Unit 4: Quantum Physics

POOJA PREMNATH
S01

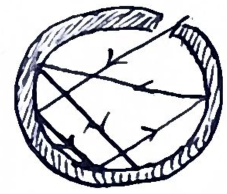
* Black body radiation:

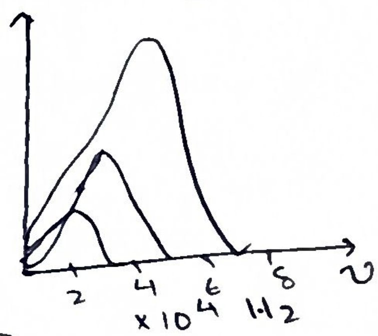
- **Black body**: absorbs all light and reflects none of the light that is incident on it.
- **making a black body**: a spherical cavity, painted black within, completely sealed but for a narrow aperture. light entering through the aperture would undergo multiple reflections inside the cavity. when heated, the black body would emit more per unit area than any other body.
- **spectral energy distribution of black body radiation**:

(i) area under the curve $\Rightarrow$ total energy emitted by a black body at a given temperature.

area $\propto$ increase in temperature

(ii) Peak frequency also shifts towards the right





* Planck's Theory (Derivation)

Assumptions (i) According to Planck, a black body consists of a no. of oscillators, vibrating with a specific frequency.

(ii) The frequency of vibration = frequency of radiation emitted by it.

(iii) The oscillators cannot radiate energy in a continuous fashion, but only in the form of discrete quanta. If the frequency is ν, the energy emitted would always be an integral multiple of $h\nu$.

To find: energy density over a particular frequency range, i.e from ν to $\nu + d\nu$.

Let there be N oscillators, and let E be the total energy.

Average energy of each oscillator:

$$\overline{\varepsilon} = \frac{E}{N} \quad - (1)$$

Also: $N = N_0 + N_1 + N_2 + \cdots N_r$ $\quad (2)$

and $E = 0 + \varepsilon N_1 + 2\varepsilon N_2 + 3\varepsilon N_3 + \cdots r\varepsilon N_r \quad \cdots (3)$

By using the Maxwell - Boltzmann distribution law; the no. of oscillators of energy $r\varepsilon$ is given by:

$$N_r = N_0 \exp\left(\frac{-r\varepsilon}{kT}\right) \quad (4)$$

Substituting eqn. (4) in (2)

$$N = N_0 + N_0 \exp\left(\frac{-\varepsilon_p}{kT}\right) + N_0 \exp\left(\frac{-2\varepsilon_p}{kT}\right) + \dots \; N_0 \exp\left(\frac{-n\varepsilon_p}{kT}\right)$$

$$\Rightarrow N = N_0\left[1 + x + x^2 + \dots\right]$$

where $x = \exp\left(\frac{-\varepsilon_p}{kT}\right)$

$$\Rightarrow \boxed{N = \frac{N_0}{1-x}} \quad - (5)$$

Substituting (4) in (3)

$$E = 0 + N_0\varepsilon_p \exp\left(\frac{-\varepsilon_p}{kT}\right) + 2\varepsilon_p N_0\left(\frac{-2\varepsilon_p}{kT}\right) + 3\varepsilon_p N_0\left(\frac{-3\varepsilon_p}{kT}\right) + \dots \; r\varepsilon_p N_0\left(\frac{-r\varepsilon_p}{kT}\right)$$

$$\Rightarrow E = N_0 \varepsilon_p\left[1 + 2x + 3x^2 + 4x^3 + \dots \; r x^{r-1}\right]$$

where $x = \exp\left(\frac{-\varepsilon_p}{kT}\right)$

$$\therefore \boxed{E = \frac{N_0 \varepsilon_p \cdot x}{(1-x)^2}} \quad - (6)$$

Substituting (5), (6) in (1)

$$\bar{\varepsilon_p} = \frac{N_0 \varepsilon_p x}{(1-x)^2} \times \frac{1-x}{N_0}$$

$$\bar{\varepsilon_p} = \frac{\varepsilon x}{1-x}$$

$$\bar{\varepsilon_p} = \frac{\varepsilon_p \exp\left(\frac{-\varepsilon_p}{kT}\right)}{1 - \exp\left(\frac{-\varepsilon_p}{kT}\right)}$$

$$\bar{\varepsilon_p} = \frac{\varepsilon_p}{\frac{1}{\exp\left(\frac{-\varepsilon_p}{kT}\right)} - 1} \Rightarrow \boxed{\bar{\varepsilon_p} = \frac{\varepsilon_p}{\exp\left(\frac{\varepsilon_p}{kT}\right) - 1}} \quad - (7)$$

$$\boxed{\bar{\varepsilon} = \frac{h\nu}{\exp\left(\frac{h\nu}{kT}\right) - 1}} \Rightarrow (8)$$

when $\exp\left(\frac{h\nu}{kT}\right) >> 1$

$$\exp\left(\frac{h\nu}{kT}\right) \sim \frac{h\nu}{kT} + 1$$

$$\Rightarrow \bar{\varepsilon} = \frac{h\nu}{\frac{h\nu}{kT} + 1 - 1}$$

$$\Rightarrow \boxed{\varepsilon = kT} \quad - (9)$$ (when ε is small)

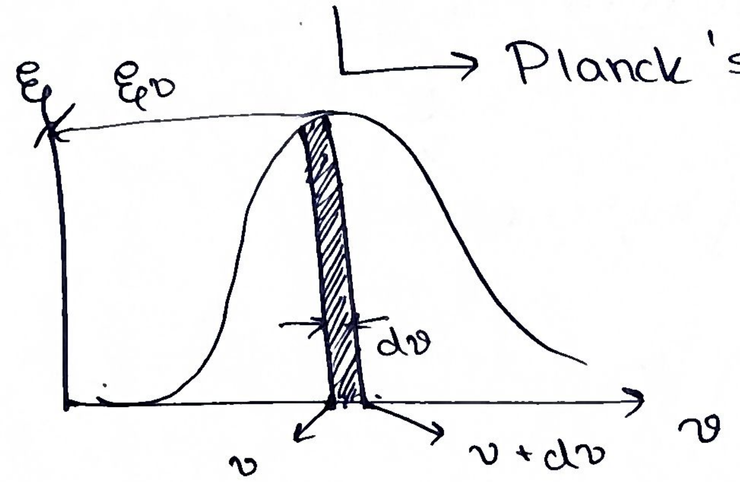
It can be shown that the no. of oscillators per unit volume in the frequency range ν to $\nu + d\nu$ is $N = \frac{8\pi\nu^2 d\nu}{c^3}$

$$\therefore \varepsilon_\nu d\nu = \frac{8\pi\nu^2 d\nu}{c^3} \cdot \frac{h\nu}{\exp\left(\frac{h\nu}{kT}\right) - 1}$$

$$\therefore \boxed{\varepsilon_\nu d\nu = \frac{8\pi h\nu^3}{c^3} \cdot \left(\frac{1}{\exp\left(\frac{h\nu}{kT}\right) - 1}\right) d\nu} \quad - (10)$$

→ Planck's Radiation Law

Graph



Planck's Radiation Law in Terms of λ

$$\nu = \frac{c}{\lambda}, \quad d\nu = \frac{d}{d\lambda}\left(\frac{c}{\lambda}\right) = \frac{-c}{\lambda^2} d\lambda$$

$$|d\nu| = \frac{c}{\lambda^2} d\lambda$$

Substituting values for ν, $|d\nu|$ in (10)

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

$$E_\lambda d\lambda = \frac{8\pi}{\cancel{c^3}}\frac{h\cancel{c^3}}{\lambda^3}\left(\frac{1}{\exp\left(\frac{hc}{\lambda kT}\right)-1}\right)\cdot\frac{c}{\lambda^2}$$

$$\boxed{E_\lambda d\lambda = \frac{8\pi hc}{\lambda^5}\left(\frac{1}{\exp\left(\frac{hc}{\lambda kT}\right)-1}\right)d\lambda} \quad (11)$$

* Deduction of Wien's displacement law by Planck's Radiation law

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

The product of wavelength corresponding to maximum energy & absolute temperature is a constant.

