

Quantum Mechanics

Module - 1

- Microscopic Domain

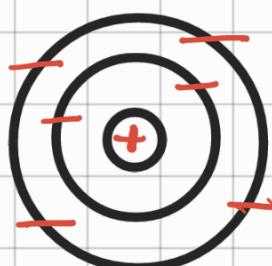
Stability of atoms, properties of sub-atomic particles

- Blackbody Radiation
- Photoelectric effect
- Compton effect
- Atomic stability and spectroscopy

- Limitations of Classical Theory

↳ Blackbody radiation

↳ Stability of atom



The e^- collapse into the nucleus which is not possible

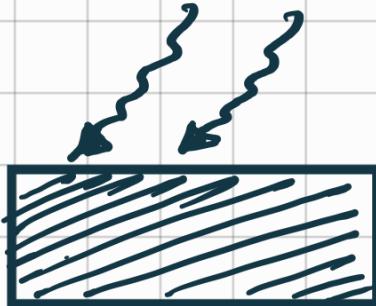
↳ Hydrogen atom spectra

$$\overline{\nu} = R_H \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

Lyman, Balmer, Paschen,
Brackett & Pfund series

[The following limitations of classical theory can be explained through Bohr's Theory]

- Photoelectric effect



↳ photoelectric effect can only occur only if $\nu \geq \nu_0$.

↳ It can be explained through Einstein's eqⁿ.

PE effect is an instantaneous process, i.e

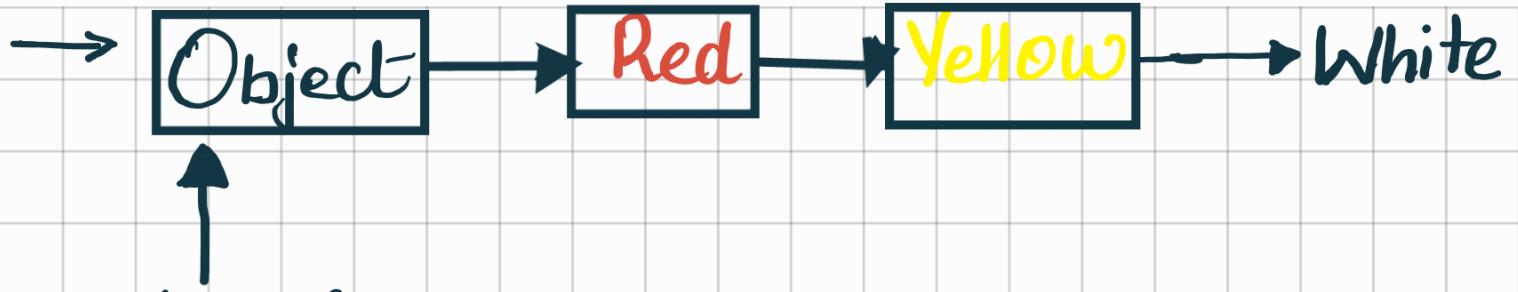
$$h\nu = h\nu_0 + K_{\max}$$

there is no time lag between the incidence of light and emission of electron.

- Blackbody Radiation

→ interaction b/w radiation & matter

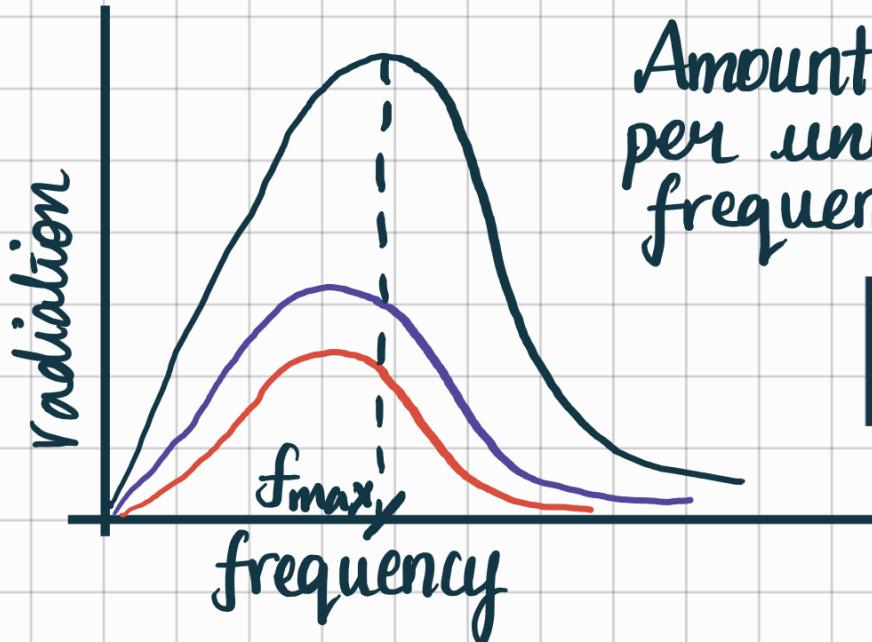
→ The radiation can be reflected, transmitted or adsorbed.



Heat {continuous distribution of frequencies from UV to IR}

EMI is emitted due to thermal agitation of e^- on the surface.

Spectral Energy Density



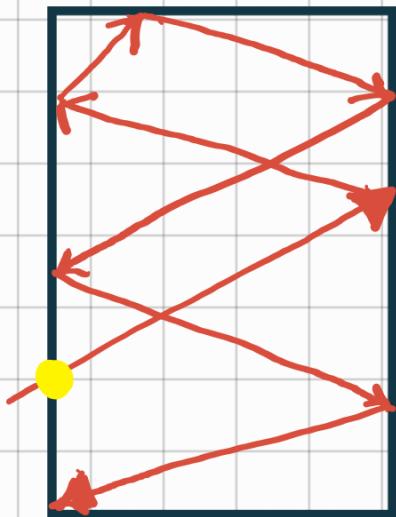
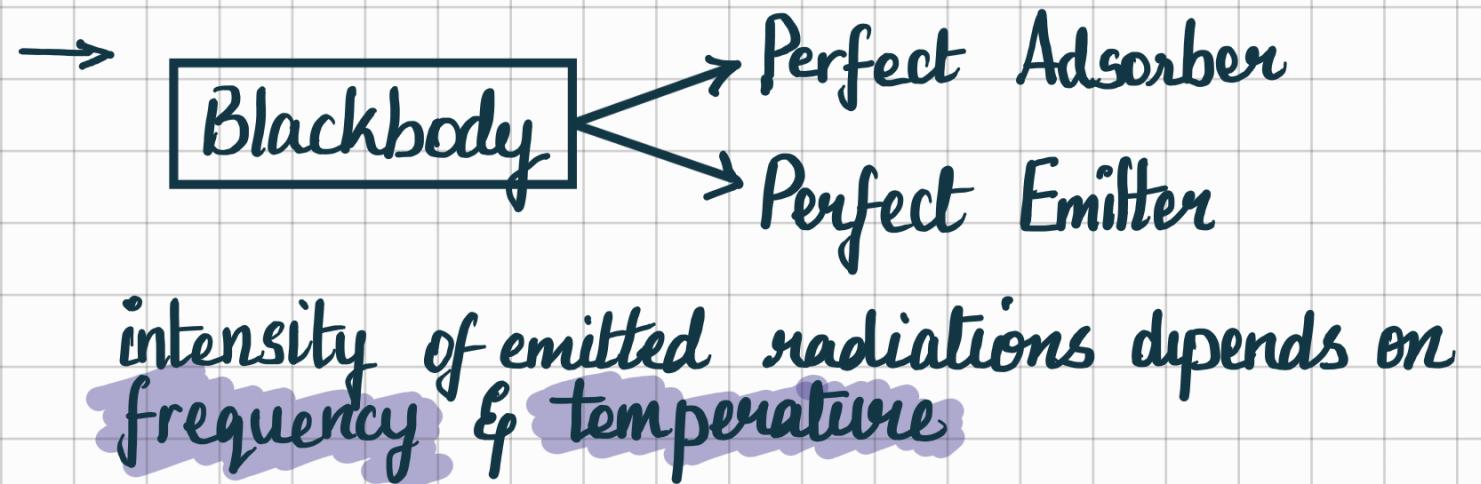
Amount of energy emitted per unit volume per frequency: $J/m^3/Hz$

$$\lambda_{\max} T = b$$

→ Wien's Law

- "wavelength of radiation emitted is directly proportional to the fourth power of temperature" is called Stephen's law.

$$P = \sigma T^4$$

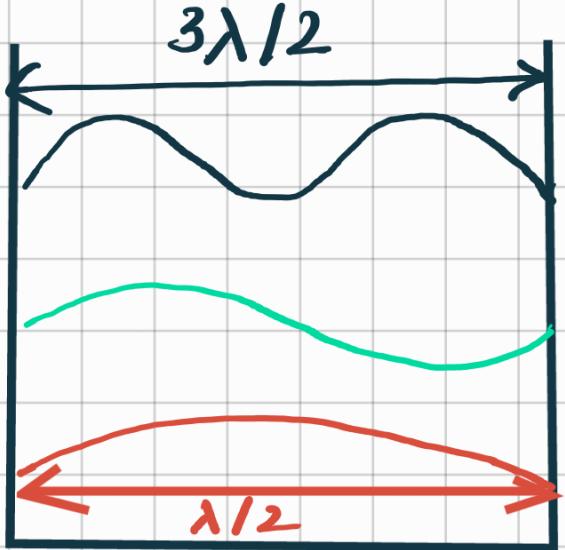


- ↳ Internal walls are perfectly reflecting except a small hole on its surface.
- ↳ Radiation gets completely trapped inside the cavity i.e. completely adsorbed.

Radiations emitted by a blackbody when it is heated : Blackbody Radiation

• Rayleigh's - Jeans formula :

The radiation of standing waves having a temperature T with nodes at metallic surfaces.



No of independent standing waves $G(v)dv$, in frequency interval v and $v+dv$ per unit volume of the blackbody cavity is given by :

$$G(v)dv = \frac{8\pi v^2}{c^3} dv$$

↓
Independent of the shape
of the cavity.

Higher frequency leads to more number of standing waves.

→ Average energy of standing wave

average energy per degree of freedom = $\frac{1}{2} k_B T$

$$\therefore \text{Average energy/oscillator} = \frac{1}{2} mv^2 + \frac{1}{2} kx^2 \\ = \underline{\underline{KT}}$$

Spectral density = $u(v) dv = \frac{8\pi v^2 K T d\nu}{c^3}$

At $v \rightarrow \infty \Rightarrow u(v)dv \rightarrow \infty \Rightarrow$ UV Catastrophe

→ Planck's Radiation Theory

Energy exchange b/w radiation & matter occurs in a discrete manner.

"Energy of radiation emitted by oscillating charges must only come in integral multiples of $h\nu$."

$$E = nh\nu \text{ where, } n=1, 2, 3\dots$$

$$h = 6.6 \times 10^{-34} \text{ J}\cdot\text{s}$$

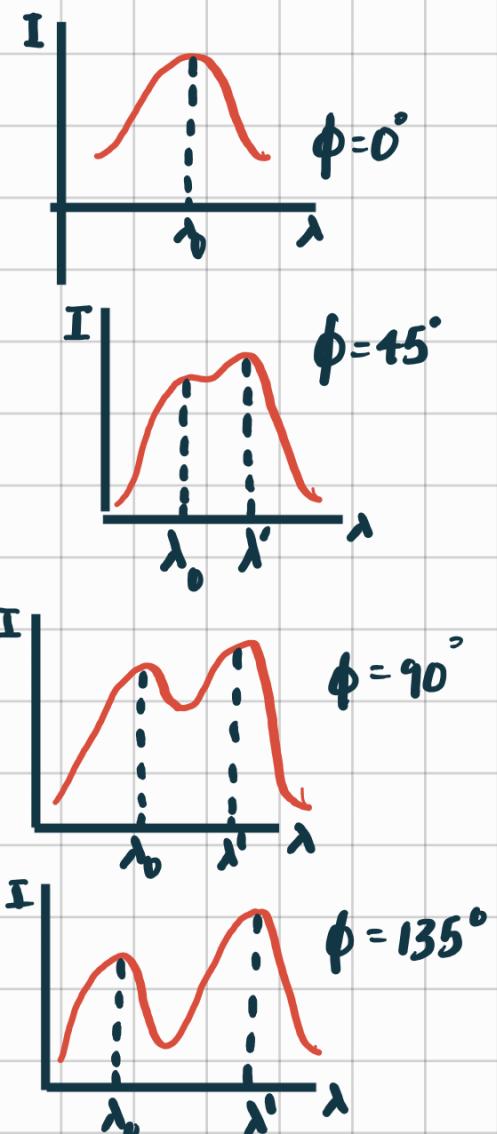
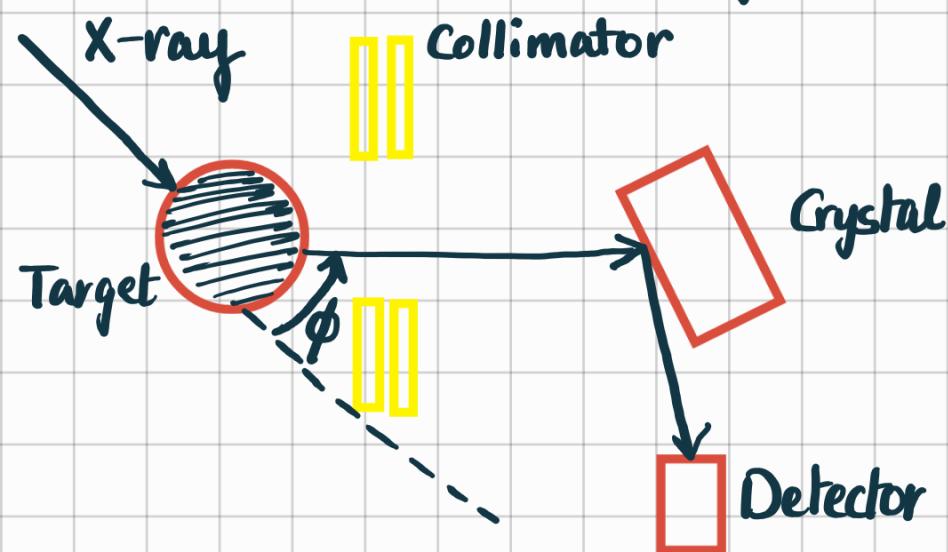
Emission or adsorption of radiation occurs only when there is a change in quantum state

$$\mu(v) = \frac{8\pi v^3}{c^3} \frac{h v}{\exp\left(\frac{h v}{k T}\right) - 1}$$

Planck's Radiation formula

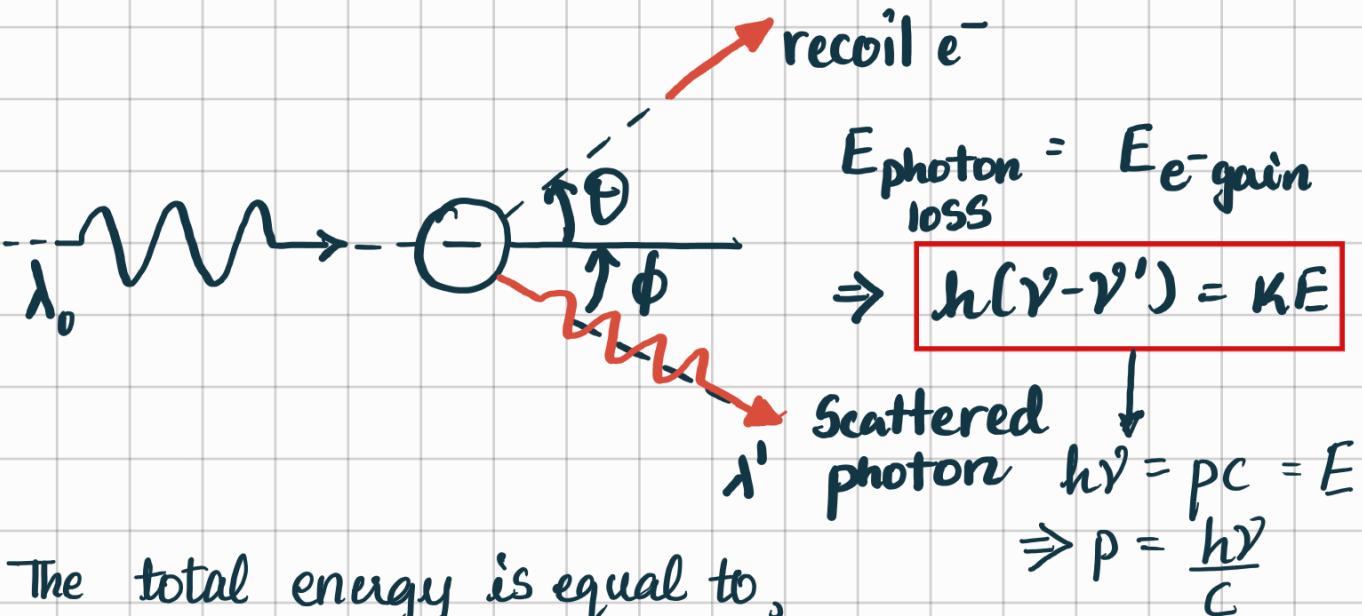
$$d \rightarrow E$$

→ Compton Scattering :



Result : Scattered radiation peak shifts to longer wavelength than source. Wavelength shift only depends on scattering angle.

classically, λ_0 and λ' must be the same. But, experimentally the wavelength of X-rays increased by $\Delta\lambda$, which depends on scattering angle.



