2. Quantum Physics

1.0 Introduction:

During 17^{th} to 19^{th} centuries, Newtonian mechanics along with the Maxwell's electromagnetic wave theory and thermodynamics provided a path for the development of science and engineering. All the scientific results were explained successfully with these theories. These developments are termed as Classical Physics or Classical Mechanics or Newtonian Mechanics.

According to Classical Physics, the properties of light such as reflection, refraction, interference, diffraction and polarization are explained satisfactorily this stresses on wave nature of light. Upto the end of 19^{th} century, it was fixed that light has only one nature i.e. wave nature. But during first quarter of 20^{th} century, new invented properties challenged the wave nature of light.

From one of the first experimental result of black body radiation indicated that wave theory was not sufficient to explain the concept of black body radiation. Further in 1896, Wien made attempts to explain the spectrum of black body radiation only for the shorter wavelengths. In 1900, Rayleigh and Jeans attempted to explain the spectrum of black body radiation for longer wavelengths.

In 1900, Max Planck, a German Physicist, proposed his quantum theory for the explanation of experimental results of black body radiation and he succeeded in it. His idea was totally against to the classical physics. He proposed that light has particle nature. This quantum theory further supported by photoelectric effect, Compton Effect, line spectra etc.

In 1887, Heinrich Hertz first observed photoelectric effect and details was studied by Philipp Lenard. The photoelectric effect could not explained by the classical physics. In 1905, Albert Einstein successfully explained photoelectric effect by his photo-electric equation with the help of Planck's quantum theory. In 1913, Niels Bhor, Denmark Physicist accounted for the spectral lines of hydrogen atom using Planck's quantum theory. Later in 1926, A. H. Compton, an American Physicist discovered the scattered X-rays associated with increase in wavelength. It is known as Compton Effect. It was satisfactorily explained on the basis of Planck's quantum theory. In the same year, Gilbert Lewis, an American Physicist named the quantum of wave of light as 'Photon'.

During 1900 to 1930, all these developments in physics led to conflict that whether the light behaves as a wave or particle. The propagation of properties of light such as reflection, refraction, interference, diffraction and polarization can be explained by considering the wave nature of light. On the other hand black body radiation, photoelectric effect, Compton Effect and emission of spectral line are the properties of light which interact with matter can be explained by considering the particle nature of light. The wave nature and particle nature are contradictor to each other. But it is seen that both natures are not observed simultaneously in any one property of light. All properties of light indicated that light behave as wave or particle one at a time. This led to idea that light has dual nature: wave as well as particle. These aspects of light are compliment to each other.

The wave-particle dualism of light triggers the minds of French Physicist, Lousis de Broglie. In 1924, he proposed the wave-particle dualism of matter. In 1927, Davison and Germen gave experimental proof of matter waves.

Wave aspect of matter which is spreading whereas particle aspect of matter which is localized in space led to problem of accepting the dual nature of matter. This problem was simplified by Germen Physicist, Warner Heisenberg, in 1927, with discovery of "Uncertainty Principle". In uncertainty principle, wave packets have been considered instead of the particles.

All these discoveries were related to micro-world and are explained by Planck's quantum theory. These developments gave birth to 'Quantum Mechanics' which is foundation of modern Physics.

Upto 19th century classical mechanics based on Newton's equation governed laws of physics. To govern quantum mechanics the equation was proposed by Austrian Physicist, Erwin Schrödinger in 1926. Schrödinger equations include all important elements of Planck, de-Broglie and Heisenberg.

2.0 Black Body Radiation:

A perfect black body is one which absorbs radiation of all wavelengths incident upon it. Further, such a body cannot transmit or reflect any radiation, and therefore it appears black. A black body can radiate energy in all possible wavelengths when it is heated to a suitable temperature. These radiations are called black body radiations.

2.1 Characteristic of Black Body Radiation:

Black body radiations are characterized by Kirchhoff's law, Stefan's law and Wien's law. According to these laws, black body radiations are stated as follows:

A) Kirchhoff's Law: The ratio of emissive power (e_λ) to the coefficient of absorption (a_λ) of a given wavelength is the same for all bodies at a given temperature is equal to the emissive power (E_b) of a perfectly black body at that temperature.

$$\frac{e_\lambda}{a_\lambda} = E_b - - - - - - -(1)$$

B) Stefan's Law: The radiant energy (Q) emitted per unit time per unit area of a perfectly black body is directly proportional to the fourth power of its absolute temperature (T).

$$Q \; \alpha \; T^4$$

$$Q = \sigma T^4 - - - - - - -(2)$$

where σ is constant of proportionality also known as Stefan's constant and its value is 5.78 x 10^{-8} $Wm^{-2}K^{-4}$.

C) Wein's Law: Wein's law state that the wavelength corresponds to the maximum energy is inversely proportional to absolute temperature (T).

$$\lambda_m T = constant - - - - - - -(3)$$

The wavelength of energy radiated from the body is shifted from maximum to minimum value during the increase in temperature of black body. The value of constant is 2.982 x 10^{-3} mK.

2.2 Energy Distribution of Black Body:

Series of attempts have been made to explain the distribution of energy among different wavelengths in black body radiation. Stefan's fourth power law is used to explain this, but it does not explain how the energy is distributed among the different wavelengths.

The energy distribution from black body was explained by Lummer and Pringsheim as shown in figure 1.

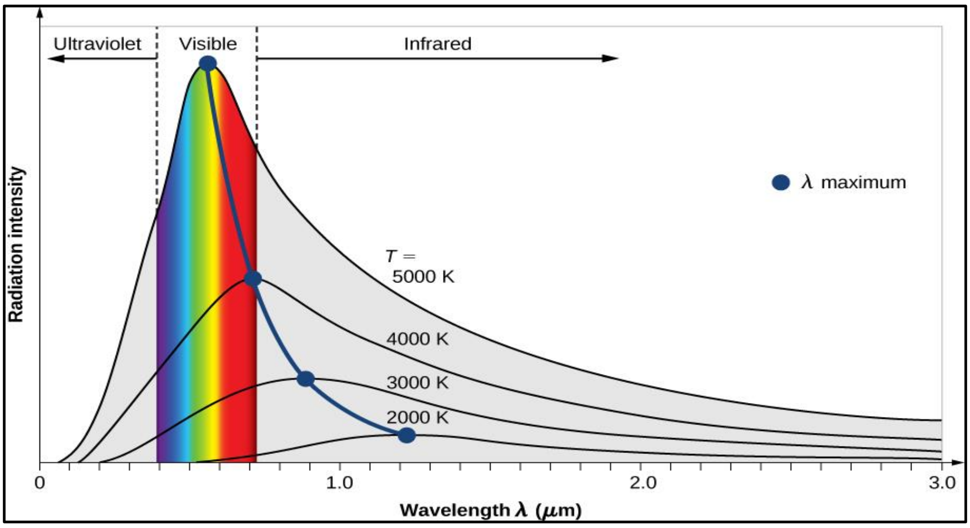


Figure 1: Energy spectrum of black body radiation

From above graph the following observations are made:

i) The distribution of energy is not uniform.

ii) For a particular temperature, the intensity of radiation increases up to a particular wavelength and then it is found to decrease with increase in wavelength.

iii) As temperature increases, the peak energy shifts towards shorter wavelengths.

3.0 Plank's Quantum Theory:

The quantum theory was proposed by Max Planck in 1900 (awarded Nobel Prize in 1918) to explain the distribution of energy in the spectrum of black body radiation.

The following hypothesis made by Planck for the derivation of radiation law.

i) Planck assumed that the black body is made up of number of oscillating particles. The particles can vibrate in all possible frequencies. The frequency of radiation from the body is the same as that of the vibrating particles.

ii) The oscillatory particles cannot emit energy continuously but they radiate energy only in the form of discrete packets. These energy packets are called 'quanta' or 'photons'.

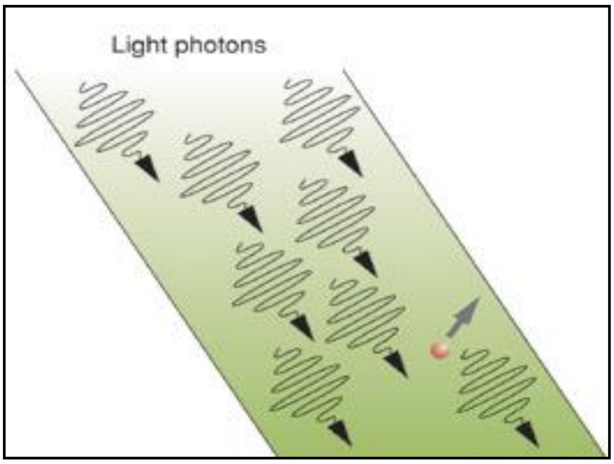


Figure 2: Radiation in form of quanta

The energy (E) associated with each photon of frequency (ν) is given by

$$E = h\nu ------(4)$$

where h is Planck's constant and the value of h = 6.625 x 10^{-34}Js

iii) The vibrating particles can radiate energy when oscillators move from one state to another. The radiation of energy is not continuous, but discrete in nature. The values of energy of the oscillators are like 0, hν, 2hν, 3hν,……., nhν.

Properties of Photon:

1. Photon energy is hν, which is different for different kinds of radiations.
2. Energy of photon is independent of intensity. The intensity depends upon the number of photons.
3. The momentum of photon is hν/c or h/λ.
4. Photons are electrically neutral.

