Unit-4

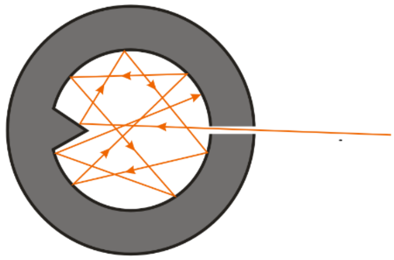
Quantum Mechanics

Syllabus:

Black body radiation, ultraviolet catastrophe, Crompton effect, plates theory of radiation, phase and group velocity, particle in a box, uncertainty principle, well-behaved wave equation, Schrodinger equation, application to particle in a box.

Black body:

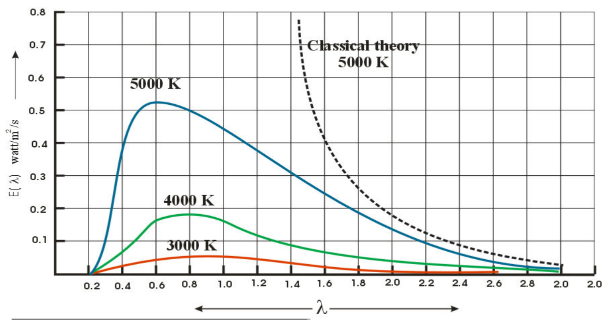
A black body is one which absorbs all types of heat radiation incident on it when radiations are permitted to fall on black body they are neither reflected nor transmitted.
A black body is known as black body due to the fact that whatever may the colour of the incident radiation the body appears black by absorbing all kind of radiations incident on it.
A perfect black does not exists thus a body representing close proximity to perfect black body so it can be considered as a black body.
A hollow sphere is taken with fine hole and a point projection in front of the hole and is coated with lamp black on its inner surface shows the close proximity to the black body, when the radiation enter through hole, they suffer multiple reflection and are totally absorbed.



Figure(1): Black body

Black Body radiation:

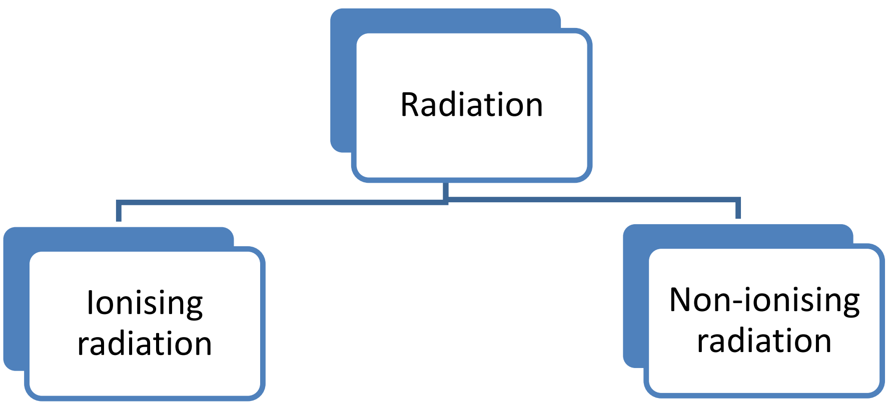
A body which completely absorbs radiation of all radiations of all wavelength/frequencies incident on it and emits all of them when heated at higher temperature is called black body. The radiation emitted by such a body is called black body radiation. So the radiation emitted form a black body is a continuous spectrum i.e. it contains radiation of all the frequencies.
Distributions of the radiant energy over different wavelength in the black body radiation at a given temperature are shown in the figure.
Black body radiation is a common synonym for thermal radiation.



Figure(2): Black body radiation

Radiation:

Radiation is a process which the surface of an object radiates its thermal energy in the form of the electromagnetic waves.



Radiations are of two types

Emissivity:

The emissivity of a material is the irradiative power of its surface to emit heat by radiation, usually it is shown by e or ε. It is the ratio of energy radiated by a material to the energy radiated by the black body.
True black body has maximum emissivity $\varepsilon = 1$ (highly polished silver has an emissivity for about 0.02 at least.)

Plank's Quantum Hypothesis:

Plank assumes that the atoms of the wall of blackbody behave as an oscillator and each has a characteristic frequency of oscillation. He made the following assumption-

1) An oscillator can have any arbitrary value of energy but can have only discrete energies as per the following relation
$$E = nh\nu$$
Where $n = 0,1,2,3$ and ν and h are known as frequency and Plank's constant.
2) The oscillator can absorb or emit energy only in the form of packets of energy $(h\nu)$ but not continuously.
$$\Delta E = \Delta h\nu$$

Average energy of Plank's Oscillators:

If N be the total number of oscillations and E as the total energy of these oscillators, then average energy will be given by the relation.

$$\bar{E} = \frac{E}{N} \quad \ldots\ldots\ldots \quad (1)$$

Now consider $N_0, N_1, N_2 \ldots \ldots \ldots N_n$ as the number of oscillators having the energy values $0, h\nu, 2h\nu \ldots nh\nu$ respectively. Then by the Maxwell's distribution formula

$$N = N_0 + N_1 + N_2 + \cdots \ldots \ldots \ldots \ldots ..$$

$$N = N_0\left(1 + e^{-\frac{h\nu}{kT}} + e^{-\frac{2h\nu}{kT}} + \cdots \ldots \ldots .\right)$$

$$N = \frac{N_0}{\left(1 - e^{-\frac{h\nu}{kT}}\right)} \quad \ldots\ldots\ldots \quad (2)$$

And the total energy

$$E = (N_0 \times 0) + (N_1 \times h\nu) + (N_2 \times 2h\nu) + \cdots \ldots .$$

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

$$E = N_0 e^{-\frac{h\nu}{kT}} \times \left[h\nu + 2e^{-\frac{h\nu}{kT}} + 3e^{-\frac{2h\nu}{kT}} + \cdots \ldots\right] . . .$$

$$E = N_0 e^{-\frac{h\nu}{kT}} \frac{h\nu}{\left(1 - e^{-\frac{h\nu}{kT}}\right)^2} \quad \ldots\ldots\ldots \quad (3)$$

Putting the value of N and E from above equations in equation (1) we get-

$$\bar{E} = \frac{E}{N}$$

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

$$\bar{E} = \frac{h\nu}{\left(e^{\frac{h\nu}{kT}} - 1\right)} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (4)$$

This is the expression for the average energy in Plank's oscillators.

Plank's radiation formula:

The average density of radiation (u_ν) in the frequency range ν and $\nu + d\nu$ depending upon the average of an oscillator is given by-

$$u_\nu d\nu = \frac{8\pi\nu^2}{c^3} d\nu \times \bar{E} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (5)$$

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

$$u_\nu d\nu = \frac{8\pi h}{c^3} \frac{\nu^3}{\left(e^{\frac{h\nu}{kT}} - 1\right)} d\nu \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (6)$$

The above relation is known as the Plank's radiation formula in terms of the frequency. This law can also be expressed in terms of wavelength λ of the radiation. Since $\nu = \frac{c}{\lambda}$ for electromagnetic radiation, $d\nu = -\frac{c}{\lambda^2} d\lambda$. Further we know that the frequency is reciprocal of wavelength or in other words an increase in frequency corresponds to a decrease in wavelength. therefore

$$u_\lambda d\lambda = -u_\nu d\nu$$

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

$$u_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} \frac{1}{\left(e^{\frac{hc}{\lambda kT}} - 1\right)} d\lambda \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (7)$$

The above relation is known as the Plank's law in terms of wavelength (λ)

Wien's law and Rayleigh-Jeans law:

With the help of Plank's radiation Wien's law and Rayleigh-Jens law can be derive. When the wavelength (λ) and temperature (T) are very small, then $e^{\frac{hc}{\lambda kT}} \gg 1$. Therefore, 1 can be neglected in the denominator of equation (7).

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

By substituting $8\pi hc = A$ and $\frac{hc}{k} = B$, we get

$$u_\lambda d\lambda = \frac{A}{\lambda^5} e^{-\frac{B}{\lambda T}} d\lambda \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (8)$$

This is known as Wien's law, which is valid at low temperature T and small wavelength λ.

For higher temperature T and large wavelength λ, $e^{\frac{hc}{\lambda kT}}$ can be approximated to $1 + \frac{hc}{\lambda kT}$. Then we have from equation (7)

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

$$u_\lambda d\lambda = \frac{8\pi kT}{\lambda^4} d\lambda \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (9)$$

This is known as Rayleigh-Jeans law.