The total energy is equal to,

$$E = m_0 c^2 + KE = \sqrt{p^2 c^2 + m_0^2 c^4}$$

$$\Rightarrow h(\nu - \nu') = KE$$

$$\Rightarrow \frac{h\nu}{c} + 0 = \frac{h\nu'}{c} \cos\phi + p \cos\theta$$

$$\Rightarrow pc \cos\theta = h\nu(1 - \cos\phi) \quad \text{--- (1)}$$

$$\frac{h\nu'}{c} \sin\phi - p \sin\theta = 0 \Rightarrow p \sin\theta = \frac{h\nu'}{c} \sin\phi \quad \text{--- (2)}$$

adding eqⁿ(1) & (2)

$$p^2 c^2 = h^2 \nu^2 + h(\nu')^2 - 2h\nu\nu' \cos\phi$$

$$\Rightarrow (KE)^2 + 2(KE)m_0 c^2 = h^2 \nu^2 + h(\nu')^2 - 2h\nu\nu' \cos\phi$$

~~$$\Rightarrow h^2(\nu^2 + (\nu')^2) - 2h\nu\nu' + 2h\nu m_0 c^2 - 2h\nu' m_0 c^2 = h^2 \nu^2 + h(\nu')^2 - 2h\nu\nu' \cos\phi$$~~

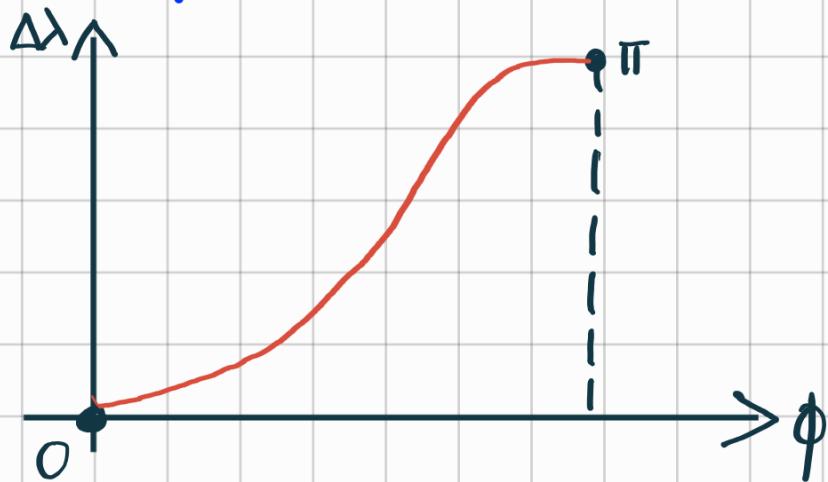
$$\Rightarrow \cancel{2h}(\gamma m_0 c^2 - \gamma' m_0 c^2) = \cancel{2h\gamma\gamma'}(1 - \cos\phi)$$

$$\Rightarrow h m_0 c^2 \left[\frac{c}{\lambda} - \frac{c}{\lambda'} \right] = \frac{c^2}{\lambda\lambda'} (1 - \cos\phi) h$$

$$\Rightarrow m_0 \left[\frac{c(\lambda' - \lambda)}{\lambda\lambda'} \right] = \frac{[1 - \cos\phi] h}{\cancel{\lambda\lambda'}}$$

$$\Rightarrow \boxed{\lambda' - \lambda = \frac{h}{m_0 c} (1 - \cos\phi)} \quad \text{where, } \frac{h}{m_0 c} = \underline{2.43 \text{ pm}}$$

$\Delta\lambda$ is minimum at $\phi = 0^\circ$ and maximum at $\phi = 180^\circ$



- De-Broglie's Hypothesis

Matter can exhibit wave-like & particle-like properties.

This wave-like property of matter is called matter waves

$$E = \sqrt{p^2 c^2 + m_0^2 c^4}$$

since rest mass of photon is zero

$$E = \sqrt{p^2 c^2} = pc \Rightarrow p = \frac{E}{c} \quad \text{--- (1)}$$

According to Planck's law, $E = \frac{hc}{\lambda} \quad \text{--- (2)}$

from eqⁿ (1) & (2)

$$\frac{E}{c} = \frac{h}{\lambda} \Rightarrow \lambda = \frac{hc}{E} = \frac{hc}{pc} \Rightarrow \boxed{\lambda = \frac{h}{P}}$$

The corresponding wavelength for the matter wave is the

De-Broglie wavelength

Applies to moving particles

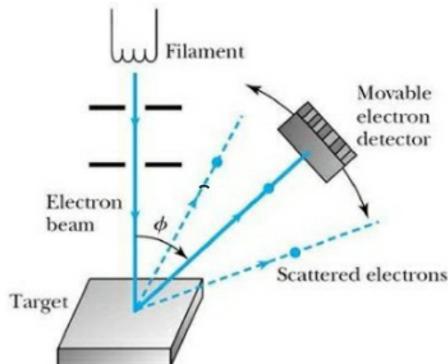
Properties of Matter Waves

Matter waves are not real waves. The quantity whose periodic variations makes up matter waves is called wavefunction (ψ).

particles with high momenta have small DB wavelength

Davinson-Germer Experiment

The experiment consisted of firing an electron beam from an electron gun on a Ni crystal at normal incidence. The electron gun consisted of a heated filament that released thermally excited electrons which were then accelerated through p.d., V and kinetic energy, eV. The angular dependence of the reflected electron intensity was measured and was determined to have the same diffraction pattern as predicted by Bragg in X-Ray.



→ According to De-Broglie relation, a beam of **54eV** had a wavelength of **0.165nm**. This matched the prediction of Bragg's Law.

Here, ϕ is the angle between the incident beam and the Bragg's plane so that is Bragg's condition of diffraction.

$$2d \sin \phi = n\lambda$$

here, $\phi = 65^\circ$, for a Ni crystal,

$$d = 0.091\text{nm}$$

Hence the wavelength of incident radiation should be

$$\lambda = 0.165\text{ nm}$$

The following experiment proves the De-Broglie hypothesis & the existence of matter waves.

• Wavefunction :

Quantity whose periodic variation make up matter waves is called wavefunction (Ψ).

- Ψ must be continuous and single valued everywhere. The 1st derivative of Ψ must also be continuous and single valued
- $\Psi \rightarrow 0$ as $x, y, z \rightarrow \infty$ and Ψ must be finite when $x, y, z = 0$

→ Physical Significance of Ψ :

- Ψ is the amplitude of matter waves
- $|\Psi|^2$ gives the probability of finding a particle at a given point (x, y, z) in space at a particular instant, t.

$$|\Psi|^2 dx dy dz$$

→ Probability of a particle being present in a volume $dx dy dz$.

The total probability of finding the particle somewhere is unity i.e. the particle is certainly found in space.

$$\iiint |\Psi|^2 dx dy dz = 1$$

if Ψ doesn't satisfy this condition, then Ψ' will.

Ψ' satisfying the above condition is called **Normalized wavefunction**

$$\Psi' = A \Psi$$

Two wavefunctions $\phi_1(x)$ and $\phi_2(x)$ are said to be orthogonal to each other in the interval (a, b) iff :

$$\int_a^b \psi_2^*(x) \psi_1(x) dx = 0$$

• Heisenberg's Uncertainty Principle

The quantum world is not deterministic, unlike classical physics.

The Heisenberg's principle is a direct consequence of the **wave-particle duality**.

"It is impossible to specify precisely and simultaneously the value of both members of particular pair of variables which are canonically conjugate to each other in the Hamiltonian sense."

$(x, p_x), (\phi, J_z), (E, t)$ are the canonically conjugate pair of variable.

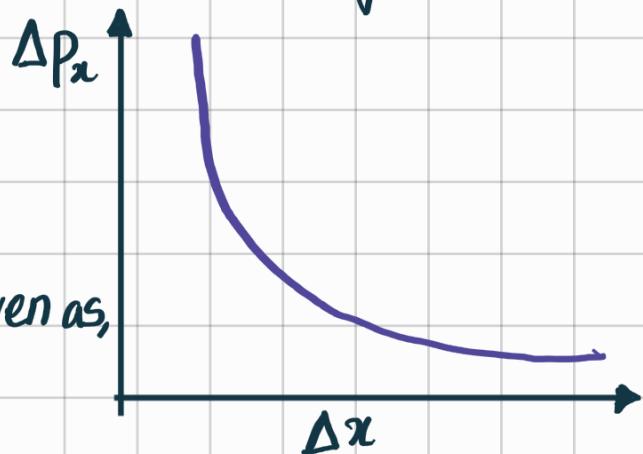
"The position and momentum of a particle cannot be determined simultaneously with arbitrary precision."

$\rightarrow \Delta x \rightarrow$ Uncertainty in position
 'x'

$$\Delta x \Delta p_x = \Delta E \Delta t = \Delta \phi \Delta J \geq \frac{\hbar}{2}$$

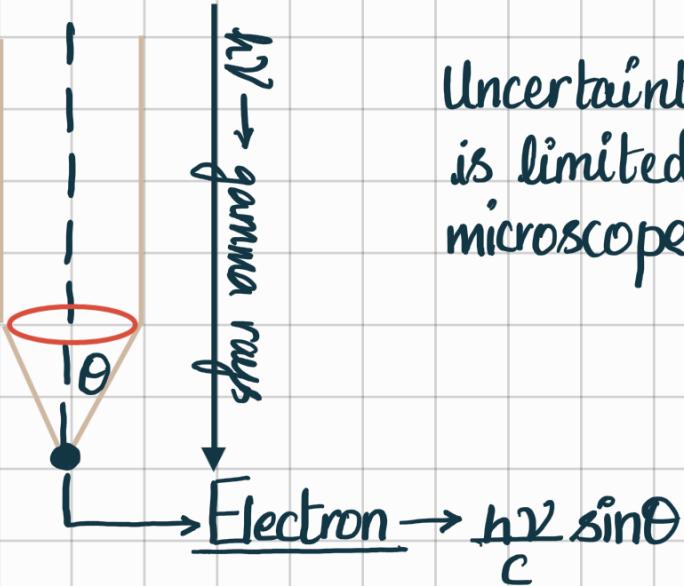
Uncertainty of any quantity A is given as,

$$\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$$



→ Experimental verification

1. Localization experiment -



Uncertainty in the position of the electron is limited by resolving power of microscope.

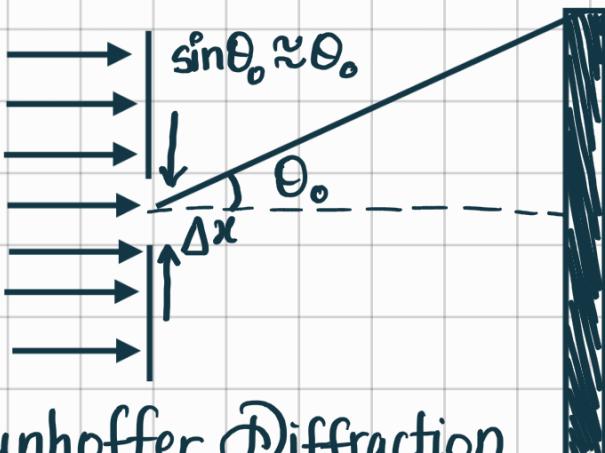
$$\Delta x = \frac{\lambda}{2 \sin \theta}$$

Recoil momentum of the electron due to incident γ -rays is $\frac{h\nu}{c}$ and its x -component is:

$$P_x = \Delta p_x = \frac{h\nu \sin\theta}{c}$$

$$\rightarrow \Delta x \Delta p_x \sim \frac{\hbar}{2}$$

2. Electron Diffraction through a narrow slit -



$$\begin{aligned} & \text{for 1st minimum:} \\ & d \sin \theta = n\lambda \\ & \Rightarrow \Delta x \cdot \Theta_0 \sim \lambda \\ & \Rightarrow \Delta x \sim \frac{\lambda}{\Theta_0} \end{aligned}$$

Fraunhofer Diffraction

Due to the presence of slit, the electron beam suffers diffraction and each electron acquires the X -components of momentum.

$$\Delta p_x = p \sin \theta_0 \sim p \theta_0 \Rightarrow \therefore \Delta x \cdot \Delta p_x \sim \lambda p = h$$

→ Application of Uncertainty relation :

1. Ground state & Bohr's energy

Total energy of electron in the electric field of a proton.

$$E = \frac{p^2}{2m} - \frac{e^2}{r} = \frac{p^2}{2m} - \frac{e^2 p}{\hbar}$$

$$\text{Condition for minimization of energy: } \left. \frac{dE}{dp} \right|_{p=p_0} = 0$$

$$\Rightarrow p_0 = \frac{me^2}{\hbar}$$

$$r_0 \sim \frac{\hbar}{p_0} = \frac{\hbar^2}{me^2} \sim 0.0529 \text{ nm}$$

$$E_0 \sim -\frac{me^4}{2\hbar} \sim -13.6 \text{ eV}$$

• Schrodinger's Equation -

It states the relationship between the momentum and wavelength associated with matter waves, using the De-Broglie's relation.

It describes the behavior of atomic systems & their interaction with other particles and E-M radiation.

