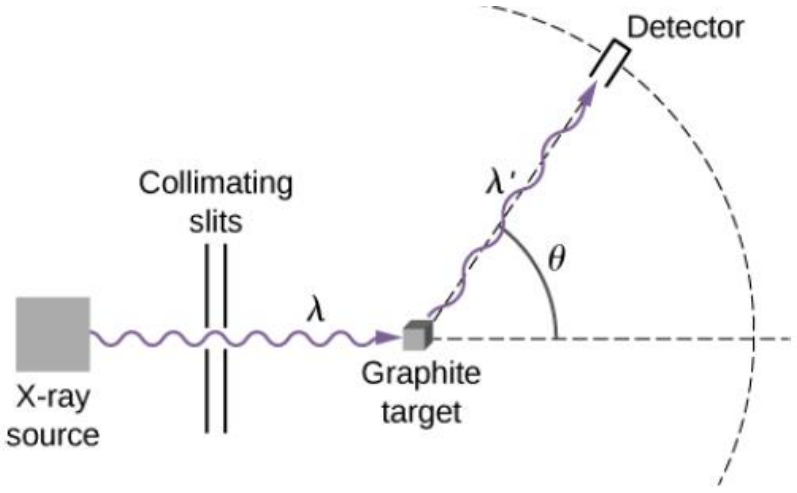


Fig.11. *Experimental of the Compton Effect*

The difference between wavelengths of initial photon and scattered photon is known as ***Compton Shift.*** The Compton Effect is an ***incoherent and inelastic scattering*** of a photon by an ***elastic collision*** with electron in which both ***relativistic energy and momentum*** are conserved. Here both photon and electron treated as *relativistic particles.*

Mathematical description of Compton Effect

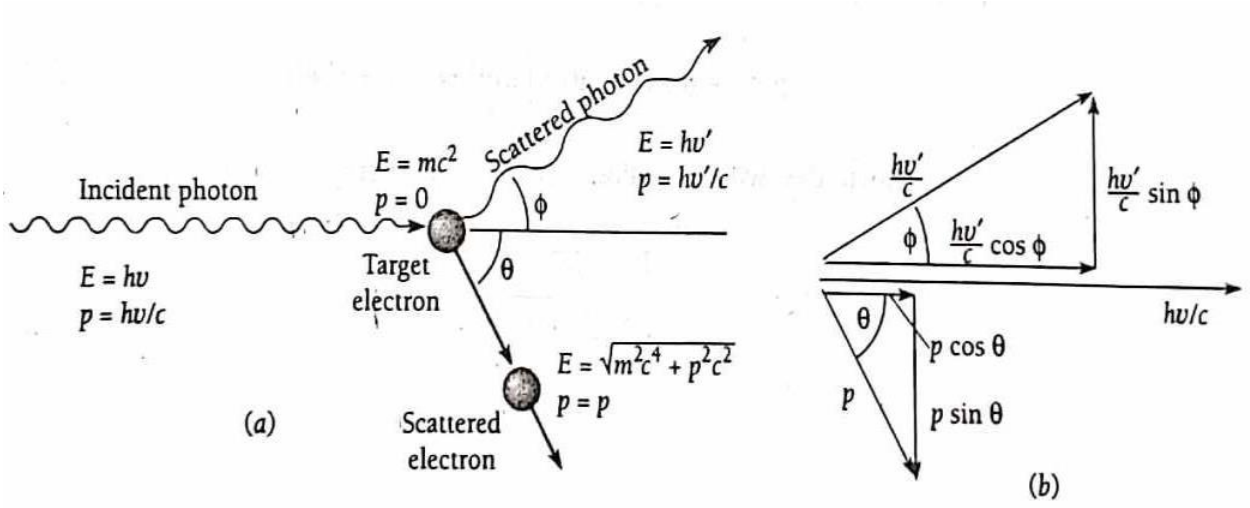


Fig.12. a) Energy and momentum are conserved b) vector diagram of the scattered photon and electron momenta.

The above figures 12 represents collision two particle: an x-ray photon (zero rest mass) and an electron (rest mass m and initially at rest). After this striking the scattered away with an angle ϕ from its original direction while the electron receives an impulse and begins to move with a speed v by making an angle ɵ with direction of incident photon . It is consider that the photon transfer some energy to

the electron. Due to energy loss, the frequency of the incident photon υ changes to a lower value υ′.

Loss in photon energy = Kinetic Energy (KE) gain by **recoil electron**

hυ−**h**υ′=**KE [h** is planck constant**]**

Momentum of a massless particle (here 'photon') is given by Theory of Relativity as: **Photon momentum=(hυ)/c** [**c** is speed of light in vacuum and υ is frequency of photon]

Momentum is a vector quantity so in this **two-body** collision momentum must be conserved in each of two mutually perpendicular directions. Now momentum of incident photon is **h**υ**⁄c** and scattered photon is **h**υ′**⁄c.** The initial and final momentum of electron is **0** and **p.**

Along direction of incident photon, the conservation of momentum gives:

Total initial momentum = Total final momentum

$$\mathbf{h\upsilon c + 0 = h\upsilon' c cos\phi + p\, cos\theta \ldots\ldots (1)}$$

Along perpendicular to the direction of incident photon, the conservation of momentum gives:

$$\mathbf{0 = h\upsilon' c sin\phi - p\, sin\theta \ldots.. (2)}$$

Multiply equations 1 and 2 by **c** we get:

$$\mathbf{pc\, cos\theta = h\upsilon - h\upsilon' cos\phi \ldots\ldots\ldots (3)}$$

$$\mathbf{pc\, sin\theta = h\upsilon' sin\phi \ldots\ldots\ldots (4)}$$

By squaring eqn. 3 and 4 and then adding them we get:

$$\boldsymbol{p^2c^2 = (h\upsilon) - 2(h\upsilon)\,(\,\upsilon')\,cos\phi + (h\upsilon')^2 \ldots\ldots\ldots (5)}$$

From the Theory of Relativity, the total energy of **recoil electron** is given by the equations:

Total Energy = KE + Rest Mass Energy

$$\mathbf{E = KE + mc^2 \ldots\ldots\ldots (6)}$$

$$\boldsymbol{E^2 = m^2c^4 + p^2c^2} \ldots\ldots\ldots\ldots (7)$$

From equation **6** an**7** it can written that,

$$\mathbf{(KE + mc^2)^2 = m^2c^4 + p^2c^2}$$

$$\mathbf{(KE)^2 + 2\,mc^2\,KE = p^2c^2 \ldots\ldots\ldots (8)}$$

Now, substituting the value **KE**=(**h**υ−**h**υ′) in equation **8** we get

$$\mathbf{p^2c^2 = (h\upsilon)^2 - 2\,(h\upsilon)\,(\,\upsilon') + (h\upsilon')^2 + 2\,mc^2\,(h\upsilon - h\upsilon') \ldots\ldots\ldots (9)}$$

Substituting the value of $\boldsymbol{p^2c^2}$ from equation **5** into **9** we finally obtain

$$\mathbf{2\,mc^2\,(h\upsilon - h\upsilon') = 2\,(h\upsilon)\,(\,\upsilon')\,(1 - cos\phi) \ldots\ldots\ldots (10)}$$

Dividing the eq. **10** by ($\mathbf{2h^2c^2}$) we obtain

$$\frac{mc}{h}\left(\frac{\upsilon}{c} - \frac{\upsilon'}{c}\right) = \frac{\upsilon}{c}\,\frac{\upsilon'}{c}\,(1 - \cos\phi) \quad \ldots$$

(11)

Now from definition of wavelength we have: $\upsilon/\boldsymbol{c} = \boldsymbol{1/\lambda}$ and $\upsilon'/\boldsymbol{c} = \boldsymbol{1/\lambda'}$ and then eq. **11** becomes

$$\frac{mc}{h}\left(\frac{1}{\lambda}-\frac{1}{\lambda'}\right)=\frac{1-\cos\phi}{\lambda\,\lambda'}$$

$$\lambda-\lambda'=\frac{h}{mc}(1-\cos\phi)$$

$$\Delta\lambda=\lambda_c\,(1-\cos\phi) \quad \ldots\ldots\ldots (12)$$

This eq. **12** was derived By A. H. Compton and it describes the phenomenon known as Compton Effect. The term $\Delta\lambda$ gives the change in photon wavelength due Scattering with a free electron and it is called **Compton Shift.**

➢ From eq. 12 it is clear that the **Compton Shift is independent of the wavelength of the incident photon and depend on scattering angle.**

➢ The term $\lambda_c = \frac{h}{m_c}$ is called **Compton Wavelength** of the **scattering particle (Here electron).**

➢ For an electron λ_c = **2.426**×10^{-12} m = **2.426** pm (10^{-12} m = 1 pm)

➢ Eq. **12** gives that Compton Shift becomes **maximum** for $\phi = 180^0$ and then

$$\Delta\lambda_{max} = 2\lambda_c$$

The maximum change in wavelength is (for scattering from an electron)

$$= 4.86\times10^{-12}\ \text{m}$$

This value would be **insignificant for visible light ($\lambda\sim 10^{-7}$ m)** but this wavelength shift is **significant for x-ray ($\lambda\sim 10^{-10}$ m).**

Numerical Problem: From

Q.1) X-rays of wavelength 10.0 pm are scattered from a target. (a) Find the wavelength of x-rays scattered through 45^0. (b) Find the maximum wavelength present in the scattered x-rays. (c) Find the maximum kinetic energy of the recoil electrons.