3.1 Average Energy of Plank's Oscillator:

Let N be the total number of vibrating particles (oscillators) in the body. The total energy of the body is E. Therefore the average energy (Ē) is given by,

$$\bar{E} = \frac{E}{N} ------(5)$$

Let us consider the number of vibrating particles in the body as N_0, N_1, N_2, N_3,……, N_n. According to Planck's hypothesis, the energy of above can be written as 0, hν, 2hν, 3hν,….., nhν. Therefore, the total number of vibrating particles is given as,

$$N = N_0 + N_1 + N_2 + N_3 + \cdots + N_n ------(6)$$

According to Maxwell's distribution formula, the number of particles in the n^{th} oscillatory system can be written as,

$$N_n = N_0 e^{\frac{-nh\nu}{kT}} ------(7)$$

where h is the Planck's constant, ν be the frequency of radiation, k is the Boltzmann's constant and T be the absolute temperature.

Extending Maxwell's distribution function to the present system, the total number of particles N can be written as,

$$N = N_0 + N_0 e^{\frac{-h\nu}{kT}} + N_0 e^{\frac{-2h\nu}{kT}} + N_0 e^{\frac{-3h\nu}{kT}} + \cdots + N_0 e^{\frac{-nh\nu}{kT}} ------(8)$$

$$N = N_0 \left[1 + e^{\frac{-h\nu}{kT}} + e^{\frac{-2h\nu}{kT}} + e^{\frac{-3h\nu}{kT}} + \cdots + e^{\frac{-nh\nu}{kT}}\right] ------(9)$$

Since equation (9) is similar to the well known mathematical expression,

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

Therefore equation (9) can be written as,

$$N = N_0 \frac{1}{1 - e^{\frac{-h\nu}{kT}}} ------(10)$$

Similarly, the total energy of the body can be written as,

$$E = (N_0 \times 0) + (N_1 \times h\nu) + (N_2 \times 2h\nu) + \cdots + (N_n \times nh\nu) ------(11)$$

$$E = (N_0 \times 0) + \left(N_0 e^{\frac{-h\nu}{kT}} \times h\nu\right) + \left(N_0 e^{\frac{-2h\nu}{kT}} \times 2h\nu\right) + \cdots + \left(N_0 e^{\frac{-nh\nu}{kT}} \times nh\nu\right) --(12)$$

$$E = N_0 e^{\frac{-h\nu}{kT}} h\nu \left[1 + 2e^{\frac{-h\nu}{kT}} + 3e^{\frac{-2h\nu}{kT}} + \cdots + ne^{\frac{-(n-1)h\nu}{kT}}\right] ------(13)$$

Since equation (13) is similar to the well known mathematical expression,

$$1 + 2x + 3x^2 + 4x^3 + \cdots + nx^{n-1} = \frac{1}{(1-x)^2}$$

Therefore equation (13) can be written as,

$$E = N_0 e^{\frac{-h\nu}{kT}} h\nu \frac{1}{\left(1 - e^{\frac{-h\nu}{kT}}\right)^2} ------(14)$$

Substituting the total number of oscillators and energy from equation (10) & (14) respectively in equation (5), we get,

$$\bar{E} = \frac{N_0 e^{\frac{-h\nu}{kT}} h\nu \frac{1}{\left(1-e^{\frac{-h\nu}{kT}}\right)^2}}{N_0 \frac{1}{1-e^{\frac{-h\nu}{kT}}}} ------(15)$$

$$\bar{E} = \frac{N_0 e^{\frac{-h\nu}{kT}} h\nu \left(1 - e^{\frac{-h\nu}{kT}}\right)^{-2}}{N_0 \left(1 - e^{\frac{-h\nu}{kT}}\right)^{-1}} ------(16)$$

After rearranging equation (16)

$$\bar{E} = \frac{e^{\frac{-h\nu}{kT}} h\nu \left(1 - e^{\frac{-h\nu}{kT}}\right)}{\left(1 - e^{\frac{-h\nu}{kT}}\right)^2}$$

$$\bar{E} = \frac{h\nu\, e^{\frac{-h\nu}{kT}}}{\left(1 - e^{\frac{-h\nu}{kT}}\right)}$$

$$\bar{E} = \frac{h\nu\, e^{\frac{-h\nu}{kT}} \Big/ e^{\frac{-h\nu}{kT}}}{\left(1 - e^{\frac{-h\nu}{kT}}\right) \Big/ e^{\frac{-h\nu}{kT}}}$$

$$\bar{E} = \frac{h\nu}{\left(e^{\frac{h\nu}{kT}} - 1\right)} - - - - - - -(17)$$

The equation (17) gives the average energy of the oscillations.

3.2 Plank's Radiation Law:

If ν and ν + dν be the frequency range, the number of oscillation can be written as,

$$N = \frac{8\pi\nu^2}{c^3} d\nu - - - - - - -(18)$$

Therefore, the total energy per unit volume (u) for a particular frequency can be obtained by multiplying equations (17) & (18) as,

$$u_\nu d\nu = \frac{8\pi\nu^2}{c^3} \frac{h\nu}{\left(e^{\frac{h\nu}{kT}} - 1\right)} d\nu - - - - - - -(19)$$

$$u_\nu d\nu = \frac{8\pi h\nu^3}{c^3} \frac{1}{\left(e^{\frac{h\nu}{kT}} - 1\right)} d\nu - - - - - - -(20)$$

Equation (20) is known as Planck's equation for radiation law in terms of frequency.

It can also be written in terms of wavelength as,

$$u_\lambda d\lambda = -u_\nu d\nu - - - - - - -(21)$$

The negative sign indicate that as increase in frequency corresponds to the decrease in its wavelength.

Since,

$$\nu = \frac{c}{\lambda} - - - - - - -(22)$$

Differentiating equation (22)

$$dv = -c\frac{d\lambda}{\lambda^2} ------(23)$$

Using equation (20), (22) & (23) in equation (21),

$$u_\lambda d\lambda = -\frac{8\pi h\left(\frac{c}{\lambda}\right)^3}{c^3}\frac{1}{\left(e^{\frac{hc}{\lambda kT}}-1\right)}\left(-c\frac{d\lambda}{\lambda^2}\right) ------(24)$$

$$u_\lambda d\lambda = \frac{8\pi hc}{\lambda^5}\frac{1}{\left(e^{\frac{hc}{\lambda kT}}-1\right)}d\lambda ------(25)$$

Equation (25) is known as Planck's equation for radiation law in terms of wavelength.

3.3 Wein's Law:

Using Planck's radiation law from equation (25), we can derive Wein's law as,

When wavelength (λ) and temperature (T) are very small, the value of $e^{\frac{hc}{\lambda kT}} \gg 1$

$$u_\lambda d\lambda = \frac{8\pi hc}{\lambda^5}e^{-\frac{hc}{\lambda kT}}d\lambda ------(26)$$

$$8\pi hc = A \;\&\; \frac{hc}{k} = B$$

$$u_\lambda d\lambda = \frac{A}{\lambda^5}e^{-\frac{B}{\lambda T}}d\lambda ------(27)$$

Equation (27) is the Wein's law and this formula holds good only for short wavelength.

3.4 Rayleigh and Jean's Law:

Using Planck's radiation law from equation (25), we can derive Rayleigh & Jean's law,

When wavelength (λ) and temperature (T) are longer, the value of $e^{\frac{hc}{\lambda kT}} \cong 1 + \frac{hc}{\lambda kT}$

$$u_\lambda d\lambda = \frac{8\pi hc}{\lambda^5}\frac{1}{\left(1+\frac{hc}{\lambda kT}-1\right)}d\lambda ------(28)$$

$$u_\lambda d\lambda = \frac{8\pi kT}{\lambda^4}d\lambda ------(29)$$

Equation (29) is the Rayleigh and Jean's law and this formula holds good only for longer wavelength.

4.0 Compton Effect:

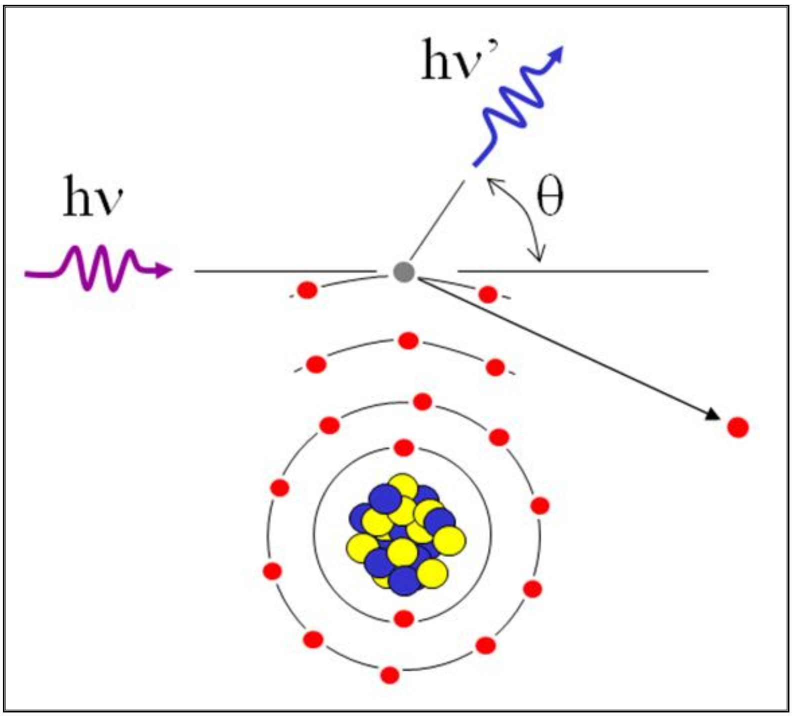


Figure 3: Compton Effect

According to classical electromagnetic theory, when electromagnetic radiation of frequency ν is incident on free charges like electron, the free charges absorb this radiation and start oscillating at frequency ν. Then these oscillating charges radiate electromagnetic waves with same frequency ν. This type of scattering where the change in frequency or wavelength does not take place is called as **Coherent Scattering or Thomson Scattering**. The coherent scattering has been observed in visible range at longer wavelength.