Consider a group of waves associated with a moving particle

$\Psi(\vec{r}, t) \rightarrow$ Displacement of these waves at position \vec{r} and time t .

Let the wave motion be represented by the classical wave equation.

$$\nabla^2 \Psi(\vec{r}, t) = \frac{1}{v^2} \frac{\partial^2 \Psi(\vec{r}, t)}{\partial t^2}$$

$v \rightarrow$ speed of the moving particle.

where,

$$\begin{aligned}\vec{\nabla} &= \hat{i} \frac{\delta}{\delta x} + \hat{j} \frac{\delta}{\delta y} + \hat{k} \frac{\delta}{\delta z} \Rightarrow \nabla^2 = \vec{\nabla} \cdot \vec{\nabla} \\ \Rightarrow \nabla^2 &= \hat{i} \frac{\delta^2}{\delta x^2} + \hat{j} \frac{\delta^2}{\delta y^2} + \hat{k} \frac{\delta^2}{\delta z^2}\end{aligned}$$

Assume that the wave amplitude at \vec{r} is periodic in t

$$\Psi(\vec{r}, t) = \Psi(\vec{r}) e^{-i\omega t} \quad \text{①}$$

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

$$\nu = \frac{c}{\lambda} \Rightarrow \lambda = \frac{h}{mv}$$

Substitute eqⁿ ① in wave equation, we get

$$\nabla^2 \Psi(\vec{r}, t) = -\frac{\omega^2}{v^2} \Psi(\vec{r}, t) = -\frac{4\pi^2}{\lambda^2} \Psi(\vec{r}, t)$$

$$\Rightarrow \nabla^2 \Psi(\vec{r}, t) + \frac{4\pi^2}{\lambda^2} \Psi(\vec{r}, t) = 0 \quad \text{②}$$

The total energy (E) of any particle is the sum of its Potential Energy (V) & Kinetic energy ($K.E.$).

$$K.E. = \frac{1}{2} m v^2 = E - V \Rightarrow mV = \sqrt{2m(E-V)}$$

Hence, the wave equation describing the motion becomes,

$$\nabla^2 \Psi(\vec{r}, t) + \frac{8\pi^2 m^2 V^2 (E-V)}{\hbar^2} \Psi(\vec{r}, t) = 0 \quad \textcircled{A}$$

$$\text{But, } \hbar = \frac{h}{2\pi}$$

$$\nabla^2 \Psi(\vec{r}, t) + \frac{2m}{\hbar^2} (E-V) \Psi(\vec{r}, t) = 0 \quad \textcircled{B}$$

The Schrodinger's Time-Independent Equation is :-

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

from eqⁿ \textcircled{A}

$$\nabla^2 \Psi(\vec{r}) e^{-i\omega t} + \frac{8\pi^2 m}{\hbar^2} (E-V) \Psi(\vec{r}) e^{-i\omega t} = 0$$

$$\Rightarrow \nabla^2 \Psi(\vec{r}) e^{-i\omega t} + \frac{8\pi^2 m}{\hbar^2} V \Psi(\vec{r}) e^{-i\omega t} = \frac{8\pi^2 m}{\hbar^2} E \Psi(\vec{r}) e^{-i\omega t}$$

∇^2 involves differentiation w.r.t space coordinates only

$$\Rightarrow -\nabla^2 \Psi(\vec{r}, t) + \frac{8\pi^2 m}{h^2} V \Psi(\vec{r}, t) = \frac{8\pi^2 m E}{h^2} \Psi(\vec{r}, t)$$

C

R.H.S of eqⁿ C can be written as follows :

$$\frac{8\pi^2 m}{h^2} E \Psi(\vec{r}) e^{-i\omega t} = \frac{8\pi^2 m}{h^2} \left(\frac{E}{-i\omega} \right) \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \frac{8\pi^2 m}{h^2} \left(\frac{i\hbar}{2m} \right) \times \frac{\partial \Psi(\vec{r}, t)}{\partial t}$$

Now, eqⁿ C becomes.

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

Energy operator (E)

↓

Hamiltonian Operator (\hat{H})

Schrodinger's Time Dependant Equation

In general,

$$\boxed{\hat{H}\Psi = E\Psi}$$

Eigenvalue Equation

where, $\hat{H} \rightarrow$ Eigen Operator
 $E \rightarrow$ Eigen Value
 $\Psi \rightarrow$ Eigen function

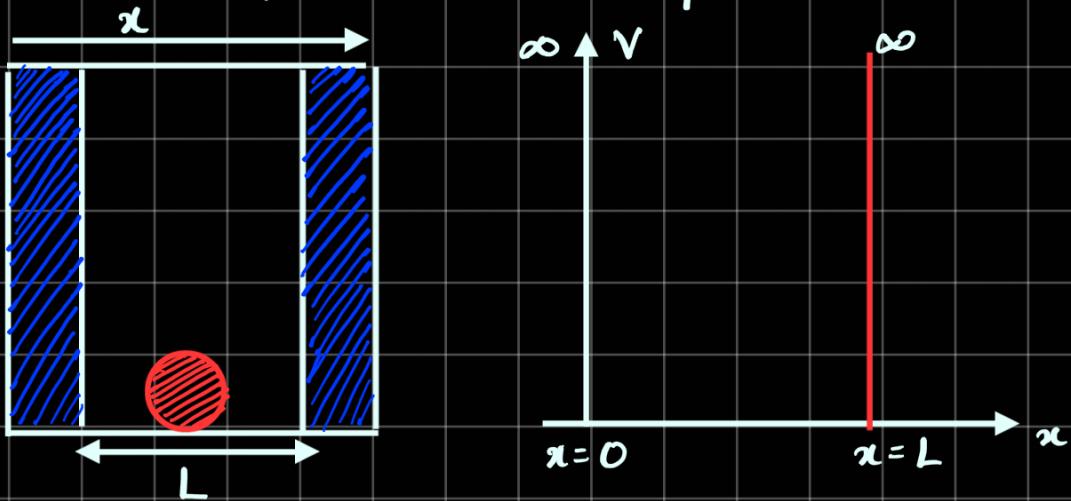


Application of Schrodinger's Equation

Module - 2

• Particle in a box (1-D) :

Consider a particle of mass m is confined to move inside a box along x -direction only. The particle is trapped inside the infinitely hard walls of the walls and cannot penetrate it.



The potential can be written as -

$$V(x) = \begin{cases} \infty & |x \leq 0, x \geq L \\ 0 & |0 < x < L \end{cases}$$

Wavefunction corresponding to the particle must be zero where the potential is infinity.

$$\Psi = 0 \text{ for } x \leq 0 \text{ and } x \geq L$$

The Schrodinger's time independent equation for the particle is :

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

$$\Rightarrow \frac{d^2\Psi}{dx^2} + k^2 \Psi(x) = 0, \text{ where } k = \sqrt{\frac{2mE}{\hbar^2}} \rightarrow \text{Wave vector}$$

The general solution of this equation is :

$$\Psi(x) = Ae^{ikx} + Be^{-ikx}$$

The boundary conditions are used to evaluate the constants A and B.

$$\Psi(x) = 0 \text{ at } x=0 \text{ and } x=L$$

$$\Rightarrow 0 = A(1) + B(1) \Rightarrow A = -B$$

$$\therefore \Psi(x) = A(e^{ikx} - e^{-ikx}) = 2iA \sin(kx) \Rightarrow \boxed{\Psi(x) = C \sin kx}$$

$$\Psi(x) = 0 \text{ at } x=L \Rightarrow C \sin(kL) = 0$$

$$\Rightarrow kL = n\pi$$

$$\Rightarrow k = \frac{n\pi}{L} \text{ and } E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

$$\boxed{\Psi_n(x) = C \sin\left(\frac{n\pi}{L}x\right)}$$

where, n is the principle quantum no.

Since, the probability of finding the particle inside the box is unity, using the normalization procedure.

$$\int_0^L \Psi^*(x) \Psi(x) dx = 1$$

$$\Rightarrow C^2 \int_0^L \sin^2\left(\frac{n\pi}{L}x\right) dx = 1$$

$$\Rightarrow C^2 \int_0^L 1 - \cos\left(\frac{2\pi nx}{L}\right) dx = 1$$

$$\Rightarrow \frac{C^2}{2} \left[x - \frac{L}{2\pi n} \sin\left(\frac{2\pi nx}{L}\right) \right]_0^L = 1$$

$$\boxed{C = \sqrt{2}}$$

$$\boxed{[-\frac{\hbar^2}{L} \leq]}$$

Hence, from eqⁿ 1 & 2

$$\boxed{\Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)}$$

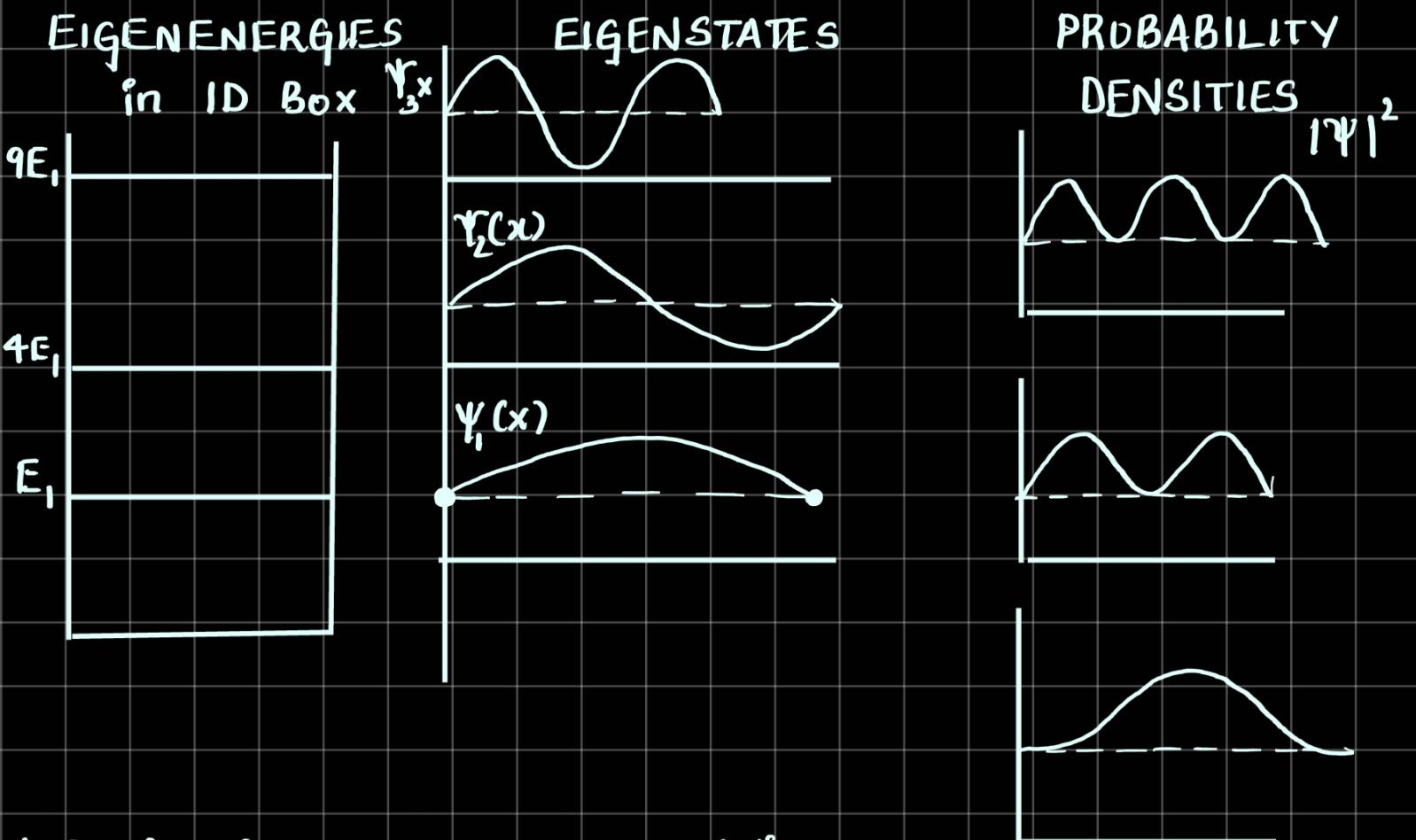
but, we know that,

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

$$E_{n+1} - E_n = (2n+1) \left[\frac{\pi^2 \hbar^2}{2mL^2} \right]$$

i.e the energy is quantized and
the ground state energy is given as:

$$\boxed{E_1 = \frac{\pi^2 \hbar^2}{2mL^2}}$$



↳ Particle in a Box - 3D extrapolation

(n_x, n_y, n_z)

$$\Psi(x, y, z) = \Psi(x) \Psi(y) \Psi(z)$$

$$\Psi(x, y, z) = \sqrt{\frac{2}{L_x}} \sqrt{\frac{2}{L_y}} \sqrt{\frac{2}{L_z}} \sin\left(\frac{n_x \pi}{L_x}\right) \sin\left(\frac{n_y \pi}{L_y}\right) \sin\left(\frac{n_z \pi}{L_z}\right)$$

$$E_n = \frac{\pi^2 \hbar^2}{2m} \left[\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right]$$

Quantum Tunneling:

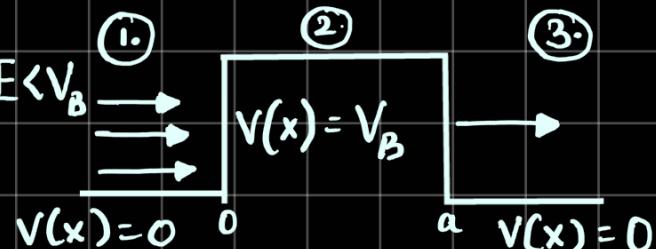
Ability to penetrate and tunnel through a classical forbidden region is called quantum tunneling.