Solution: (a) From the expression of Compton shift we can write: $\Delta\lambda = \lambda_c\ (1 - \cos\phi)$ where, λ and λ' are wavelengths of incident and scattered x-ray respectively and ϕ is scattering angle.

λ_c = Compton wavelength of recoil electron = 2.426 pm and given that, $\phi = 45^0$; λ = 10.0 pm

$\lambda' = \lambda + \lambda_c\ (1 - \cos\phi) = [10.0 + 2.426\ (1 - \cos 45^0)]$ pm = = $[10.0 + 2.426\ (1 - 0.707)]$ pm

$\lambda' = [10.0 + (2.426 \times 0.293)]$ pm = 10.71 pm

(b) Maximum wavelength of scattered x-ray = $\lambda'_{max} = \lambda + \Delta\lambda_{max} = \lambda + 2\ \lambda_c = [10.0 + (2 \times 2.426)]$ pm = 14.9 pm

(c) From the of kinetic energy of recoil electron KE = hc $(\frac{1}{\lambda} - \frac{1}{\lambda'})$ it clear that KE is becomes maximum for maximum λ'. Here h is Planck constant and c is speed of light in vacuum. From (b) we have λ'_{max} = 14.9 pm

Therefore, $KE_{max} = (6.62 \times 10^{-34})$ J-s (3×10^8) ms^{-1} $[\frac{1}{10\ pm} - \frac{1}{14.9\ pm}]$

$$KE_{max} = (6.62 \times 10^{-34}) \text{ J-s } (3 \times 10^8) \text{ ms}^{-1} \left[\frac{1}{10\ m} - \frac{1}{14.9\ m}\right] \times 10^{12} = 6.54 \times 10^{-15} \text{ Joule} = 40.8 \text{ keV}$$

[1 Joule = 1.6×10^{-19} eV]

Q. 2) At what scattering angle will incident 100 keV x-rays leave a target with an energy of 90 keV.

Solution: The energy of incident x-ray E = 100 keV= 1.6×10^{-14} Joule and that of scattered x-ray

$E' = 90$ keV = 1.44×10^{-14} Joule. Let us consider that the scattering angle = ϕ

Wavelength of incident x-ray $\lambda = \frac{hc}{E}$, here h is Planck constant and c is speed of light in vacuum.

$\lambda = [(6.626 \times 10^{-34}$ J-s) $(3 \times 10^8$ m)] /(1.6×10^{-14}) J = 12.42×10^{-12} m = **12.42 pm** [10^{-12} m = 1 pm]

Similarly, wavelength of incident x-ray λ' = [$(6.626 \times 10^{-34}$ J-s) $(3 \times 10^8$ m)] /(1.44×10^{-14}) J = **13.8 pm**

From the expression of Compton shift we can write: $\Delta\lambda = \lambda_c\ (1 - \cos\phi)$

λ_c = Compton wavelength of recoil electron = 2.426 pm

Here $\Delta\lambda = (\lambda' - \lambda) = (13.8 - 12.42)$ pm = 1.38 pm

$(1 - \cos\phi) = \Delta\lambda\ /\ \lambda_c = {}^{(1.38\ pm}/_{2.426\ pm}) = 0.56$

$\cos\phi = (1 - 0.5688) = 0.4311 = \cos 64^0$ ⟹ **$\phi = 64^0$**

2.6 Electromagnetic Spectrum

Depending on their characteristics (wavelength, frequency and wave number) electromagnetic radiations are of many types and constitute what is called as an electromagnetic spectrum (Fig. 10). The part of the spectrum that we can see is called visible spectrum and is a very small part of the overall spectrum.

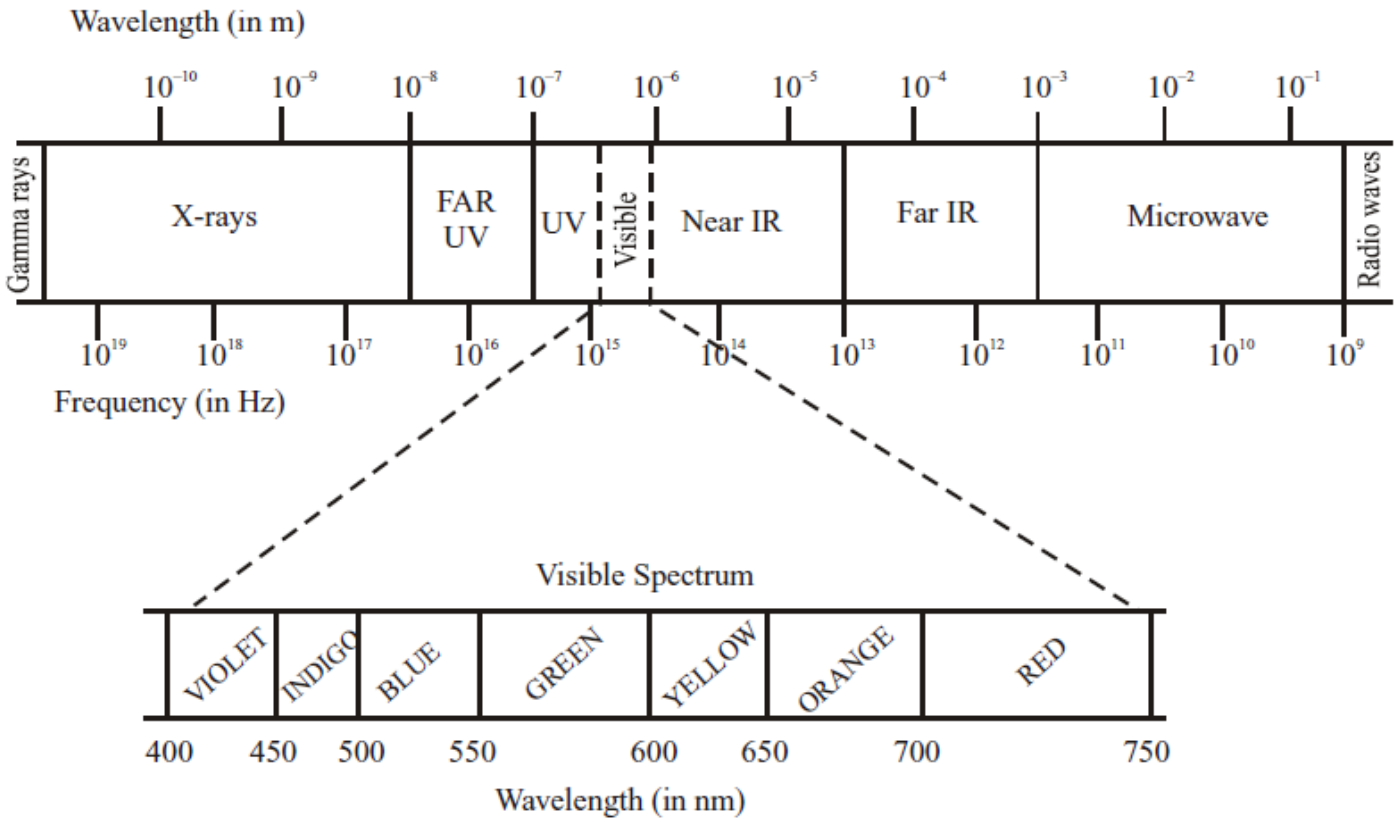


Fig. 13: *The electromagnetic spectrum*

Wave Particle Duality

As you are aware that some of the properties of light e.g., diffraction and interference can be explained on the basis of its wave nature. On the other hand

some other properties like photoelectric effect and scattering of light can be explained only on the basis of particle nature of light. Thus light has a dual nature possessing the properties of both a wave and a particle, i.e., light could under some conditions behave like a particle and other conditions behave as a wave.

In 1923 a young French physicist, Louis de Broglie, argued that if light can show wave as well as particle nature, why should particles of matter (e.g., electron) not possess wave like characteristics? He proposed that matter particles should indeed have a wave nature and said that a particle of mass *m* moving with a velocity *v* has an associated wavelength, λ (some times called *de Broglie wavelength)* given by the formula;

$$\lambda = \frac{h}{mv} \qquad \text{or} \qquad \lambda = \frac{h}{p}$$

Where (p = *mv*) is the momentum of the particle. The de Broglie wavelength of a body is inversely proportional to its momentum. Since the magnitude of *h* is very small, the wavelength of the objects of our everyday world would be too small to be observed. Let us make a calculation to see this.