Ultraviolet Catastrophe:

One of the nagging questions at the time concerned the spectrum of radiation emitted by a so-called black body. A perfect black body is an object that absorbs all radiation that is incident on it. Perfect absorbers are also perfect emitters of radiation, in the sense that heating the black body to a particular temperature causes the black body to emit radiation with a spectrum that is characteristic of that temperature. Examples of black bodies include the Sun and other stars, light bulb filaments, and the element in a toaster. The colours of these objects correspond to the temperature of the object. Examples of the spectra emitted by objects at particular temperatures are shown in Figure 3

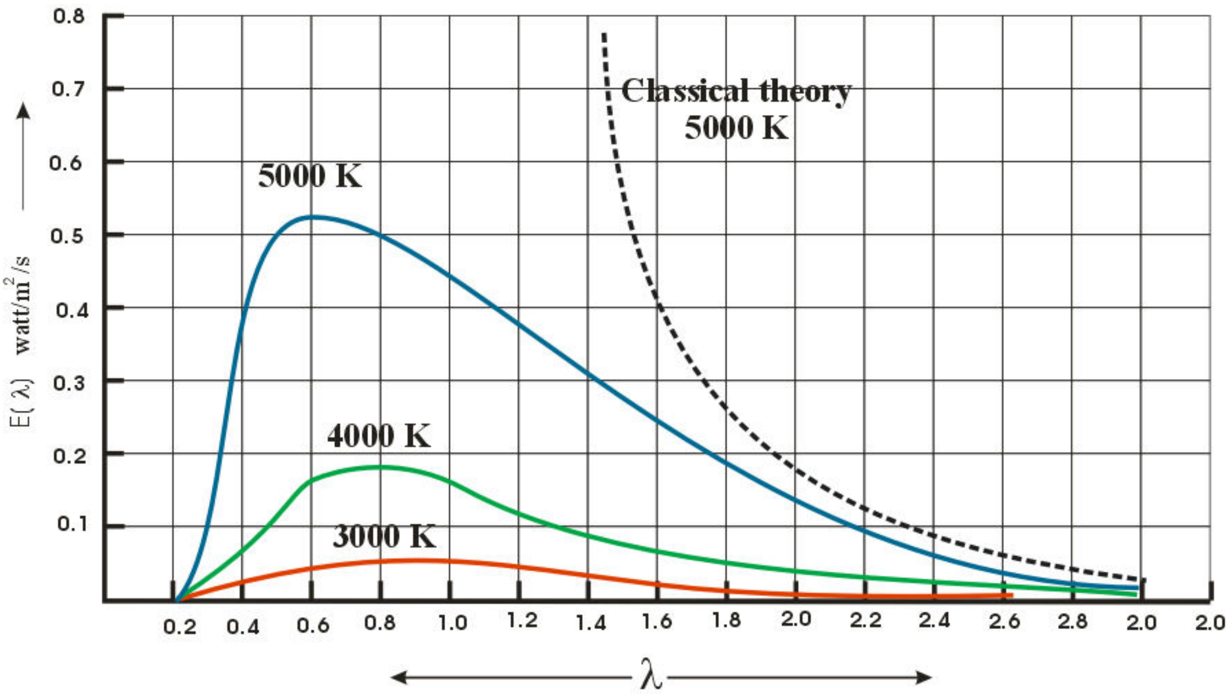


Figure 3: The spectra of electromagnetic radiation emitted by hot objects. Each spectrum corresponds to a particular temperature. The black curve(dotted line) represents the predicted spectrum of a 5000 K black body, according to the classical theory of black bodies

At the end of the 19th century, the puzzle regarding blackbody radiation was that the theory regarding how hot objects radiate energy predicted that an infinite amount of energy is emitted at small wavelengths, which clearly makes no sense from the perspective of energy conservation. Because small wavelengths correspond to the ultraviolet end of the spectrum, this puzzle was known as the ultraviolet catastrophe. Figure 27.1 shows the issue, comparing the theoretical predictions to the actual spectrum for an object at a temperature of 5000 K. There is clearly a substantial disagreement between the curves

Matter wave:

According to Louis de-Broglie every moving matter particle is surrounded by a wave whose wavelength depends up on the mass of the particle and its velocity. These waves are known as matter wave or de-Broglie waves.

Wavelength of the de-Broglie wave:

Consider a photon whose energy is given by $E = h\vartheta = \frac{hc}{\lambda}$ $[\because c = \vartheta\lambda]$ .... (1)

Where h is Plank's constant $6.623 \times 10^{-34} J\ sec$, ϑ is the frequency and λ is the wavelength of photon. Now by Einstein's mass energy relation

$$E = mc^2 \qquad \text{..} \quad (2)$$

By equation (1) and (2)

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

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

$$\lambda = \frac{h}{p} \qquad \text{Where } p = r$$

In place of the photon a material particle of mass m is moving with velocity v then

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

(i)

Now we know that the kinetic energy of the material particle of mass m moving with velocity ϑ is given by-

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

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

$$E = \frac{p^2}{2m} \qquad [\because p = n$$

$$p = \sqrt{2mE}$$

So by equation (3)

$$\lambda = \frac{h}{\sqrt{2mE}}$$

(ii)

According to kinetic theory of gasses the average kinetic energy of the material particle is given by $E = \frac{3}{2} KT$ where $K = 1.38 \times 10^{-23} J/K$ i.e. Boltzmann constant

$$\frac{1}{2}mv^2 = \frac{3}{2}KT$$

$$m^2v^2 = 3mKT$$

$$P^2 = 3mKT \qquad \boxed{\because E \ \frac{1}{2}mc^2}$$

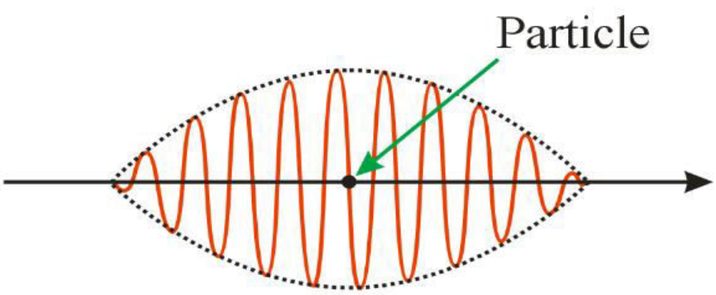
$$p = \sqrt{3mKT}$$

So by equation (3)

$$\lambda = \frac{h}{\sqrt{3mKT}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (4)$$

Group or Envelope of the wave:

When a mass particle moves with some velocity than it emits the matter waves, those waves interacts each other and where there they interfere constructively they form an envelope around the particle which is known as wave group or simply envelope.



Figure(2): Formation of the wave packet

Group velocity:

Group velocity of a wave is the velocity with which the overall shape of the wave's amplitudes (modulation or envelope) of the wave propagates through space. It is denoted by v_g.

Phase velocity:

The phase velocity of a wave is the rate at which the phase or the wave propagates in the space. It is denoted by v_p.

Expression for Group velocity and phase velocity:

Let us suppose that the wave group arises from the combination of two waves that have some amplitude A but differ by an amount $\Delta\omega$ in angular frequency and an mount Δk in wave number.

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

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

By the principle of superposition

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

$$y = A[\cos(\omega t - kx) + \cos\{(\omega + \Delta\omega)t - (k + \Delta k)x\}]$$

Using the identity

$$\cos A + \cos B = 2\cos\left(\frac{A+B}{2}\right)\cos\left(\frac{A-B}{2}\right)$$

And $\cos(-\theta) = \cos\theta$

$A + B = \frac{(\omega t - kx) + \{\omega t + \Delta\omega t - kx - \Delta kx\}}{2}$	$A - B = \frac{(\omega t - kx) - \{\omega t + \Delta\omega t - kx - \Delta kx\}}{2}$
$A + B = \frac{2\omega t - 2kx + \Delta\omega t - \Delta kx}{2}$	$A - B = \frac{\omega t - kx - \omega t - \Delta\omega t + kx + \Delta kx}{2}$
$A + B = \frac{2\omega t + \Delta\omega t - 2kx - \Delta kx}{2}$	$A - B = \frac{-\Delta\omega t + \Delta kx}{2}$
$A + B = \frac{(2\omega + \Delta\omega)t - (2k + \Delta k)x}{2}$	$A - B = -\frac{\Delta\omega t - \Delta kx}{2}$

$$y = A\left[2\cos\left\{\frac{(2\omega + \Delta\omega)t - (2k + \Delta k)x}{2}\right\} \cdot \cos\left\{\frac{\Delta\omega t - \Delta kx}{2}\right\}\right]$$

Let $2\omega + \Delta\omega = 2\omega$ and $2k + \Delta k = 2k$

So we have

$$y = 2A\left[\cos\left(\frac{2\omega t - 2kx}{2}\right) \cdot \cos\left(\frac{\Delta\omega t - \Delta kx}{2}\right)\right]$$

$$\Rightarrow \quad y = 2A\left[\cos(\omega t - kx)\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)\right] \ldots\ldots\ldots\ldots\ldots \quad (4)$$

This is the resultant wave equation of superposition of two waves having the amplitude $2A\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)$ and phase $\cos(\omega t - kx)$ where ω and k are mean values of angular frequency and prapogation constant of the wave.