Consider a particle in the simple P.E of the form.

$$V(x) = 0, -\infty < x < 0$$

$$V(x) = V_B, 0 < x < a$$

$$V(x) = 0, a < x < \infty$$



$$\text{region 1} \rightarrow \frac{\partial^2 \Psi_1(x)}{\partial x^2} + \frac{2mE}{\hbar^2} \Psi_1(x) = 0$$

$$\text{region 2} \rightarrow \frac{\partial^2 \Psi_2(x)}{\partial x^2} + \frac{2m(E - V_B)}{\hbar^2} \Psi_2(x) = 0$$

$$\text{region 3} \rightarrow \frac{\partial^2 \Psi_3(x)}{\partial x^2} + \frac{2mE}{\hbar^2} \Psi_3(x) = 0$$

$$\Psi_1(x) = Ae^{ik_1 x} + Be^{-ik_1 x}$$

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\Psi_2(x) = Ce^{-k_2 x} + De^{k_2 x}$$

$$k_2 = \sqrt{\frac{2m(V_B - E)}{\hbar^2}}$$

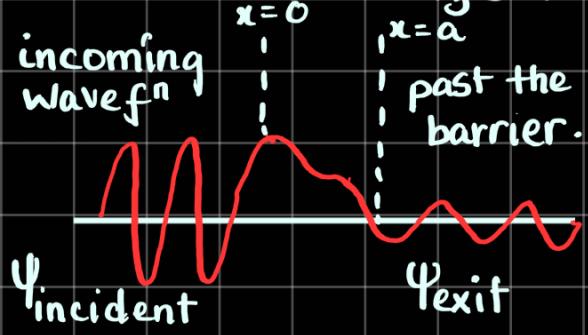
$$\Psi_3(x) = Ee^{ik_1 x} + F e^{-ik_1 x}$$

But in $\Psi_2(x), \Psi_3(x)$

$$D=0 \leftrightarrow F=0$$

$$\text{Therefore, } \Psi_1(x) = A e^{i k_1 x} + B e^{-i k_1 x} \quad \Psi_2(x) = C e^{-i k_2 x}$$

$$\Psi_3(x) = E e^{-i k_1 x}$$



Transmission probability :

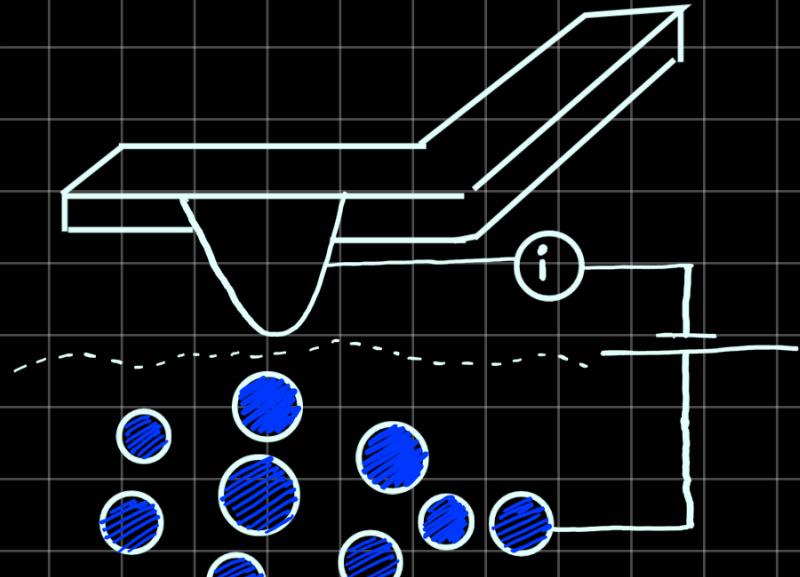
$$T = \frac{|\Psi_2(x=a)|^2}{|\Psi_2(x=0)|^2} \sim \exp(-2k_2 a)$$

$$V_B, a \rightarrow \infty \\ T \rightarrow 0$$

→ Scanning Tunneling Microscope :

Uses the principle of Quantum Mechanical tunneling.
It was invented in 1981 by Gerd Binnig and Heinrich Rohrer
at IBM Zurich.

an electrically conducting probe with a very sharp edge is brought near the surface



The empty space between the tip and the surface is called the barrier. The tip and surface are the two walls of the potential well.

STM: Atomically sharp needle and terminates in a single atom.

Pure Metals [W, Au]

$$E_F - E_A = 1$$

Alloys L_PF - Rh, Ph-Ir]
Chemically modified conductors [W/S, Pt-Rh/S, W/C]

- Raster the tip across the surface, and using the current as a feedback signal
- The tip-surface separation is controlled to be constant by keeping the tunneling current to be constant.
- The voltage necessary to keep the tip at a constant separation is used to form a comp. image.

Note: STM can either be used in Constant Current Mode or Constant Height Mode.



We can either probe at a constant height or look at the current variations.

Nanotechnology

Nano-sized materials exhibit some remarkable properties that may be different from the properties of bulk materials. Nanotechnology is the creation of fundamental materials, devices and systems through the understanding & control of matter at dimensions in nanoscale, where new functionalities and new properties of matter are observed & harnessed.

→ Device Miniturization : Moore's Law

"The number of transistors incorporated in a chip will approximately double every 24 months."

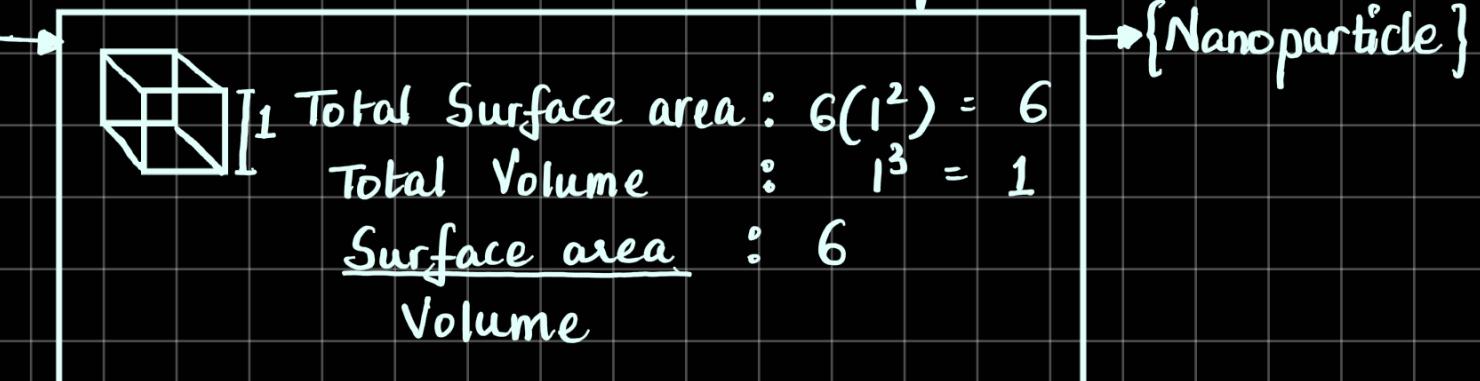
The law / statement given by Gordon Moore is amazingly accurate and is essentially the gospel of microelectronics today & hence drives the industry today.

The evidence of Moore's Law is everywhere, embedded in devices like: Laptops, mobiles, automobiles, life saving medical devices, space crafts etc.

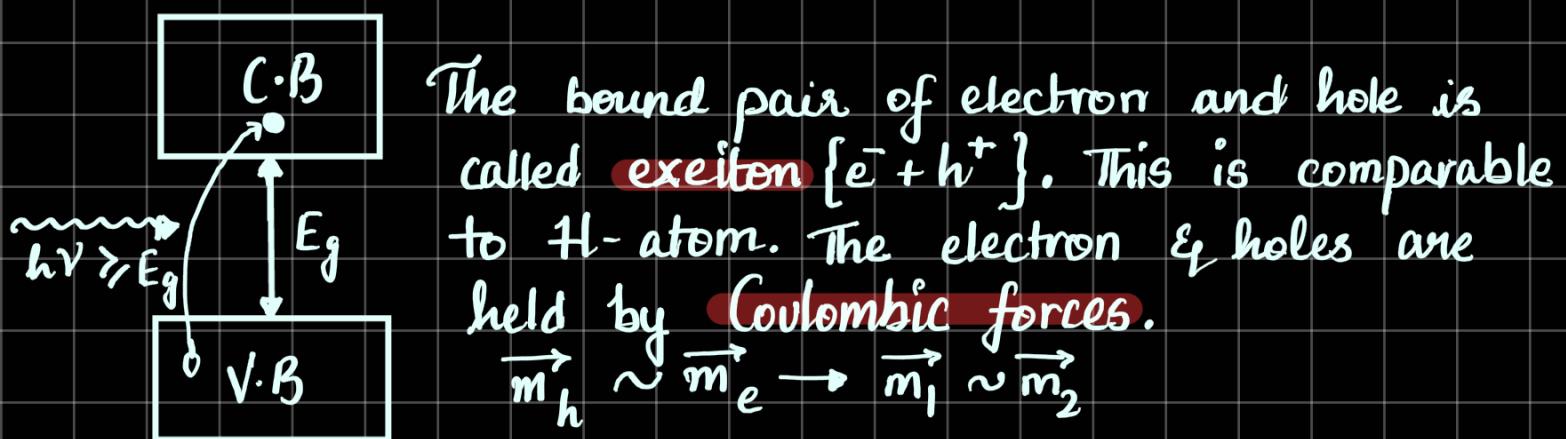
→ Some Nanoscale Terms

- Cluster - A collection of units (atoms or reactive molecules) of upto 50 units.
- Colloids - A stable liquid phase containing particles in the 1-1000 nm range. A colloid particle is one such 1-1000 nm particle.

- Nanoparticle - A solid particle in the 1-1000 nm range that could be noncrystalline, aggregate of crystallite or a single crystallite.
- Nanocrystal - A solid particle that is a solid crystal in the nanometer range.



→ Quantum Confinement
 It applies to nanomaterials only.



$$m \rightarrow M \text{ (reduced mass)} = \frac{m_1 m_2}{m_1 + m_2}$$

$$\Rightarrow M = \frac{1}{m_1} + \frac{1}{m_2}$$

when $m_1 \rightarrow m_e$
 $m_2 \rightarrow m_h$

when $m_1 \rightarrow m_e$ and $m_2 \rightarrow m_p$

$$\Rightarrow M \sim m_1 \text{ since } m_1 \ll m_2$$

Exciton binding energy, $E = -\frac{13.6 M}{C e^2}$

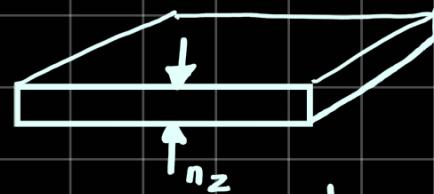
$$\text{Bohr's excitonic radius, } r = \frac{0.529 E_s}{M} n^2 \text{ Å}$$

Quantum Dots - Wires - Wells

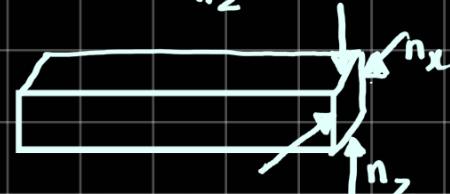
for a bulk semiconductor, electrons in CB (and holes in VB) are free to move in all 3D - space

Quantum Confinement in :

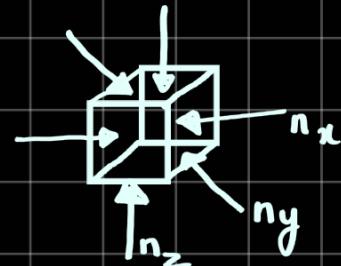
1 direction :- Quantum well
 {2D electron}



2 directions :- Quantum wire
 {1D electron}

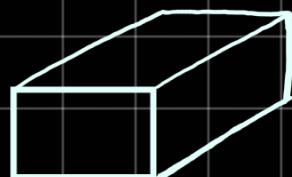


3 direction :- Quantum dot
 {Zero D electron}



{ Each confinement converts a continuous k in a discrete q·n (n) } $[k \rightarrow k_x \text{ or } k_y \text{ or } k_z]$

Three - Dimension



$$\text{density} \propto \sqrt{E}$$

d

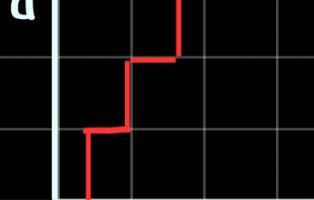


Two - D



$$\text{density} \propto E^0$$

d

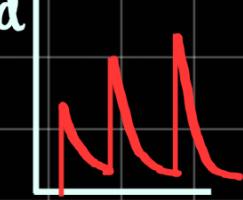


One - D



$$\text{density} \propto \frac{1}{\sqrt{E}}$$

d

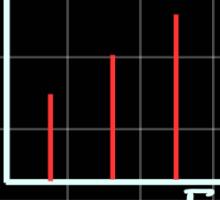


Zero - D



$$\text{density} \propto \delta E$$

d



E

E

E

Density of states ($P_{DOS}(E)$) allows us to determine the total no. of states/unit volume in an energy band with energies E_1 (bottom of band) & E_2 (top of band) according to :-

$$N = \int_{E_1}^{E_2} P_{DOS}(E) dE$$

- Discrete Energy Levels

The energy levels depends on size and shape of the quantum dot.

Smaller quantum dots

↳ Higher energy required to confine excitons to a smaller volume

- Energy levels increases in energy & spread out
- Higher band gap energy.

Three ways to confine excitons :-

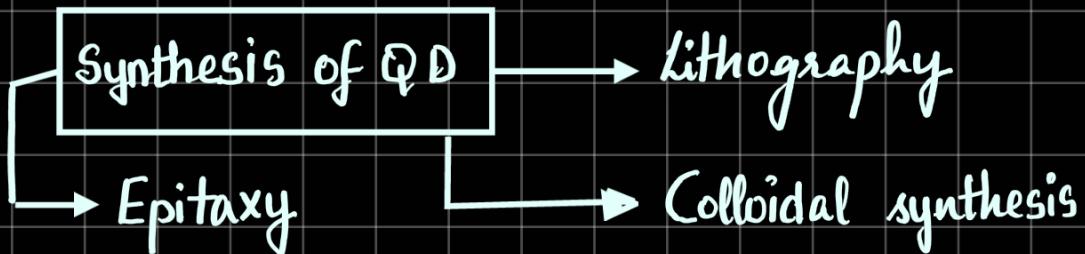


Photo detectors
and LASERS

Photovoltaic devices

Memory
elements

Applications
of Q.D's

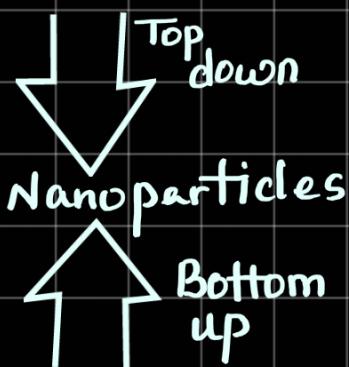
Biosensors and
imaging

Flat - panel
displays

Quantum
Computation

LED's

Synthesis of Nanomaterials



Mechanical grinding & Ball milling: top down
Wet Chemical synthesis

Top - down → single crystals are etched in an aqueous solⁿ.

Bottom - down → Sol-gel, Combustion precipitation etc.

Gas-phase synthesis:- Chemical Vapour Deposition (CVD)

Physical Vapour Deposition (PVD)

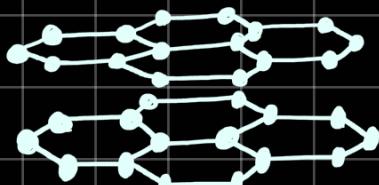
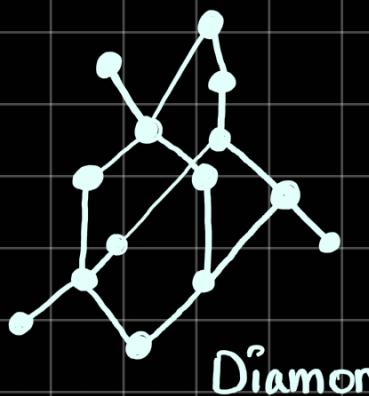
Sputtering

Thermal evaporation

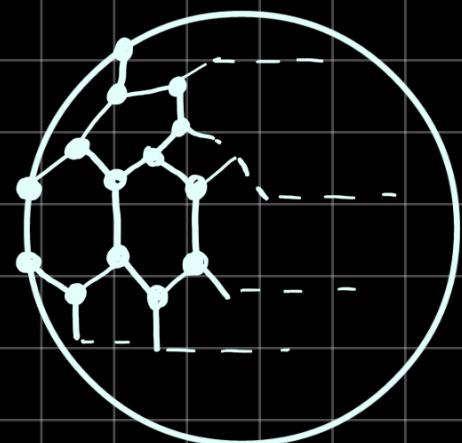
Pulsed Laser Deposition

→ Carbon Nanotubes

The allotropes of carbon are :-



Graphite



Buckminster fullerene (C_{60})

The fullerenes can also form cylindrical structure called as 'bucky-tubes'. CNT's also known fullerenes are allotropes of carbon with a cylindrical nanostructure.