Example: Calculate the de Broglie wavelength associated with a cricket ball weighing 380 g thrown at a speed of 140 km per hour?

Solution: Mass of the cricket ball = 380 g = 380 $\times 10^{-3}$ kg = 0.38 kg

Speed or Velocity = 140 km/hr = (140 $\times$1000)/3600

$= 38.89 \text{ m s}^{-1}$

The wavelength associated with the cricket ball will be

$$\lambda = \frac{h}{mv} = \frac{6.626 \times 10^{-34} \text{ JS}}{(0.380kg)\,(38.89\text{m s}^{-1})}$$

$$= 4.48 \times 10^{-35} \text{ m} \quad (\text{J} = \text{kg m}^2 \text{ s}^{-2})$$

Exercise:

A 2 g bullet is moving at the velocity of 3×10^2 m s^{-1}. Calculate the wavelength of the material wave associated with this bullet?

Heisenberg's Uncertainty Principle

An important consequence of the wave-particle duality of matter and radiation was discovered by Werner Heisenberg in 1927 and is called the **uncertainty principle**. According to this principle it is not possible to simultaneously measure both the ***position*** and ***momentum (or velocity)*** of an electron accurately. In simple words we may state that more accurately you measure a particle's position, the less accurately you're able to measure its momentum, and vice versa. Mathematically, the Heisenberg principle can be expressed in terms of an inequality.

$$\Delta x \Delta p = h$$

Where Δx and Δp are the uncertainties in the measurements of position and momentum respectively. If the position of an object is known exactly (i.e., $\Delta x = 0$), then the uncertainty in the momentum must be infinite, meaning that we cannot say

anything about the velocity. Similarly, if the velocity is known exactly, then the position would be entirely uncertain and the particle could be anywhere. It means that we cannot say anything about the position of the particle. In actual practice none of the two properties can be measured with certainty. Due to the small value of the Planck's constant , *h* (6.626 x 10^{-34} J s) this principle is not relevant while making measurements of large objects like car, bus or aeroplane etc.. It is relevant, only when you are making measurements on very small objects such as electrons.

Exercise:

Suppose you want to determine the position of an electron to a precision of about 5 x 10^{-12} m. Estimate the uncertainty of velocity under this condition?

Chapter three

Atomic spectra and Bohr's Model

Atomic spectrum

You know that when we pass a beam of sunlight through a prism we get a range of colours from violet to red (VIBGYOR) in the form of a spectrum (like rainbow). This is called a ***continuous spectrum*** because the wavelengths of the light varies continuously that is without any break (Fig. 14).

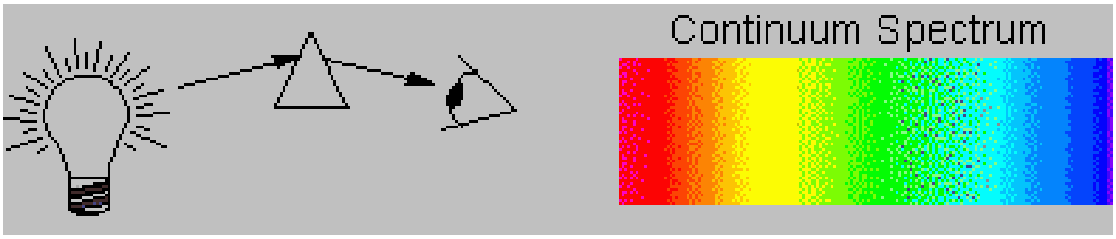


Fig. 14. ***continuous spectrum***

If a metal or one of its compounds is heated in the flame of a burner, a color characteristic of the metal appears. This is the well-known **flame reaction**. If the colored light is separated by means of a prism, a few strong line spectra are observed, and the wavelength of each line is characteristic of the metal involved. For instance, the yellow flame reaction of Na corresponds to two yellow lines of its spectrum in the visible region, and the wavelengths of these two lines are 5.890 x 10^{-7} m and 5.896 x 10^{-7} m, respectively. If a gas is sealed in a high vacuum tube, and a high voltage is applied, the gas discharges and emits light. Separation of this light by means of a prism will give a series of discontinuous line spectra. Since the wavelengths of this light are characteristic of the atom, the spectrum is called its ***atomic spectrum.***

Atomic spectrum is a spectrum that has been shined through or originates from a material (usually a gas) and contains patterns that are characteristic of the elements present in the material.

Kinds of atomic spectra:

Emission spectra: an atomic gas is excited, usually by an electric current, and emits radiation of specific wavelengths.

Absorption spectra: an atomic gas absorbs radiation of specific wavelengths. Of course, molecules can have emission and absorption spectra too. For example, if we put a high voltage current through hydrogen gas, we see light. The light is not a continuous spectrum, but a series of discrete, monoenergetic lines (fig.15).

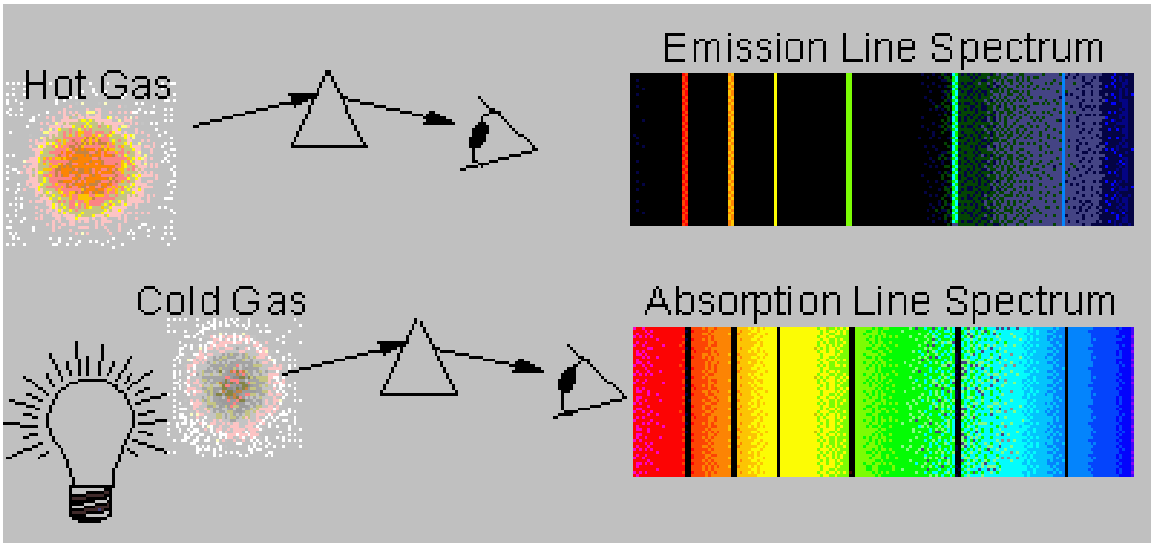


Fig.15 ***Emission and absorption spectrum***

Line Spectrum of Hydrogen Atom

When an electric discharge is passed through a discharge tube containing hydrogen gas at low pressure, it emits some light. When this light is passed through a prism it splits up into a set of five lines. This spectrum is called the ***line spectrum of hydrogen*** (Fig. 16).

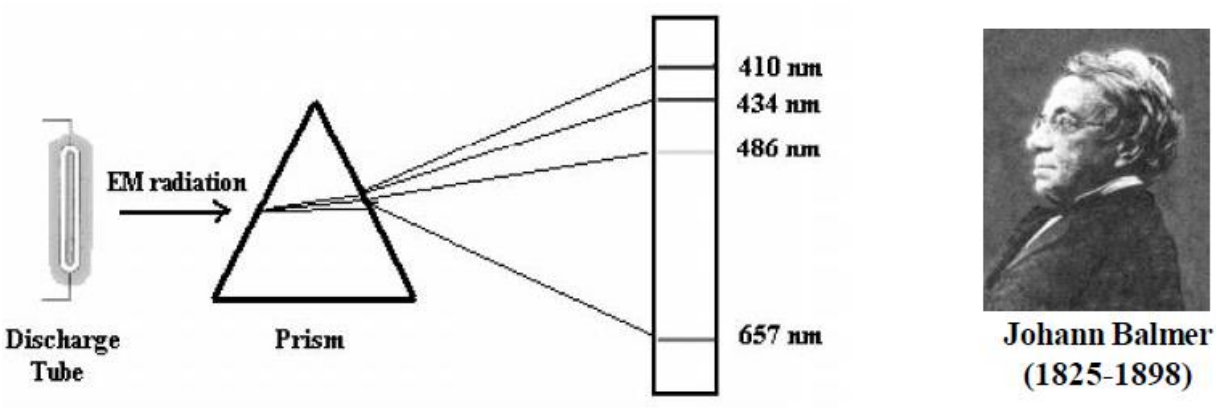


Fig. 16: *A schematic diagram showing line spectrum of hydrogen in the visible range*

On careful analysis of the hydrogen spectrum it was found to consist of a few sets of lines in the ultraviolet, visible and infrared regions. These sets of lines were observed by different scientists. The Swiss physicist Johann Jakob Balmer (1825-1898) separated the light emitted during discharge from low-pressure hydrogen. He realized that the wavelength λ of a series of spectral lines could accurately be expressed by a simple equation (1885). The Swedish physicist Johannes Robert Rydberg (1854-1919) found that the wavenumber ῡ (*The number of waves contained in a unit length*) of a spectral line could be expressed by an equation as indicated below (1889).

$$\bar{v} = \frac{1}{\lambda} = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \text{ cm}^{-1} \; ; \; R_H = 109677 \text{ cm}^{-1}$$

Where n1 and n2 are positive integers (n1 < n2) and RH is called Rydberg's constant. The different sets of lines observed in the hydrogen atom spectrum, their discoverers and the values of n1 and n2 are given in the following Table.