$\lambda_m T$ = constant

For short wavelengths: $\exp\left(\frac{hc}{\lambda kT}\right) \gg 1$

$$\therefore E_\lambda d\lambda = \frac{8\pi hc}{\lambda^5}\left(\frac{1}{\exp\left(\frac{hc}{\lambda kT}\right)}\right)d\lambda$$

Let $c_1 = 8\pi hc$

$c_2 = \frac{hc}{k}$

$$\therefore \boxed{E_\lambda d\lambda = c_1\lambda^{-5}\exp\left(\frac{-c_2}{\lambda T}\right)d\lambda}$$ Wien's displacement law.

* Deduction of Rayleigh Jean's Law from Planck's Radiation Law

For longer wavelengths: ν is small $\rightarrow \frac{h\nu}{kT}$ is small

$\exp\left(\frac{h\nu}{kT}\right) \Rightarrow 1+\frac{h\nu}{kT}$ (ignoring higher powers)

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

$$= \frac{8\pi \cancel{hc}}{\lambda^{\cancel{5}}}\cdot\frac{kT}{\frac{\cancel{hc}}{\cancel{\lambda}}}\cdot d\lambda$$

$$\boxed{E_\lambda d\lambda = \frac{8\pi kT}{\lambda^4}d\lambda}$$ $\Rightarrow$ Rayleigh-Jeans Law

Compton Effect :

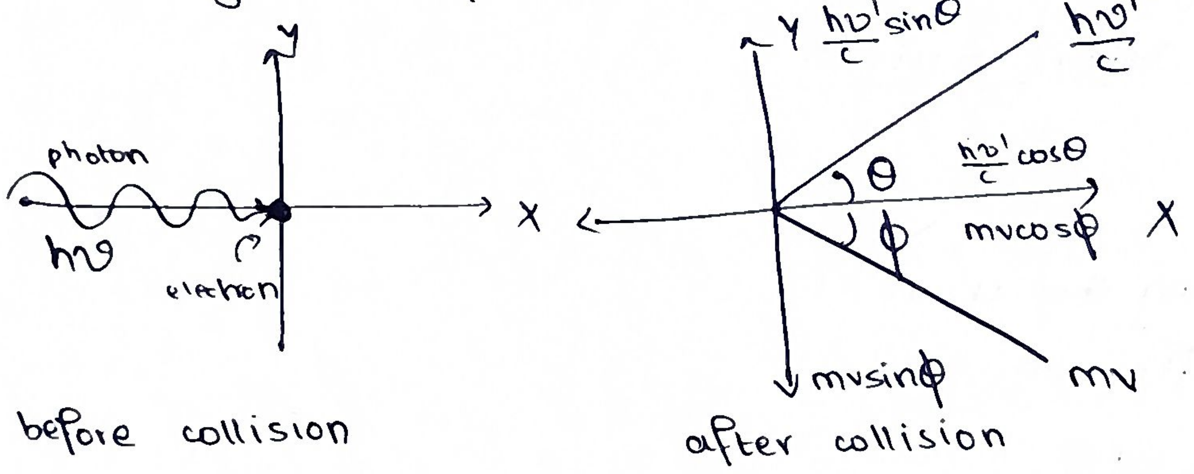
Statement: When a beam of high frequency radiation, say X rays / γ rays ~~sta~~ is scattered by a substance of low atomic no, the scattered radiation has 2 wavelengths; one identical to the incident wavelength, while the other has a slightly longer wavelength. This phenomenon of the change in wavelength of scattered X-rays, γ-rays is called Compton shift, and the effect is called the Compton effect.

Explanation: It can be explained on the basis of the quantum theory. An X-radiation consists of light quanta / photons which each have an energy $h\nu$. When a photon collides with a free electron, it transfers some of this energy to it. This means that the scattered photon would have a lower energy, than the incident one.

Theoretical proof of the Compton effect

(i) Consider an X-ray photon striking an electron. The electron is initially at rest, and the collision is assumed to be elastic.

(ii) After collision, the photon is scattered from its initial direction of motion by an angle θ, and the electron by an angle ϕ.



Energy before collision

energy of photon $= h\nu$

energy of electron $= m_0c^2$

Total initial energy $= h\nu + m_0c^2$

Energy after collision

energy of photon $= h\nu'$

energy of electron $= mc^2$

Total final energy $= h\nu' + mc^2$

By law of conservation of energy

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

$$\boxed{h(\nu - \nu') = mc^2 - m_0c^2} \quad - (1)$$

Momentum along x-axis before collision

momentum of photon : $\frac{h\nu}{c}$

momentum of electron $= 0$

Total initial momentum along x-axis : $\frac{h\nu}{c}$

Momentum along x-axis after collision

momentum of photon along x axis : $\frac{h\nu'}{c}\cos\theta$

momentum of electron along x axis : $mv\cos\phi$

Total final momentum $= \frac{h\nu'}{c}\cos\theta + mv\cos\phi$

By law of conservation of momentum :

initial momentum along x axis = final momentum along x axis

$$\frac{h\nu}{c} = \frac{h\nu'}{c}\cos\theta + mv\cos\phi \quad - (2)$$

Momentum along y-axis before collision

momentum of photon $= 0$

momentum of electron $= 0$

Total initial momentum along the y axis $= 0$

Momentum along y-axis after collision

momentum of photon $= \frac{h\nu'}{c}\sin\theta$

momentum of electron $= -mv\sin\phi$

Total final momentum along y-axis $= \frac{h\nu'}{c}\sin\theta - mv\sin\phi$

By law of conservation of momentum :

momentum before collision along y axis = momentum after collision along y axis

$$0 = \frac{h\nu'}{c}\sin\theta - mv\sin\phi. \quad - (3)$$

multiplying eqn (2), (3) by c throughout;

$h\nu = h\nu'\cos\theta + mvc\cos\phi$ — (4)

and $\Rightarrow h(\nu - \nu'\cos\theta) = mvc\cos\phi$

$0 = h\nu'\sin\theta - mvc\sin\phi$ — (5)

$\Rightarrow h\nu'\sin\theta = mvc\sin\phi$

squaring and adding (4) (5)