However, prediction of classical theory fails in scattering of radiation of very short wavelengths like X-rays. The scattered X-rays are found to consist of two frequencies (ν & ν'). The wavelength λ corresponds to the frequency ν is called unmodified wavelength whereas the wavelength λ' corresponds to the frequency ν' is called modified wavelength. This type of scattering is called as **Incoherent Scattering or Compton Scattering**.

"When a monochromatic beam of X-rays of wavelength λ is allowed to fall on a solid material (such as paraffin or carbon), the scattered beam consist of two components: one whose wavelength equal to incident wavelength and the other with a higher wavelength. The phenomenon of increase in wavelength (or decrease in frequency) of X-ray radiations by scattering is called as Compton Effect."

This effect is based on the quantum theory of radiations.

4.1 Derivation of Compton Shift:

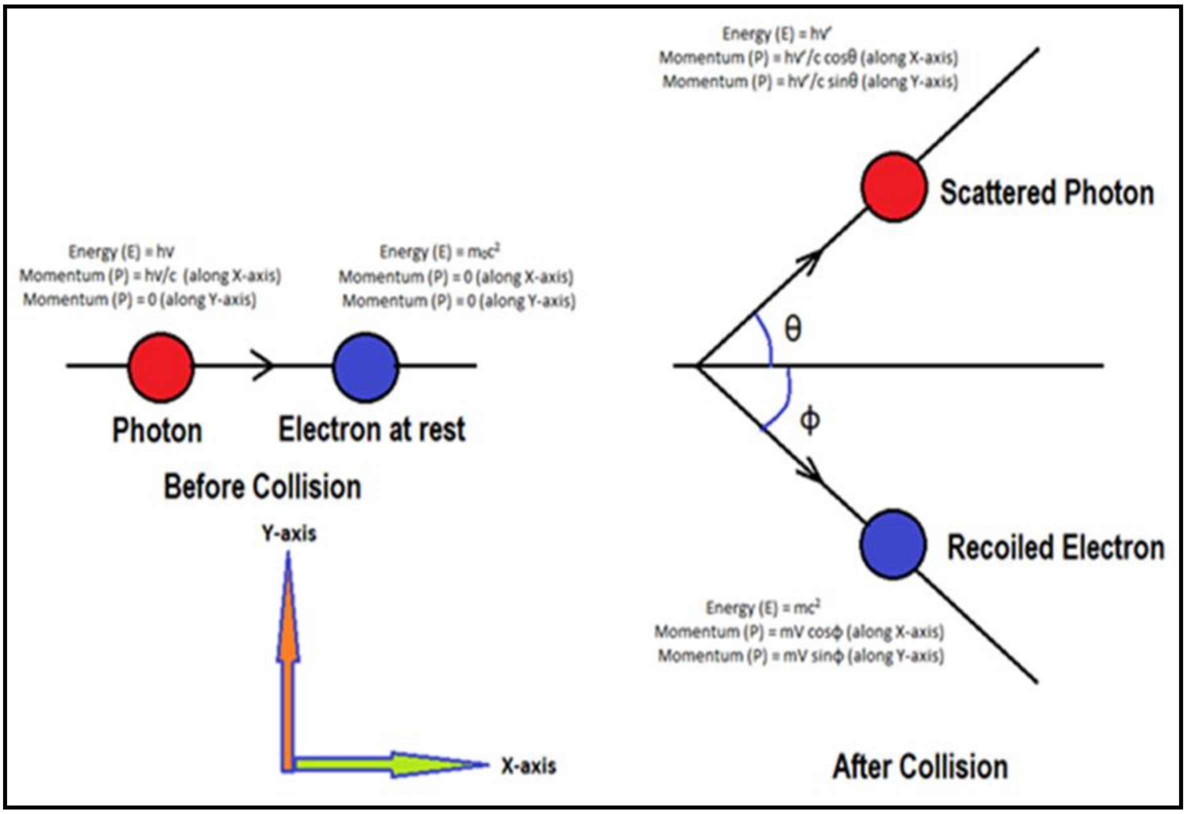


Figure 4: Compton scattering

According to quantum theory of radiations, X-rays consist of photons whose energy is hν. When a photon (hν) collides with a free electron in the solid material, the incident photon transfers some of its energy to the free electron. By the energy transfer, the electron acquires kinetic energy and recoiled with velocity V. After the collision, the scattered photon comes out with reduced energy hν' or increased wavelength λ'.

Let us calculate the **total energy** before and after collision.

Before collision:

$$Energy\ of\ incident\ photon : h\nu$$

$$Energy\ of\ electron\ at\ rest : m_0c^2$$

$$Total\ Energy\ before\ collision : h\nu + m_0c^2 ------(30)$$

After collision:

$$Energy\ of\ scattered\ photon : h\nu'$$

$$Energy\ of\ recoiled\ electron : mc^2$$

$$Total\ Energy\ after\ collision : h\nu' + mc^2 ------(31)$$

Similarly, x and y components of **momentum** before and after collision can be calculated as follows.

Before collision:

X-component

$$Momentum\ of\ incident\ photon : \frac{h\nu}{c}$$

$$Momentum\ of\ electron\ at\ rest : 0$$

$$Total\ Momentum\ along\ x-axis\ : \frac{h\nu}{c} ------(32)$$

Y-component

$$Momentum\ of\ incident\ photon : 0$$

$$Momentum\ of\ electron\ at\ rest : 0$$

$$Total\ Momentum\ along\ y-axis\ : 0 ------(33)$$

After collision:

X-component

$$Momentum\ of\ scattered\ photon : \frac{h\nu'}{c}cos\theta$$

$$Momentum\ of\ recoiled\ electron\ : mVcos\Phi$$

$$Total\ Momentum\ along\ x-axis\ : \frac{h\nu'}{c}cos\theta + mVcos\Phi ------(34)$$

Y-component

$$Momentum\ of\ scattered\ photon : \frac{h\nu'}{c}sin\theta$$

$$Momentum\ of\ recoiled\ electron\ : -mVsin\Phi$$

$$Total\ Momentum\ along\ y-axis\ : \frac{h\nu'}{c}sin\theta - mVsin\Phi ------(35)$$

Then, according to the law of conservation of momentum,

Along x- axis $$\frac{h\nu}{c} = \frac{h\nu'}{c}cos\theta + mVcos\Phi ------(36)$$

Along y- axis $$0 = \frac{h\nu'}{c}sin\theta - mVsin\Phi ------(37)$$

Rearranging equation (36)

$$h\nu = h\nu' cos\theta + cmVcos\Phi$$

$$cmVcos\Phi = h(\nu - \nu' cos\theta) ------(38)$$

Rearranging equation (37)

$$cmV sin\Phi = h\nu' sin\theta -------- (39)$$

Squaring and adding equations (38) & (39)

$$c^2m^2V^2cos^2\Phi + c^2m^2V^2sin^2\Phi = h^2(\nu - \nu' cos\theta)^2 + h^2\nu'^2 sin^2\theta ------(40)$$

$$c^2m^2V^2(cos^2\Phi + sin^2\Phi) = h^2(\nu^2 - 2\nu\nu' cos\theta + {\nu'}^2 cos^2\theta) + h^2\nu'^2 sin^2\theta$$

$$c^2m^2V^2 = h^2\nu^2 - 2h^2\nu\nu' cos\theta + h^2{\nu'}^2 cos^2\theta + h^2\nu'^2 sin^2\theta$$

$$c^2m^2V^2 = h^2\left(\nu^2 - 2\nu\nu' cos\theta + {\nu'}^2\right) ------(41)$$

According to the law of conservation of energy,

$$h\nu + m_0c^2 = h\nu' + mc^2$$

$$mc^2 = h(\nu - \nu') + m_0c^2 ------(42)$$

Squaring equation (42)

$$m^2c^4 = [h(\nu - \nu') + m_0c^2]^2$$

$$m^2c^4 = h^2\left(\nu^2 - 2\nu\nu' + {\nu'}^2\right) + 2h(\nu - \nu')m_0c^2 + {m_0}^2c^4 ------(43)$$

Subtracting equation (41) from (43)

$$\begin{aligned} m^2c^4 - c^2m^2V^2 & \\ &= h^2\left(\nu^2 - 2\nu\nu' + {\nu'}^2\right) + 2h(\nu - \nu')m_0c^2 + {m_0}^2c^4 \\ &- h^2\left(\nu^2 - 2\nu\nu' cos\theta + {\nu'}^2\right) \end{aligned}$$

$$\begin{aligned} m^2c^2(c^2 - V^2) & \\ &= h^2\nu^2 - 2h^2\nu\nu' + h^2{\nu'}^2 + 2h(\nu - \nu')m_0c^2 + {m_0}^2c^4 - h^2\nu^2 + 2h^2\nu\nu' cos\theta \\ &- h^2{\nu'}^2 \end{aligned}$$

$$m^2c^2(c^2 - V^2) = -2h^2\nu\nu' + 2h(\nu - \nu')m_0c^2 + {m_0}^2c^4 + 2h^2\nu\nu' cos\theta$$

$$m^2c^2(c^2 - V^2) = -2h^2\nu\nu'(1 - cos\theta) + 2h(\nu - \nu')m_0c^2 + {m_0}^2c^4 ------(44)$$

According to theory of relativity,

$$m = \frac{m_0}{\sqrt{1 - \frac{V^2}{c^2}}} ------(45)$$

Squaring of equation (45)