Table: Summary of the emission lines observed in hydrogen spectrum

Series	n_1	n_2	Region of spectrum
Lyman	1	2,3,4…..	Ultraviolet
Balmer	2	3,4,5…..	Visible
Paschen	3	4,5,6…..	Infrared
Bracket	4	5,6,7…..	Infrared
Pfund	5	6,7,8…..	Infrared

The line spectrum of hydrogen atom was explained by Bohr's model, which is discussed below.

Bohr's Model

In 1913, Niels Bohr (1885-1962) proposed another model of the atom where electrons move around the nucleus in circular paths. Bohr's atomic model is built upon a set of postulates, which are as follows :

1. The electrons move in a definite circular paths around the nucleus (Fig 3.10). He called these circular paths as **orbits** and postulated that ***as long as the electron is in a given orbit its energy does not change*** (or energy remains

fixed). These orbits were therefore referred to as **stationary orbits** or **stationary states** or **non radiating orbits.**

2. The ***electron can change its orbit by absorbing or releasing energy***. An electron at a lower (initial) state of energy, E_i can go to a (final) higher state of energy, E_f by absorbing (Fig 17) a single photon of energy given by

$$E = h\nu = E_f - E_i$$

Similarly, when electron changes its orbit from a higher initial state of energy E_i to a lower final state of energy E_f , a single photon of energy hν is released.

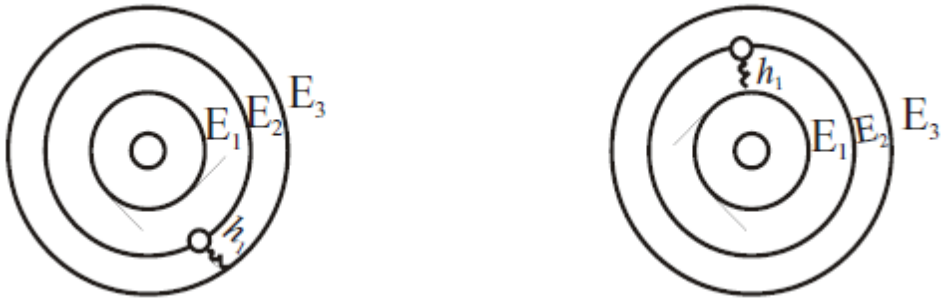


Fig. 17: *Absorption and emission of photon causes the electron to change its energy level.*

3. The **angular momentum of an electron** of mass m_e moving in a circular orbit of radius r and velocity v is an integral multiple of $h/2\pi$.

$$m_e v r = \frac{nh}{2\pi}$$

where n is a positive integer, known as the **principal quantum number**.

SIZES OF ALLOWED ORBITS (orbit radius determination):

Classically, for an orbiting electron (mass m, charge $-e$ and speed v), the centripetal force is balanced by the electric (Coulomb) force:

$$\frac{mv^2}{r} = \frac{Ze^2}{4\pi\varepsilon_0 r^2}$$

For hydrogen, $Z = 1$, so:

$$\frac{mv^2}{r} = \frac{e^2}{4\pi\varepsilon_0 r^2}$$

$$\frac{mv^2}{r} = \frac{m^2v^2r^2}{mr^3} = \frac{n^2h^2}{4\pi^2mr^3}$$

$$\frac{n^2h^2}{4\pi^2mr^3} = \frac{e^2}{4\pi\varepsilon_0 r^2}$$

The orbit radius

$$r = n^2\left(\frac{\varepsilon_0 h^2}{\pi m e^2}\right) = n^2 a_0$$

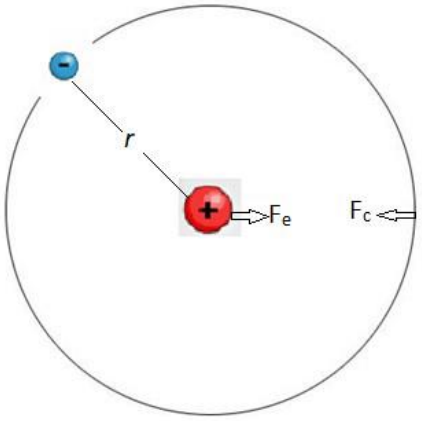
a_0 is called the **Bohr radius** - radius of the innermost ($n = 1$) orbit of the hydrogen atom. $a_0 = \varepsilon_0 h^2/(\pi m e^2) = 5.29\times10^{-11}$ m = 0.529 Å.

ENERGIES OF ALLOWED ORBITS

Assume a circular orbit for electrons for convenience, the centripetal force

$$F_c = \frac{mv^2}{r}$$

This force holding the electrons in an orbit of radius r from the nucleus is provided by the centripetal force.



$$F_e = \frac{1}{4\pi\varepsilon_o}\frac{e^2}{r^2}$$

For stable orbits $F_c = F_e$ $\quad \frac{mv^2}{r} = \frac{1}{4\pi\varepsilon_o}\frac{e^2}{r^2}$

The electron velocity v is related to the orbit radius r by the formula

$$v = \frac{e}{\sqrt{4\pi\varepsilon_o mr}}$$

The Kinetic energy of the atomic electron is

$$\mathrm{KE} = \frac{1}{2}mv^2 = \frac{e^2}{8\pi\varepsilon_0 r}$$

Potential (Coulomb) energy is

$$\mathrm{PE} = -\frac{e^2}{4\pi\varepsilon_0 r}$$

PE is **negative** because electron and proton charges are of opposite sign.

Total energy E = PE + KE

$$E = -\frac{e^2}{4\pi\varepsilon_0 r} + \frac{e^2}{8\pi\varepsilon_0 r} = -\frac{e^2}{8\pi\varepsilon_0 r}$$

 The minus sign means energy is **required** to remove the electron

 This energy is called the **binding energy**. If the energy is zero or positive the electron is not bound to the nucleus.

Substituting for *r* gives the energies of other allowed states:

$$E_n = -\frac{1}{n^2}\left(\frac{me^4}{8\varepsilon_0^2 h^2}\right) = -\frac{E_1}{n^2}$$

You may note here that the energies of the Bohr orbits are inversely proportional to the square of the **quantum number** *n*. As *n* increases the value of the energy increases (becomes lesser negative or more positive). It means that as we go farther from the nucleus the energy of the orbit goes on increasing. Experiments show that 13.6 ev energy is needed to remove the electron from the hydrogen atom orbit. Lowest (ground) state of hydrogen: $E1 = -13.6$ eV

Explanation of Line Spectrum of Hydrogen Atom

According to the second postulate, the energy emitted in the transition of a single electron from an initial stationary state of energy E_i to a final stationary state of energy E_f is given as $h\upsilon = E_i - E_f$. Substituting the expressions for energy from we can get the formula given by Rydberg. Thus Bohr's model provides an explanation for the observed line spectrum of hydrogen as summarized in the previous Table. Fig. 17 shows the energy level diagram for hydrogen atom and the transitions responsible for the observed line spectrum