Phase velocity:

Since phase $\omega t - kx = constant$

Differentiating with respect to t we get

$$\omega dt - k\,dx = 0$$

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

But $v_p = \frac{dx}{dt}$ phase velocity

$$\Longrightarrow \quad v_p = \frac{dx}{dt} = \frac{\omega}{k} \quad \text{...} \quad (5)$$

Group Velocity:

$$\Longrightarrow \quad \frac{\Delta\omega}{2}dt \quad \frac{\Delta k}{2}dx = 0$$

$$\Longrightarrow \quad \frac{\Delta\omega}{2}dt = \frac{\Delta k}{2}dx$$

$$\Longrightarrow \quad \frac{\Delta\omega}{\Delta k} = \frac{dx}{dt}$$

So the group velocity

$$v_g = \frac{dx}{dt} = \frac{d\omega}{dk} \quad \text{...} \quad (6)$$

Relation between Group velocity and phase velocity

1. For dispersive and non-dispersive medium:

But by equation (5) i.e. $v_p = \frac{\omega}{k} \Longrightarrow \quad \omega = k v_p$

Putting into equation (6) we get

$$\Longrightarrow \quad v_g = \frac{d(k v_p)}{dk}$$

$$\Longrightarrow \quad v_g = v_p .\ 1 + k\frac{dv_p}{dk}$$

$$\Longrightarrow \quad v_g = v_p + \left(\frac{2\pi}{\lambda}\right)\frac{dv_p}{d\left(\frac{2\pi}{\lambda}\right)}$$

$$\Longrightarrow \quad v_g = v_p + \left(\frac{\cancel{2\pi}}{\lambda}\right)\frac{dv_p}{\cancel{2\pi}\, d(\lambda^{-1})}$$

$$\Longrightarrow \quad v_g = v_p + \left(\frac{1}{\lambda}\right)\left(\frac{dv_p}{(-\lambda^{-2}).\ d\lambda}\right)$$

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

Different cases:

1) If $\frac{dv_p}{d\lambda} = 0$ i.e. if the phase velocity does not depends on the wavelength then $v_g = v_p$ such a medium is called the non dispersive medium.

2) If $\frac{dv_p}{d\lambda} \neq 0$ i.e. if it has positive values then $v_g < v_p$ then such a medium is called the dispersive medium.

2. Relativistic particle:

Let us consider a de-Broglie wave associated with a moving particle of rest mass m_0 and velocity v, then the ω and k will be given by

$$\Longrightarrow \quad \omega = 2\pi\vartheta$$

$$\Longrightarrow \quad \omega = \frac{2\pi mc^2}{h} \qquad \boxed{\because \ \vartheta = \frac{mc^2}{h}}$$

$$\Longrightarrow \quad \omega = \frac{2\pi c^2}{h} . \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \qquad (8)$$

And

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

$$\Longrightarrow \quad k = \frac{2\pi}{\left(\frac{h}{mv}\right)} \qquad \boxed{\because \ \lambda = \frac{h}{mv}}$$

$$\Rightarrow \quad k = \frac{2\pi m_0 v}{h\sqrt{1-\frac{v^2}{c^2}}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots (9) \qquad \boxed{\because \quad m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}}$$

Now phase velocity $v_p = \frac{\omega}{k}$

So

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

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

$$v_p = \frac{c^2}{v} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (10)$$

Now group velocity $v_g = \frac{d\omega}{dk}$

The expression can be written as

$$v_g = \frac{\left(\frac{d\omega}{dv}\right)}{\left(\frac{dk}{dv}\right)} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (11)$$

In order to find the value of v_g we have to solve the following terms-

$$\Rightarrow \quad \frac{d\omega}{dv} = \frac{d}{dv}\left[\frac{2\pi c^2}{h} . \frac{m_0}{\sqrt{1 \quad \frac{v^2}{c^2}}}\right] \qquad \boxed{\text{[By equation (8)]}}$$

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

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

$$\Rightarrow \quad \frac{d\omega}{dv} = \frac{2\pi c^2 m_0}{h}\left(\frac{v}{c^2}\right)\left(1 \quad \frac{v^2}{c^2}\right)^{-\frac{3}{2}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (12)$$

Again

$$\Rightarrow \quad \frac{dk}{dv} = \frac{d}{dv}\left[\frac{2\pi m_0 v}{h\sqrt{1 \quad \frac{v^2}{c^2}}}\right]$$

$$\Rightarrow \quad \frac{dk}{dv} = \frac{2\pi m_0}{h}\left[\frac{d}{dv}\frac{v}{\sqrt{1 \quad \frac{v^2}{c^2}}}\right]$$

$$\Rightarrow \qquad \frac{dk}{dv} = \frac{2\pi m_0}{h} . \left[\frac{\sqrt{1 \quad \frac{v^2}{c^2}} . \quad 1 \quad \frac{1}{2}\left(1. \quad \frac{v^2}{c^2}\right)^{-\frac{1}{2}} . \quad \left(\frac{2v}{c^2}\right)}{\left(1 \quad \frac{v^2}{c^2}\right)} \right]$$

$$\Rightarrow \qquad \frac{dk}{dv} = \frac{2\pi m_0}{h} . \left[\frac{\sqrt{1 \quad \frac{v^2}{c^2}} \quad + \frac{v^2}{c^2} . \frac{1}{\sqrt{1 \quad \frac{v^2}{c^2}}}}{\left(1 \quad \frac{v^2}{c^2}\right)} \right]$$

$$\Rightarrow \qquad \frac{dk}{dv} = \frac{2\pi m_0}{h} . \left[\frac{1 \quad \frac{v^2}{c^2} + \frac{v^2}{c^2}}{\left(\frac{1 \quad -^2}{c^2}\right) v \sqrt{1 \quad \frac{v^2}{c^2}}} \right]$$

$$\Rightarrow \qquad \frac{dk}{dv} = \left[\frac{2\pi m_0}{h} \left(\frac{1 \quad -^2}{c^2}\right)^{-\frac{3}{2}} v^2 \right] \qquad \ldots\ldots\ldots\ldots\ldots\ldots \qquad (13)$$

Putting the value from (13) and (14) into (11) we get

$$\Rightarrow \qquad v_g = \left[\frac{\left\{ \frac{2\pi c^2 m_0}{h} \left(\frac{v}{c^2}\right) \quad \left(1 \quad \frac{v^2}{c^2}\right)^{-\frac{3}{2}} \right\}}{\left\{ \frac{2\pi m_0}{h} \left(1 \quad \frac{v^2}{c^2}\right)^{-\frac{3}{2}} \right\}} \right]$$

Group velocity $\qquad v_g = v \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \qquad (14)$

By equation (10) we have

$$v_p . \quad \imath = c^2$$

By equation (14) i.e. $v_g = \quad v$

So $\qquad v_p . \; {}_g v = c^2$

3. Non-Relativistic free Particle:

According to the de-Broglie hypothesis

$$\lambda = \frac{h}{m v_g}$$

Now the total energy

$$E = \frac{1}{2} m v_g^2 \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \qquad (1)$$

And $\qquad E = h\vartheta \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \qquad (2)$

By equation (1) and (2)

$$h\vartheta = \frac{1}{2} m v_g^2$$

$$h\vartheta = \frac{mv_g^2}{2h}$$

And phase velocity $v_p = \vartheta\lambda$

So we have

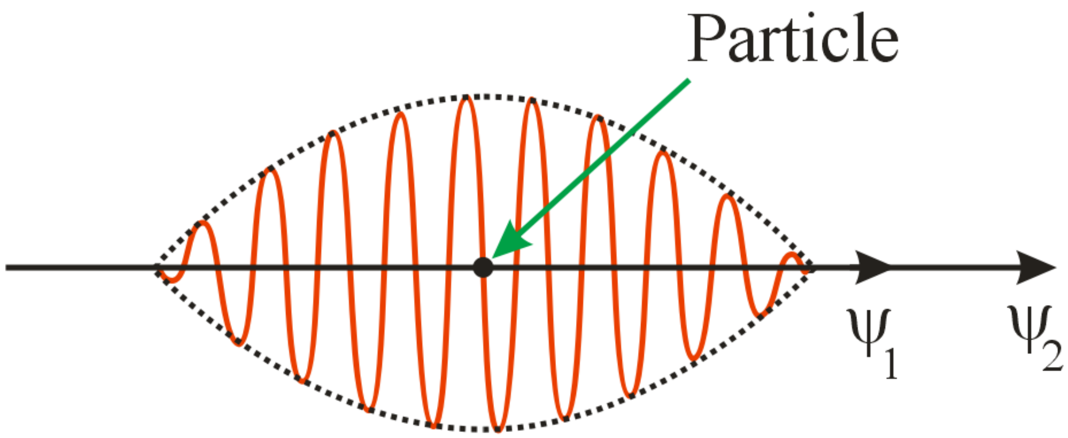
$$v_p = \frac{mv_g^2}{2h} \times \frac{h}{mv_g}$$

$$v_p = \frac{v_g}{2}$$

Uncertainty Principle:

It is impossible to determine the exact position and momentum of a particle simultaneously.