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

$$m^2 = \frac{{m_0}^2}{\frac{c^2-V^2}{c^2}}$$

$$m^2 = \frac{{m_0}^2c^2}{c^2-V^2}$$

$$m^2(c^2-V^2) = {m_0}^2c^2 ------(46)$$

Multiplying c^2 on both sides of equation (46)

$$m^2c^2(c^2-V^2) = {m_0}^2c^4 ------(47)$$

Using equation (47) in equation (44) we get,

$${m_0}^2c^4 = -2h^2\nu\nu'(1-cos\theta) + 2h(\nu-\nu')m_0c^2 + {m_0}^2c^4$$

$$0 = -2h^2\nu\nu'(1-cos\theta) + 2h(\nu-\nu')m_0c^2$$

$$2h(\nu-\nu')m_0c^2 = 2h^2\nu\nu'(1-cos\theta)$$

$$\frac{(\nu-\nu')}{\nu\nu'} = \frac{h}{m_0c^2}(1-cos\theta)$$

$$\frac{\nu}{\nu\nu'} - \frac{\nu'}{\nu\nu'} = \frac{h}{m_0c^2}(1-cos\theta)$$

$$\frac{1}{\nu'} - \frac{1}{\nu} = \frac{h}{m_0c^2}(1-cos\theta) ------(48)$$

Multiplying c on both sides of equation (48)

$$\frac{c}{\nu'} - \frac{c}{\nu} = \frac{h}{m_0c}(1-cos\theta)$$

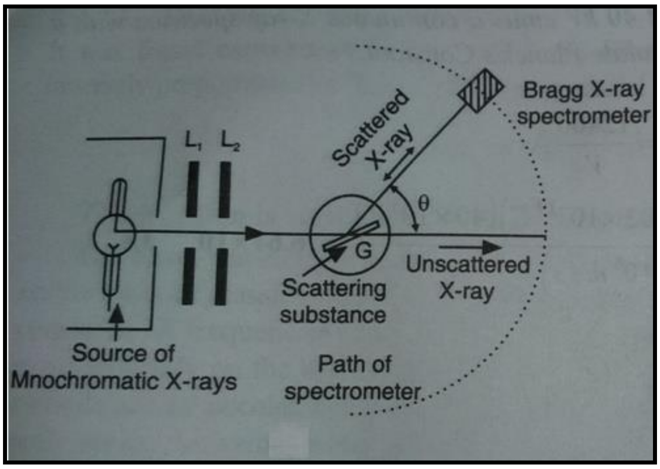
$$\lambda' - \lambda = \frac{h}{m_0c}(1-cos\theta) ------(49)$$

Therefore the change in wavelength (dλ) is given as,

$$d\lambda = \frac{h}{m_0c}(1-cos\theta) ------(50)$$

The equation (50) gives the Compton shift. The Compton shift (dλ) is independent on the wavelength of incident radiation and nature of scattering substance but it depends only on the scattering substance.

4.2 Verification of Compton Effect:



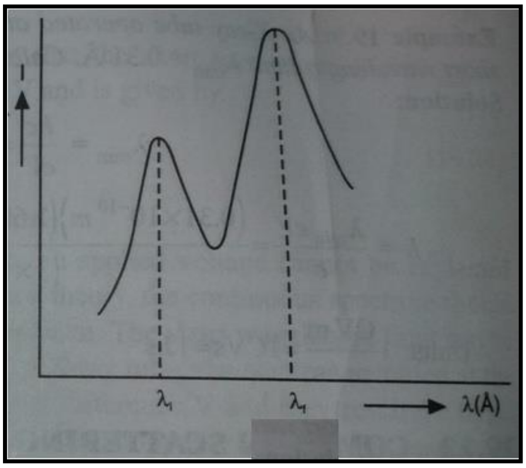


Figure 5(A): Compton Apparatus for Scattered X-ray's **Figure 5(B): Unmodified & Modified Components**

A beam of monochromatic X-ray of known wavelength is made incident on a graphite target is shown in figure 5(A). The intensity distribution with wavelength of monochromatic X-ray scattered at different angles is measured by Bragg's X-ray spectrometer. The intensity distribution with wavelength for different angles is shown in figure 6. It may be noted that diffraction pattern has two diffraction peaks: one corresponding to modified radiation and other corresponding to unmodified radiation are shown in figure 5(B). The difference between two peaks on the wavelength axis provides the Compton shift. It can be concluded from diffraction pattern that greater scattering angle yields greater Compton shift.

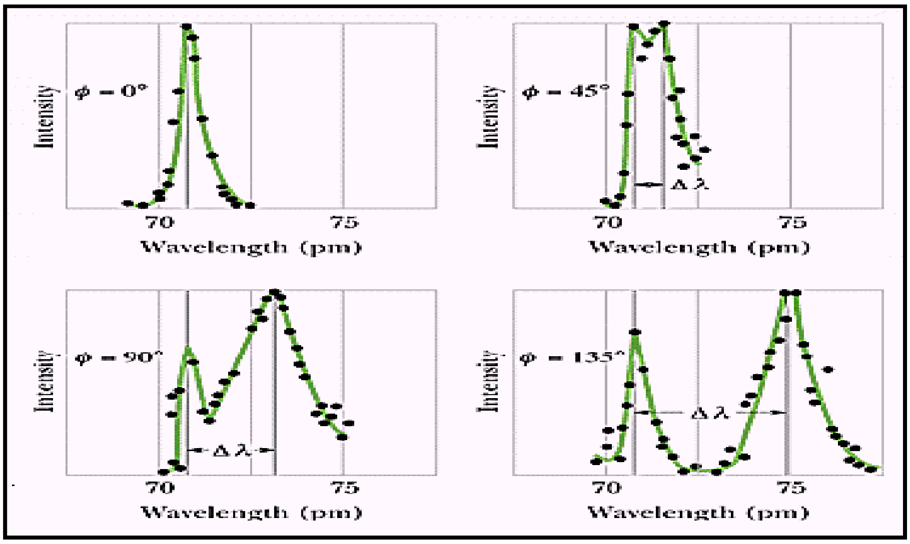


Figure 6: Compton shift for different angles between two peaks

E.g. $$d\lambda = \lambda' - \lambda = \frac{h}{m_0 c}(1 - cos\theta)$$

$$If\ \theta = 0^o \ldots\ldots\ldots\ldots then \quad d\lambda = \lambda' - \lambda = 0$$

$$If\ \theta = 45^o \ldots\ldots\ldots\ldots then \quad d\lambda = \lambda' - \lambda = 0.0070\ A^o$$

$$If\ \theta = 90^o \ldots\ldots\ldots\ldots then \quad d\lambda = \lambda' - \lambda = 0.0242\ A^o$$

$$If\ \theta = 180^o \ldots\ldots\ldots\ldots then \quad d\lambda = \lambda' - \lambda = 0.0484\ A^o$$

Hence, Compton Effect is experimentally verified.

4.3 Compton Effect in Visible Range:

Compton Effect is observed significantly with X-rays which are very short wavelength. If we use visible light (λ = 4000 to 7000A^o) in place of X-rays and calculate the Compton shift.

$$d\lambda = \frac{h}{m_0 c}(1 - cos\theta) = 0.0242(1 - cos\theta)\ A^o$$

$$If\ \theta = 90^o \ldots\ldots\ldots\ldots then \quad d\lambda = \lambda' - \lambda = 0.0242\ A^o$$

$$If\ \theta = 180^o \ldots\ldots\ldots\ldots then \quad d\lambda = \lambda' - \lambda = 0.0484\ A^o$$

The percentage of Compton Shift,

for λ = 1 A^o Compton shift = 5%

for λ = 5 A^o Compton shift = 1%

for λ = 5000 A^o Compton shift = 0.001%

So, we can see that the Compton Shift for the case of visible light is not significant. For this reason, the X-rays are appropriate for realizing the Compton Effect.

5.0 Simple Concept of Quantum Theory:

According to Plank’s quantum hypothesis, the radiation does not emit in continuous fashion rather it gets emitted in discrete packets of energy equal to hν. These packets are referred to as quanta or photons. Therefore, it can be said that the exchange of energy between the radiation and the matter takes place in discrete set of values. In view of the application of quantum theory, it is necessary to be aware of the photon.

5.1 Photon:

Photon is an elementary particle that is mass less and has no charge. It is a bundle of energy or packet of energy emitted by a source of radiation. It moves with velocity of light. It can carry energy and momentum.

As per the special theory of relativity, the mass m of the particle moving with velocity v comparable to the velocity of light c is given by,

$$m = \frac{m_0}{\sqrt{1 - \frac{V^2}{c^2}}} ------(51)$$

where, m is the relativistic mass of the particle and m_0 is its rest mass.

Since the photon is moving with velocity of light, we substitute v = c in equation (51).

So that, the moving mass m of photon becomes infinity $i.e. (m = \infty)$, which is not possible. So, if photon moves with velocity of light then zero in the numerator balances the zero in the denominator i.e. $(m = 0/0)$, this is an indeterminate quantity. It means if we take rest mass of the photon to be zero, this value should not particularly disturb us due the fact that the photons are never at rest and always keep moving with the velocity of light.

The energy of photon is given as,

$$E = h\nu ------(52)$$

If m is the moving mass of the photon, then energy of photon from energy mass relation is given as,

$$E = mc^2 ------(53)$$

From equation (52) & (53),

$$mc^2 = h\nu$$

$$m = \frac{h\nu}{c^2} ------(54)$$

Now the energy relation,

$$E^2 = p^2c^2 + {m_0}^2c^4 ------(55)$$

Since $m_0 = 0$, E = pc and the momentum of photon is given by,

$$p = \frac{E}{c} = \frac{mc^2}{c} = mc ------(56)$$

or

$$p = \frac{E}{c} = \frac{h\nu}{c} ------(57)$$

Thus, if photon of frequency ν, is to e treated as a particle, then the characteristics of the photon are given as,

$$m_0 = 0, E = h\nu, m = \frac{h\nu}{c^2}\ and\ p = \frac{h\nu}{c}$$

These characteristic of photons are useful in the application of quantum theory.