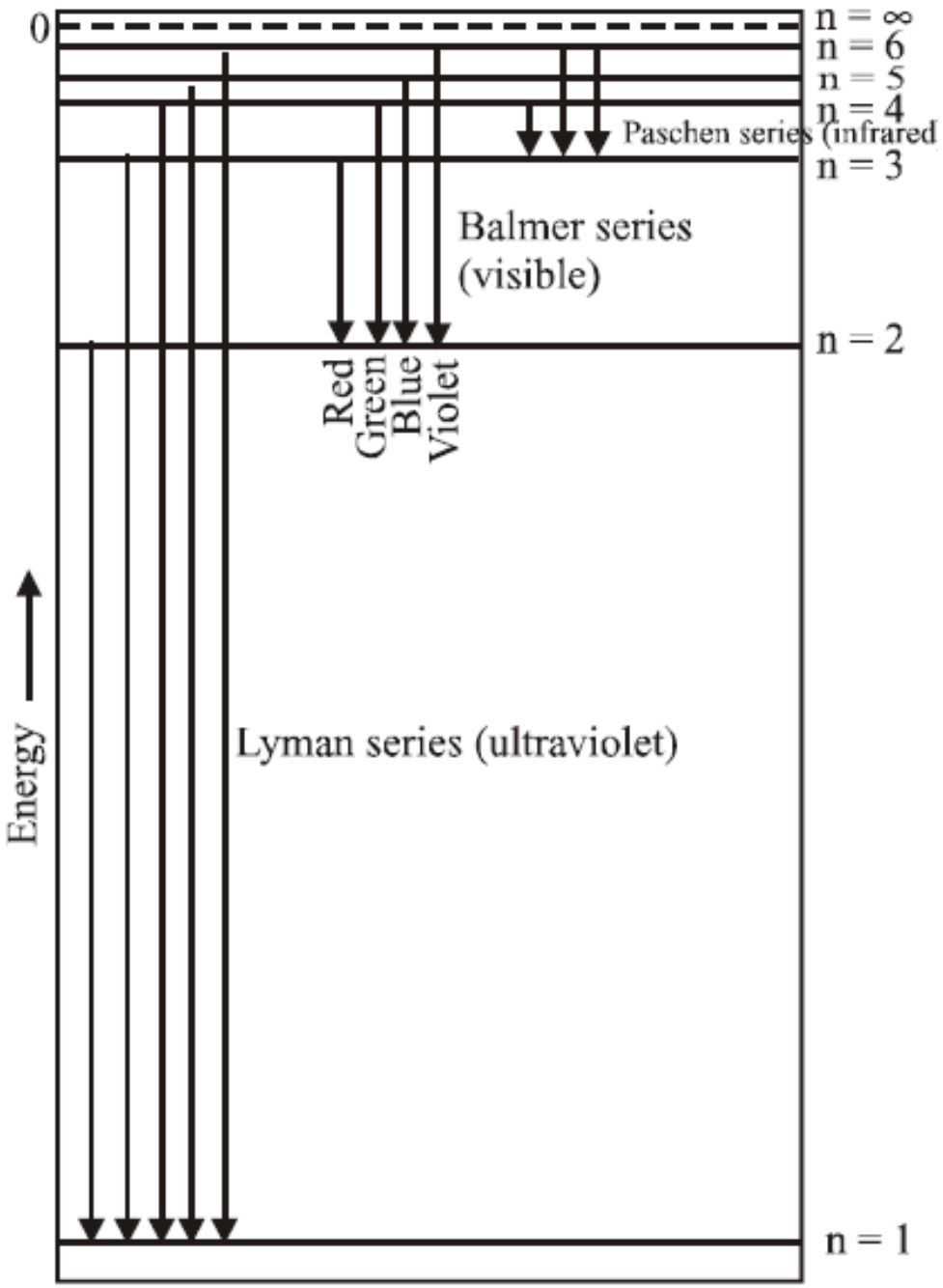


Fig. 17 Energy level diagram for H-atom, showing various transitions responsible for the observed line spectrum

Wave behaviour of electron in the Bohr orbit

An electron in orbit around hydrogen nucleus has wavelength $\lambda=h/mv$ and a velocity as given previously:

$$v = \frac{e}{\sqrt{4\pi \varepsilon_0 mr}}.$$

You can solve these two equations for the wavelength:

$$\lambda = \frac{h}{e}\sqrt{\frac{4\pi \varepsilon_0 r}{m}}.$$

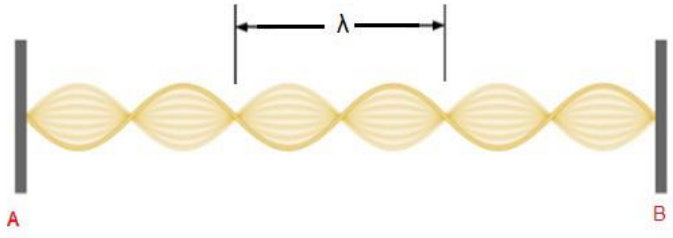
Plugging in the electron mass, $r=5.3\times10^{-11}$ m for the radius of an electron orbit in hydrogen, $e=1.6\times10^{-19}$ C, and $\varepsilon_0=8.85\times10^{-12}$, you get a wavelength $\lambda=33\times10^{-11}$ m, which is the circumference of the electron orbit.

The orbit of the electron in a hydrogen atom corresponds to one complete electron wave joined on itself. The fact that the electron orbit in a hydrogen atom is one electron wavelength in circumference provides the clue needed to construct a theory of the atom.

Using the concept of the electron matter wave, de Broglie provided a rationale for the quantization of the electron's angular momentum in the hydrogen atom, which was postulated in Bohr's quantum theory.

The physical explanation for the first Bohr quantization condition comes naturally when we assume that an electron in a hydrogen atom behaves not like a particle but like a wave.

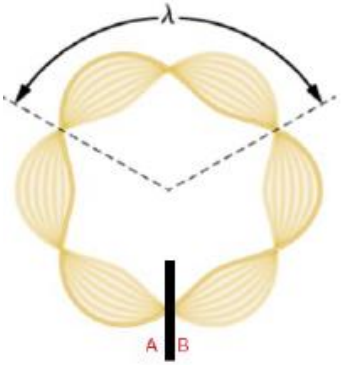
Imagine a stretched string that is clamped at both ends and vibrates in one of its normal modes. If the length of the string is l, the wavelengths of these vibrations cannot be arbitrary but must be such that an integer k number of half-wavelengths fit exactly on the distance l between the ends. This is the condition for a standing wave on a string.



Now suppose we bend its length into a circle and fasten its ends to each other.

This produces a circular string that vibrates in normal modes, satisfying the same standing-wave condition, but the number of half-wavelengths must now be an even number and the length l is now circumference of the circle. This means that the radii in Bohr model are not arbitrary but must satisfy the following standing-wave condition:

$$2\pi r_n = 2n\tfrac{\lambda}{2}.$$



If an electron in the nth Bohr orbit moves as a wave, its wavelength should be equal to

$$\lambda = 2\pi r_n / n.$$

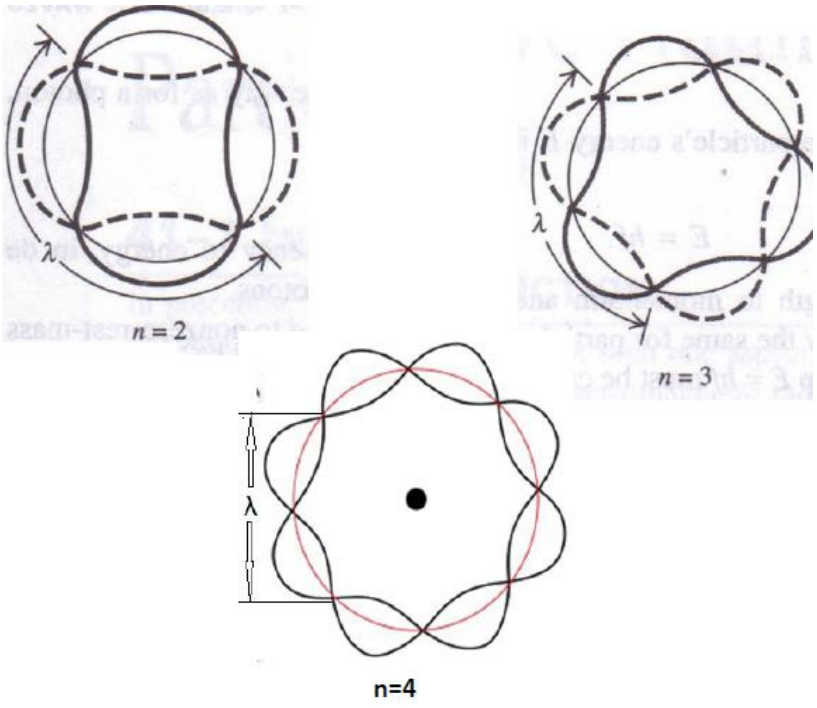
The electron wave of this wavelength corresponds to the electron's linear momentum,

$$p = h/\lambda = nh/\ (2\pi r_n) = n\hbar/r_n.$$

In a circular orbit, therefore, the electron's angular momentum must be

$$L_n = r_n p = r_n \frac{n\hbar}{r_n} = n\hbar.$$

This equation is the first of Bohr's quantization conditions. It provides physical explanation for Bohr's quantization condition. It is a convincing theoretical argument for the existence of matter waves.