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

$$h^2\nu^2 + h^2\nu'^2 - 2\nu\nu'\cos\theta h^2 = m^2v^2c^2 \quad -(6)$$

squaring eqn (1) $\quad \{ \text{eqn (1)} = h(\nu - \nu') + m_oc^2 = mc^2 \}$

$\cancel{h^2(\nu^2 + \nu'^2 - 2\nu\nu') = mc^2 - m_oc}$

$\cancel{h^2(\nu^2 + \nu'^2 - 2\nu\nu') + m_o^2c^4 = m^2c^4 \quad -(7)}$

$$(h(\nu - \nu') + m_oc^2)^2 = m^2c^4$$

$$h^2(\nu^2 + \nu'^2 - 2\nu\nu') + m_o^2c^4 + 2h(\nu - \nu')m_oc^2 = m^2c^4 \quad -(7)$$

Subtracting (6) from (7)

$$m^2c^4 - m^2v^2c^2 = h^2(\nu^2 + \nu'^2 - 2\nu\nu') + m_o^2c^4 + 2h(\nu - \nu')m_oc^2 - h^2\nu^2 - h^2\nu'^2 + 2h^2\nu\nu'\cos\theta$$

$$\Rightarrow m^2c^2(c^2 - v^2) = -2h^2\nu\nu' + m_o^2c^4 + 2h(\nu - \nu')m_oc^2 + 2h^2\nu\nu'\cos\theta$$

$$\Rightarrow m^2c^2(c^2 - v^2) = -2h^2\nu\nu'(1 - \cos\theta) + m_o^2c^4 + 2h(\nu - \nu')m_oc^2$$

(8)

By means of Einstein's Theory of Relativity

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

squaring,

$$m^2 = \frac{m_o^2}{1 - \frac{v^2}{c^2}} \Rightarrow m^2 = \frac{m_o^2c^2}{c^2 - v^2} \Rightarrow m^2(c^2 - v^2) = m_o^2c^2$$

multiplying both sides by c^2

$$m^2c^2(c^2 - v^2) = m_o^2c^4 \quad -(9)$$

sub eqn (9) in (8)

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

$$\cancel{2}h^{\cancel{2}}\nu\nu'(1-\cos\theta) = \cancel{2h}(\nu-\nu') m_0 c^2.$$

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

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

multiplying throughout by c.

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

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

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

(OR) $$\boxed{d\lambda = \frac{h}{m_0 c}(1-\cos\theta)}$$

Case1 : when $\theta = 0$

$\cos\theta = 1$

$d\lambda = 0$

Case2 when $\theta = 90°$

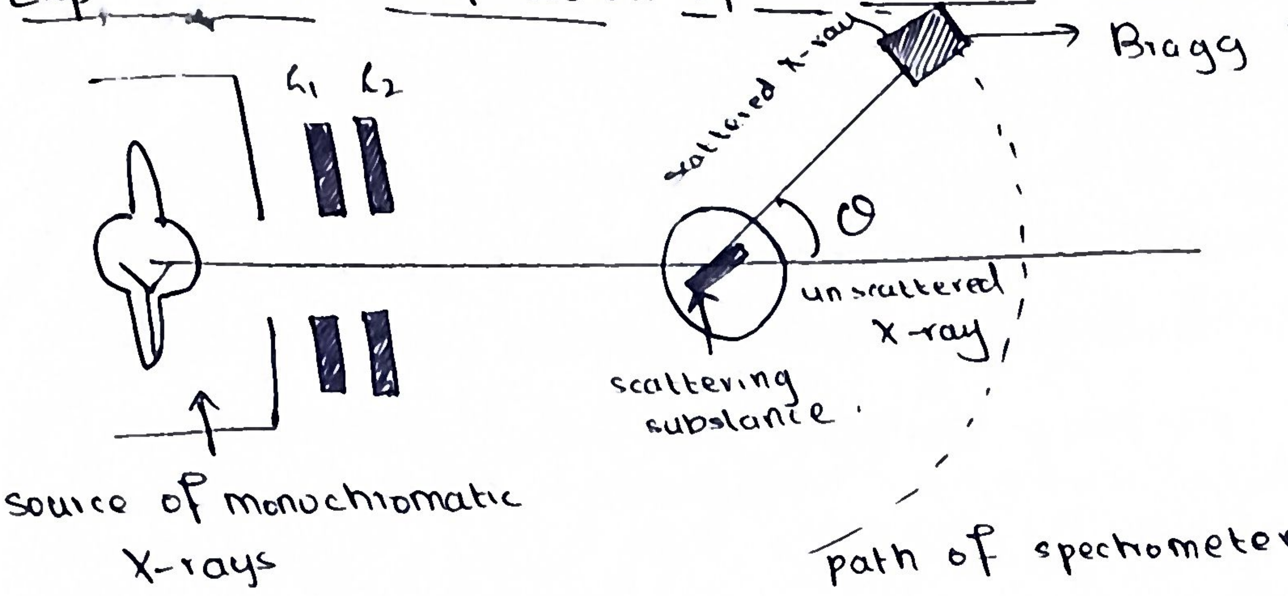
$d\lambda = \frac{h}{m_0 c} = 0.0243\,\mathring{A} \Rightarrow$ Compton wavelength