6.0 de-Broglie hypothesis:

Louis de-Broglie in 1924 extended the wave particle parallelism of light radiations to all the fundamental entities of Physics such as electrons, protons, neutrons, atoms and molecules etc. He put a bold suggestion that the correspondence between wave and particle should not confine only to electromagnetic radiation, but it should also be valid for material practices, i.e. like radiation, matter also has a dual (i.e., particle like and wave like) character. In his doctoral thesis de-Broglie wrote that there is an intimate connection between waves and corpuscles not only in the case of radiation but also in the case of matter. **A moving particle is always associated with the wave and the particle is controlled by waves.** This suggestion was based on the fact that nature loves symmetry, if radiation like light can act like wave some times and like a particle at other times, then the material particles (e.g., electron, neutron, etc.) should act as waves at some other times. These waves associated with particles are named de- Broglie waves or matter waves.

6.1 Expression for de- Broglie wavelength:

The expression of the wavelength associated with a material particle can be derived on the analogy of radiation as follows:

Considering the plank's theory of radiation, the energy of photon (quanta)

$$E = h\nu = \frac{hc}{\lambda} ------(58)$$

where c is the velocity of light in vacuum and λ is its wave length.

According to Einstein energy – mass relation

$$E = mc^2 ------(59)$$

Comparing equation (58) & (59)

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

$$\lambda = \frac{h}{mc} = \frac{h}{p} ------(60)$$

where, mc = p is the momentum associated with photon.

In case of material particle of mass m moving with a velocity v , the momentum is mv, therefore the wavelength associated with this particle (in analogy to wavelength associated with photon) is given by,

$$\lambda = \frac{h}{mv} = \frac{h}{p} ------(61)$$

6.2 Different expressions for de-Broglie wavelength:

(a) If E is the kinetic energy of the material particle then

$$E = \frac{1}{2}mv^2 = \frac{1}{2}\frac{m^2v^2}{m} = \frac{p^2}{2m} ------(62)$$

$$p^2 = 2mE$$

$$p = \sqrt{2mE} ------(63)$$

Therefore de-Broglie's wavelength is given by

$$\lambda = \frac{h}{\sqrt{2mE}} ------(64)$$

(b) When a charged particle carrying a charge 'q' is accelerated by potential difference V, then its kinetic energy K.E. is given by

$$E = qV ------(65)$$

Hence, de-Broglie's wavelength associated with this particle is

$$\lambda = \frac{h}{\sqrt{2mqV}} ------(66)$$

For an electron q = 1.602 x 10^{-19} c, mass m = 9.1 X 10^{-31} kg

$$\lambda = \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.602 \times 10^{-19} \times V}} ------(67)$$

$$\lambda = \frac{12.26}{\sqrt{V}}\ A^{o} ------(68)$$

6.3 Properties of Matter Waves:

a) Lighter is the particle, greater is the wavelength associated with it.

b) Smaller is the velocity of the particle, greater is the wavelength associated with it.

c) When v = 0, then λ = ∞, i.e. wave becomes indeterminate and if v = ∞ then λ = 0. This shows that matter waves are generated only when material particles are in motion.

d) Matter waves are produced whether the particles are charged particles or not ($\lambda = \frac{h}{mv}$ is independent of charge). i.e., matter waves are not electromagnetic waves but they are a new kind of waves.

e) It can be shown that the matter waves can travel faster than light i.e. the velocity of matter waves can be greater than the velocity of light.

f) No single phenomenon exhibits both particle nature and wave nature simultaneously.

6.4 Distinction between Matter waves and Electromagnetic waves:

Matter waves	**Electromagnetic waves**
1. Matter waves are associated with moving particles (charged or uncharged)	1. Electromagnetic waves are produced only by accelerated charged particles.
2. Wavelength depends on the mass of the particle and its velocity. $\lambda = \frac{h}{mv}$	2. Wavelength depends on the energy of photon
3. Matter waves can travel with a velocity greater than the velocity of light.	3. Travel with velocity of light c = 3×10^{8} m/s.
4. Matter wave is not electromagnetic wave.	4. Electric field and magnetic field oscillate perpendicular to each other.
5. Matter wave require medium for propagation, i.e. they cannot travel through vacuum.	5. Electromagnetic waves do not require any medium for propagation, i.e., they can pass through vacuum.

7.0 Phase Velocity and Group Velocity:

A) Phase Velocity:

The phase velocity (u) is defined as the ratio of angular frequency (ω) to the propagation constant (k).

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

We can write the equation of de-Broglie's wave travelling along positive x direction as,

$$y = a\ \sin(\omega t - kx) ------(69)$$

where 'a' is the amplitude, ω (=2πν) is the angular frequency, k (=2π/λ) is the propagation constant and (ωt-kx) is the phase of wave motion.

It means the particle of the constant phase travels such that (ωt-kx) = constant.

Therefore differentiation of constant phase is

$$\frac{d}{dt}(\omega t - kx) = 0 ------ (70)$$

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

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

But $\frac{dx}{dt} = u$ which is phase or wave velocity.

$$u = \frac{\omega}{k} ------(71)$$

Thus the wave velocity is the velocity of planes of constant phase which advances through the medium.

We can write the phase velocity

$$u = \nu\lambda ------(72)$$

For electromagnetic wave

$$E = h\nu$$

$$\nu = \frac{E}{h} ------(73)$$

and for de-Broglie wavelength.

$$\lambda = \frac{h}{p} = \frac{h}{mv} - - - - - - -(74)$$

Put the values from (73) and (74) in (72)

$$u = \frac{E}{h} \times \frac{h}{mv} = \frac{E}{mv} = \frac{mc^2}{mv} = \frac{c^2}{v} - - - - - - -(75)$$

Since c>>v, equation (75) implies that the phase velocity of de-Broglie wave associated with the particle moving with velocity v is greater than velocity of light c.

B) Group Velocity:

As we have seen in the earlier part, the phase velocity of a wave associated with a particle comes out to be greater than the velocity of light. This problem can overcome by assuming each moving particle is associated with group of wave or a wave packet rather than single wave. In this context, de-Broglie waves are represented by a wave packet and hence we have group velocity associated with them. In order to realize the concept of group velocity, we consider the combination of two waves, resultant of which is shown in figure 7.

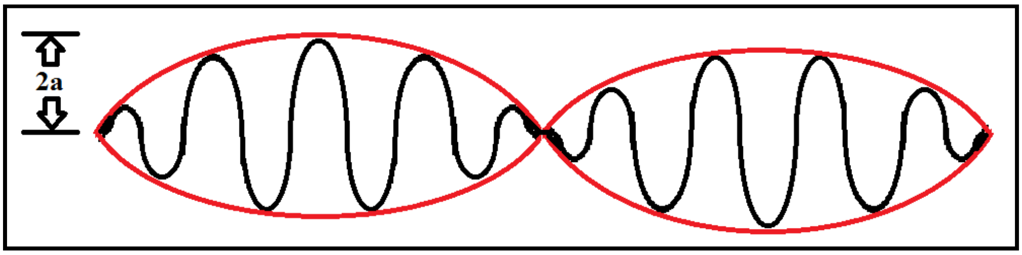


Figure 7: wave packets

The two waves are represented by

$$y_1 = a\sin(\omega_1 t - k_1 x) - - - - - - -(76)$$

$$y_2 = a\sin(\omega_2 t - k_2 x) - - - - - - -(77)$$

The resultant wave due to superposition of these waves is given by,

$$y = y_1 + y_2$$

$$y = a\sin(\omega_1 t - k_1 x) + a\sin(\omega_2 t - k_2 x)$$

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

$$y = 2a\sin[\omega t - kx]\cos\left[\frac{(\Delta\omega)t}{2} - \frac{(\Delta k)x}{2}\right] - - - - - - -(78)$$

where, $\omega = \frac{(\omega_1+\omega_2)}{2}$, $k = \frac{(k_1+k_2)}{2}$, $\Delta\omega = \omega_1 - \omega_2$, $\Delta k = k_1 - k_2$.

The resultant wave from equation (78) has two parts,

i) A wave of frequency ω, propagation constant k & velocity u is given by,

$$u = \frac{\omega}{k} = \frac{2\pi\nu}{2\pi/\lambda} = \nu\lambda$$

which is phase velocity or wave velocity.

ii) Another wave of frequency Δω/2, propagation constant Δk/2 & velocity G = Δω/Δk. This velocity is the velocity of envelop of group of waves i.e. velocity of wave packet known as group velocity.

$$G = \frac{\Delta\omega}{\Delta k} = \frac{\partial\omega}{\partial k} = \frac{\partial(2\pi\nu)}{\partial(2\pi/\lambda)} = \frac{\partial\nu}{\partial(1/\lambda)} = -\lambda^2\frac{\partial\nu}{\partial\lambda} = -\frac{\lambda^2}{2\pi}\frac{\partial\omega}{\partial\lambda}$$

This is the expression for the group velocity.

7.1 Relation between Phase Velocity and Group Velocity:

If u be phase or wave velocity, then group velocity can be written as,

$$G = \frac{d\omega}{dk} = \frac{d(uk)}{dk}$$

$$G = u + k\frac{du}{dk} - - - - - - -(79)$$

As we know, $k = \frac{2\pi}{\lambda}$

By differentiating, $dk = -\frac{2\pi}{\lambda^2}d\lambda$

By taking ratio of above two equations

$$\frac{k}{dk} = -\frac{\lambda}{d\lambda} - - - - - - -(80)$$

Substituting equation (80) in equation (79)

The group velocity is given by,

$$G = u + \left(-\frac{\lambda}{d\lambda}\right) du$$

$$G = u - \lambda \frac{du}{d\lambda} ------(81)$$

This relation shows that the group velocity G is less than phase velocity u in a dispersive medium where u is a function of k or λ. However in a non-dispersive medium, the velocity u is independent of k, i.e. wave of all wavelength travel with same speed du/dλ=0. Therefore G = u.