Drawbacks of the Bohr's model

Bohr model had several limitations and was replaced by the quantum mechanics model.

- The model stood strong in explaining spectra of lighter atoms similar to hydrogen. It could not explain the spectral lines for heavier atoms.
- The model could not account for hyperfine structures like doublets and triplets.
- As per the Bohr's model, the angular momentum of the electron in the ground state of a hydrogen atom is equal to the reduced Planck constant ($h/2\pi$). The modern quantum theory says it is zero.
- The model didn't stand to the advent of the dual nature (wave particle duality) of the electron.
- The model was in contradiction to the later development of the Heisenberg uncertainty principle that says that the position and momentum of a particle cannot be determined simultaneously. However, Bohr model defined the position (orbits) and momentum of the electron at the same time

Chapter four

Wave Mechanical Model of Atom

Wave Mechanical Model of Atom

Wave Mechanical Model of atom was proposed by Erwin Schrödinger- an Austrian physicist in 1926. This model is basically a formalism or a mathematical recipe, which is based on some postulates that have no foundation in classical physics. The correctness of these postulates can be justified in terms of the correctness of the results predicted by them. According to this Model, the motion of electron inside the atom could be described in terms of a mathematical function called, **wave function**, ψ (Greek letter, psi). The wave functions are assumed to contain all the information about the electron and are obtained by solving a differential equation called Schrödinger wave equation (SWE). The square of the wave function ψ^2 is a measure of the probability of finding an electron in a three dimensional space around the nucleus.

On solving the SWE for hydrogen atom we get a number of wave functions, which are characterized by three quantum numbers.

- ***Principal quantum number, n***
- ***Azimuthal quantum number, l***
- ***Magnetic quantum number, ml***

These quantum numbers arise in the process of logically solving the wave equation. Every electron in an atom has a unique (different) set of quantum numbers which help to describe the three dimensional region where there is

maximum probability of finding the electron. This region is called as ***atomic orbital*** or simply ***orbital***.

Significance of Quantum Numbers

The three quantum numbers describe the size, shape, and orientation of the atomic orbitals in space. There is an additional quantum number which does not follow from the Schrödinger wave equation but is introduced to account for electron spin. The fourth quantum number thus help in designating the electrons present in the atom. Let us understand the significance of each of these quantum numbers.

Principal quantum number, n

The principal quantum number, *n* describes the energy level (or principal shell) of the electron within the atom. *n* can have only positive non zero integral values (i.e., *n* = 1,2,3,4……). This means that in an atom, the electron can have only certain energies. Thus we may say that n quantizes energy of the electron. The principal quantum number also determines the mean distance of the electron from the nucleus, i.e., its size. Greater the value of ***n*** farther is the electron from the nucleus.

Each principal shell can accommodate a maximum of $2n^2$ electrons, i.e.,

n =1 number of electrons : 2

n =2 number of electrons : 8

n =3 number of electrons : 18 and so on…

Azimuthal quantum number, l

The azimuthal quantum number, *l* is related to the geometrical shape of the orbital.

The value of *l* may be zero or a positive integer less than or equal to n–1 (n is the principal quantum number), i.e., *l* = 0,1,2,3…… (n–1). Different values of *l* correspond to different types of **subshells** and each subshell contains orbitals of a given shape.

***l* = 0**, corresponds to **s**-subshell and contains the orbital with **spherical shape** called as ***s* orbital**.

***l* = 1**, corresponds to **p**-subshell and contains the orbitals with a **dumb-bell shape** called as ***p*-orbitals**. There are three p-orbitals in each p-subshell

***l* = 2**, corresponds to **d**-subshell and contains the orbitals with a **cloverleaf shape** called as ***d*-orbitals.**

***l* = 3**, corresponds to **f**-subshell and contain ***f* orbitals.** There are seven *f*-orbitals in each *f*-subshell.

The shapes of s, p and d orbitals will be discussed in the next subsection.

Magnetic quantum number, m_l

The quantum number, m_l, describes the direction or orientation of the orbital in space. The quantum number $\boldsymbol{m_l}$ may have any integral value from – *l* to + *l*. For example, for *l* = 1 ; m_l can have the values as –1,0 and 1.

Magnetic spin quantum number, m_s

The quantum number, m_s, describes the spin of the electron i.e., whether it is clockwise or anticlockwise. The quantum number, m_s does not arise while solving SWE. The clockwise and anticlockwise direction of electron spin has arbitrarily been assigned the values as +1/2 and –1/2 respectively. To sum up, let us take an example of an electron belonging to the third shell (n = 3). This electron can be in an *s*-subshell (l = 0) or a *p*-subshell (l = 1) or a *d*-subshell (l = 2). If it happens to be in a *p*-subshell it may be in any of the three possible *p* orbitals (corresponding to m_l = –1, 0 + 1 directed along *x*, *y* or *z*– axis. And within the orbital it may have clockwise (m_s = + ½) or anti-clockwise (m_s = -½) direction of electron spin. The possible values of different quantum numbers for an electron belonging to the third shell are given in the following Table.

You may note here that the third shell can contain a maximum of 18 electrons and each of them, has a distinct set of four quantum numbers.

The quantum numbers for an electron belonging to the third shell

Principal quantum number, n	Azimuthal quantum number, l	Magnetic quantum number, m_l	Magnetic spin quantum number, m_s
3	0	0	+1/2
			–1/2
	1	–1	+1/2
			–1/2
		0	+1/2
			–1/2
		+1	+1/2
			–1/2
	2	–2	+1/2
			–1/2
		–1	+1/2
			–1/2
		0	+1/2
			–1/2
		+1	+1/2
			–1/2
		+2	+1/2
			–1/2

Difference between orbit and orbital

An **orbit** refers to ***definite circular paths of fixed energy around a central stationary nucleus*** while an **orbital** refers to ***the three dimensional region of space around the nucleus where there is a probability of finding the electron***.

Shapes of Orbitals

We have defined an orbital as "***the three dimensional region of space around the nucleus where there is maximum probability of finding the electron***". Let us try to understand the meaning of an orbital by taking the example of 1*s* orbital (*n* =1; *l* =0). This can be understood in terms of a radial probability curve. Such a curve gives the variation of the probability of finding the electron as a function of distance from the nucleus. For 1s orbital the radial probability curve (Fig. 18 (a)) shows that the probability of finding the electron in 1s orbital increases as we move away from the nucleus and reaches a maximum at a certain distance (= 0.0529 nm or 52.9 pm for hydrogen atom) and then decreases as we go further away from it and at a certain distance it becomes close to zero. The curve shows the radial probability for a given direction.

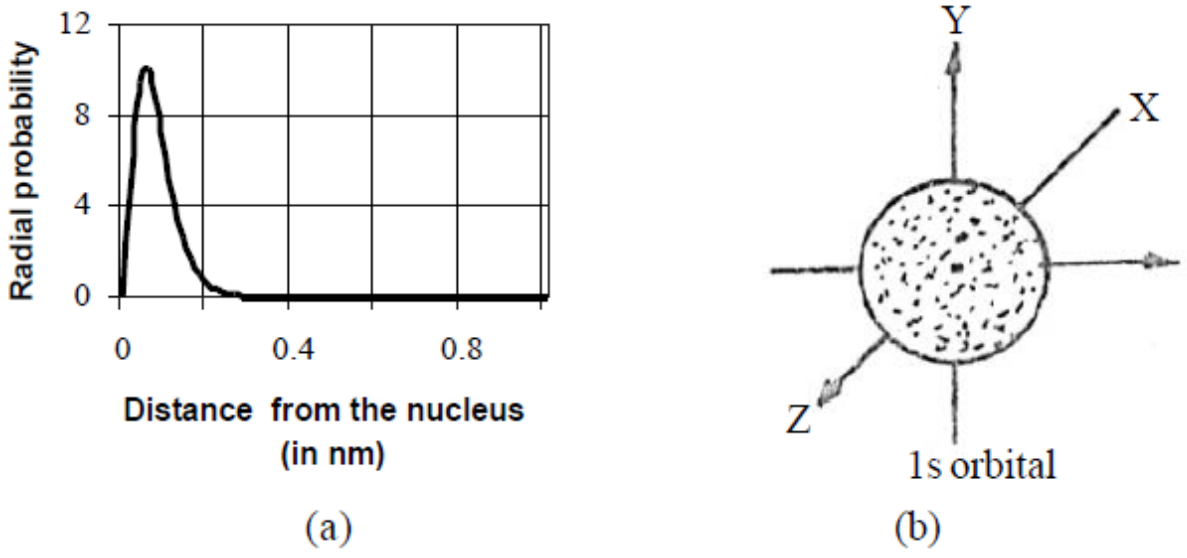


Fig.18: *(a) Radial probability curve for 1s orbital (b) Boundary surface diagram for 1s orbital*

The probability would be same for all possible directions. If we put all such curves together it would give a spherical distribution of the electron probability. Since the radial probability does not become zero at any distance, we cannot specify the size of the sphere. Therefore, the orbital is represented as a boundary surface diagram, which may be thought as a region of space, which contains 95 % of the probability of finding the electron, as indicated in Fig.18(b). Thus the 1s orbital is represented as a sphere.