case 3 when $\theta = 180°$

$d\lambda = \frac{2h}{m_0 c} = 0.0485\,\mathring{A}$

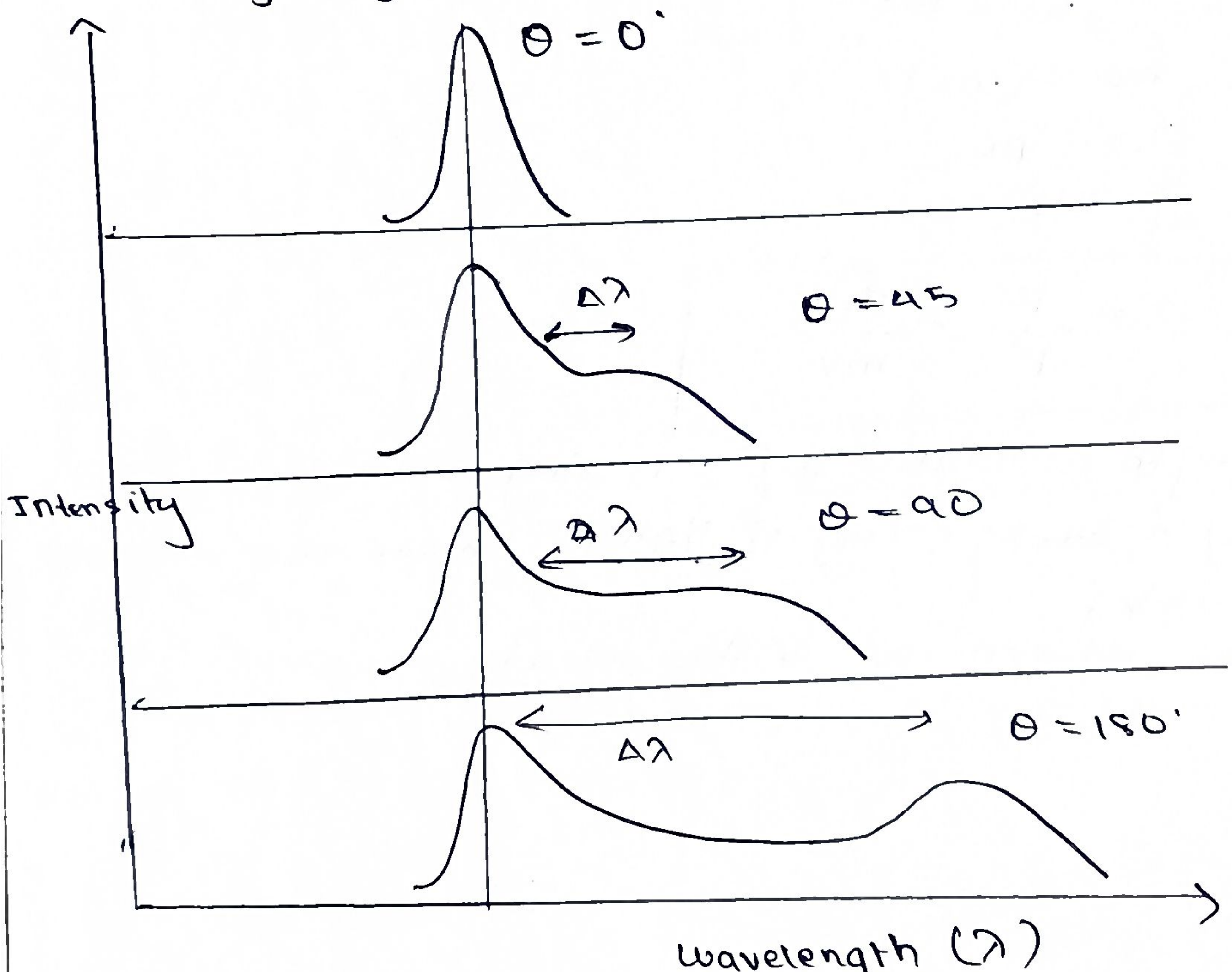
The change in wavelength is maximum when the scattering angle $\theta = 180°$.

Experimental verification of the Compton effect



Experiment (i) A beam of mono-chromatic X-rays of wavelength λ is made to fall on a scattering material like a block of carbon.
The spectrometer can freely swing in an arc about the scattering beam.

(ii) The intensity and wavelength are measured for different scattering angles, and graphs are plotted.



Inference: From the graphs, it is evident that along with the incident wavelength that is scattered, there also exists a longer wavelength (λ').
The Compton wavelength ($d\lambda$) is seen to vary with the angle of scattering, and the shift is larger for a larger scattering angle.

The experimentally found Compton wavelength nearly coincides with the theoretical value (0.0243 Å). Thus the Compton effect is experimentally verified and it proves the corpuscular nature of radiation and the validity of the quantum concept.

*Wave Particle Duality? : de Broglie suggested that an electron or any other material particle should also exhibit wave like properties when they are in motion. This property is called particle duality.
The waves associated w/ these particles are called matter waves / de Broglie waves.

* De-Broglie Wavelength

(i) Considering light as a wave of frequency ν, the energy associated w/ it would be : $E = h\nu$.

(ii) Considering it to be a particle of mass m, travelling w/ a velocity c, the energy would be $E = mc^2$.

Comparing both eqns : $h\nu = mc^2$

$$h\nu = (mc)c$$

$$h\nu = pc$$

$\nu = c\lambda$

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

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

* de-Broglie wavelength associated w/ a moving electron.

Consider an electron w/ a kinetic energy of $\frac{1}{2}mv^2$, under the influence of a potential difference V.
m is the mass of the electron and v the velocity.

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

$$mv^2 = 2eV$$

multiplying both sides by m

$$m^2v^2 = 2eV.m$$

$$(mv)^2 = 2eV.m$$

$$mv = \sqrt{2eV.m}$$

$$\frac{h}{\lambda} = \sqrt{2eV.m}$$

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

$$\rightarrow \boxed{\lambda = \sqrt{\frac{150}{V}}\ \mathring{A}}$$

* Properties of Matter Waves

(i) A material particle has matter waves just as light quanta has light waves.

(ii) The wavelength of these matter waves is given by: $\lambda = \frac{h}{mv} = \frac{h}{p}$

(iii) If the mass / velocity is large, the wavelength would be small.

(iv) These matter waves are generated when the particle is in motion.

(v) There is no charge associated w/ the wavelength of the particle.

(vi) The existence of matter waves confirms the dual nature of the particle.

(vii) Matter waves are not electromagnetic waves.

$$E = h\nu = mc^2$$

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

$$v_w = \nu\lambda$$

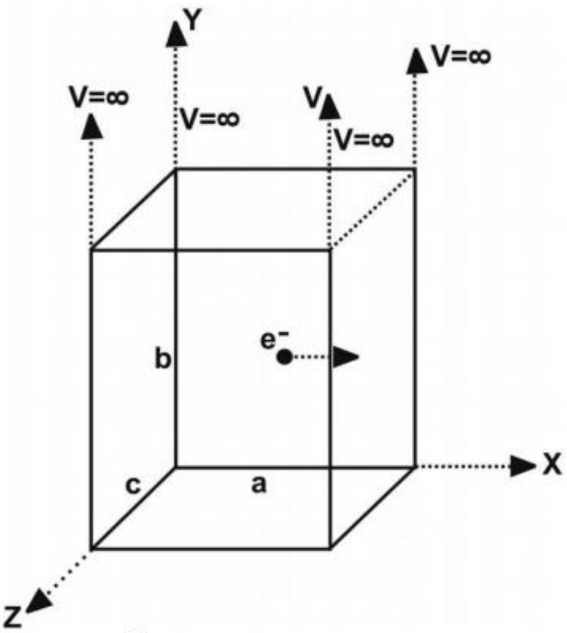
$$= \frac{mc^2}{h} \times \lambda$$

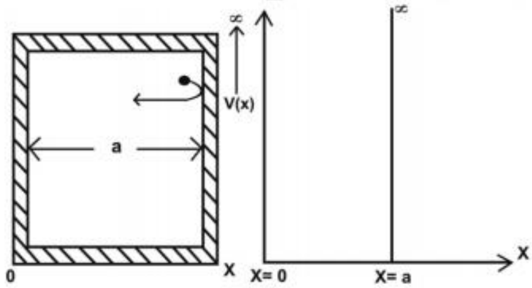
$$= \frac{mc^2}{h} \times \frac{h}{mv_p}$$

$$\boxed{v_w = \frac{c^2}{v_p}}$$

(viii) In a single expt / phenomenon, both wave and particle nature do not exist simultaneously.

PATICLE IN A ONE DIMENSIOAL BOX





1. Consider a particle of mass "m" moving inside a one dimensional box.
2. The walls of the box are between x=0 and x=a.
3. The potential energy (V) is assumed to be 0 inside the box.
4. The potential function is : $V(x) = 0\ for\ 0 < x < a$ and $V(x) = \infty\ for\ 0 \geq x \geq a$
5. This function is known as the square well potential.
6. The value of ψ the wave function of the particle is found by applying the boundary conditions to the one dimensional Schrodinger equation.