7.2 Relation between Group Velocity and Particle:

Consider a material particle of rest mass m_0. Let its mass be m when it moves with velocity v. Then its total energy E is given by,

$$E = mc^2 = \frac{m_0 c^2}{\sqrt{1 - \frac{V^2}{c^2}}} ------(82)$$

Its momentum is given by,

$$p = mv = \frac{m_0 v}{\sqrt{1 - \frac{V^2}{c^2}}} ------(83)$$

The frequency of the associated de-Broglie wave is given by,

$$\nu = \frac{E}{h} = \frac{m_0 c^2}{\sqrt{1 - \frac{V^2}{c^2}}} \frac{1}{h}$$

$$\omega = 2\pi\nu = \frac{2\pi m_0 c^2}{h\sqrt{1 - \frac{V^2}{c^2}}}$$

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

$$\frac{d\omega}{dv} = \frac{2\pi m_0 v}{h\left(1 - \frac{V^2}{c^2}\right)^{3/2}} ------(84)$$

The wavelength of the associated de-Broglie wave is given by,

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

Hence propagation constant,

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

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

$$\frac{dk}{dv} = \frac{2\pi m_0}{h}\left[\left(1-\frac{V^2}{c^2}\right)^{-1/2} + \frac{V^2}{c^2}\left(1-\frac{V^2}{c^2}\right)^{-3/2}\right]$$

$$\frac{dk}{dv} = \frac{2\pi m_0}{h}\left(1-\frac{V^2}{c^2}\right)^{-3/2}\left[1-\frac{V^2}{c^2}+\frac{V^2}{c^2}\right]$$

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

$$\frac{dk}{dv} = \frac{2\pi m_0}{h\left(1-\frac{V^2}{c^2}\right)^{3/2}} ------(85)$$

Since the group velocity,

$$G = \frac{d\omega}{dk} = \frac{d\omega/dv}{dk/dv}$$

$$G = \frac{d\omega}{dk} = \frac{\frac{2\pi m_0 v}{h\left(1-\frac{V^2}{c^2}\right)^{3/2}}}{\frac{2\pi m_0}{h\left(1-\frac{V^2}{c^2}\right)^{3/2}}}$$

$$G = v ------(86)$$

Thus the wave group associated with the moving material particle travels with the same velocity as the particle. It proves that a material particle in motion is equivalent to group of wave packet.

8.0 Heisenberg Uncertainty Principle:

In 1927, Heisenberg German physicist (awarded Nobel Prize in 1932) proposed a very interesting principle, which is direct consequence of the dual nature of matter known as Uncertainty principle.

According to classical mechanics, the position and velocity or momentum of a body can be determined very accurately depending on the precision of the measuring device. Similarly angular position, angular momentum & energy at a given moment can be theoretically measured with infinite accuracy. But classical mechanics completely fails when it comes to microscopic & submicroscopic particles like electrons, protons etc.

De-Broglie introduced the concept of matter wave i.e. material particles are associated with wave packets or wave groups. The wave concept introduces a limit to the accuracy with which we can measure the particle properties like position & momentum of moving particles. According to Born's probability interpretation the particle may be found anywhere within the wave packet.

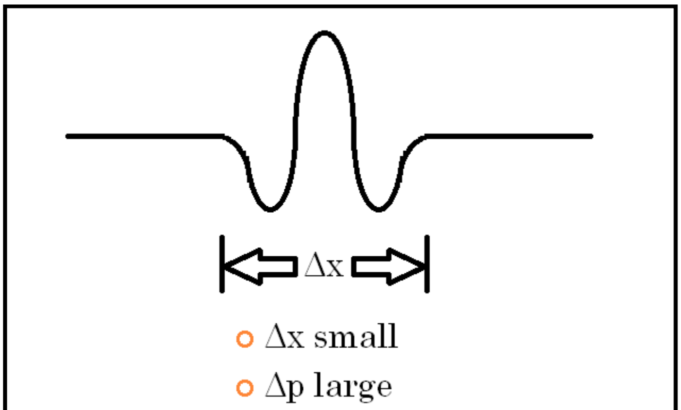


Fig (a)

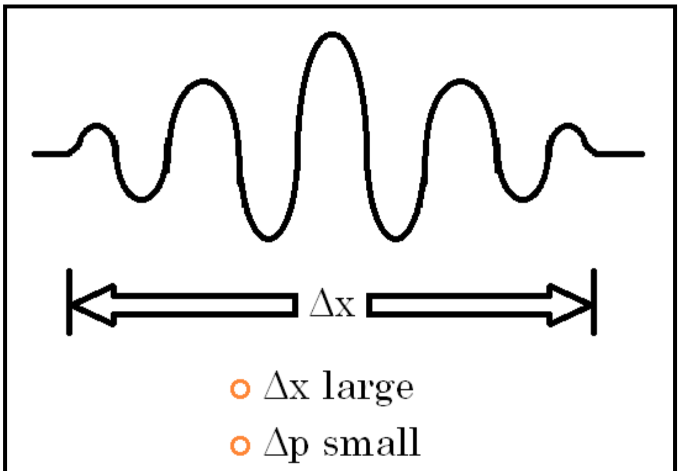


Fig (b)

If a wave packet is very narrow as shown in fig. a, position of associated particle is readily found but measure of its wavelength is impossible. So associated momentum is difficult to be measured since de-Broglie wavelength $\lambda = h/p$.

If a wave packet of associated particle is wide enough as shown in fig. b, wavelength can be estimated more accurately hence the momentum of the particle can be found out very accurately. But the position or location of the particle is anywhere within this wave group, indicating large uncertainty in location of particle.

Certainty in position involves uncertainty in momentum. Certainty in momentum involves uncertainty in position. This shows that it is impossible to know the location of a particle in a wave packet & its momentum accurately and simultaneously.

The Heisenberg's uncertainty principle states that "it is impossible to specify precisely and simultaneously the values of both members of particular pairs of physical variables that describes the behavior of an atomic system."

Qualitatively this principle states that the order of magnitude of the product of the uncertainties in the knowledge of two variables must be at least $h/2\pi$.

Considering the pair of physical variables as position and momentum, we have

$$\Delta p.\Delta x \geq \hbar ------(86)$$

where,

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

Δp is the uncertainty in determining the momentum.

Δx is the uncertainty in determining the position of the particle.

Similarly, we have

$$\Delta E.\Delta t \geq \hbar ------(87)$$

Where, ΔE is the uncertainty in determining the energy and Δt is the uncertainty in determining the time.

$$\Delta J.\Delta \theta \geq \hbar ------(88)$$

Where, ΔJ is the uncertainty in determining the angular momentum and $\Delta \theta$ is the uncertainty in determining the angle.

8.1 Mathematical Proof of HUP:

Heisenberg's uncertainty principle can be proved on the basis of de-Broglie's wave concept. According to de-Broglie's wave a material particle in motion is equivalent to the wave group or wave packet. The group velocity G being equal to the particle velocity V.

Consider a simple case of wave packet formed by superposition of two simple harmonic plane waves of equal amplitude 'a' and having nearly equal frequencies ω_1 and ω_2.

The two waves can be represented by the equations,

$$y_1 = a\sin(\omega_1 t - k_1 x) ------(89)$$

$$y_2 = a\sin(\omega_2 t - k_2 x) ------(90)$$

where k_1 & k_2 are their propagation constants and ω_1/k_1 & ω_2/k_2 are their respective phase velocities.

The resultant wave due to superposition of these waves is given by,

$$y = y_1 + y_2$$

$$y = a\sin(\omega_1 t - k_1 x) + a\sin(\omega_2 t - k_2 x)$$

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

$$y = 2a\sin[\omega t - kx]\cos\left[\frac{(\Delta\omega)t}{2} - \frac{(\Delta k)x}{2}\right] ------(91)$$

where, $\omega = \frac{(\omega_1+\omega_2)}{2}$, $k = \frac{(k_1+k_2)}{2}$, $\Delta\omega = \omega_1 - \omega_2$, $\Delta k = k_1 - k_2$.

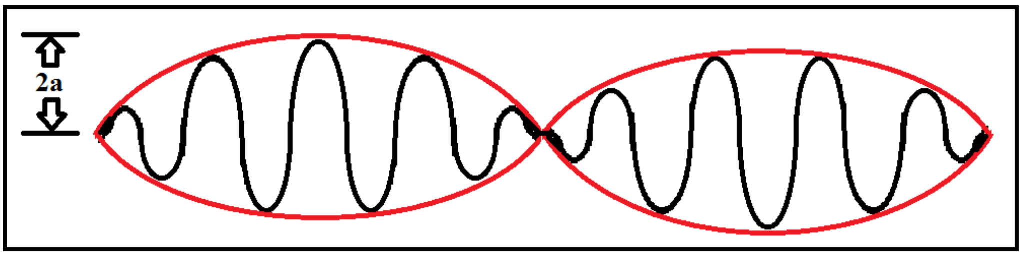


Figure 8: wave packets

The resultant wave is as shown in figure 8. Envelop of this wave travels with the group velocity G is given by,

$$G = \frac{\Delta\omega}{\Delta k} = \frac{\omega_1 - \omega_2}{k_1 - k_2} ------(92)$$

Since the group velocity of de-Broglie wave packet associated with the moving particle is equal to the particle velocity, the loop so formed is equivalent to the position of the particle. Then the particle may be anywhere within the loop.