Types of Carbon Nanotubes

→ Single Walled Nanotubes (SWNT) -

✓ diameter ~ 1nm with tube length that can be

millions long.

- ✓ The structure of SWNT can be seen by wrapping a 1-atom thick layer of graphite called graphene.
- ✓ The way the graphene sheet is wrapped is represented by indices (m, n) called chiral vector.
SWNT show superior electric properties.

→ MultiWalled Nanotubes (MWNT) -

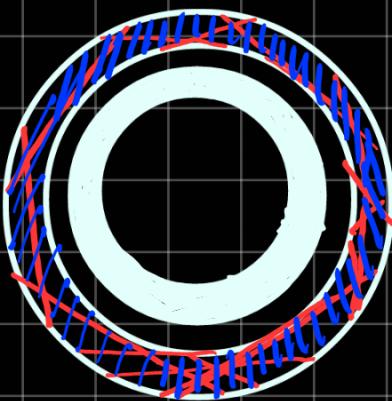
MWNT consist of multiple rolled layers (concentric layers) of graphite.

There are two models of description of MWNT - :

- Russian Doll Model, where sheets of graphite are arranged in concentric cylinders
- Parchment Model, a single sheet of graphite is rolled in around itself, resembling a scroll of parchment.

→ Torus -

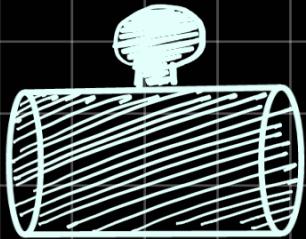
A nanotorus is theoretically described as carbon nanotubes bent into a torus. They are predicted to have many unique properties like magnetic properties which describes the interaction with an applied field to a mechanical moment.



Carbon
Nanotubes

→ Nanobud -

Carbon nanobuds are formed by combining two allotropes of carbon : carbon nanotubes and buckyballs. Nanobuds has useful properties of CNT and buckyballs.



Carbon
nanotubes

Synthesis of CNT's → Arc Discharge, Laser Ablation
Ball Milling, Chemical Vapour Deposition

Applications

of CNT's → Solar Cells, Ultracapacitors, Paper batteries,
nanoelectromechanical systems like NRAM.

→ Nanoscale Size Effect :-

Realization of miniaturized devices & systems while providing more functionality. Attainment of high surface area to volume ratio. Nanomaterials show the following types of properties :-

- Physical Properties
- Chemical Properties
- Electrical Properties
- Mechanical Properties
- Optical Properties

Advantages

of Nanotechnology :- 1. Material - with NT, we can create unique materials/products which are :-

2. Industrial -

- ✓ Computers can be a billion times faster & a million times smaller
- ✓ Automatic Pollution Cleanup
- ✓ Manufacturing cost ~ 0

- ✓ Stronger
- ✓ Lighter
- ✓ Cheaper
- ✓ Durable
- ✓ Precise

3. > Medical - ✓ End of illnesses (cancer, heart disease etc)
✓ Universal immunity
✓ Body Sculpting

→ Properties of Nanomaterials

The properties of N.m are significantly different from bulk solid. This is due to N.m size of the material which render them :

- ✓ Large fraction of surface atoms
- ✓ High surface energy
- ✓ Spatial confinement
- ✓ Reduced imperfections

LASER

Module - 4

Modern light sources convert electrical signals to optical signal.

LED source → Monochromatic ; not coherent ; discrete

LASER → Monochromatic ; coherent ; discrete

Characteristics of LASERS

→ High Directionality

LASER's are highly directional & emit in one direction. Directionality of lasers is expressed in terms of full angle beam divergence



It is defined as twice the angle that the outer edge of the beam makes with the axis of the beam

→ High Intensity

- LASER gives out light in a narrow range and it's energy is concentrated in a narrow range. (both spatially & spectrally)

• Greater intensity

• No of photons/sec = $10^{16} - 10^{28}$

• Output power of LASER varies from mW (continuous) and GW (pulsed).

→ High degree of Monochromativity

High degree of non-monochromaticity

- Much more monochromatic than any conventional light sources
- Absolute monochromatic is impossible because of Uncertainty relation b/w energy and time. $\Delta E \Delta t \geq \frac{h}{2}$
- Degree of non-monochromaticity,

$$\xi = \frac{\Delta\nu}{\nu_0} \rightarrow \Delta\nu \sim 100 - 1000 \text{ Hz and } \Delta\lambda \sim 10^{-8} - 10^{-2} \text{ Å}$$

High Contrast

Same phase or constant phase

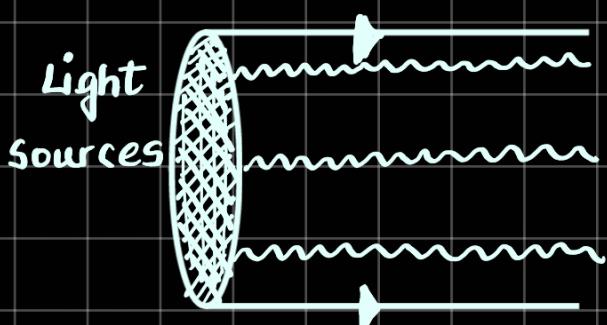
Light coming out of a laser is highly ordered

High degree of coherence results in tremendous optical concentration.

Coherence:

Conventional light sources: light consists of tiny separate waves that reinforce or cancel each other randomly.

Wavefront produced varies in phase from point to point (spatial) or time to time (temporal)



Temporal Coherence

- Correlation b/w the field at a point and field at the same point at a later.

- If phase difference b/w the two fields remains constant during the period of observation, then the source is temporally coherent.

Spatial Coherence

- Two fields at two different points on a wavefront of an e.m wave are said to be spatially coherent if they preserve a constant

phase difference over a time period, t .

Temporal coherence is a characteristic of a single beam of light whereas Spatial coherence concerns the relationship b/w two separate beams of light.

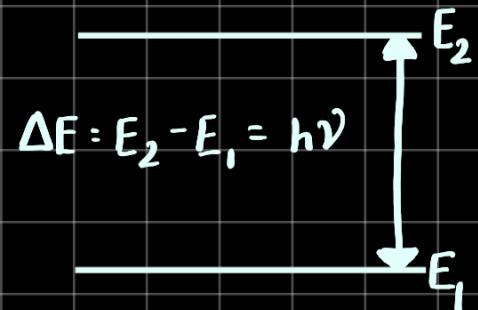
Average time upto which the ideal sinusoidal behavior remains is called Coherence time (T_c).
The corresponding length is called Coherence length (L_c)

$$L_c = c T_c$$

There is no correlation b/w the phase of the waves after T_c .

Adsorption and Emission

Interaction of light with matter takes place in discrete packets of energy called photons (quanta).



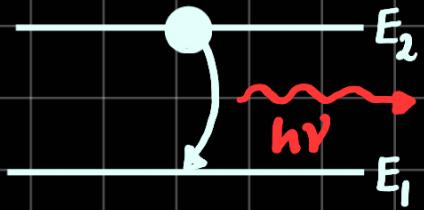
Different energy states for an atom corresponds to different electronic configuration.

The frequency of adsorbed or emitted radiation is related to the difference in energy b/w higher and lower energy states.

Adsorption \rightarrow always stimulated

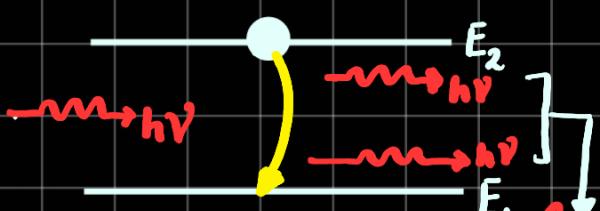
Emission \rightarrow spontaneous or stimulated

Spontaneous Emission:



Random incoherent radiation occurs when the nature of a large no. of atoms is random.
Hence the emission occurs without any external help

Stimulated Emission:



There are only two types of processes in nature: stimulated adsorption and emission. Spontaneous emission **Coherent** is just a special type of random stimulated emission due to zero point energy of vacuum.

Light associated with the stimulating and stimulated photon is in same phase and same polarization:

Coherent Radiation

When an atom is stimulated to emit light, the energy liberated is used constructively to provide amplification.

Einstein's Relation

Rates of 3 transition processes in a collection of atoms are mathematically related:

- Adsorption
- Spontaneous Emission
- Stimulated Emission

Assumption

Atomic system is in thermal equilibrium

Rate of upward = Rate of downward transitions

→ Population of energy levels can be described by Maxwell-Boltzmann distribution

Suppose N_1 and N_2 are the density of atoms in energy levels E_1 and E_2 respectively.

E_2, N_2

$$\Delta E = E_2 - E_1 = h\nu$$

E_1, N_1

$$N = g \exp\left(\frac{-E}{k_B T}\right)$$

$$\frac{N_1}{N_2} = \frac{g_1 \exp\left(-E_1/k_B T\right)}{g_1 \exp\left(-E_2/k_B T\right)}$$

g -degeneracy factor

Quantum mechanical states having same energy are degeneracy factor.

M-B Distribution

$$\frac{N_1}{N_2} = \left(\frac{g_1}{g_2} \right) \exp\left[\frac{h\nu}{k_B T} \right]$$

Rate of adsorption : R_{12} (electron transition from $1 \rightarrow 2$)

$$R_{12} \propto N_1$$

$$R_{12} \propto P_v \text{ (spectral energy density)}$$

$$R_{12} = B_{12} N_1 P_v$$

$B_{12} \rightarrow$ Einstein's coefficient for Adsorption

Rate of Spontaneous Emissions (G_{21})

Average time an electron spends in the excited state before spontaneous emission takes place is called spontaneous lifetime T_{21} .

$$G_{21} = N_2 \left[\frac{1}{T_{21}} \right] = N_2 A_{21}$$

$$\text{Rate of Stimulated Emission} \rightarrow F_{21} = B_{21} N_2 P_r$$

rate of downward emission: R_{21} (electron transition from 2 → 1)

$$R_{21} = N_2 A_{21} + B_{21} N_2 P_r$$

for a system in thermal equilibrium →

$$R_{12} = R_{21}$$

$$B_{12} N_1 P_r = A_{21} N_2 + B_{21} N_2 P_r$$

$$\Rightarrow P_r = \frac{A_{21} N_2}{N_1 B_{12} - N_2 B_{21}}$$

$$P_r = \frac{\left(A_{21} / B_{21} \right)}{\left(\frac{g_1 B_{12}}{g_2 B_{21}} \exp\left(\frac{h\nu}{k_B T}\right) \right) - 1}$$

$$\Rightarrow P_r = \frac{8\pi h\nu^3 n_0^3}{c^3} \left(\frac{1}{\exp\left(\frac{h\nu}{k_B T}\right) - 1} \right)$$

$$\text{where; } B_{12} = \left(\frac{g_2}{g_1} \right) B_{21} \text{ and } \frac{A_{21}}{B_{21}} = \frac{8\pi h\nu^3 n_0^3}{c^3}$$

Hence, when the degeneracies of the two levels are same;

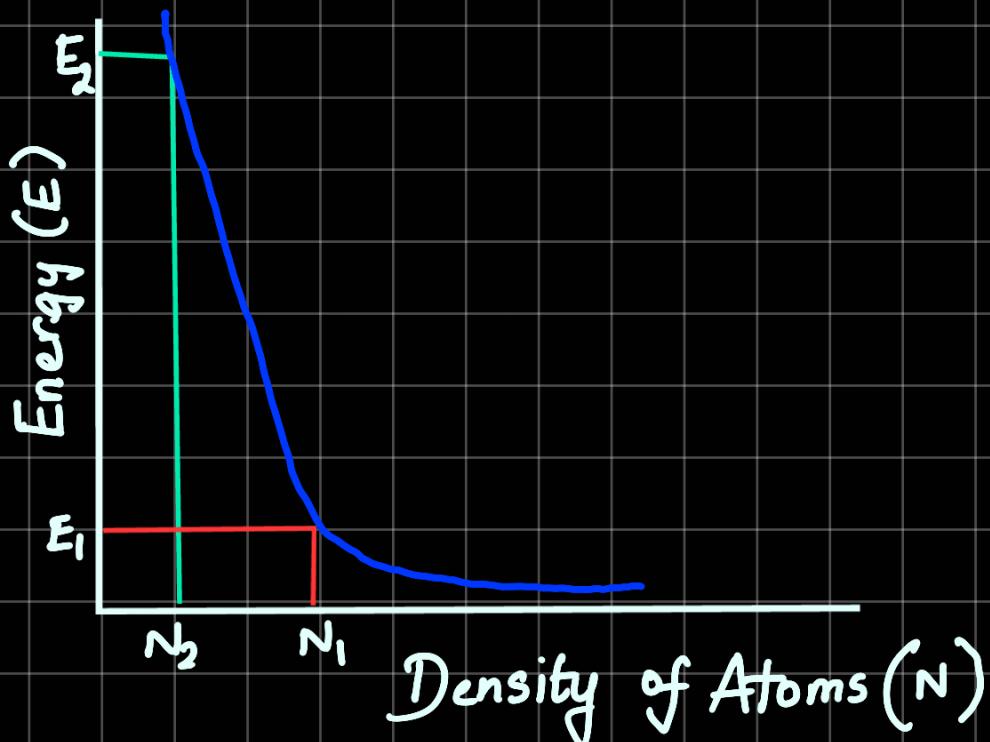
$B_{12} = B_{21}$, then the probability of absorption and stimulated emission are the same.

$$\frac{\text{Stimulated emission rate}}{\text{Spontaneous emission rate}} = \frac{B_{21} \times P_r}{A_{21}} = \frac{1}{\exp\left(\frac{h\nu}{kT}\right) - 1}$$

→ Population Inversion -

- For a system under thermal equilibrium, spontaneous emission is the dominant one

- Radiation emitted in the spectrum in a random manner is Incoherent source.
- Rate of stimulated emission \rightarrow ↑ Es \rightarrow Coherent source
- Popⁿ density (upper level) $>$ Popⁿ density (lower level)



Methods to achieve Population Inversion

- Medium in which P.I is achieved : Active Medium
- Active medium is placed b/w the two mirrors of optical cavity .(Fabry - Perot - Etalon)
- It is practically impossible to achieve P.I thermally
- The method by which P.I is achieved is called Pumping.

→ Optical Pumping

Xe or Kr flash lamp is used to supply the luminous energy to the system. Ex: Ruby (Cr:Al₂O₃ laser)

→ Direct electron excitation

- Similar to electric discharge
- Used in gaseous ion lasers

- Electrons are released from atoms due to high voltage electric discharge thru a gas
- Ionized medium & population (higher) increases

→ Inelastic atom-atom collision

- Pumping by electric discharge provides the initial excitation which raises one type of atom (A) to its excited form (A^*).
- These atoms collide in- elastically with another atom $B \rightarrow B^*$

Ex: He-Ne laser, He-Cd laser

→ Chemical Reaction

- Molecules undergo chem. changes in which the product is a molecule or atom in excited state

Ex: H-F laser

→ Direct Conversion

- Electrical energy is directly converted into radiation.