Let us consider a particle surrounded by a wave group of de-Broglie wave as shown in the figure



Figure(3): particle surrounded by a wave packet

Let us consider two such waves of angular frequency ω_1 and ω_2 and prapogation constant k_1 and k_2 traviling along the same direction are-

$$\psi_1 = A \sin(\omega_1 t - k_1 x) \quad \text{..........} \quad (1)$$

$$\psi_2 = A \sin(\omega_2 t - k_2 x) \quad \text{..........} \quad (2)$$

According to the principal of superposition

$$\psi = \psi_1 + \psi_2$$

$$\psi = A \sin(\omega_1 t - k_1 x) + A \sin(\omega_2 t - k_2 x)$$

$$\psi = A[\sin(\omega_1 t - k_1 x) + \sin(\omega_2 t - k_2 x)]$$

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

$$\because \sin C + \sin D = 2 \sin\left(\frac{C+D}{2}\right) \cos\left(\frac{C-D}{2}\right)$$

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

Let $\omega = \frac{\omega_1 + \omega_2}{2}$

And $k = \frac{k_1 + k_2}{2}$

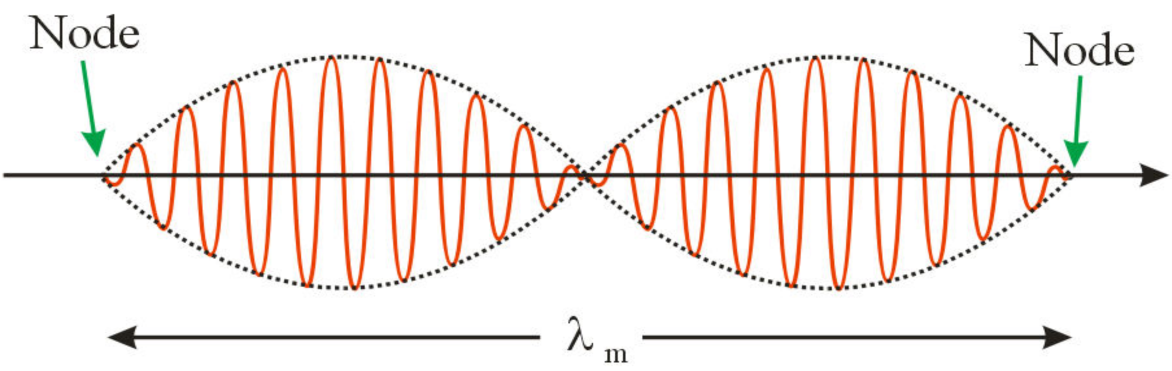
And $\Delta\omega = \omega_1 - \omega_2$

And $\Delta k = k_1 - k_2$ .... (3)

So we have

$$\psi = 2A\left[\sin(\omega t - kx)\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)\right] \quad \text{.. (4)}$$

The resultant wave is plotted in the figure (4). The position of the particle cannot be given with certainty it is somewhere between the one node and the next node. So the error in the measurement of the position of the particle is therefore equal to the distance between these two nodes.



Figure(4): The envelope created by the superposition of two waves.

The node is formed when

$$\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right) = 0 \qquad \because \cos A = 0 \Rightarrow A = (2n+1)\frac{\pi}{2}$$

$$\Rightarrow \quad \frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x = (2n+1)\frac{\pi}{2}$$

Thus x_1 and x_2 represents the positions of two successive nodes, then at any instant t, we get-

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_1 = (2n+1)\frac{\pi}{2} \quad \text{.. (5)}$$

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_2 = (2n+3)\frac{\pi}{2} \quad \text{.. (6)}$$

Now on subtracting (5) from (6) we get

$$\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x_2 - \frac{\Delta\omega}{2}t + \frac{\Delta k}{2}x_1 = 2n.\frac{\pi}{2} + \frac{3\pi}{2} - 2n.\frac{\pi}{2} - \frac{\pi}{2}$$

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

$$\Delta k\, \Delta x = 2\pi \quad \text{.. (7)}$$

But $k = \frac{2\pi}{\lambda_m}$

$$\Delta\left(\frac{2\pi}{\lambda_m}\right)\ \Delta x = 2\pi$$

Again $\lambda_m = \frac{h}{mv} = \frac{h}{p}$

So $$2\pi\,\Delta\left\{\frac{1}{\left(\frac{h}{p}\right)}\right\}\Delta x = 2\pi$$

$$\frac{1}{h}.\ \Delta p.\ \Delta x = 1$$

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

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

Where $\hbar = h/2\pi$

Energy and time uncertainty principle:

Let Δx be the width of the wave packet moving along the x-axis, let v_g be the group velocity of the wave packet and v_x is the particle velocity along x-axis. Now if the wave packet moves through Δx in Δt time. Since Δx is the uncertainty in the x-coordinates of the particle and Δt is the uncertainty in the time i.e. given by

$$\Delta t = \frac{\Delta x}{v_g}$$

$$\Delta x = v_g.\ \Delta t \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (1)$$

If the rest mass of the particle is m_0 then the kinetic energy is given by

$$E = \frac{1}{2}m_0 v_x^2$$

$$E = \frac{1}{2m_0}.\ m_0^2 v_x^2$$

$$E = \frac{1}{2m_0}.\ (m_0 v_x)^2$$

$$E = \frac{1}{2m_0}.\ p_x^2$$

$$E = \frac{p_x^2}{2m_0} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (2)$$

If Δp_x and ΔE are the uncetainity in the momentum and energy respectively, then differentiating (2) we get

$$\Delta E = \frac{2p_x.\Delta p_x}{2m_0}$$

$$\Delta E = \frac{p_x.\Delta p_x}{m_0}$$

$$\Delta P_x = \frac{m_0 \Delta E}{p_x}$$

But $p_x = m_0 v_x$

So $$\Delta P_x = \frac{m_0}{m_0 v_x}\Delta E \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (3)$$

Now by(1) and (3)

$$\Delta x.\ \Delta p_x = v_g.\ \Delta t.\ \frac{1}{v_x}\Delta E$$

But $v_g = v_x$ so we have

$$\Delta x \Delta p_x = \Delta t. \ \Delta E \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (4)$$

We know that

$$\Delta x \Delta p_x \geq \hbar \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (5)$$

So by (4) and (5)

$$\Delta t. \ \Delta E \geq \hbar$$

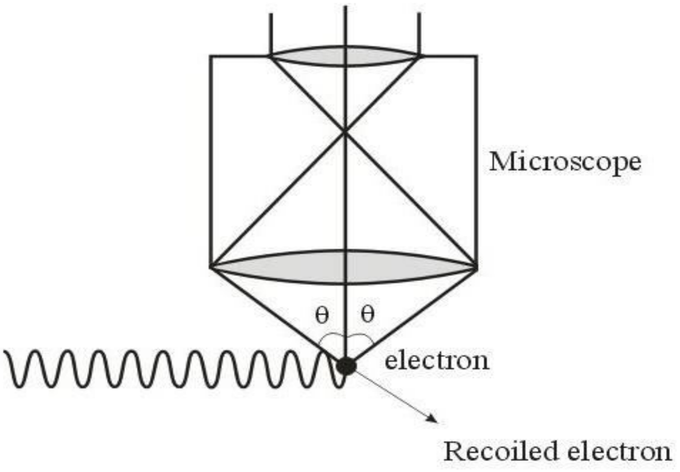
Application of uncertainty Principle:

Determination of the position of a particle with the help of a microscope:

Let us consider the case of the measurement of the position of an electron is determined. For this the electron is illuminated with light (photon). Now the smallest distance between the two points that can be resolved by microscope is given by

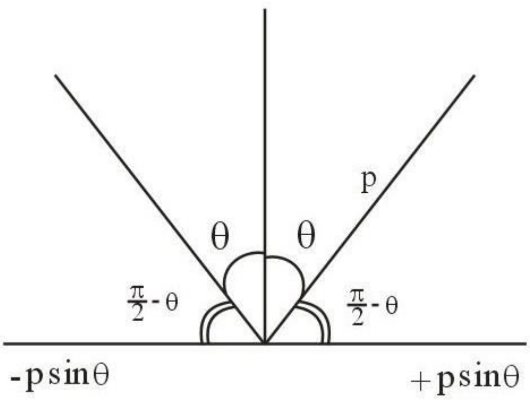
$$\Delta x = \frac{\lambda}{2 \sin \theta} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (1)$$

From the above equation it is clear that for exactness of position determination improves with a decrease in the wavelength (λ) of liaght. Let us imagine that we are using a $(\gamma - ray)$ microscope of angular aperture 2θ.



Figure(5): microscope

In order to observe the electron, it is necessary that at least one photon must strike the electron and scattered inside the microscope. The scattered photon can enter in the field of view $+\theta$ to $-\theta$ as shown in the figure.