The Schrodinger equation is

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2m(E-V)}{\hbar^2}\Psi = 0 --- (1)$$

Since V is 0 between the walls ,

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2mE}{\hbar^2}\Psi = 0 --- (2)$$

Substituting

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

$$\frac{\partial^2 \Psi}{\partial x^2} + k^2\Psi = 0 --- (3)$$

The general solution is of the form $\Psi(x) = A sin\ kx + B\ cos\ kx --- (4)$

A and B are unknown constants.

.Applying the boundary condition (i) ψ=0 at x=0, to (4)

$$0 = A sin\ kx + B\ cos\ kx --- (4)$$

$$0 = A\ X\ 0 + B\ X\ 1$$

$$Hence\ B = 0$$

$$Therefore\ \ 0 = A sin\ ka$$

That is either A=0 or sin ka=0.

Since B is already zero, A cannot be zero. Therefore sin ka = 0.

Hence ka = nπ, where n = 1,2,3,........ or,

$$k = \frac{n\pi}{a} - - - (5)$$

Substituting (5) in (4),

$$\Psi(x) = A \sin \frac{n\pi}{a} x - - - - (6)$$

Squaring (5)

$$k^2 = \frac{n^2\pi^2}{a^2} - - - (7)$$

.From (2)

$$k^2 = \frac{2mE}{\hbar^2} = \frac{2mE}{\frac{h^2}{4\pi^2}} = \frac{8\pi^2 mE}{h^2} - -(8) since\ \hbar^2 = \frac{h^2}{4\pi^2}$$

Equating (7) & (8)

$$\frac{8\pi^2 mE}{h^2} = \frac{n^2\pi^2}{a^2}$$

$$E_n = \frac{n^2 h^2}{8ma^2} \quad - - - (9)$$

For each value of n,(n=1,2,3..) there is an energy level.

Thus the particle in a box can have only a discrete energy level given by (9).

Each energy value is called Eigen value and the corresponding wave function is called Eigen function.

"Eigenvalue" and "eigenvector" come from the meaning "inherent, characteristic"

Normalization of Wave function:

Probability density is =$\psi^* \psi$

The eigen function is

$$\Psi(x) = A \sin \frac{n\pi}{a} x \quad from\ (6)$$

Therefore

$$\psi^{*}\psi = A\,sin\frac{n\pi}{a}x \quad X\,A\,sin\frac{n\pi}{a}x$$

$$\psi^{*}\psi = A^{2}\,sin\left[\frac{n\pi}{a}x\right]^{2} - - - (10)$$

The probability of finding the particle anywhere inside the box is given by:

$$\int_{0}^{a}\psi^{*}\psi\,dx = 1$$

Substituting the value from (1) in (2)

$$\int_{0}^{a}A^{2}\,sin\left[\frac{n\pi}{a}x\right]^{2}dx = 1$$

$$A^{2}\int_{0}^{a}\frac{1-cos2\frac{n\pi}{a}x}{2}dx = 1$$

$$A^{2}\left[\int_{0}^{a}\frac{1}{2}dx - \frac{1}{2}\int_{0}^{a}cos2\frac{n\pi}{a}x\,dx\right] = 1$$

$$A^{2}\left[\frac{x}{2} - \frac{2sin\frac{n\pi}{a}x}{2\frac{n\pi}{a}}\right]_{0}^{a} = 1$$

$$A^{2}\left[\frac{x}{2}\right]_{0}^{a} = 1$$

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

Therefore

$$A^{2} = \frac{2}{a}\ \ or\ A = \sqrt{\frac{2}{a}}\ - - - -(11)$$

Substituting in (6) , the eigen function ψ_n belonging to is eigen values E_n is expressed as

$$\Psi_n(x) = \sqrt{\frac{2}{a}}\, sin\frac{n\pi}{a}x - - - (12)$$

Equation (12) is called Normalized wave function.

Special Cases:

<u>Case1:</u> For n=1,

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

$$\Psi_1(x) = \sqrt{\frac{2}{a}}\, sin\frac{\pi}{a}x$$

<u>Case2:</u> For n=2,

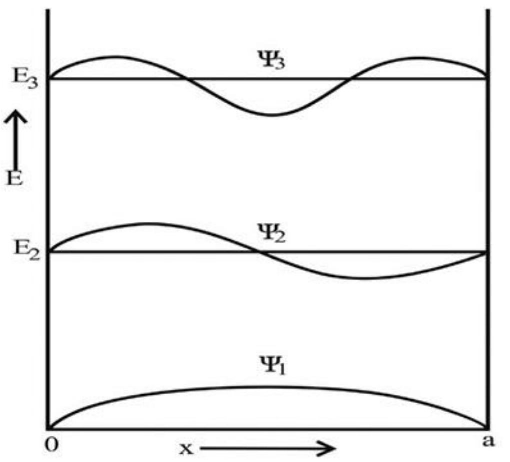
$$E_2 = \frac{4h^2}{8ma^2} = 4E_1$$

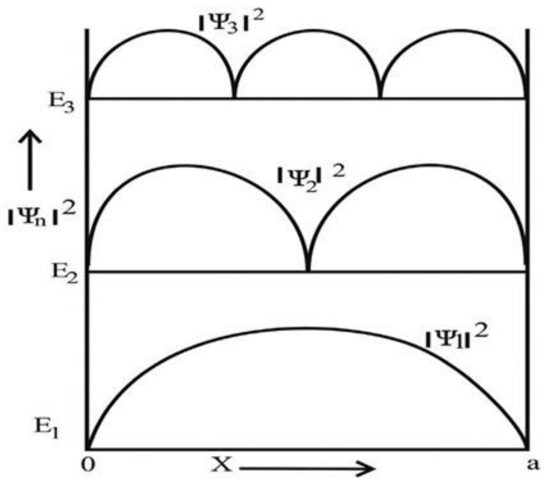
$$\Psi_2(x) = \sqrt{\frac{2}{a}}\, sin\frac{2\pi}{a}x$$

<u>Case3:</u> For n=3,

$$E_2 = \frac{9h^2}{8ma^2} = 9E_1$$

$$\Psi_2(x) = \sqrt{\frac{2}{a}}\, sin\frac{3\pi}{a}x$$





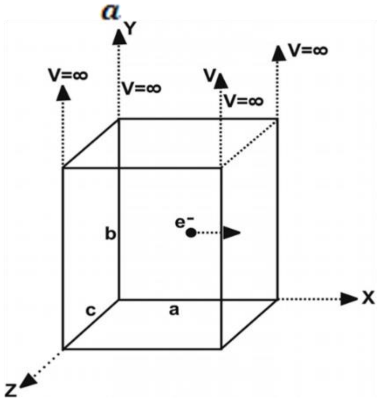
PATICLE IN A THREE DIMENSIOAL BOX

$$\Psi_{(n_x n_y n_z)} = \sqrt{\frac{2}{a}}\, sin\, \frac{n_x \pi}{a} x \sqrt{\frac{2}{a}}\, sin\, \frac{n_y \pi}{a} y \sqrt{\frac{2}{a}}\, sin\, \frac{n_z \pi}{a} z$$

$$\Psi_{(n_x n_y n_z)} = \sqrt{\frac{8}{a^3}}\, sin\, \frac{n_x \pi x}{a}\, sin\, \frac{n_y \pi y}{a}\, sin\, \frac{n_z \pi z}{a}$$

$$E_n = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8ma^2} + \frac{n_z^2 h^2}{8ma^2}$$

$$= \frac{h^2}{8ma^2}(n_x^2 + n_y^2 + n_z^2)$$



DEGENERACY AND NON-DEGENERACY

Degeneracy

When different quantum states of particle have the same energy Eigen value but different Eigen functions and quantum states are said to exhibit degeneracy the quantum states are called degenerate states.