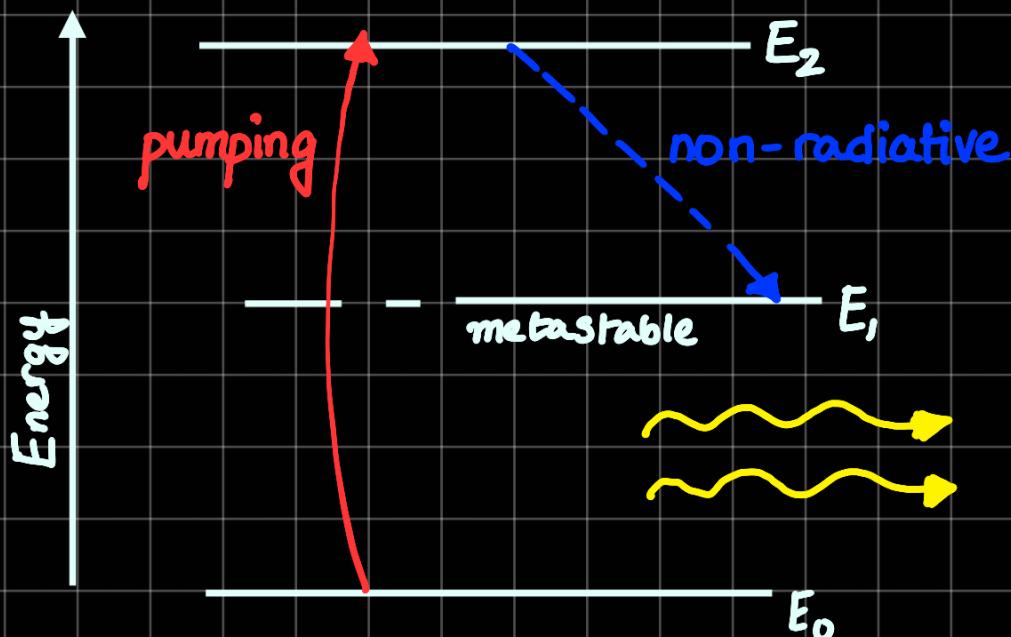
Ex: Semiconductor diode lasers

For a two-level system it is impossible to attain P.I., because $B_{12} = B_{21}$.

- Probability of adsorption & stimulated emission is same and at best 1:1 ratio can be obtained even with an ideal pumping mechanism.
- Population inversion however can occur only in a system with 3 or 4 levels.
- They contain a central metastable state in which atoms spend unusually longer time. From this metastable state, stimulated emission or lasing action takes place.

place.

Ex: 3 level laser (Ruby laser)



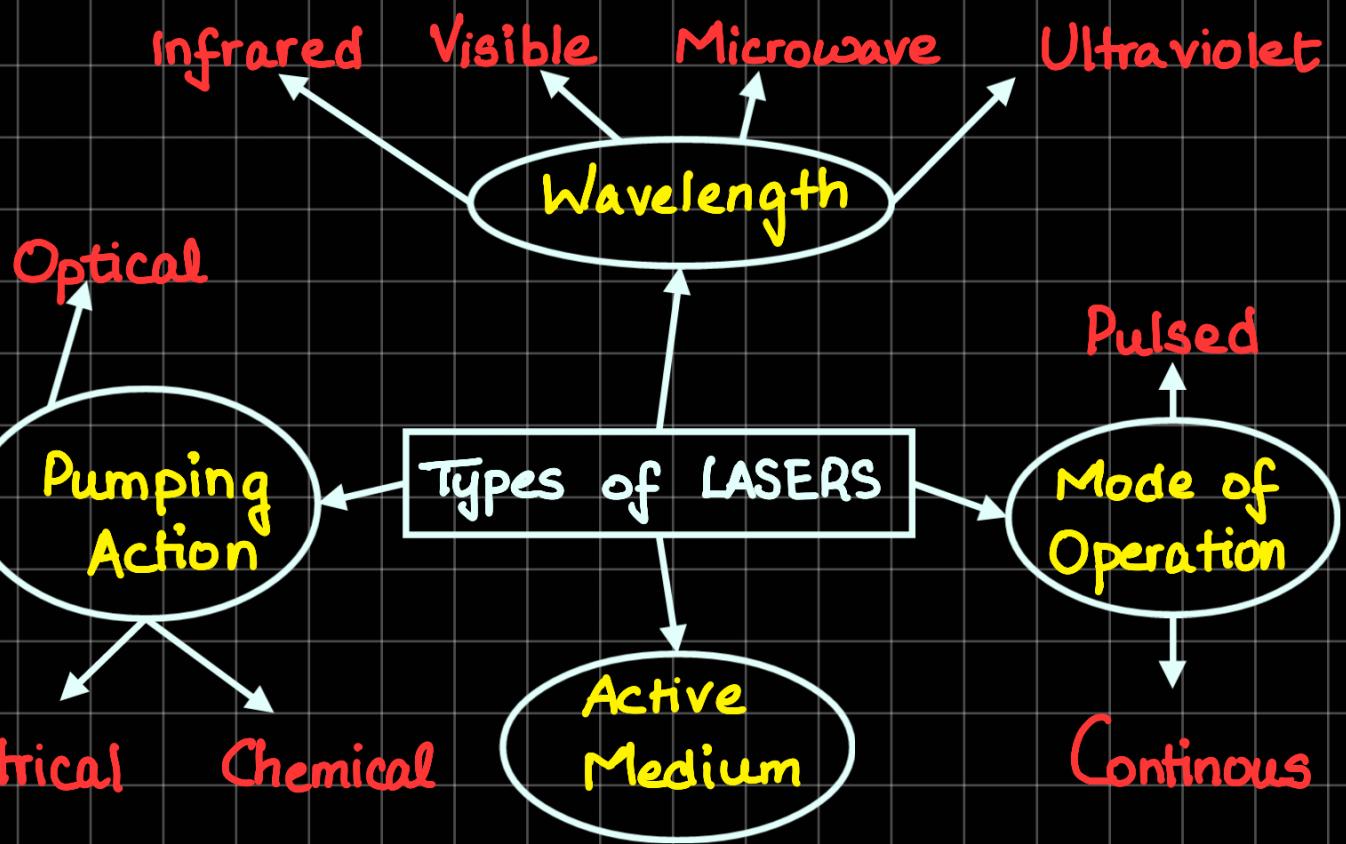
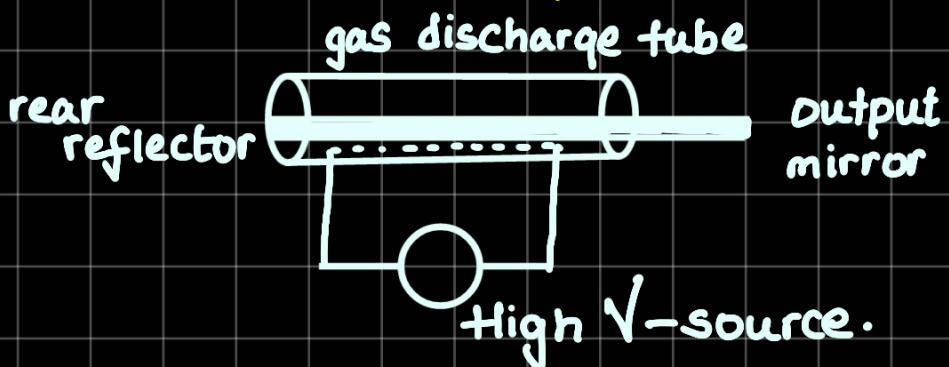
→ LASERs :-

Principle : Stimulated emission can lead to a chain reaction & laser emission.

Components :

1. **Active Medium** - Main component for lasing action.
P.I among the atoms is achieved in this medium.
2. **Excitation Mechanism (Pumping) -**
Pump energy to the active medium to achieve population inversion (Optical/Electrical/Chemical)
3. **Optical Cavity** - Setup for obtaining amplification of stimulated photons, by oscillating them back & forth b/w two reflecting concave mirrors placed coaxially. One of the mirrors is highly reflected (rear) and the partially reflected (output coupler)

4. The two coaxial mirrors facing each other constitute the **Optical Resonator**.



Laser Threshold Condition :

Attenuation Factor

$$\frac{dI}{dz} = -\alpha I$$

$$\Rightarrow \alpha = \frac{c^2}{\gamma^2 I_{sp} 8\pi n_0^2} g(\gamma) [N_1 - N_2] = -\gamma$$

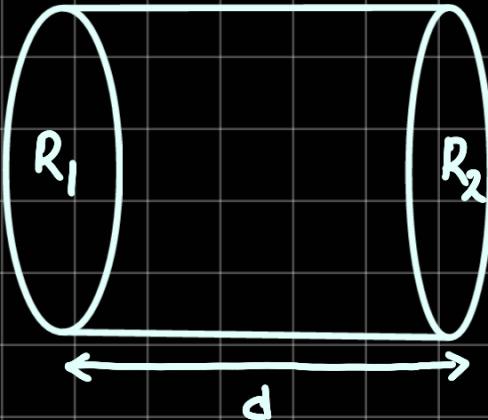
$$\Rightarrow I(z) = I_0 \exp(-\alpha z)$$

where, $\alpha \rightarrow$ Attenuation factor

$\gamma \rightarrow$ Amplification (gain) factor

$g(\gamma) \rightarrow$ Broadening function

- P.I is required for Amplification
- In order to generate radiation, this amplifying medium is placed in an optical resonator which consists of a pair of mirrors facing each other: **Fabry-Perot-etalon**
- α_1 = Average loss/ length due to all loss mechanism except reflectivity.



- If the oscillation need to be sustained in the cavity, losses must be compensated by the gain.
- Hence, a minimum population inversion is required to overcome the losses.
- For LASER oscillations to begin

$$R_1 R_2 e^{2(\gamma - \alpha_1)d} \geq 1$$

- For a continuous steady state, equality holds good \rightarrow Threshold
- If P.I is T_{ed} , then $LHS \gg 1$
Roundtrip gain > Round trip loss

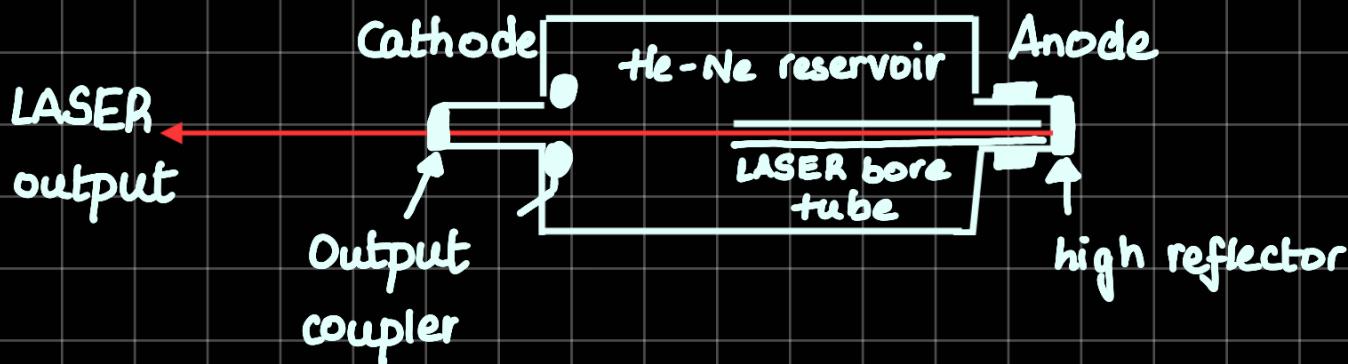
$$\gamma \geq \left[\alpha_1 - \frac{1}{2d} \ln(R_1 R_2) \right]$$

Depends on passive cavity parameters.

→ Types of LASERS -

1. He - Ne LASER

- Active Medium - Mixture of He & Ne gas
- Operational wavelength - 632.8 nm
- Four Level Laser Scheme
- More directional & monochromatic than solid state lasers
- Output is moderate when compared to solid state laser



- ✓ Setup consists of discharge tube of 80cm and bore diameter of 1.5 cm.
- ✓ Gain medium is a mixture of He and Ne at low pressure (50 Pa/cm^2).
- ✓ The pumping is provided electrically by creating a discharge. The electrical discharge is created by applying $\sim 1 \text{ KV}$ through an anode and cathode present at each end of the glass tube.
- ✓ Optical cavity of the laser typically consists of a plane, high reflecting mirror at one end & a convex output mirror at the other.
- ✓ Cavity lengths = 15 - 20cm
- ✓ Typical power = 1 - 100 mW
- Working of He-Ne laser
 - Gas is ionized when voltage is applied to electrode,

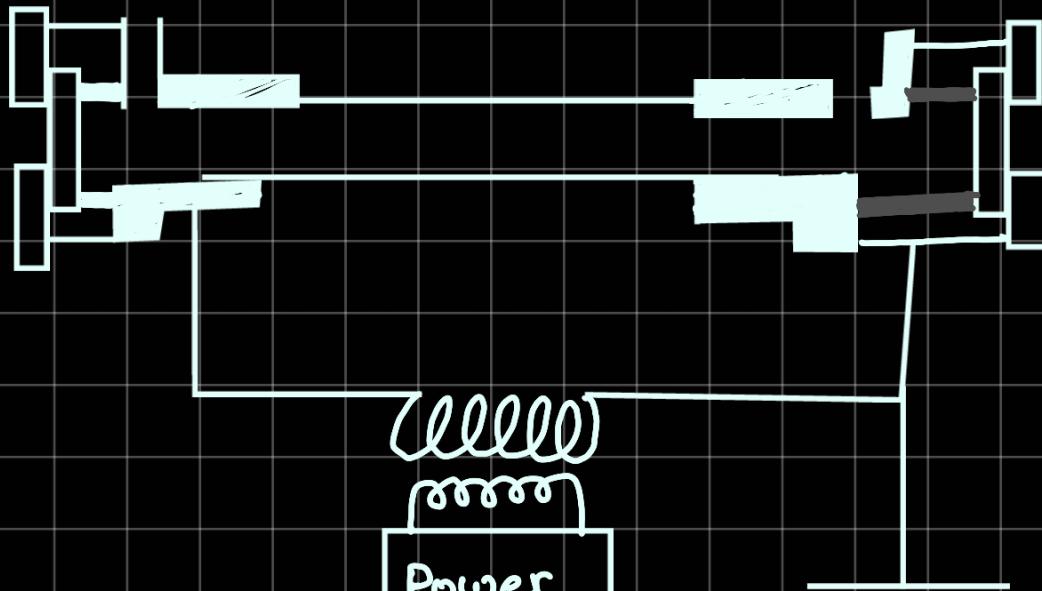
thus accelerating the electrons / ions.

- Electrons acquire higher velocity & hence transfer K.E to He thru inelastic collisions.
- He atoms are readily excited due to electron impact. Thus these He atoms are excited to F_2 and F_3 at 19.81 and 20.61 eV which are metastable states.
- These atoms return to the ground state by transferring energy to Ne in identical energy state. called as resonant transfer of energy.
Ne levels E_4 & E_6 nearly coincide with F_1 & F_2 ↗
- An additional energy of 0.05 eV is provided as K.E to He atom.