Now condition of the formation of node from equation (91) is given by,

$$cos\left[\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right] = 0$$

$$i.e.\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right) = \frac{\pi}{2}, \frac{3\pi}{2}, \ldots, \frac{(2n+1)\pi}{2} ------(93)$$

where n = $0, 1, 2$.....

If x_1 and x_2 be the values of positions of two consecutive nodes, then from equation (93) by putting n and n+1, we get,

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_1 = \frac{(2n+1)\pi}{2} ------(94)$$

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_2 = \frac{(2n+3)\pi}{2} ------(95)$$

Subtracting equation (95) from (94) we get,

$$\frac{\Delta k}{2}(x_1 - x_2) = \pi$$

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

$$\therefore \Delta x = \frac{2\pi}{\Delta k} ------- (96)$$

But

$$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = \frac{2\pi p}{h} ------- (97)$$

Differentiating equation (97)

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

where Δp is the uncertainty in the measurement of momentum p.

From equation (96),

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

$$\Delta p \,.\, \Delta x = h$$

$$\therefore \Delta p \,.\, \Delta x \geq \hbar \,-------\, (98)$$

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

The sign $\geq$ is due to the fact that wave packets or wave groups may have different shapes.

8.2 Application of HUP:

A) Uncertainty principle applied to the pair of variable energy time:

Uncertainty in time and energy can be described with the help of Heisenberg's uncertainty principle.

Consider the particle of mass m and velocity v therefore it possess kinetic energy E which is given by,

$$E = \frac{1}{2}mv^2 \,-------\, (99)$$

In order to obtain the uncertainty in energy ΔE and time Δt, differentiate equation (99) we get,

$$\Delta E = \frac{1}{2}mv.2\Delta v = v\,(m.\Delta v) = v\,.\,\Delta p \,-------\, (100)$$

But we know that $v = \frac{\Delta x}{\Delta t}$ Hence equation (100) becomes,

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

$$\Delta E.\Delta t = \Delta x.\Delta p \,-------\, (101)$$

But according to the Heisenberg's uncertainty principle for position and momentum,

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

The equation (101) becomes,

$$\Delta E.\Delta t \geq \hbar \,-------\, (102)$$

Thus from above result it is seen that the product of uncertainties in energy and time measurement is of the order of Planck's constant.

B) Non Existence of Electron in the Nucleus:

The important results of atomic configuration can be verified by using uncertainty principle. In this sense we can prove that the electron cannot exist inside the nucleus.

We know that radius of the nucleus is 10^{-14}m and it is clear that, if the electron is to exist in the nucleus, then its uncertainty in its position will be equal to diameter of the nucleus which is $\Delta x \cong 2 \times 10^{-14}\ m$.

According to Heisenberg's Uncertainty principle, the uncertainty in momentum is given by,

$$\Delta x . \Delta p_x \geq \hbar$$

$$\Delta x . \Delta p_x \geq \frac{h}{2\pi}$$

$$\Delta p_x \geq \frac{h}{2\pi . \Delta x}$$

$$\Delta p_x \geq \frac{6.625 \times 10^{-34}}{2 \times 3.14 \times 2 \times 10^{-14}}$$

$$\therefore \Delta p_x \geq 5.275 \times 10^{-21}\ kg\frac{m}{s} - - - - - - - - (103)$$

This is the uncertainty in momentum of the electron. It means that momentum of the electron would not be less than Δp_x, rather it could be comparable to Δp_x.

$$p = 5.275 \times 10^{-21}\ kg\frac{m}{s}$$

The K.E. (E) of the electron can be obtained in terms of momentum as,

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m} - - - - - - - - (104)$$

$$E = \frac{(5.275 \times 10^{-21})^2}{2 \times 9.1 \times 10^{-31}}\ J$$

$$E = \frac{(5.275 \times 10^{-21})^2}{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19}}\ eV = 95.55 \times 10^6\ eV \approx 96\ MeV - - - - - (105)$$

From the above result, it is clear that the electrons inside the nucleus may exist only when it possess the energy of the order of 96 MeV. However the maximum possible K.E. of an electron emitted by radioactive nuclei is about 4 MeV. Hence it is concluded that the electron cannot reside inside the nucleus.

9.0 Wavefunction and its physical significance:

We are familiar with light wave, sound waves and water waves. A wave implies a variation of some quantity with space and time. A sound wave is characterized by the pressure or density variation in the medium. A light wave consists of variations of electric and magnetic field vectors in space. Then one question is raised that, what varies when a particle described by a wave or what constitutes the variation in case of matter waves.

The quantity whose variations make up matter waves is called as wave function and it is denoted by ψ.

ψ describes the wave as a function of position and time. However it has no direct physical significance, as it is not an observable quantity.

The value of wave function is related to the probability of finding the particle at a given place at a given time.

In general, ψ is a complex valued function. According to Heisenberg's Uncertainty principle, we can only know the probable value in the measurement. The probability cannot be negative. Hence ψ cannot be measure the presence of the particle at the location (x, y, z) but it is certain that it is in some way an index of the presence of the particle at around (x, y, z, t).

A probability interpretation of the wave function was given by Max Born in 1926. He suggested that the square of the magnitude of the wave function $|\psi|^2$ evaluated in a particular region represents the probability of finding the particle in that region.

Probability, P, of finding the particle in an infinitesimal volume dV (= dxdydz) is proportional to $|\psi\ (x,y,z)|^2$ dxdydz at time t.

$$P \propto |\Psi(x,y,z)|^2 dv - - - - - - - - (106)$$

$|\psi|^2$ is the probability density and ψ is the probability amplitude.

Since the particle is certainly somewhere in the space, the probability P = 1 and the integral of $|\psi|^2$ dV over entire space must be equal to unity.

$$\int_{-\infty}^{\infty} |\Psi|^2 dv = 1 - - - - - - - - (107)$$

The wave function ψ is in general a complex function. But the probability must be real. Therefore to make probability a real quantity, ψ is to be multiplied by its complex conjugate ψ*. The probability density in such a case is taken as ψ*.ψ

The quantity ψ*.ψ will be always a positive real quantity.

The quantity $|\psi|^2$ represents the probability density, is a positive real quantity, it can be replaced by $\psi^*.\psi$ if ψ is complex.

Since the probability of finding a particle somewhere is finite. We have the total probability over all space equal to unity.

$$\int_{-\infty}^{\infty} \Psi\Psi^* dv = 1 - - - - - - - - (108)$$

Equation (108) is called the normalization condition & a wave function that obeys this equation is said to be normalized.

Thus ψ has no physical significance but $|\psi|^2$ gives the probability of finding the atomic particle in a particular region.

Normalization Condition:

If at all the particle exists, it must be found somewhere in the universe. Since we are sure that the particle must be somewhere in space, the sum of all the probabilities over all values of x, y, z must be unity.

If ψ (x, y, z, t) is multiplied by a constant C such that,

ψN (x, y, z, t) = C ψ (x, y, z, t)

where ψN (x, y, z, t) satisfies the relation

$$\int_{-\infty}^{\infty} |\Psi_N(x,y,z,t)|^2 dxdydz = |C|^2 \int_{-\infty}^{\infty} |\Psi(x,y,z,t)|^2 dxdydz = 1 - - - - - - - - (109)$$

then ψN (x, y, z, t) is said to be normalized wave function and C is the normalized constant. This condition (109) is known as the normalization condition.

From equation (109) we have,

$$|C|^2 = \frac{1}{\int_{-\infty}^{\infty} |\Psi(x,y,z,t)|^2 dxdydz} - - - - - - - - (110)$$

$|\psi N$ (x, y, z, t)$|^2$dxdydz is called probability density.
Whenever wave function are normalized $|\psi|^2$dV equals to the probability that a particle will be found in an volume dV.
Thus probability P = $|\psi(x,y,z)|^2$dV

10.0 Schrödinger Wave Equations:

10.1 Schrödinger Time Dependent Wave Equation (for free particle in one dimension):

Consider a free particle moving with velocity v, momentum p = mv = h/λ and energy E in one direction i.e. in positive x-direction.

The free particle means no forces acting on it and its total energy is essentially kinetic, so that

$$E = \frac{1}{2}mv^2 = \frac{1}{2m}(m^2v^2) = \frac{p^2}{2m} - - - - - - - - (111)$$

But the de-Broglie waves associated with the moving particle due to the wave function ψ(r, t) also called continuous travelling harmonic wave having the wavelength (λ) and frequency (ν) can be described by,

$$p = \frac{h}{\lambda} = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \hbar k - - - - - - - - (112)$$

$$E = h\nu = \frac{h}{2\pi}2\pi\nu = \hbar\omega - - - - - - - - (113)$$

where, ħ = h / 2π, k = 2π / λ called the propagation constant and ω be the angular frequency of wave.

Combining eq. (111) & (113) we get,

$$E = \hbar\omega = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} - - - - - - - - (114)$$

Now there is a need of wave equation to describe the continuous travelling harmonic waves which will involve the equation (114) in it. The wave function ψ(r, t) must be harmonic one. Since such functions can be superimposed to form a wave packet representing the particle and will travel with velocity equal to the velocity of the particle i.e. wave packet velocity or group velocity ω = v, then it is expected to have one of the following forms:

$cos(kx - \omega t),\ sin(kx - \omega t), e^{i(kx-\omega t)}, e^{-i(kx-\omega t)}$ or some linear combination of them.

Also, the expected equation of ψ(r,t) must have two basic properties.

First, it must be linear, in order that the solution of it can be superposed to produce interference effects (in three dimensional case) and to be permit the construction of wave packets.