Figure(6): Scattering of an photon by an electron

Rough

$E = h\vartheta$

$but\ \vartheta\lambda = c$

So

$E = \frac{hc}{\lambda} \ldots \ldots \ldots \ldots \ldots \ldots \ldots$

And

$E = mc^2 \ldots \ldots \ldots \ldots \ldots \ldots$ (2

So

$mc^2 = \frac{h\vartheta}{\lambda}$

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

The momentum (p) of the scattered photon is $\left(\frac{h}{\lambda}\right)$ then the momentum along the x-axis is $(-p \sin\theta)$ and $(+p \sin\theta)$. But when the photon of wavelength λ' collied to the electron then this photon recoile the electron by giving some momentum to it.

Now the uncertainty in the momentum transfer to the electron will be $\Delta p = [p + p_x] - [p - p_x]$

$$\Delta p = \left(\frac{h}{\lambda'} + \frac{h}{\lambda}\sin\theta\right) - \left(\frac{h}{\lambda'} - \frac{h}{\lambda}\sin\theta\right)$$

$$\Delta p = \frac{2h}{\lambda}\sin\theta \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (2)$$

By equation (1) and (2)

$$\Delta p.\ \Delta x = \frac{\lambda}{2\sin\theta} \times \frac{2h\sin\theta}{\lambda}$$

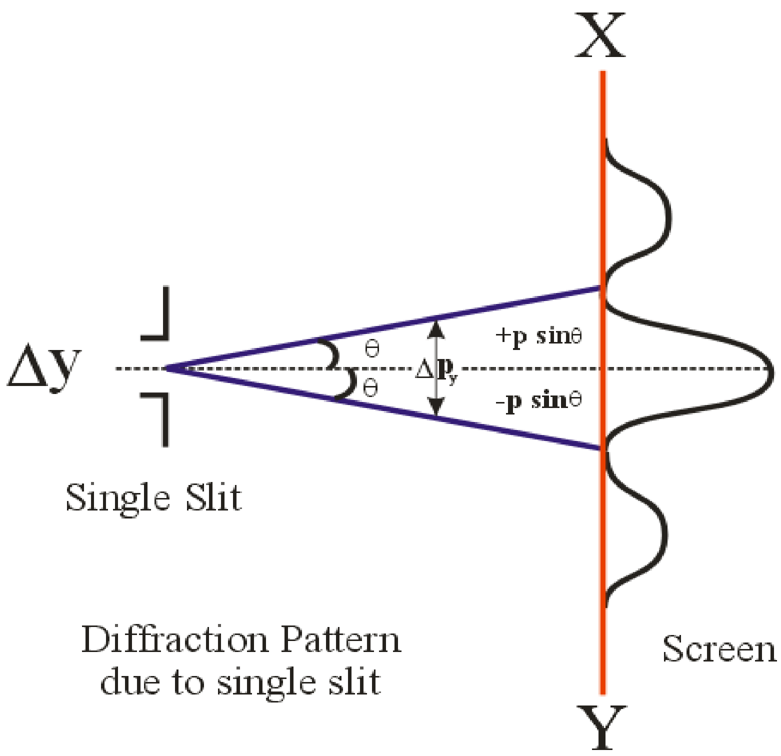
$$\Delta p.\ \Delta x = h$$

$$\Delta p.\ \Delta x \geq \frac{\hbar}{2}$$

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

<u>Diffraction of electron beam by a single slit:</u>

Suppose a narrow beam of electron passes through a narrow single slit and produces a diffraction on the screen as shown in figure.



Figure(7): Diffraction pattern of electron beam by single slit

But the theory of Fraunhofer's diffraction at a single slit $(2d \sin\theta = \pm n\lambda)$ the first minima is given by

$$2\Delta y \sin = \lambda \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (1)$$

In producing the diffraction pattern on the screen, all the electrons have passed through the slits but we can-not say definitely at what place of the slit. Hence the uncertainty in determining the position of electron is equal to the width of the slit (Δy) then by equation (1)

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

Initially the electrons are moving x-axis and hence they have no component of momentum along y-axis. After diffraction on the slit, they are deviated from their initial path to form the pattern. Now they have a component $p \sin \theta$. As y component of momentum may be anywhere between $(p \sin \theta)$ and $(-p \sin \theta)$. Hance the uncertainty in y component is

$$\Delta p_y = p \sin \theta - (-p \sin \theta)$$

$$\Delta p_y = 2p \sin \theta$$

$$\Delta p_y = 2 \left(\frac{h}{\lambda}\right) \sin \theta \qquad \left[\because p = \frac{h}{\lambda}\right] \quad \ldots\ldots\ldots\ldots \quad (3)$$

By equation (2) and (3)

$$\Delta y . \Delta p_y = \frac{\lambda}{2 \sin \theta} \times \frac{2h}{\lambda} \sin \theta$$

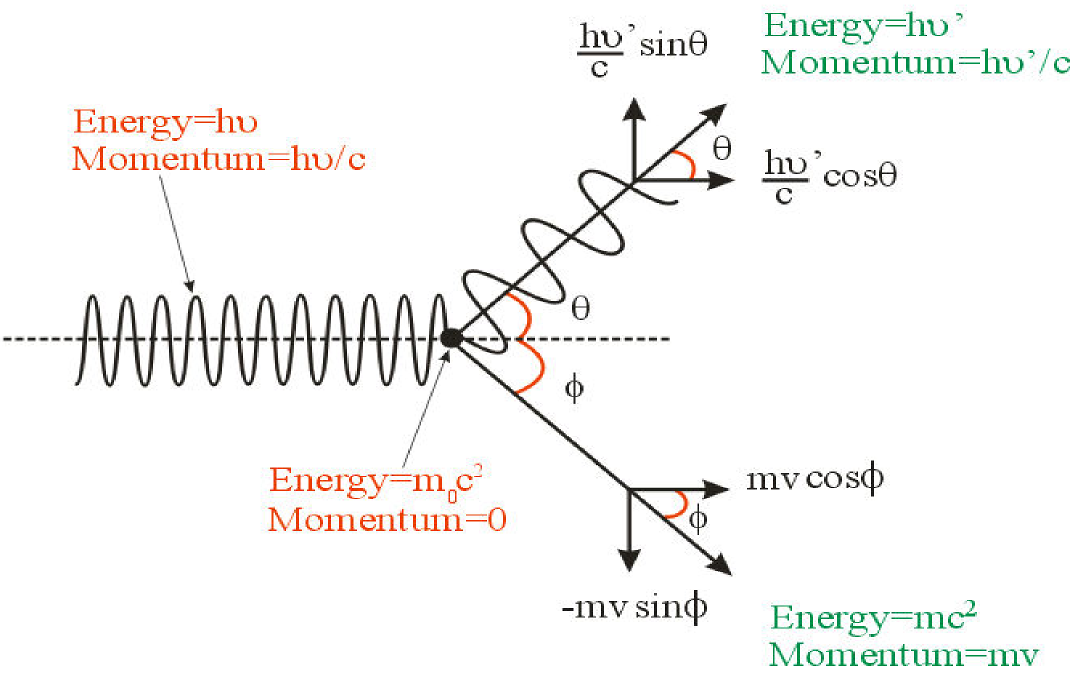
$$\Delta y . \Delta p_y \geq h$$

$$\Delta y . \Delta p_y \geq \frac{\hbar}{2}$$

Compton Scattering:

When a beam of monochromatic radiation of sharply define frequency incident on materials of low atomic number, the rays suffers a change in frequency on scattering. This scattered beam contains two beams one having lower frequency or greater wavelength other having the same frequency or wavelength.

The radiation of unchanged frequency in the scattered beam is known as unmodified radiation while the radiation of lower frequency or slightly higher wavelength is called a modified radiation. This phenomenon is known as Compton effect.