2. Carbon di-oxide (CO_2) laser -

In molecular lasers, oscillations are achieved by electronic transition b/w vibrational & rotational states of all molecules. These transitions cause the laser effect in CO_2 lasers. $CO_2 \rightarrow$ linear structure. Three different modes of vibration are possible

- Symmetric stretching mode
- Bending mode
- Asymmetric stretching mode.



Discharge tube of diameter, **2.5cm** and length **5m**

- Working

- N_2 plays a similar role to He in He-Ne laser

- N_2 gets excited due to collision with electron



- Excited N_2 can readily transfer energy to CO_2 in resonant collisions since the lowest vibrational energy of N_2 has nearly as much energy as the asymmetric stretching mode of CO_2 .

Electromagnetic Theory

Module - 5

$$\nabla = \frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j} + \frac{\partial}{\partial z} \hat{k}$$

- Operator
- Can function on scalars or vectors.

→ Gradient of a scalar field -

The gradient of the scalar field, $f(x, y, z)$ is given as :-

$$\vec{\nabla} f = \frac{\partial f}{\partial x} \hat{i} + \frac{\partial f}{\partial y} \hat{j} + \frac{\partial f}{\partial z} \hat{k} \rightarrow \text{Gives dir^n to vector}$$

Magnitude of $f(x, y, z)$:-

$$\vec{\nabla} f(x_0, y_0, z_0) = \frac{\partial f}{\partial x}(x_0, y_0, z_0) \hat{i} + \frac{\partial f}{\partial y}(x_0, y_0, z_0) \hat{j} + \frac{\partial f}{\partial z}(x_0, y_0, z_0) \hat{k}$$

→ Divergence of a vector field -

This divergence of a vector field $\vec{F} = [F_1, F_2, F_3]$ is a scalar field, $\text{div } F$ which is -

$$\text{div } F = \vec{\nabla} \cdot \vec{F} = \frac{\partial F_1}{\partial x} + \frac{\partial F_2}{\partial y} + \frac{\partial F_3}{\partial z}$$

div : Smooth Vectors field $\vec{F} \rightarrow$ Scalar Vector field

$$\vec{F} \rightarrow \frac{\partial F_1}{\partial x} + \frac{\partial F_2}{\partial y} + \frac{\partial F_3}{\partial z}$$

\rightarrow Curl of a Vector field

The curl of a vector field, $\text{curl } \vec{F}$ is another vector defined as :-

$$\text{curl } \vec{F} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ F_1 & F_2 & F_3 \end{vmatrix}$$

- $\text{div } \vec{F} = \vec{\nabla} \cdot \vec{F} = 0 \longrightarrow$ The vector field is **solenoidal**
- $\text{curl } \vec{F} = 0 \longrightarrow$ The vector field is **irrotational**
- Basic Theorem of Calculus

The integral of the derivative of a function over a region is equal to the value of the function at the boundary.

Gauss Divergence Theorem

$$\int_V \{ \vec{\nabla} \cdot \vec{F} \} dV = \oint_S \vec{F} \cdot d\vec{A}$$

Stokes Theorem

$$\oint_S \{ \vec{\nabla} \cdot \vec{F} \} dA = \oint_C \vec{F} \cdot d\vec{l}$$

- Maxwell's Equation -

\rightarrow Integral form -

$$\text{Gauss Law of Electrostatic} \rightarrow \oint_S \vec{E} \cdot d\vec{A} = \frac{1}{\epsilon_0} \cdot Q_{\text{enc}}$$

Gauss Law of Magnetostatics $\rightarrow \oint_S \vec{B} \cdot d\vec{A} = 0$

Faraday law of emi $\rightarrow \oint_C \vec{E} \cdot d\vec{l} = -\frac{d\phi_B}{dt}$

Ampere's Law $\rightarrow \oint_C \vec{B} \cdot d\vec{l} = \mu_0 I + \mu_0 E_0 \frac{d\phi_E}{dt}$

→ Differential form -

Gauss Law of electrostatics

$$\text{we know, } Q_{\text{enc}} = \int_V \rho dV \quad \text{--- (1)}$$

From the Gauss divergence theorem,

$$\oint_S \vec{E} \cdot d\vec{A} = \int_V (\nabla \cdot \vec{E}) dV \quad \text{--- (2)}$$

$$\Rightarrow \int_V (\nabla \cdot \vec{E}) dV = \frac{1}{\epsilon_0} \int_V \rho dV$$

$$\Rightarrow \boxed{\nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0}}$$

Gauss Law of magnetostatics

$$\boxed{\nabla \cdot \vec{B} = 0}$$

Faraday's law of emi

$$\oint \vec{B} \cdot d\vec{A} = \oint \vec{B} \cdot d\vec{A}$$

$$\Rightarrow \oint \vec{E} \cdot d\vec{l} = - \oint \frac{\partial \vec{B}}{\partial t} \cdot d\vec{A}$$

$$\Rightarrow \boxed{\vec{\nabla} \times \vec{E} = - \frac{\partial \vec{B}}{\partial t}}$$

Ampere's Law modified by Maxwell

$$\oint \vec{B} \cdot d\vec{l} = \mu_0 I + \mu_0 \epsilon_0 \frac{d\phi_E}{dt}$$

$$\Rightarrow \boxed{\vec{\nabla} \times \vec{B} = \mu_0 \left[\vec{J} + \epsilon_0 \frac{d\vec{E}}{dt} \right]}$$

Just as changing magnetic field induces an electric field, a changing electric field also induces a magnetic field.

$$\vec{J}_d = \epsilon_0 \frac{d\vec{E}}{dt}$$

Maxwell's equation represent a set of 1st order coupled partial differential equations. The 4 equations along with Lorentz force, $\vec{F} = q[\vec{E} + (\vec{v} \times \vec{B})]$ summarizes the entire theoretical content of classical electrodynamics.

→ Wave equation of EM waves -

For Simplicity , assume that the charges & currents are limited to a small region surrounding the origin.

Always analyze the fields at regions far away from origin : **FREE SPACE**

$$\vec{\nabla} \cdot \vec{E} = 0$$

$$\vec{\nabla} \cdot \vec{B} = 0$$

$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

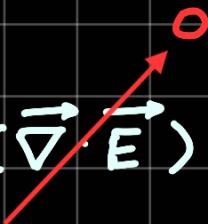
$$\vec{\nabla} \times \vec{B} = \mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t}$$

$$\Rightarrow \vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\Rightarrow \vec{\nabla} \times (\vec{\nabla} \times \vec{E}) = \vec{\nabla} \cdot (\vec{\nabla} \times \vec{E}) - \nabla^2 \vec{E}$$

$$\Rightarrow \vec{\nabla} \times \left[-\frac{\partial \vec{B}}{\partial t} \right] = \nabla^2 \vec{E}$$

$$\Rightarrow \boxed{\nabla^2 \vec{E} - \mu_0 \epsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2} = 0}$$



$$\boxed{\left(\nabla^2 - \mu_0 \epsilon_0 \frac{\partial^2}{\partial t^2} \right) \vec{E} = 0}$$

$$\boxed{\left(\nabla^2 - \mu_0 \epsilon_0 \frac{\partial^2}{\partial t^2} \right) \vec{B} = 0}$$

{Wave equation of E·M waves}
in free space

$$V = \frac{1}{\sqrt{\mu_0 \epsilon_0}} = C \rightarrow \text{speed of light}$$

E and B propagate in free space as the wave travels with speed 'c'.

$$\vec{E}(\vec{r}, t) = \vec{E}_0 \exp[i(\vec{k} \cdot \vec{r} - \omega t)]$$

$$\vec{B}(\vec{r}, t) = \vec{B}_0 \exp[i(\vec{k} \cdot \vec{r} - \omega t)]$$

Surface of constant phase determines the nature of wave.

At a fixed time, t and for a monochromatic wave (fixed ω).

$$\vec{k} \cdot \vec{r} = \text{const.}$$

$$k_x x + k_y y + k_z z = \text{const.}$$

{Represents a plane \perp to \vec{k} }

$\therefore E$ and B represent plane wave solution.

- Requirement of satisfying wave eqn's -

$$\nabla^2 \cdot \vec{E} = -k^2 \vec{E} \Rightarrow \mu_0 \epsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2} = -\mu_0 \epsilon_0 \omega^2 \vec{E}$$

$$\Rightarrow k = \sqrt{\mu_0 \epsilon_0} \omega$$

$$\vec{\nabla} \cdot (f \vec{d}) = f(\vec{\nabla} \cdot \vec{d}) + \vec{\nabla} f \cdot \vec{d}$$

$$\begin{aligned}\vec{\nabla} \cdot \vec{E} &= 0 \Rightarrow \vec{k} \cdot \vec{E} = 0 \\ \vec{\nabla} \cdot \vec{B} &= 0 \Rightarrow \vec{k} \cdot \vec{B} = 0\end{aligned}$$

E and B ^{are} oscillating perpendicular to direction of propagation :- **Transverse Waves**

$$\vec{\nabla} \times (f \vec{d}) = f(\vec{\nabla} \times \vec{d}) + \vec{\nabla} f \times \vec{d}$$

we know $\rightarrow \vec{\nabla} \times \vec{E} = \frac{-\partial \vec{B}}{\partial t}$

$$\Rightarrow \vec{B} = \sqrt{\mu_0 \epsilon_0} \frac{\vec{k} \times \vec{E}}{|\vec{k}|}$$

But $\vec{E} \perp \vec{B}$, then

$$\Rightarrow |\vec{B}| = \sqrt{\mu_0 \epsilon_0} |\vec{E}|$$

\rightarrow Phase velocity -

Phase of em. waves propagating along z-axis is given by : $kz - \omega t$

Phase velocity is defined as the rate at which the phase of a wave propagates in free space :

$$v_p = \frac{\partial z}{\partial t} = \frac{\omega}{k} = f\lambda$$

→ Group velocity -

for a sin curve/waveform comprised of many sin curves that all propagate with same velocity, the waveform will move at the phase velocity of sin component.

The waveform moves at a rate that depends on the relative position of the component wavefronts as func. of time. This is group velocity.

$$v_g = \frac{d\omega}{dk} \rightarrow \omega = vk = \frac{c}{n(\lambda)} \cdot \frac{2\pi}{\lambda}$$

phase velocity = const → free space

$$\omega = ck \text{ and } \frac{d\omega}{dk} = c$$

Velocity of light in a medium depends on wavelength → dispersion

$$\frac{dn}{d\lambda} = \frac{dn}{dk} \cdot \frac{dk}{d\lambda}$$

$$\Rightarrow n = \frac{c}{v_p} = \frac{ck}{\omega} \rightarrow \frac{dn}{dk} = \frac{c}{\omega} - \frac{ck}{\omega^2} \frac{d\omega}{dk}$$

$$\Rightarrow k = \frac{2\pi}{\lambda} \rightarrow \frac{dk}{d\lambda} = -\frac{2\pi}{\lambda^2} = -\frac{k}{\lambda}$$

$$v_g = v_p \left(1 + \frac{\lambda}{n} \frac{dn}{d\lambda} \right)$$

→ for dispersive medium

Group index (N_g) is :

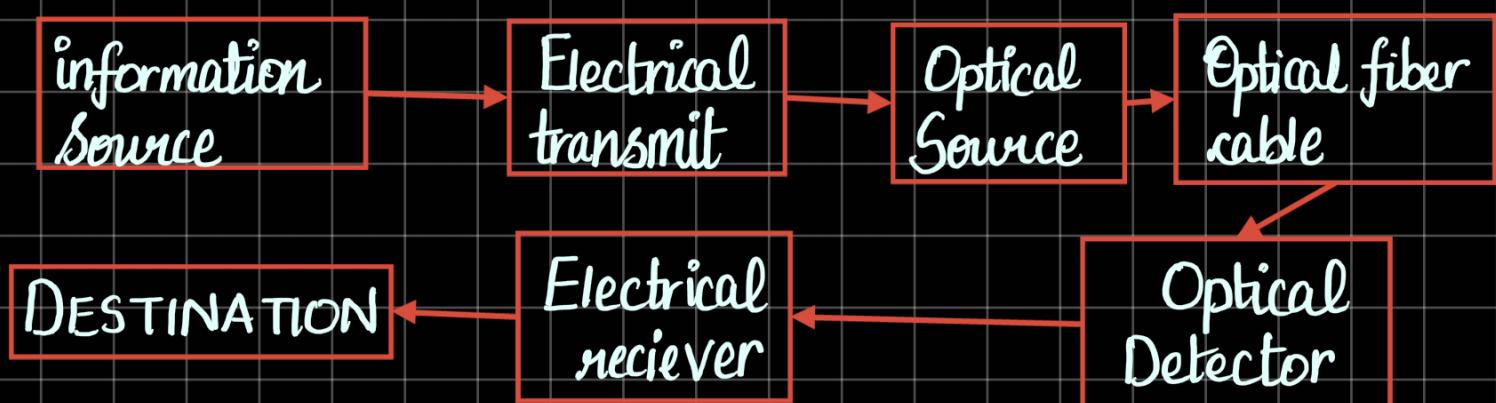
$$N_g = \frac{c}{v_g}$$

Optical Fibres Communication

module - 1

The proposals for optical communication via dielectric waveguides or optical fibers from glass to avoid signal degradation was given by Kao and Hockham and Werts in 1966.

Schematic Diagram :



Electrical
isolation

Small size and
weight

Enormous
potential band-
width

Advantages of Optical
Communications

Immunity
to interference and
crosstalk

Signal security,
ruggedness, flexible

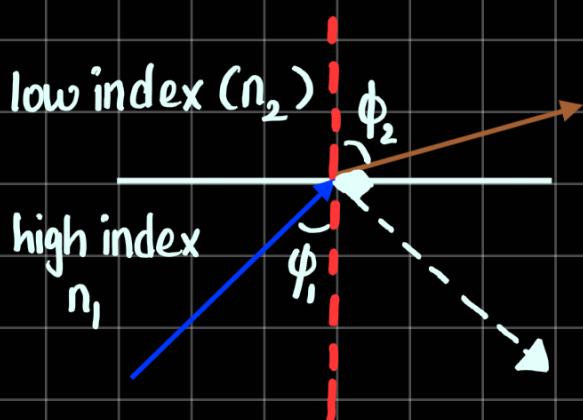
Low transmission
loss : 0.2 dB/km

and low cost

Basic Principle of Opticals fibres:

The basic principle of light propagation in an optical fibres is Total Internal Reflection.