DEGENERATE ENERGY STATES

have same eigen value but different eigen function

$n_x = 1$; $n_y = 1$; $n_z = 2$

$$\Psi_{(112)} = \sqrt{\frac{8}{a^3}}\, sin\, \frac{\pi x}{a}\, sin\, \frac{\pi y}{a}\, sin\, \frac{2\pi z}{a} \qquad E_{(112)} = \frac{6h^2}{8ma^2}$$

$n_x = 1$; $n_y = 2$; $n_z = 1$

$$\Psi_{(121)} = \sqrt{\frac{8}{a^3}}\, sin\, \frac{\pi x}{a}\, sin\, \frac{2\pi y}{a}\, sin\, \frac{\pi z}{a} \qquad E_{(121)} = \frac{6h^2}{8ma^2}$$

$n_x = 2$; $n_y = 1$; $n_z = 1$

$$\Psi_{(211)} = \sqrt{\frac{8}{a^3}}\, \sin\frac{2\pi x}{a}\, \sin\frac{\pi y}{a}\, \sin\frac{\pi z}{a}$$

$$E_{(211)} = \frac{6h^2}{8ma^2}$$

the above equations are same Eigen value Eigen function

NON DEGENERACY

have same eigen value and same eigen function

$n_x = 1$; $n_y = 1$; $n_z = 1$

$$\Psi_{(111)} = \sqrt{\frac{8}{a^3}}\, \sin\frac{\pi x}{a}\, \sin\frac{\pi y}{a}\, \sin\frac{\pi z}{a}$$

$$E_{(111)} = \frac{3h^2}{8ma^2}$$

$$E_{(111)} = \frac{3h^2}{8ma^2}$$

QUANTUM PHYSICS

Schrodinger equation is basic equation of matter waves.

The two forms of the wave equation are:

1. Time independent wave equation
2. Time dependent wave equation

I. Schrodinger time independent equation:

- Consider a wave associated with a particle.
- Let x,y,z be the coordinates of the particle.
- Let ψbe the displacement for the de Broglie wave at any time,
- The 3D wave equation for wave motion is given by:

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} = \frac{1}{v^2}\frac{\partial^2 \Psi}{\partial t} - - - (1)$$

- v is the velocity of the wave.
- Equation is rewritten as

$$\nabla^2 \Psi = \frac{1}{V^2}\frac{\partial^2 \Psi}{\partial t} - - - (2)$$

- Where

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

- ∇ is a Laplacian's operator.
- The solution equation of this equation is of the form

$$\Psi(x, y, z, t) = \Psi_0(x, y, z, t)e^{-i\omega t}$$
$$\Psi = \Psi_0 e^{-i\omega t} - - - -(3)$$

- $\Psi_0(x, y, z, t)$ is a function of x,y,z,t and gives the amplitude with respect to time t.
- Differentiating twice with respect to t

$$\frac{\partial \Psi}{\partial t} = -i\omega \Psi_0 e^{-i\omega t}$$
$$\frac{\partial^2 \Psi}{\partial t^2} = (-i\omega)(-i\omega)\Psi_0 e^{-i\omega t}$$
$$\frac{\partial^2 \Psi}{\partial t^2} = (i^2 \omega^2)\Psi_0 e^{-i\omega t}$$

$$\frac{\partial^2 \Psi}{\partial t^2} = -\omega^2 \Psi_0 e^{-i\omega t}$$

$$\frac{\partial^2 \Psi}{\partial t^2} = -\omega^2 \, \Psi - - - (4)$$

Since

$$\Psi_0 e^{-i\omega t} = \Psi_0$$

- Substituting (4) in (2),

$$\nabla^2 \Psi = -\frac{\omega^2}{v^2} \Psi$$

$$\nabla^2 \Psi + \frac{\omega^2}{v^2} \Psi = 0 - - - (5)$$

- Angular frequency is

$$\omega = 2\pi \nu = 2\pi \frac{v}{\lambda}$$

- Therefore

$$\frac{\omega}{v} = \frac{2\pi}{\lambda} - - - (6)$$

- Squaring (6)

$$\frac{\omega^2}{v^2} = \frac{4\pi^2}{\lambda^2} - - - (7)$$

- Substituting (7) in (5), $\nabla^2 \Psi + \frac{4\pi^2}{\lambda^2} \Psi = 0 - - - -(8)$
- Putting $\lambda = \frac{h}{mv}$, in equation (8)

$$\nabla^2 \Psi + \frac{4\pi^2}{\frac{h^2}{m^2 v^2}} \Psi = 0 - - -$$

$$\nabla^2 \Psi + \frac{4\pi^2 m^2 v^2}{h^2} \Psi = 0 - - - (9)$$

- If E is the energy of the particle and V is the potential energy and ½ mv^2 is the kinetic energy, then Total energy (E)= potential energy (V) + kinetic energy (½ mv^2).

$$E = V + \frac{1}{2}mv^2$$
$$E - V = \frac{1}{2}mv^2$$
$$2(E - V) = mv^2$$

- Multiplying by on both sides,

$$m^2v^2 = 2m(E - V) - - - (10)$$

- Substituting (10) in (9),

$$\nabla^2\Psi + \frac{4\pi^2 2m(E - V)}{h^2}\Psi = 0$$
$$\nabla^2\Psi + \frac{8\pi^2 m(E - V)}{h^2}\Psi = 0 - - - - (11)$$

- This equation is called Schrodinger Time independent equation.
- Substituting $\hbar = \frac{h}{2\pi}$,

$$\hbar^2 = \frac{h^2}{4\pi^2} - - - (12)$$

, where $\hbar$ is called reduced Planck's constant.

- Substituting (12) in (11),

$$\nabla^2\Psi + \frac{2m(E - V)}{\hbar^2}\Psi = 0 - - - - (13)$$

- Equation (13) has no term representing time and hence it is called Time independent Schrodinger equation.