Second, the coefficient of equation must involve only constants such as mass and charge of the particle and not the parameters of the particular kind of motion of the particle.

To satisfy all these conditions, the suitable form of wave function out of these four forms is,

$$\Psi(x,t) = Ae^{i(kx-\omega t)} -------(115)$$

where, A constant called the amplitude of wave.

$$\Psi(x,t) = Ae^{i\left(\frac{p}{\hbar}x-\frac{E}{\hbar}t\right)} = Ae^{\frac{i}{\hbar}(px-Et)} -------(116)$$

Equation (116) is the mathematical description of wave which is equivalent of the unrestricted particle of total energy E and momentum p moving in positive x-direction.

Differentiating equation (116) w. r. t. x we get,

$$\frac{\partial\Psi}{\partial x} = Ae^{\frac{i}{\hbar}(px-Et)}\frac{ip}{\hbar} = \Psi\frac{ip}{\hbar} = \frac{i}{\hbar}p\Psi -------(117)$$

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

$$-i\hbar\frac{\partial\Psi}{\partial x} = p\Psi -------(118)$$

Differentiating equation (118) w. r. t. x we get,

$$-i\hbar\frac{\partial^2\Psi}{\partial x^2} = p\frac{\partial\Psi}{\partial x} = p\left(\frac{i}{\hbar}p\Psi\right)$$

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

$$-\hbar^2\frac{\partial^2\Psi}{\partial x^2} = p^2\Psi -------(119)$$

Dividing 2m on both sides, where m is the mass of particle in motion, we get

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = \frac{p^2\Psi}{2m} = E\Psi -------(120)$$

Again differentiating equation (116) w. r. t. t we get,

$$\frac{\partial\Psi}{\partial t} = Ae^{\frac{i}{\hbar}(px-Et)}\left(-\frac{i}{\hbar}E\right) = -\Psi\frac{i}{\hbar}E$$

$$i\hbar\frac{\partial\Psi}{\partial t}=E\Psi - - - - - - - - (121)$$

Comparing equation (120) & (121) we get,

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} - - - - - - - - (122)$$

Equation (122) is the Schrödinger's wave equation for a free particle moving in positive x-direction (i.e. in one dimension)

10.2 Schrödinger Time Dependent Wave Equation (for particle under external force in one dimension):

When a particle moves in the positive x direction under influence of external force, like one dimensional motion of electron in a crystal under the influence of nuclear potential field.

The total energy E of the particle is given by,

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

$$E=\frac{1}{2}mv^2+V(x,t)$$

$$E=\frac{p^2}{2m}+V(x,t) - - - - - - - - (123)$$

Multiplying ψ on both sides of equation (123), we get

$$E\Psi=\left[\frac{{p_x}^2}{2m}+V(x,t)\right]\Psi$$

Replacing the dynamical variables by their operators in equation (123) we get

$$\hat{E}\Psi=\left[\frac{{\hat{p}_x}^2}{2m}+\hat{V}(x,t)\right]\Psi$$

Or

$$i\hbar\frac{\partial\Psi}{\partial t}=\left[\frac{\left(-i\hbar\frac{\partial}{\partial x}\right)^2}{2m}+V(x,t)\right]\Psi$$

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x,t)\Psi \text{ ------- } (124)$$

Equation (124) is the Time-dependent Schrödinger's wave equation for the particle under the influence of external force in one dimension.

10.3 Schrödinger Time Dependent Wave Equation (for particle under external force in three dimensions):

In this case the particle move in any direction under the influence of external force, therefore the total energy E of the particle is given by,

$$E = \frac{p^2}{2m} + V(\bar{r},t) \text{ ------- } (125)$$

where,

$\bar{r} = ix + jy = kz$ be the position vector of particle,

$p^2 = {p_x}^2 + {p_y}^2 + {p_z}^2$ components of momentum.

Multiplying ψ(r, t) on sides of equation (125) and writing in terms of operators is given as,

$$\hat{E}\Psi(r,t) = \left[\frac{\hat{p}^2}{2m} + \hat{V}(r,t)\right]\Psi(r,t)$$

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t) = \left[\frac{1}{2m}\left({\hat{p}_x}^2 + {\hat{p}_y}^2 + {\hat{p}_z}^2\right) + \hat{V}(r,t)\right]\Psi(r,t)$$

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t) = \left\{\frac{1}{2m}\left[\left(-i\hbar\frac{\partial}{\partial x}\right)^2 + \left(-i\hbar\frac{\partial}{\partial y}\right)^2 + \left(-i\hbar\frac{\partial}{\partial z}\right)^2\right] + \hat{V}(r,t)\right\}\Psi(r,t)$$

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t) = \left\{-\frac{\hbar^2}{2m}\left[\left(\frac{\partial^2}{\partial x^2}\right) + \left(\frac{\partial^2}{\partial y^2}\right) + \left(\frac{\partial^2}{\partial z^2}\right)\right]\Psi(r,t) + \hat{V}(r,t)\Psi(r,t)\right\}$$

$$i\hbar\frac{\partial}{\partial t}\Psi(r,t) = -\frac{\hbar^2}{2m}\nabla^2\Psi(r,t) + \hat{V}(r,t)\Psi(r,t) \text{ ------- } (126)$$

where $\nabla^2 = \left(\frac{\partial^2}{\partial x^2}\right) + \left(\frac{\partial^2}{\partial y^2}\right) + \left(\frac{\partial^2}{\partial z^2}\right)$ called the Laplacian Operator in cartesian coordinates.

$$\nabla^2\Psi(r,t) + \frac{2m}{\hbar^2}\left[E - \hat{V}(r,t)\right]\Psi(r,t) = 0 \text{ ------- } (127)$$

Equations (126) & (127) are the Time-dependent Schrödinger's wave equation in three dimensions for non-relativistic velocity of the particle.

10.4 Schrödinger Time Independent Wave Equation:

The wave function ψ involved in equation (124) & (126) contains all information regarding a quantum mechanical system. We have seen that in such a system the total probability of finding the particle does not change with time, although it can state where the probability density at each point remains independent of time and in consequence of this, expectation or average values of all dynamical variables are also constant in time. Such states are called stationary states and the wave function ψ, the stationary state solution. Such states also possess a definite constant value of energy and the potential field in which the particle moves does not depend on time i.e. it is only a function of position vector r. The corresponding wave equation is called the stationary state Schrödinger wave equation or time-independent Schrödinger wave equation.

Now when the P.E. of the particle is independent of time and probability density of finding the particle is constant or independent of time, equation (126) decomposes into two ordinary differential equations,

One in the space variables (x,y,z) and other in time t. This separation can be done by the method of separation of variables.

Therefore, the general wave function ψ(r,t) may be written as

$$\Psi(x,y,z,t) = \Psi(\bar{r},t) = \Psi(r).f(t) - - - - - - - (128)$$

ψ(r) is the function of r and f(t) is the function of t only.

Using equation (128) in equation (126) we get,

$$i\hbar\frac{\partial}{\partial t}[\Psi(r).f(t)] = -\frac{\hbar^2}{2m}\nabla^2[\Psi(r).f(t)] + \hat{V}(r,t)[\Psi(r).f(t)]$$

$$i\hbar\Psi(r)\frac{\partial}{\partial t}f(t) = -\frac{\hbar^2}{2m}f(t)\nabla^2\Psi(r) + \hat{V}(r,t)[\Psi(r).f(t)]$$

Dividing throughout by ψ(r).f(t), we get,

$$i\hbar\frac{1}{f(t)}\frac{\partial}{\partial t}f(t) = -\frac{\hbar^2}{2m}\frac{1}{\Psi(r)}\nabla^2\Psi(r) + \hat{V}(r,t) - - - - - - (129)$$

In this equation LHS depends only on t & RHS only on ŕ i.e. x,y,z.

However, ŕ & t are independent of each other. Hence equation (129) can be true only if each side is equal to some constant.

We denote this constant by E, which has the dimensions of energy of the system.

$$R.H.S. = -\frac{\hbar^2}{2m}\frac{1}{\Psi(r)}\nabla^2\Psi(r) + \hat{V}(r,t) = E$$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(r) + \hat{V}(r,t)\Psi(r) = E\Psi(r) ------(130)$$

$$\hat{H}\Psi(r) = E\Psi(r) ------(131)$$

$$Where, \hat{H} = Hamiltonian\ Operator = -\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(r,t)$$

$$Corresponding\ to\ the\ energy\ E = T + \hat{V}(r,t) = \frac{P^2}{2m} + \hat{V}(r,t)$$

Equation (130) may be written as,

$$\nabla^2\Psi(r) + \frac{2m}{\hbar^2}\left[E - \hat{V}(r,t)\right]\Psi(r) = 0 ------(131)$$

Equation (131) is called Time-independent Schrödinger's wave equation. In this equation the potential V is independent of time.

11.0 Eigenvalues and Eigenfunction:

If ψ be a well behaved function of the state of the system and this be operated by the operator Â so that it satisfies the equation.

$$\hat{A}\Psi(x) = \lambda\Psi(x)$$

Then we say that the number λ is an Eigen value of the operator Â and the operand ψ(x) is an Eigenfunction of the operator Â and the Eigen value λ & Eigenfunction ψ(x) of the operator Â belongs to each other.

e.g. If sin4x is well behaved function and is operated by an operator $\frac{d^2}{dx^2}$ it gives the following result.

$$\frac{d^2}{dx^2}(sin4x) = -16(sin4x)$$

Here -16 is the Eigen value of the operator $\frac{d^2}{dx^2}$ and operand (sin4x) is an Eigen function of an operator $\frac{d^2}{dx^2}$. And that the Eigen value -16 and Eigen function (sin4x) of the operator $\frac{d^2}{dx^2}$ belongs to each other.