Similarly, the Fig 19 (a) gives the radial probability curve for a 2s orbital while the Fig 19 (b) shows the boundary surface diagram for the same. You can note two things here. First you may note that for a 2s orbital the boundary surface diagram is bigger as compared to a 1*s* orbital. Secondly, the radial probability curve shows two maxima.

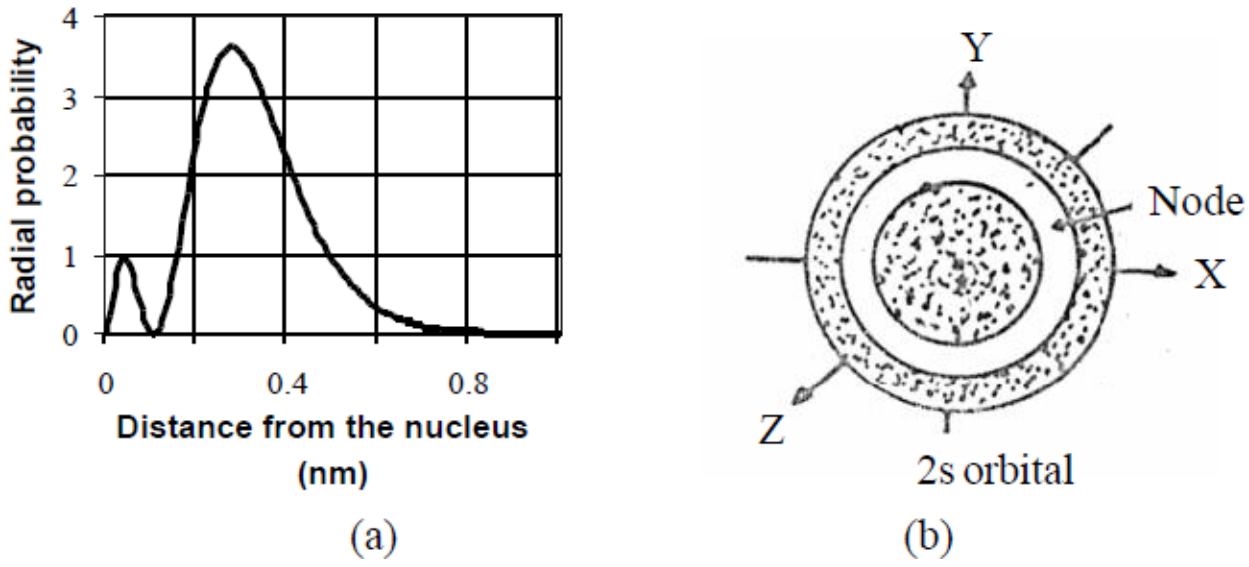


Fig. 19: *(a) Radial probability curve for 2s orbital (b) Boundary surface diagram for 2s orbital*

The probability initially increases, reaches a maxima then it decreases and comes close to zero. It increases again and decreases as we move further away from the nucleus. The region where the probability comes close to zero (before increasing again) is called a ***spherical node***. There are *n*–*l*–1 spherical nodes in an orbital.

A node is a region in space where the probability of finding the electron is close to zero.

p*- orbital:** Now when we draw the shape of a *p* orbital (n =1 ; l =1) we get a shape as shown in the Fig. 20. This picture shows the shape of one of the three possible *p* orbitals which is directed towards the z-axis; pz. You may note that the probability picture for a pz orbital consists of two lobes ; one along the positive z-axis and the other along the negative z-axis. Another important feature of a p-orbital is the absence of the electron probability in the XY- plane. Such a plane is called a ***nodal plane. The shapes of the three p-orbitals are given in Fig.21.

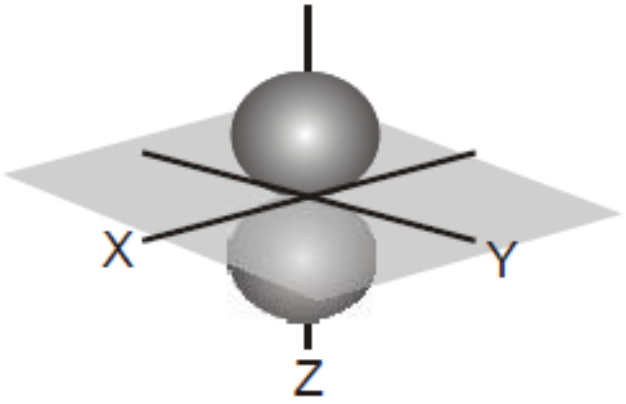


Fig.20 *A p orbital surface diagrams (Shapes)*

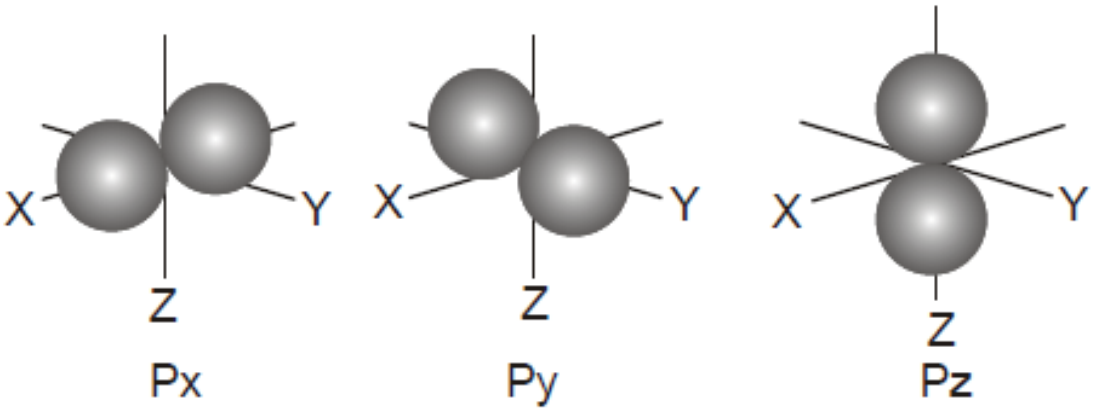


Fig.21 *The boundary showing a nodal plane of the p-orbitals*

The Fig.22 gives the shapes of five possible *d*-orbitals. The d-orbitals also contain nodal planes. The five d- orbitals have different shapes but they all have same energies i.e., these are degenerate.

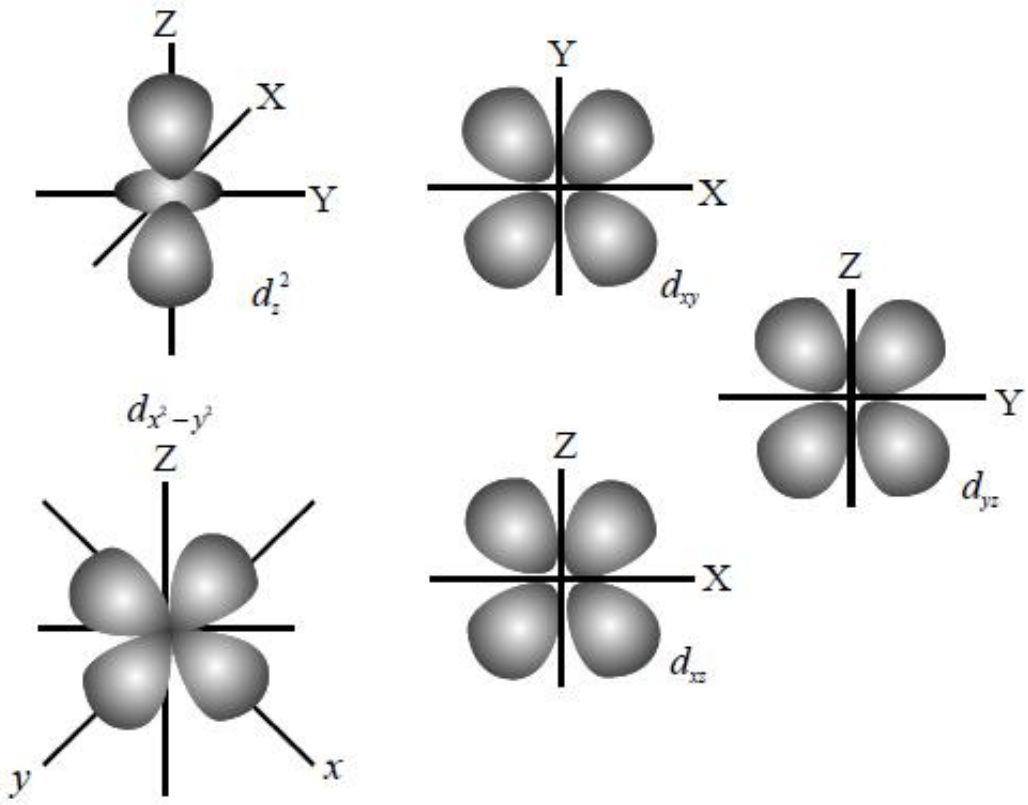


Fig.22 *The boundary surface diagrams (shapes) of the five d-orbitals*

Electronic Configuration of Elements

You have so far learnt that an atom consists of a positively charged nucleus surrounded by electrons present in orbitals of different shapes and sizes. These orbitals are part of different shells and sub-shells and are characterized by the three quantum numbers via. *n*,*l* and *ml*. Let us now take up the distribution of electrons in these shells and sub-shells. Such a distribution of electrons is called **Electronic Configuration** and is governed by three basic rules or principles.