Figure(8): Compton Scattering

The energy and momentum

S.N.	Quantity	Before collision	After collision
1.	Momentum of radiation	$\frac{h\vartheta}{c}$ (Where ϑ is the frequency of radiation)	$\frac{h\vartheta'}{c}$
2.	Energy of radiation	$E = h\vartheta$ (Where ϑ is the frequency of radiation)	$E = h\vartheta'$
3.	Momentum of electron	0	mv
4.	Energy of electron	$E = m_0c^2$ (Where m_0 is the rest mass of the electron)	$E = mc^2$ (Where m is the moving mass of the electron)

By the principle of the conservation of momentum along and perpendicular to the direction of the incidence, we get

In x-direction

$$momentum\ before\ collision = mometum\ after\ collision$$

$$h\vartheta + 0 = \frac{h\vartheta'}{c}\cos\theta + mv\cos\phi \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

In y-direction

$$0 + 0 = \frac{h\vartheta'}{c}\sin\theta - mv\sin\phi \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (2)$$

By equation (1)

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

By equation (2)

$$mvc\sin\phi = h\vartheta'\sin\theta \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

Squaring equation (3) and (4) then adding we get

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

$$m^2v^2c^2 = h^2\vartheta^2 + h^2\vartheta'^2\cos^2\theta - 2h^2\vartheta\vartheta'\cos\theta + h^2\vartheta'^2\sin^2\theta$$

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

$$m^2v^2c^2 = h^2\vartheta^2 + h^2\vartheta'^2 - 2h^2\vartheta\vartheta'\cos\theta$$

$$h^2\vartheta^2 + h^2\vartheta'^2 - 2h^2\vartheta\vartheta'\cos\theta = m^2v^2c^2 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (5)$$

Now by conservation of energy

$$Energy\ before\ collision = Energy\ after\ collision$$

$$h\vartheta + m_0c^2 = hv' + mc^2 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (6)$$

$$h\vartheta + m_0c^2 - hv' = mc^2$$

$$h\vartheta - h\vartheta' + m_0c^2 = mc^2$$

Squaring both side

$$[h\vartheta - h\vartheta' + m_0c^2]^2 = m^2c^4$$

As we know that $(a + b + c)^2 = a^2 + b^2 + c^2 + 2ab + 2bc + 2ca$

so $(a - b + c)^2 = a^2 + b^2 + c^2 - 2ab - 2bc + 2ca$

$$h^2\vartheta^2 + h^2\vartheta'^2 + m_0^2c^4 - 2h^2\vartheta\vartheta' - 2h\vartheta' m_0c^2 + 2h\vartheta m_0c^2 = m^2c^4$$

$$h^2\vartheta^2 + h^2\vartheta'^2 - 2h^2\vartheta\vartheta' + m_0^2c^4 + 2h(\vartheta - \vartheta').m_0c^2 = m^2c^4 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (7)$$

Subtracting equation (5) from (7) we get

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

$$h^2\vartheta^2 + h^2\vartheta'^2 - 2h^2\vartheta\vartheta' + m_0^2c^4 + 2h(\vartheta - \vartheta').m_0c^2 - h^2\vartheta^2 - h^2\vartheta'^2 + 2h^2\vartheta\vartheta'\cos\theta = m^2c^2(c^2 - v^2)$$

$$-h^2.\,2\vartheta\vartheta'(1 - \cos\theta) + 2h(\vartheta - \vartheta')m_0c^2 + m_0^2c^4 = m^2c^2(c^2 - v^2)$$

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

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

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

So

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

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

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

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

$$(\vartheta-\vartheta') = \frac{2h^2\vartheta\vartheta'}{2hm_0c^2}(1-\cos\theta)$$

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

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

$$\frac{1}{\vartheta'}-\frac{1}{\vartheta} = \frac{h}{m_0c^2}(1-\cos\theta) \quad \text{..............................} \quad (8)$$

Multiplying by c both side

$$\frac{c}{\vartheta'}-\frac{c}{\vartheta} = \frac{hc}{m_0c^2}(1-\cos\theta)$$

$$\lambda'-\lambda = \frac{h}{m_0c}(1-\cos\theta) \quad \text{..............................} \quad (9)$$

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

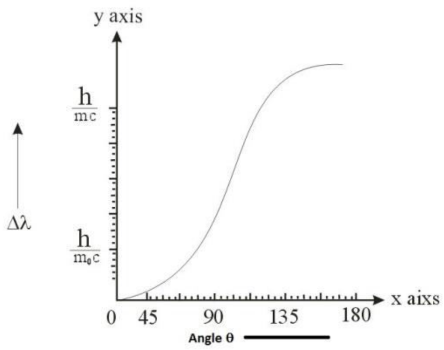
$$\Delta\lambda = \frac{h}{m_0c}2\sin^2\left(\frac{\theta}{2}\right)$$

$$\Delta\lambda = \frac{2h}{m_0c}\sin^2\left(\frac{\theta}{2}\right) \quad \text{............................} \quad (10)$$

Where $\Delta\lambda$ is the change in the wavelength

Equation (10) shows that

1) If $\theta = 0 \Longrightarrow \Delta\lambda = 0$ i.e. there is no scattering along the direction of incidence.
2) If $\theta = \frac{\pi}{2} \Longrightarrow \Delta\lambda = \frac{h}{m_0c} = \frac{6.6\times10^{-34}}{9\times10^{-31}\times3\times10^{8}} = 0.2426\ \text{Å}$ this wavelength is known as Compton wavelength and it is a constant quantity.
3) If $\theta = \pi \Longrightarrow \Delta\lambda = \frac{2h}{m_0c} = 0.4852\ \text{Å}$ so the change in the wavelength waries in accordance to the scattering angle θ and this is shown in figure.



Figure(9): Graph between angle of incidence and wavelength

Importance of Compton effect:

1) It provides the evidence of particle nature of the electromagnetic radiation.
2) This verifies the Plank's quantum hypothesis.
3) This provides an indirect verification of the following relation $m = \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}}$ and $E = mc^2$

Direction of the recoil electron:

We know that

$$mvc \cos \phi = h\vartheta - h\vartheta' \cos \theta \quad \text{..} \quad (3)$$

$$mvc \sin \phi = h\vartheta' \sin \theta \quad \text{..} \quad (4)$$

Dividing (4) by (3) we get

$$\tan \phi = \frac{h\vartheta' \sin \theta}{h\vartheta - h\vartheta' \cos \theta}$$

$$\tan \phi = \frac{\vartheta' \sin \theta}{\vartheta - \vartheta' \cos \theta}$$

Again by equation (8) i.e.

$$\frac{1}{\vartheta'} - \frac{1}{\vartheta} = \frac{h}{m_0 c}(1 - \cos \theta)$$

$$\frac{1}{\vartheta'} = \frac{1}{\vartheta} + \frac{h}{m_0 c} 2\sin^2\left(\frac{\theta}{2}\right)$$

Multiplying by ϑ we get

$$\frac{\vartheta}{\vartheta'} = 1 + \frac{h\vartheta}{m_0 c} 2\sin^2\left(\frac{\theta}{2}\right)$$

$$\frac{1}{\vartheta'} = \frac{1 + \frac{h\vartheta}{m_0 c} 2\sin^2\left(\frac{\theta}{2}\right)}{\vartheta}$$

$$\vartheta' = \frac{\vartheta}{1 + \frac{h\vartheta}{m_0 c} 2\sin^2\left(\frac{\theta}{2}\right)}$$

Then by equation (11) and (12) we have

$$\tan\phi = \frac{\left[\dfrac{\vartheta}{1 + \dfrac{h\vartheta}{m_0 c} 2\sin^2\left(\dfrac{\theta}{2}\right)}\right] .\ \sin\theta}{\vartheta - \left[\dfrac{\vartheta}{1 + \dfrac{h\vartheta}{m_0 c} 2\sin^2\left(\dfrac{\theta}{2}\right)}\right] .\ \cos\theta}$$

Let $\dfrac{h\vartheta}{m_0 c} = \alpha$

then

$$\tan\phi = \frac{\left[\dfrac{\vartheta \sin\theta}{1 + \alpha\, 2\sin^2\left(\dfrac{\theta}{2}\right)}\right]}{\vartheta - \left[\dfrac{\vartheta \cos\theta}{1 + \alpha\, 2\sin^2\left(\dfrac{\theta}{2}\right)}\right]}$$

$$\tan\phi = \frac{\left[\dfrac{\vartheta \sin\theta}{1 + \alpha\, 2\sin^2\left(\dfrac{\theta}{2}\right)}\right]}{\vartheta\left[1 - \dfrac{\cos\theta}{1 + \alpha\, 2\sin^2\left(\dfrac{\theta}{2}\right)}\right]}$$

$$\tan\phi = \frac{\left[\dfrac{\sin\theta}{1 + \alpha\, 2\sin^2\left(\dfrac{\theta}{2}\right)}\right]}{\left[\dfrac{1 + \alpha\, 2\sin^2\left(\dfrac{\theta}{2}\right) - \cos\theta}{1 + \alpha\, 2\sin^2\left(\dfrac{\theta}{2}\right)}\right]}$$

$$\tan\phi = \frac{\sin\theta}{1 + \alpha\, 2\sin^2\left(\dfrac{\theta}{2}\right) - \cos\theta}$$

$$\tan\phi = \frac{\sin\theta}{(1 - \cos\theta) + \alpha\, 2\sin^2\left(\dfrac{\theta}{2}\right)}$$

$$\tan\phi = \frac{2.\ \sin\left(\dfrac{\theta}{2}\right) .\ \cos\left(\dfrac{\theta}{2}\right)}{2.\ \sin^2\left(\dfrac{\theta}{2}\right) + \alpha\, 2\sin^2\left(\dfrac{\theta}{2}\right)}$$

$$\tan \phi = \frac{2.\ \sin\left(\frac{\theta}{2}\right).\ \cos\left(\frac{\theta}{2}\right)}{2.\ \sin^2\left(\frac{\theta}{2}\right)\ (1+\alpha)}$$

$$\tan \phi = \frac{\cot\left(\frac{\theta}{2}\right)}{[1+\alpha]}$$

$$\tan \phi = \frac{\cot\left(\frac{\theta}{2}\right)}{\left[1+\frac{h\vartheta}{m_0c^2}\right]}$$