Special case:

The one-dimensional equation is represented as

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{2m(E - V)}{\hbar^2}\Psi = 0 - - - (15)$$

II. Schrodinger time independent equation:

- Consider a wave associated with a particle.
- Let x,y,z be the coordinates of the particle.
- Let ψ be the displacement for the de Broglie wave at any time,

TIME DEPENDENT SCHRODINGER EQUATION

$$\Psi(x, y, z, t) = \Psi_0(x, y, z, t)e^{-i\omega t}$$

$$\Psi = \Psi_0 e^{-i\omega t} ----(2)$$

- Differentiating twice with respect to t

$$\frac{\partial \Psi}{\partial t} = -i\omega\Psi_0 e^{-i\omega t}$$

$$\frac{\partial \Psi}{\partial t} = -i(2\pi\nu)\Psi_0 e^{-i\omega t}$$

$$\frac{\partial \Psi}{\partial t} = -i(2\pi\nu)\Psi --- (3)$$

$$\frac{\partial \Psi}{\partial t} = -2\pi i\frac{E}{h}\Psi \qquad \left\{since\ E = h\nu, \qquad h = \frac{E}{\nu}\right\}$$

$$\frac{\partial \Psi}{\partial t} = - i2\pi\frac{E}{h}\Psi$$

$$\frac{\partial \Psi}{\partial t} = - i\frac{E}{\frac{h}{2\pi}}\Psi$$

$$\frac{\partial \Psi}{\partial t} = - i\frac{E}{\hbar}\Psi --- (4)$$

Multiplying by "i" on both sides

$$i\frac{\partial \Psi}{\partial t} = - iXi\frac{E}{\hbar}\Psi = -i^2\frac{E}{\hbar}\Psi$$

$$i\frac{\partial \Psi}{\partial t} = \frac{E}{\hbar}\Psi$$

$$E\Psi = i\hbar\frac{\partial \Psi}{\partial t} --- (5)$$

Schrodinger time independent equation(6)

$$\nabla^2\Psi + \frac{2m(E - V)}{\hbar^2}\Psi = 0 --- (6)$$

$$\nabla^2\Psi + \frac{2m}{\hbar^2}(E\Psi - V\Psi) = 0$$

Substituting (5) in the above equaton

$$\nabla^2\Psi + \frac{2m}{\hbar^2}\left\{i\hbar\frac{\partial\Psi}{\partial t} - V\Psi\right\} = 0)$$

$$\nabla^2\Psi = \frac{-2m}{\hbar^2}\left\{i\hbar\frac{\partial\Psi}{\partial t} - V\Psi\right\}$$

$$\frac{-\hbar^2}{2m}\nabla^2\Psi = \left\{i\hbar\frac{\partial\Psi}{\partial t} - V\Psi\right\}$$

$$\frac{-\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]\Psi = i\hbar\frac{\partial\Psi}{\partial t} - - - - -(7)$$

$$\mathrm{H}\Psi = \mathrm{E}\Psi - -(8)$$

$H \rightarrow \left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]$ is Hamiltonian operator and $E \rightarrow i\hbar\frac{\partial}{\partial t}$ is energy operator.

Equation (8) is called time dependent Schrodinger equation.

Physical significance of the wave function ψ

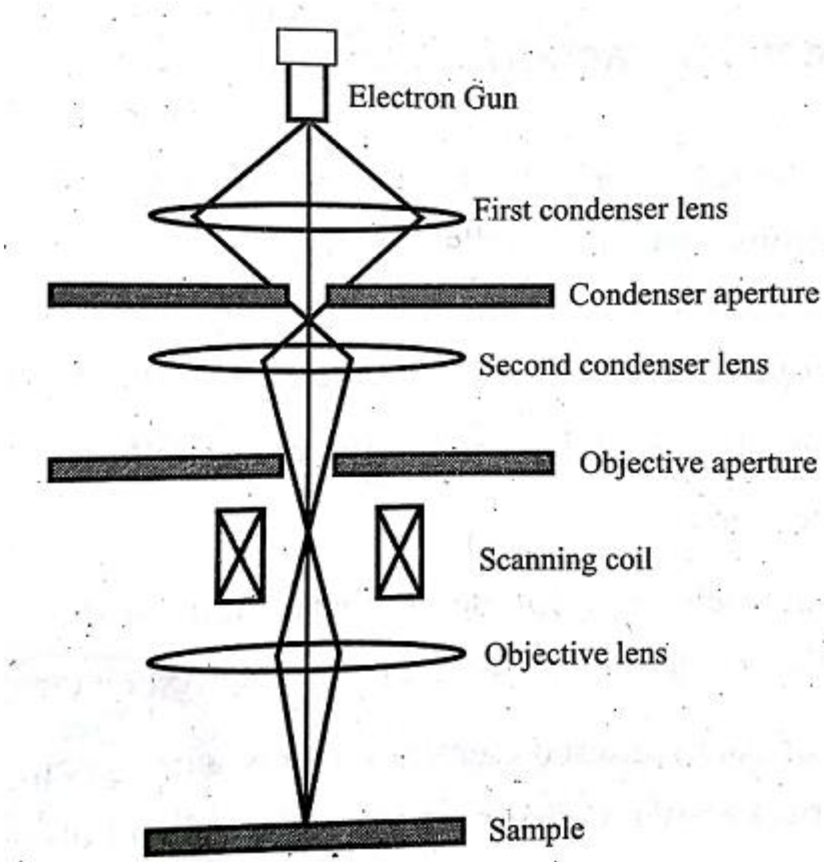
- The variable ψ characterizes the de Broglie waves is called wave function.
- The wave function connects the particle nature and the associated wave nature statistically.
- It gives the probability of finding the particle at any instant.
- The probability 1 corresponds to the certainty of finding the particle at a point at any instant.

  $\iiint \psi^*\psi d\tau = 1$, means the particle is present
- The probability 0 corresponds to the certainty of not finding the particle at a point at any instant.

  $\iiint \psi^*\psi d\tau = 0$, means the particle is not present.
- The wave function is a complex quantity that cannot be measured.
- The probability density is given by $P(\vec{r}, t) = |\psi(\vec{r}, t)|^2 = \psi^*\psi$

SCANNING ELECTRON MICROSCOPE

Scanning electron microscope, the image is produced scanning the sample with a focused electron beam and detecting the secondary (and/or) back scattered electrons. Electrons and photons are emitted at each beam location and subsequently detected.



Schematic of SEM

CONSTRUCTION AND WORKING OF A SEM

Since electrons are used instead of photons, al the lenses are electrostatic / magneto static.

1. The electron gun produces a stream of monochromatic electrons
2. The electron stream is condensed by the first condenser lens. It works in conjunction with the condenser aperture to eliminate the high angle electrons from the beam

3. The second condenser lens forms the electrons into a thin, light coherent beam
4. Objective aperture further eliminates the electrons into a thin light coherent beam.
5. A set of coils acting as electrostatic lens scans and sweeps the beam in a grid fashion. The beam dwells on points for a period of time determined by the scan speed. Dwell time is usually in microsecond.
6. When the beam strikes the sample interaction occurs. Before the beam moves to the next dwell point, the various instruments housed to measure various interactions count the number if interactions and display a pixel on a CRT. The intensity of display is determined by the interaction number. More interactions give a brighter pixel.
7. The process is repeated until the grid scan is finished and then repeated.
8. The entire pattern can be scanned 30 times per second.