1- Aufbau (or building up) Principle

This principle is concerned with the energy of the atom and states that the electrons should occupy. The electrons occupy the orbitals in such a way that the energy of atom is minimum. In other words **the electrons in an atom are filled in the increasing order of their energies**. Now, how does one know the increasing order of the orbital energies? You have learnt above that the principal quantum number determines the energy of the orbitals. Higher the value of *n* higher the energy. This is true only for hydrogen atom. For other atoms, we need to consider both *n* and *l*. This means that **different sub-shells in a given shell have different energies**. The order of orbital energies can be determined by the following (*n* + *l*) rules.

Rule 1: An orbital with a lower value for (*n* + *l*) has lower energy. For example, the 4*s* orbital (*n* + *l* = 4+0=4) will fill before a 3*d* orbital (*n* + *l* = 3 + 2 =5).

Rule 2: If the value of (n + l) is same for two orbitals then the orbital with lower value of n will be filled first. For example, the 3d orbital (n + l = 3+2=5) will fill before a 4p orbital (n + l = 4 + 1 =5).

Following these rules the increasing order of the orbital energies comes out to be

1*s* < **2*s*** < **2*p*** < **3*s*** < **3*p*** < **4*s*** < **3*d*** < **4*p*** < **5*s*** < **4*d*** < **5*p*** < **6*s***

2- Pauli's Exclusion Principle

This principle concerns the spin of electrons present in an orbital. According to the Pauli's principle, ***no two electrons can have all the four quantum numbers to be same***. For example, if a given electron in an atom has the set of four quantum numbers as n =2, l=1, m_l =1 and m_s = + ½ then no other electron in the atom can have the same set of quantum numbers. As you know that an orbital is characterized by three quantum numbers so the electrons occupying a given orbital would have same values of these three quantum numbers. These electrons are distinguished in terms of their spin quantum number, m_s. Since the spin quantum number can have only two values so ***only two electrons can occupy a given orbital***. In fact this fourth quantum number was introduced through Pauli's principle only.

3- Hund's Rule

This rule concerns the distribution of electrons in a set of orbitals of the same energy, *i.e.* constituents of a subshell. According to this rule if a number of orbitals

of the same subshell are available, then the electrons distribute in such a way that each orbital is first singly occupied with same spin. For example, the six electrons in carbon distribute as

$1s^2\ 2s^2\ 2p^1_x\ 2p^1_y 2p^0_z$ and not as $1s^2\ 2s^2\ 2p^2_x\ 2p^0_y 2p^0_z$

Since electrons repel each other, they remain as far as possible from one another by occupying different orbitals. The rules discussed above can be used to write the electronic configuration of different elements. There are two common ways of representing the electronic configurations. These are

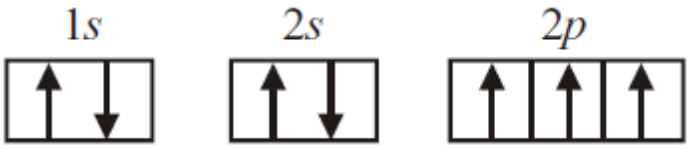
a) **Orbital notation method**:

In this method the filled orbitals are written in the order of increasing energies . The respective electrons in them are indicated as superscripts as shown in the example given below. For example, the electronic configuration of nitrogen atom (atomic number 7) is written as

$$1s^2 2s^2 2p^1_x\ 2p^1_y 2p^1_z.$$

b) **Orbital diagram method**:

In this method the filled orbitals are represented by circles or boxes and are written in the order of increasing energies. The respective electrons are indicated as arrows whose direction represents their spin. For example, the electronic configuration of nitrogen in the orbital diagram notation can be written as



Points for Revision:

- ✓ Atoms are made up of three fundamental particles namely, electrons, protons and neutrons.
- ✓ J.J Thomson made the first attempt to describe the structure of an atom in terms of a model called **plum pudding model.** According to this atoms can be considered as a large positively charged body (pudding) in which a number of small negatively charged electrons (plums) are scattered.
- ✓ According to the Rutherford's model, the positive charge of the atom and most of its mass is contained in the nucleus and the rest of the atom is empty space which contains the much smaller and negatively charged electrons.
- ✓ Electromagnetic radiation is a kind of energy, which is transmitted through space in the form of electric and magnetic fields. It travels with the speed of light and does not need any medium to travel.
- ✓ The electromagnetic radiations are characterized by a number of parameters like, amplitude, wavelength, frequency, wave number and velocity.
- ✓ Hydrogen gas gives a line spectrum consisting of distinct lines suggesting the quantisation of energy in hydrogen atom.

- ✓ In 1913, Niels Bohr proposed 'Planetary Model' for atom. According to the model the electrons move in definite circular paths of fixed energy around a central stationary nucleus. The electrons can change their orbits by absorbing or emitting a photon of energy (= h*v)* equal to the difference of the energies of the orbits.
- ✓ Bohr's model did explain for the stability of atom and the line spectrum of hydrogen. The model however was unable to explain the spectra of atoms other than hydrogen.
- ✓ Louis de Broglie, argued for the dual nature of electron and proposed that matter particles should have a wave nature. The associated wavelength, *is* given by the formula; $\lambda = \frac{h}{mv}$ or $\lambda = \frac{h}{p}$
- ✓ The wave-particle duality of matter led Werner Heisenberg to propose the **uncertainty principle**. According to which it is not possible to measure simultaneously both the ***position*** and ***momentum*** of a particle with a infinite precision.
- ✓ The dual nature of electron and Heisenberg's uncertainty principle led to the development of wave mechanical model.
- ✓ According to the Wave Mechanical Model, the motion of electron inside the atom can be described in terms of a mathematical function called, wave

function, ψ. This wave function contains all the information about the system and can be found by solving a wave equation called Schrodinger wave equation.

- ✓ The square of the wave function, ψ2 is a measure of the probability of finding the electron in a certain three dimensional space around the nucleus. This region is called as ***atomic orbital*** or simply ***orbital***.
- ✓ These wave functions are characterized by three quantum numbers. These quantum numbers describe the size, shape, and orientation of the atomic orbitals in space. Every electron in an atom has a unique set of quantum numbers.
- ✓ The principal quantum number *n* concerns the quantisation of the energy of the electron while the Azimuthal quantum number **,** *l* is related to the shape of the orbital. The magnetic quantum number *ml* describes the direction or orientation of the orbital in space.
- ✓ An additional quantum number, *ms* is introduced to account for electron spin. This quantum number does not follow from the wave mechanical model and describes the spin of the electron.
- ✓ Different orbitals have different shapes. An s orbital is spherical; *p* orbitals are dumbbell shaped ; *d* orbitals have cloverleaf shape while *f* orbitals have a eight lobed shape.

- ✓ The distribution of electrons in the shells and subshells is called **Electronic Configuration.** It is governed by three rules which are Aufbau principle ; Pauli's exclusion principle and Hund's Rule of maximum multiplicity.
- ✓ According to Aufbau principle the electrons in an atom are filled in the increasing order of their energies which is determined by ($n + l$) rules.
- ✓ According to the Pauli's exclusion principle, no two electrons can have all the four quantum numbers to be same.
- ✓ While filling electrons in the orbitals of same subshell, according to Hund's rule, each orbital is first singly occupied with same spin then the pairing up takes place.

References

1- Introduction to Atomic and Nuclear Physics, Semat and Albright, Fifth Edition.

2- Concepts of Modern Physics, Arthur Beiser, Sixth Edition.

3- Modern Physics, A. Serway, J. Moses and A. Moyer, Third Edition.

4- Modern Physics, Paul A. Tipler and Ralph A. Llewellyn, Sixth Edition.

5- Physics for Scientists and Engineers with Modern Physics, A. Serway and W. Jewett, eighth edition