Wave function and its properties:

We know that height of the water surface varies periodically in water waves, the pressure of gas varies periodically in sound waves and the electric field and magnetic field varies periodically in light waves, similarly the quantities which varies periodically in case of matter waves is called the wave function. The quantity whose variations make up the matter waves. This is represented by ψ. This has no direct physical significance and is not an observed quantity. However the value of wave function is related to the probability of finding the particle at a given place at a given time, wave function ψ is a complex quantity i.e.

$$\psi = A + iB$$

Conjugate of ψ is

$$\psi^* = A - iB$$

And

$$\psi\psi^* = |\psi|^2 = A^2 + B^2$$

$|\psi|^2$ at a time at a particular place is the probability of finding the particle there at that time and is known as probability density $|\psi|^2 = \psi\psi^*$

Let the wave function ψ is specified in x direction by the wave equation $\psi = Ae^{-i\omega\left(t-\frac{x}{v}\right)}$

Where $\omega = 2\pi\vartheta$ and $v = \vartheta\lambda$

So

$$\psi = Ae^{-2\pi\vartheta i\left(t-\frac{x}{\vartheta\lambda}\right)}$$

$$\psi = Ae^{-2\pi i\left(\vartheta t-\frac{x}{\lambda}\right)} \qquad \ldots\ldots\ldots\ldots\ldots\ldots \qquad (1)$$

As $E = h\vartheta$

$$E = \frac{h}{2\pi} . 2\pi\vartheta$$

$$E = 2\pi\, \hbar\, \vartheta$$

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

$$\lambda = \frac{2\pi . \frac{h}{2\pi}}{p}$$

$$\lambda = \frac{2\pi\, \hbar}{p}$$

$$\frac{1}{\lambda} = \frac{p}{2\pi\hbar}$$

Putting these values in (1) we get

$$\psi = Ae^{-2\pi i\left(\frac{E}{2\pi\hbar}t-\frac{p}{2\pi\hbar}x\right)}$$

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

This is the wave equation for a free particle.

Properties of wave function:

1) It must be finite everywhere: if ψ is infinite at a particular point, then it would mean an infinitely

large probability of finding the particle at that point, which is impossible. Hence ψ must have a finite or zero values at any point.

2) It must be single valued: if ψ has more than one value at any point, it means that there is more than one values of probability of finding the particle at that point, which is impossible.
3) It must be continuous: For Schrodinger equation $\frac{d^2\psi}{dx^2}$ must be finite everywhere. This is possible only where $\frac{\partial\psi}{\partial x}$ has no discontinuity at any boundary where potential changes. This implies that ψ too must be continuous across a boundary.
4) ψ must be normalised: ψ must be normalised, which means that ψ must to be zero as $x \longrightarrow \pm\infty$, $y \longrightarrow \pm\infty$, $z \longrightarrow \pm\infty$ in order that $\int|\psi|^2\, dv$ over all space be finite constant.

   If $\int_{-\infty}^{+\infty}|\psi|^2\, dv = 0 \Rightarrow$ the particle does not exists but $|\psi|^2$ over all space must be finite i.e. the body exits somewhere it

   $\therefore \int_{x_1}^{x_2}|\psi|^2\, dv = 0, \infty,$ complex are not possible.
5) Normalization: $\int_{-\infty}^{+\infty}|\psi|^2\, dv = 1$

   As $|\psi|^2 = \psi^*\psi = probability\ density(P)$
6) Probability between the limits x_1 and x_2: This is given by

   $P_{x_1x_2} = \int_{-\infty}^{+\infty}|\psi|^2\, dx\ (one\ dimensional)$
7) Expected values: To correlate experiment and theory we define the expectation values of any parameter

$$\langle x\rangle = \frac{\int_{-\infty}^{+\infty} x.\,|\psi|^2\, dx}{\int_{-\infty}^{+\infty}|\psi|^2\, dx} = \frac{\int_{-\infty}^{+\infty}\psi^*\, x\, \psi\, dx}{\int_{-\infty}^{+\infty}\psi^*\, \psi\, dx}$$

   If ψ is a normalised wave function then

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

   So

$$\langle x\rangle = \int_{-\infty}^{+\infty}|\psi|^2\, dx = 1$$

Orthonormal and Orthogonal wave function:

For two wave function $\psi_1(x)$ and $\psi_2(x)$ if the condition $\int_a^b \psi_2^*(x)\psi_1(x)\, dx = 0$ exists then they are said to be orthogonal wave function. Here $\psi_2^*(x)$ is the complex conjugate of $\psi_2(x)$.

The normalized wave function are defined by

$$\int_a^b \psi_1^*(x)\psi_1(x)\, dx = 1$$

The wave function satisfying both the conditions of normalisation and orthogonally said to be orthonormal. These two conditions simultaneously can be written as

$$\int_a^b \psi_m^*(x)\psi_n(x)d\tau = \delta_{mn} = \begin{cases} = 1 \text{ for } m = n \\ = 0 \text{ for } m \neq n \end{cases}$$

Operator:

Operator $\hat{O}$ is a mathematical rule which may applied to a function $f(x)$ which changes the function in to an other function $g(x)$.

So an operator is a rule by means of which from a given function, we can find another function for example:

$$\frac{d}{dx}\,e^{ax} = \quad a e^{ax}$$

So an operator tells us that what operation to carry out on the quantity that follows it.

Energy Operator:

We know that the wave function is given as-

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

Differentiating partially with respect to t we get

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

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

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

Hence energy operator

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

Momentum Operator:

Again by wave function i.e.

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

Differentiating equation with respect to x we get

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

$$\frac{\partial\psi}{\partial x} \quad = \quad \frac{ip}{\hbar}\,\psi$$

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

$$p\psi \qquad -i\hbar\frac{\partial\psi}{\partial x}$$

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

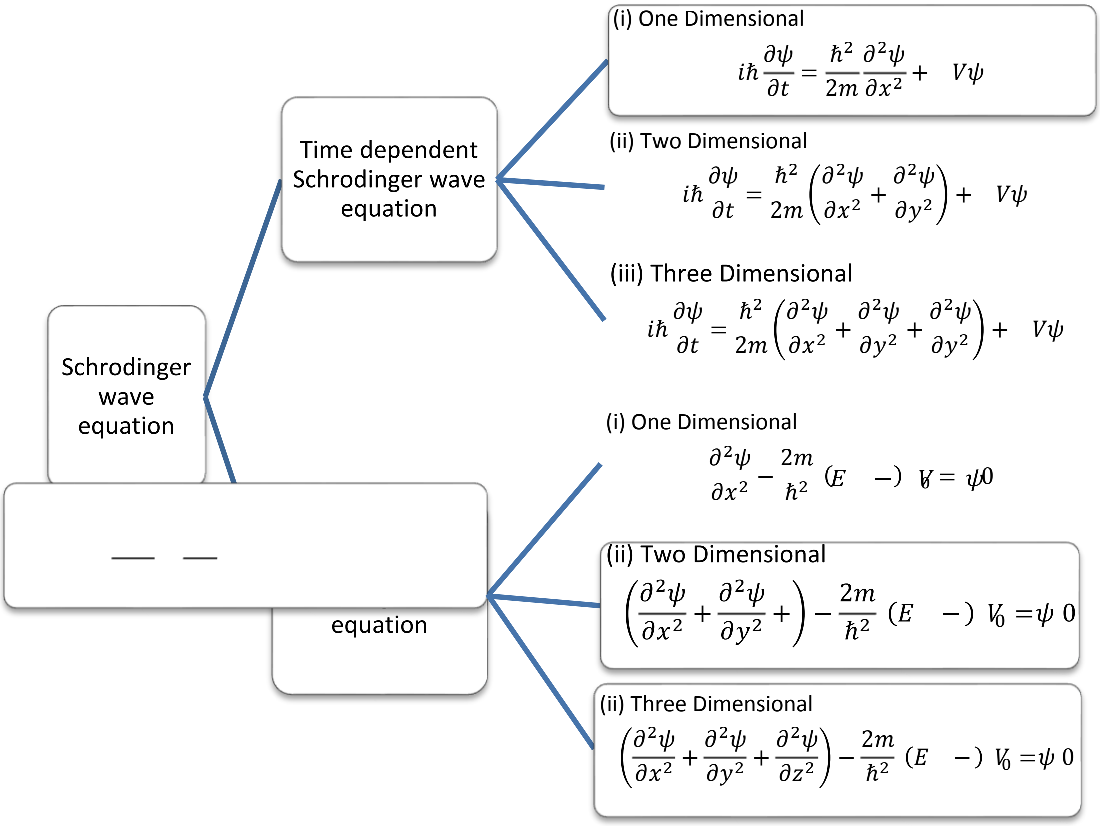
Note: $\frac{\hbar}{i}\frac{\partial\psi}{\partial x} = \quad E\psi$

Here ψ is called an eigan function of the operator $-i\hbar\frac{\partial}{\partial x}$ and E are called the corresponding energy eigan values.