SAMPLE SPECIMEN INTERACTION

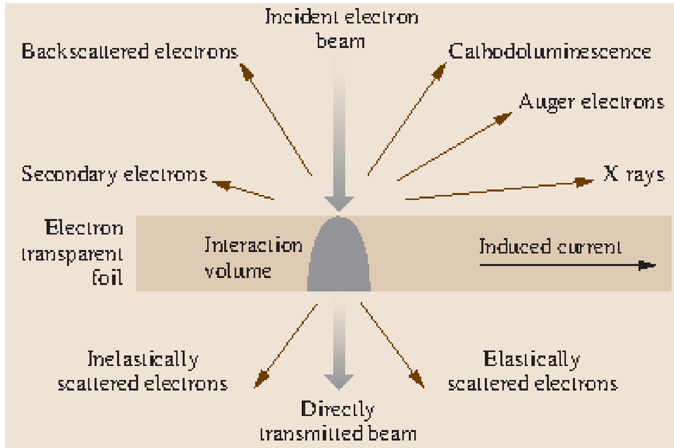
During sample – specimen interactions, the top side of the thick or bulk sample results SEM images.

BACK SCATTERED ELECTRONS

When an incident electron collides with an atom in the specimen which is nearly normal to the incident path, we get backscattered electron at nearly 180º

The intensity of backscattered electron varies with specimen's atomic number. Hence backscattered electrons are collected and imaged, high atomic number elements appear brighter than low atomic number elements.

This interactions is therefore utilized to differentiate parts of the specimen that have different average atomic number.



SECONDARY ELECTRONS

When an incident electron passes very near an atom in the specimen, it may impart some of its energy to the lower energy electron (usually in the K shell) resulting in ionization of the electron in the specimen atom. The ionized electron leaves the atom with a very small kinetic energy (5 eV) and is called secondary electrons. An change in the topography of the sample changes the yield of the secondary electrons.

Hence image formed collecting secondary electrons gives the topography of the sample

AUGER ELECTRONS

During the emission of secondary electron a lower energy electron is released thus leaving a vacancy into inner shell. A higher energy electron from the same atom can fall to the lower energy filling the vacancy. The surplus energy is released by the emission of outer orbit electron. These electrons are called Auger electrons.

They have a characteristic energy, unique to each element from which they are emitted.

These electrons are collected and sorted according to their energies to give compositional information about the sample.

X Rays

When the vacancy due to the emission of secondary electron is filled by the fall of an electron from higher orbit to lower orbit, the difference in energy may released as X-rays.

Hence X – rays thus emitted will have a characteristic energy unique to the element from which it originates.

APPLICATIONS

SEM gives useful information on

Topography: All surface features of an object.

Morphology : The shape, size and arrangement of particles on the surface of the sample

Composition : the elements and compounds the sample is composed off and their ratios.

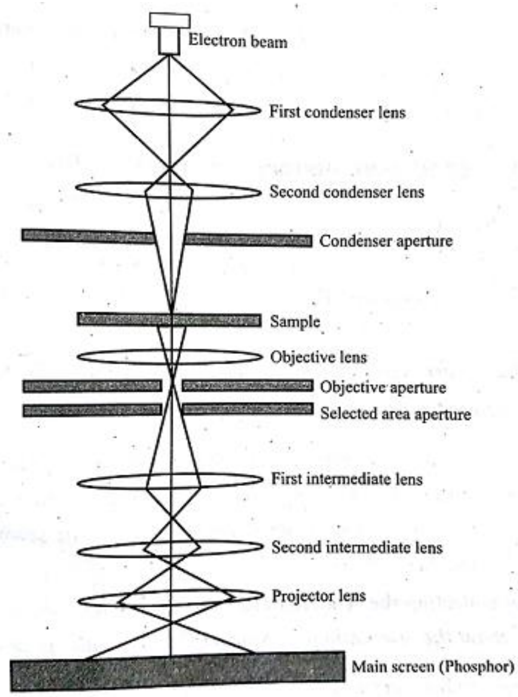
Crystallographic information: The arrangement of atoms in the specimen and their degree of order.

The most common use in the area of semiconductor applications are

1. To view the surface of the device
2. For failure analysis
3. Cross sectional analysis to determine the device dimensions such as MOSFET channel length or junction depth
4. Inspection of integrated –circuits etc

TRANSMISSION ELECTRON MICROSCOPY

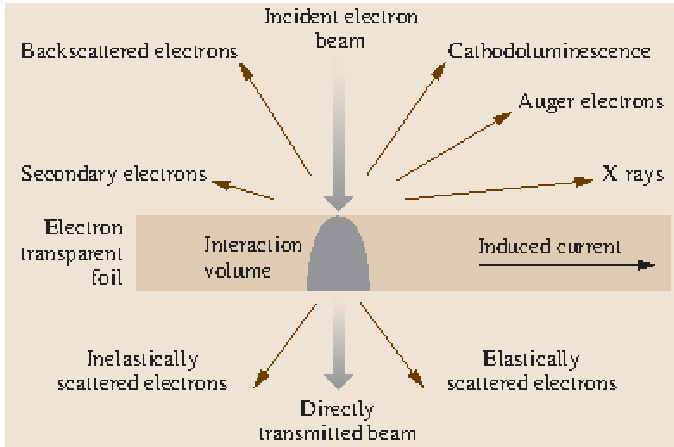
Scanning the sample with a focused electron beam and detecting and utilizing the transmitted electrons for imaging results in Transmission Electron Microscope



Schematic of TEM

CONSTRUCTION AND WORKING

1. The Electron gun produces a stream of monochromatic electrons
2. This stream is focused to a small coherent beam by the first and second condenser lenses
3. The condenser aperture knocks off high angle electrons
4. The beam strikes the specimen
5. The transmitted portion is focused by the objective lens into an image
6. Objective aperture enhances the contrast by blocking out high – angle diffracted electrons
7. Selected area aperture enables to examine by blocking out high –anle electrons by an ordered arrangement of atoms in the sample.
8. Intermediate and projector lenses enlarge the imagee
9. The beam strikes the phosphor screen and image is formed on the screen. The darker areas of the image represents thicker or denser sample areas since these areas transmit lesser electrons. The brighter areas of the image represents thinner or lesser dense sample areas since these areas transmit more electrons.



SAMPLE –ELECTRON BEAM INTERACTIONS

Specimen –beam interactions occur on the bottom side of the thin or foil sample.

UNSCATTERED ELECTRONS

These are electrons transmitted through a thin specimen without any interaction occurring inside the specimen. The intensity of transmitted scattered electrons is inversely proportional to the thickness of the specimen.

Hence thicker areas of the specimen appear darker than the thinner areas.

ELASTICALLY SCATTERED ELECTRONS

These are electrons that are scattered by atoms in the specimen without loss of energy. These scattered electrons are then transmitted though the remaining portions of the specimen. The scattered electrons follow Bragg's law: $2d \sin\theta = n\lambda$.

Hence by collecting the scattered electrons at different angles, one can get information about the orientation, atomic arrangement and phases present.

INELASTICALLY SCATTERED ELECTRONS

These are electrons that interact with specimen atoms in an inelastic manner, loosing energy. Then they are transmitted through the remaining portions of the specimen. The inelastic loss of energy is characteristic of the elements that have interacted with. These energies are unique to bonding state of each element.

Hence this can be used to extract both compositional and bonding information.

APPLICATIONS

TEM gives useful information on

Topography: All surface features of an object.

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