Schrodinger's wave equation:

Schrodinger's wave equations are the fundamental equations of quantum mechanics in the same sense as the Newton's second equation of motion of classical mechanics.

It is the differential form of de-Broglie wave associated with a particle and describes the motion of particle.



Figure(10): Schrodinger wave equations

Schrodinger's time dependent wave equation in 1-dimentional form:

Let us assume that the ψ for a particle moving freely in the positive x-direction is

$$\psi = Ae^{-\frac{i}{\hbar}(Et-px)} \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (1)$$

Now the total energy

$$E = KE + (V\ potential\ energy) \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (2)$$

And we know that the kinetic energy is related with the momentum as $KE = \frac{p^2}{2m}$

So the equation (2) in terms of wave function ψ, can be written as

$$E\psi = \left(\frac{p^2}{2m}\right)\psi + V\psi \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (3)$$

As we know that the energy and momentum operators are given by $E\psi = i\hbar\frac{d\psi}{dt}$ and $p\psi = \frac{\hbar}{i}\frac{d\psi}{dx}$

Putting the values in equation (3) we get

$$i\hbar\frac{d\psi}{dt} = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 \psi + V\psi$$

$$i\hbar\frac{d\psi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (4)$$

Schrodinger's time independent wave equation in 3-dimentional form:

$$i\hbar\frac{d\psi}{dt} = \frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}+\frac{d^2}{dz^2}\right) \psi + V\psi$$

But the Laplacian operator is given as $\nabla^2 = \left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}+\frac{d^2}{dz^2}\right)$

So the above equation can be written as-

$$i\hbar\frac{d\psi}{dt} = \frac{\hbar^2}{2m}\nabla^2\psi + V \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (5)$$

Schrodinger's time independent wave equation in 1-dimention:

Again from wave function-

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

$$\psi = Ae^{-\frac{i}{\hbar}Et}.\ e^{\frac{i}{\hbar}px}$$

$$\psi = Ae^{\frac{i}{\hbar}px}.\ e^{-\frac{i}{\hbar}Et}$$

$$\psi = \psi_0 e^{-\frac{i}{\hbar}Et}$$

Where $\psi_0 = Ae^{\frac{i}{\hbar}px}$

Now differentiating partially with respect to t we get

$$\frac{\partial\psi}{\partial t} = -\frac{iE}{\hbar}\psi_0\, e^{-\frac{i}{\hbar}Et} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (7)$$

Now differentiating partially with respect to x we get

$$\frac{\partial\psi}{\partial x} = \frac{\partial\psi_0}{\partial x}e^{-\frac{i}{\hbar}Et}$$

Again

$$\frac{\partial^2\psi}{\partial x^2} = \frac{\partial^2\psi_0}{\partial x^2}e^{-\frac{i}{\hbar}Et} \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (8)$$

Putting the value from (7) and (8) into equation (5) we get i.e. $i\hbar\frac{\partial\psi}{\partial x} = \frac{\hbar^2}{2m}\nabla^2\psi + V\psi$

$$i\hbar\left[-\frac{iE}{\hbar}\psi_0\, e^{-\frac{i}{\hbar}Et}\right] = -\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi_0}{\partial x^2}e^{-\frac{i}{\hbar}Et}\right] + V\psi_0 e^{-\frac{i}{\hbar}Et}$$

$$E\psi_0 e^{-\frac{i}{\hbar}Et} = e^{-\frac{i}{\hbar}Et}\left[\frac{\hbar^2}{2m}\frac{\partial^2\psi_0}{\partial x^2} + V\psi_0\right]$$

$$E\psi_0 = \frac{\hbar^2}{2m}\frac{\partial^2\psi_0}{\partial x^2} + V\psi_0$$

$$E\psi_0 - V\psi_0 = \frac{\hbar^2}{2m}\frac{\partial^2\psi_0}{\partial x^2}$$

$$(E - V)\psi_0 = \frac{\hbar^2}{2m}\frac{\partial^2\psi_0}{\partial x^2}$$

$$\frac{2m}{\hbar^2}(E - V)\psi_0 = \frac{\partial^2\psi_0}{\partial x^2}$$

$$\frac{\partial^2\psi_0}{\partial x^2} - \frac{2m}{\hbar^2}(E - V)\psi_0 = 0 \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (10)$$

Schrodinger's time independent wave equation in 3-dimention form:

$$\left(\frac{\partial^2\psi_0}{\partial x^2}+\frac{\partial^2\psi_0}{\partial y^2}+\frac{\partial^2\psi_0}{\partial z^2}\right) \quad \frac{2m}{\hbar^2}(E \quad - \quad V_0)\psi \;=\; 0$$

$$\nabla^2\psi_0-\frac{2m}{\hbar^2}(E \quad V)\psi_0 \;=\; 0$$

Where $\nabla^2 = \left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)$

Application of Schrodinger's wave equation:

Energy level and wave function of a particle enclosed in one dimensional box of infinite height:

Let us consider the case of a particle of mass m moving along x-axis between two rigid walls A and B at $x = 0$ and $x = L$. The potential energy V of the particle is given as

$$V = \begin{cases} 0 \; for \; 0 < x < L \\ \infty \; for \; x \leq 0 \; and \; x \geq L \end{cases}$$

Within the box, the Schrodinger wave equation is given by

$$\frac{\partial^2\psi}{\partial x^2} - \frac{2m}{\hbar^2} E\psi = 0 \qquad [\because V = 0] \text{.......................................} \quad (1)$$

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

$$\frac{\partial^2\psi}{\partial x^2} - k^2\psi = 0 \qquad \text{...} \quad (3)$$

This is a second order differential equation and its solution is given by

$$\psi = A \sin kx + B \cos kx \text{ ....} \quad (4)$$

Where A and B are constants, the value of these constants can be calculated by the boundary conditions. By first boundary condition if $x = 0 \implies \psi = 0$

Then by equation (4) we get

$$0 = A \sin k0 + B \cos k0$$

$$\implies B = 0$$

For second boundary condition $\psi = 0$ at $x = L$ then by equation (4)

$$0 = A \sin kL + 0.\cos kL$$

$$\implies A \sin kL = 0$$

But $A \neq 0$ so $\sin kL = 0 \implies kL = n\pi \; (n = 0,1,2,3 \; \ldots \; \ldots \; \ldots)$

As we know that
$$k^2 = \frac{n^2\pi^2}{L^2} \qquad \text{...} \quad (5)$$

By equation (2) and (5)

$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2}$$

For representing the n^{th} energy level replacing E BY E_n we have

$$\frac{2mE_n}{\hbar^2} = \frac{n^2\pi^2}{L^2}$$

$$E_n = \frac{n^2\pi^2}{L^2} \times \frac{\hbar^2}{2m}$$

$$E_n = \frac{n^2\pi^2}{L^2} \times \frac{h^2}{4\pi^2 \, 2m}$$

$$E_n = \frac{n^2h^2}{8mL^2} \quad \text{...} \quad (6)$$

It is clear from expression (6) that inside an infinitely deep potential well, the particle can have only discrete set of energy i.e. the energy of the particle is quantised. The discreet energies are given by

$$E_1 = \frac{h^2}{8mL^2}$$

$$E_2 = \frac{4h^2}{8mL^2} = 4E_1$$

$$E_3 = \frac{9h^2}{8mL^2} = 9E_1$$

$$E_4 = \frac{16\,h^2}{8mL^2} = 16E_1$$

$$.. = .. \quad .. \quad ..$$

$$.. = .. \quad .. \quad ..$$

The constant A of equation (4) can be obtained by applying the normalization condition i.e.

$$\int_{x=0}^{x=L} |\psi|^2\, dx = 1$$

$$\int_0^L |A \sin kx|^2\, dx = 1$$

$$A^2 \int_0^L \sin^2 kx\, dx = 1$$

$$A^2 \int_0^L \left(\frac{1-\cos 2kx}{2}\right) dx = 1$$

$$\frac{A^2}{2} \int_0^L (1 - \cos 2kx)\, dx = 1$$

$$\frac{A^2}{2}\left[\{x\}_0^L - \left\{\frac{\sin 2kx}{2k}\right\}_0^L\right] = 1$$

$$\frac{A^2}{2}\left[(L - 0) - \frac{1}{2k}(\sin 2kL - \sin\right] = 1$$

$$\frac{A^2}{2}\left[L - \frac{1}{2k}(\sin \frac{2n\pi}{L} L - \sin\right] = 1 \qquad \because k = \frac{2n\pi}{L}$$

$$\frac{A^2}{2}\left[L - \frac{1}{2k}(0 - \right] = 1 \qquad \because \sin 2n\pi$$

$$\frac{A^2}{2} L = 1$$

$$A = \sqrt{\frac{2}{L}} \quad \text{..} \quad (7)$$

Now the wave function will be given by

$$\psi = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x \qquad \boxed{(n = 1,2,3, \ldots}$$