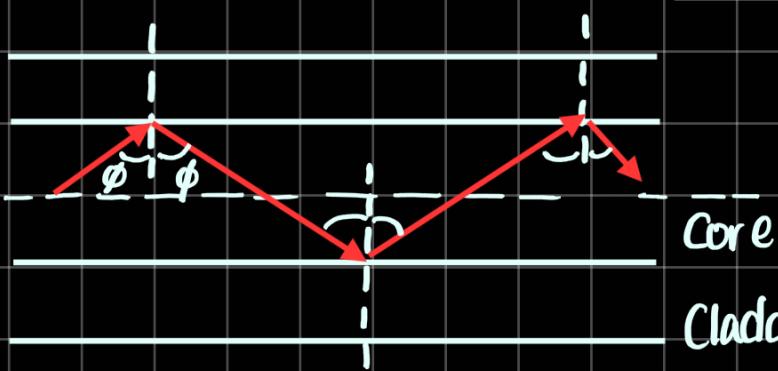
Electromagnetic waves travels between optically dense medium to optically rarer medium and the refractive index is equal to the ratio of speed of light in vacuum to the speed in the medium.



$$n_1 \sin \phi_1 = n_2 \sin \phi_2 \rightarrow \text{Snell's law}$$

when the $\phi_1 \geq \phi_c$ [critical angle], then total internal reflection occurs.

$$\sin \phi_c = \frac{n_2}{n_1}$$

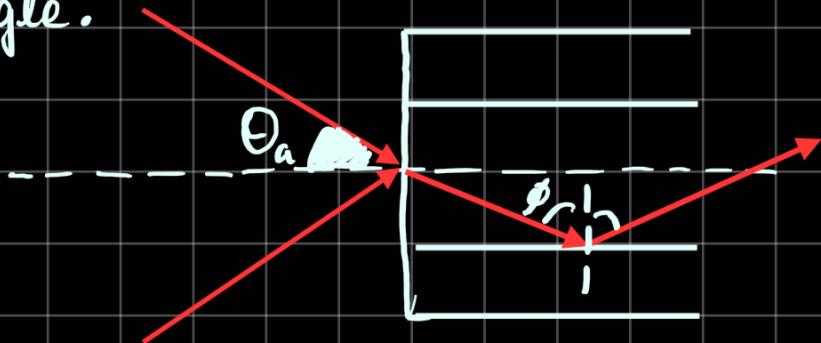


Any imperfections in the Core - cladding index will result in refraction & not a Cladding TIR.

Acceptance Angle:

Only rays with a shallow grazing angle at the core - cladding interface are transmitted by TIR. Hence, not all rays can enter the core - cladding interface.

When a ray of light at an angle θ approaches the interface, it will only enter, if and only if $\theta < \Theta_a$. Θ_a is the acceptance angle.



Any ray greater than Θ_a will not be allowed to enter the interface and any ray less than Θ_c will not be totally internally reflected.

Relation between acceptance angle & refractive index is called **Numerical Aperture**.

$$\text{Diagram: A light ray in medium } n_0 \text{ (bottom) approaches a boundary with refractive index } n_1 \text{ (core). The angle of incidence is } \Theta_1. \text{ The ray refracts into medium } n_1 \text{ at angle } \Theta_2. \text{ The angle } \phi \text{ is defined as } \phi = \frac{\pi}{2} - \Theta_2. \text{ The numerical aperture is given by:}$$

$$\begin{aligned} \phi &= \frac{\pi}{2} - \Theta_2 \\ \Rightarrow n_0 \sin \Theta_1 &= n_1 \sin \Theta_2 \\ &= n_1 \cos \phi \\ &= n_1 \sqrt{1 - \sin^2 \phi} \end{aligned}$$

$$n_0 \sin \Theta_a = \sqrt{n_1^2 - n_2^2} \Rightarrow \boxed{NA = n_0 \sin \Theta_a = \sqrt{n_1^2 - n_2^2}}$$

Numerical Aperture, in terms of relative r.i (Δ) between the core-cladding which is defined as:

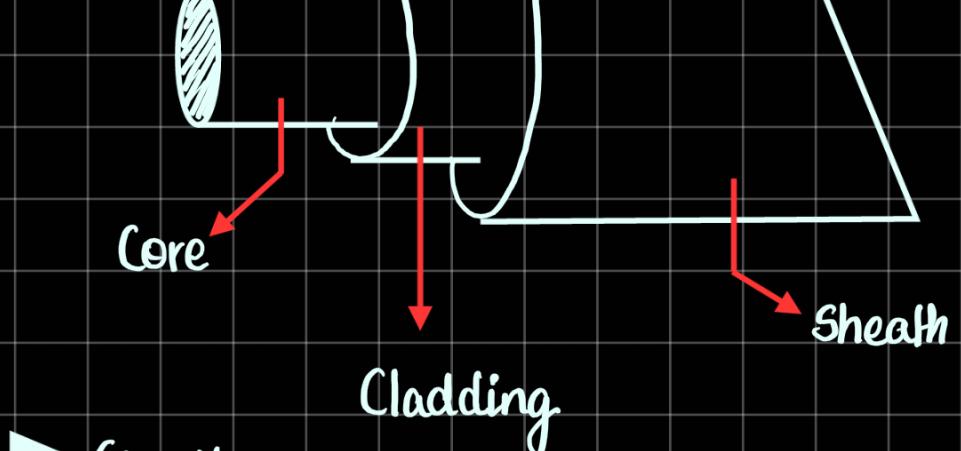
$$\Delta = \frac{n_1^2 - n_2^2}{2n_1^2} \approx \frac{n_1 - n_2}{n_1} \rightarrow \Delta \ll 1$$

$$\boxed{NA = n_1 \sqrt{2\Delta}}$$

- Structure of optical fibre



► Core



- transmission area of fiber
- Typical diameter is $50 - 500 \mu\text{m}$

► Sheath

- Has a special plastic coating that provides shocks resistance.
- Thickness ranges from 250 to 1000 μm .

► Cladding

- surrounds the core & has lesser r.i than core.
- Defines the optical boundary of the core.

• Number of Modes:

- ↳ Optical fibers is a dielectric waveguide.
- ↳ Energy in the fiber is propagated by electric and magnetic field of an e.m. wave that can be analyzed by Maxwell's eqⁿ.
- ↳ Maxwell's eqⁿ has different sets of solutions called modes. The modes gives an account of the allowed optical path in an optical fibre

Number of modes can be determined by 'horizontal wave number'(v)

$$V = \frac{2\pi a}{\lambda} (NA)$$

where, a → radius of the core.

Maximum no. of modes

step-index
fiber

graded-index
fiber

$$N_m = \frac{1}{2} V^2$$

$$N_m = \frac{1}{4} V^2$$

V

$< 2.405 = \text{step-index fiber}$

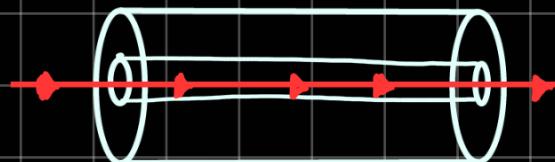
$> 2.405 = \text{graded-index fiber}$

The wavelength associated to $V = 2.405$ is known as cut-off wavelength

$$\lambda_c = \frac{\lambda V}{2.405}$$

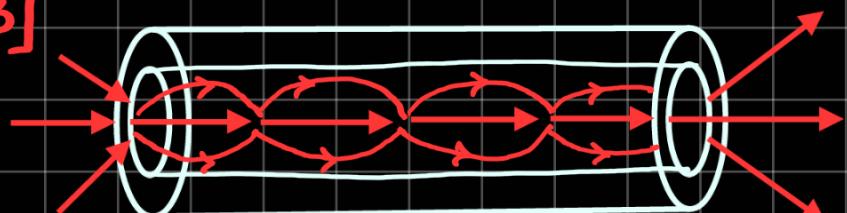
single mode fiber

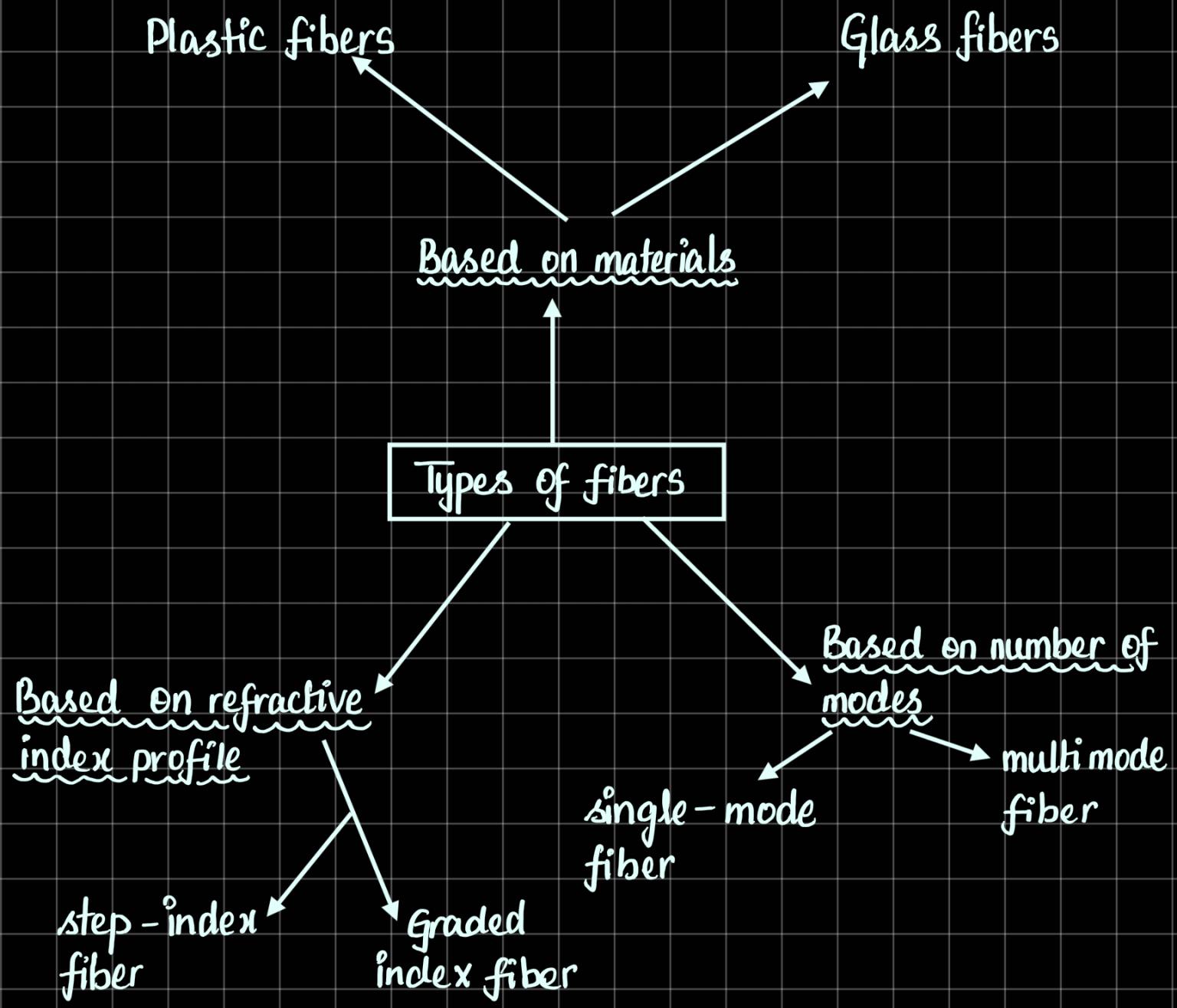
- The core is very narrow ($\sim 10\mu\text{m}$)
- NA and acceptance angle is very small. Allows only one mode
- Amount of dispersion is less
- Used for high speed, large bandwidth and transmission.



Multimode fibers

- These fibers have relatively wide core ($\sim 50\mu\text{m}$)
- There are 2 rays travelling in the core: axial rays and the marginal rays. Allows different modes to pass through together
[Marginal ray > axial rays]





Transmission Characteristics:

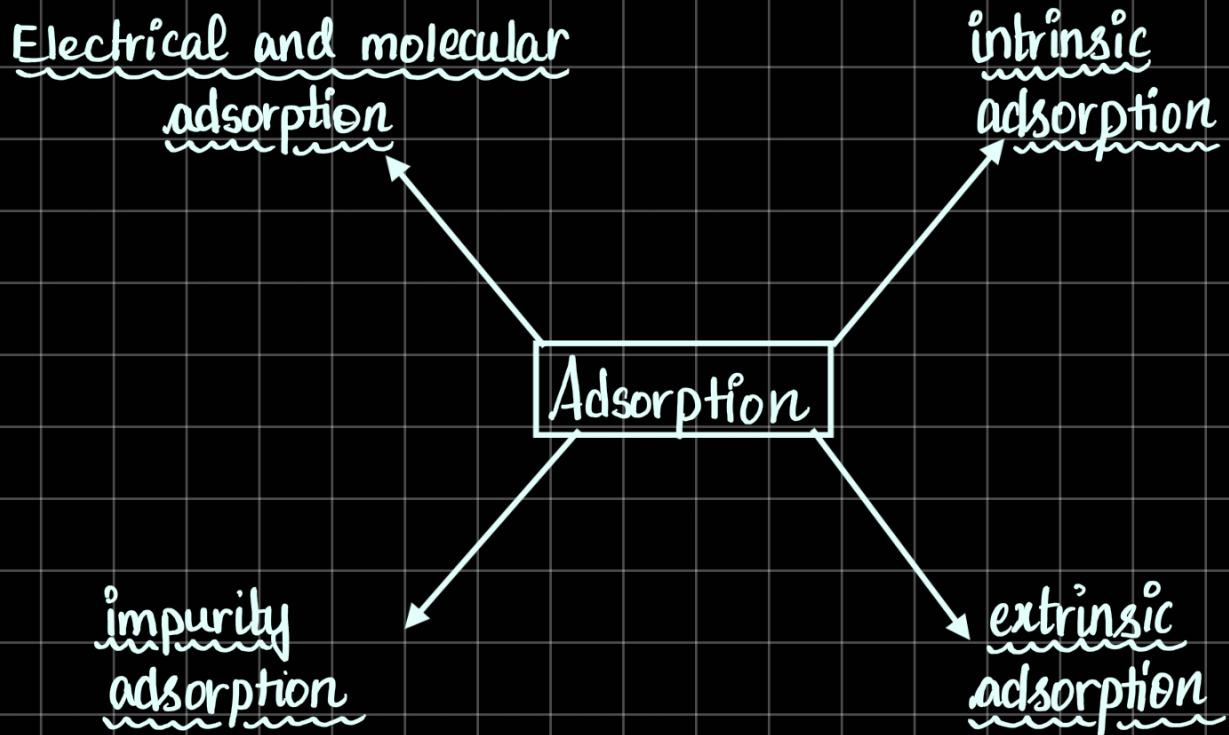
- ↳ The transmission through an optical fiber is limited by attenuation (loss) and dispersion.
- ↳ The bandwidth is mostly limited to signal dispersion within the fiber. It determines the number of bits of transmission transmitted in a given time period.

→ Attenuation :

attenuation determines the maximum transmission distance prior to signal restoration. OFC has an attenuation loss of 0.2 dB/km which is lower than metallic conductors.

Signal attenuation in optical fibers is usually expressed in decibels.

$$\alpha_{dB} L = dB = 10 \log_{10} \frac{P_i}{P_o}$$



- Scattering loss:

scattering results in attenuation, as the scattered light may not continue to satisfy total internal reflection in the fiber core.

- ↳ Rayleigh's scattering

Rayleigh's scattering results from random inhomogeneities that are small in size, compared to wavelength.

These inhomogeneities exist in the form of refraction index

These inhomogeneities exist in the form of ~~refraction index~~ fluctuation.

$$\text{Attenuation (dB/km)} \propto \frac{1}{\lambda^4}$$

↳ Mei's scattering

Imperfections in the waveguide structure of a fiber, such as non-uniformity in the shape & size of the core, perturbations in the core-cladding boundary and defects in core or cladding.

The imperfections in a fiber waveguide result in additionally scattering losses. They can also induce coupling b/w different guided modes.

Bending loss

At a bend, propagation conditions alter and the light is lost in the cladding

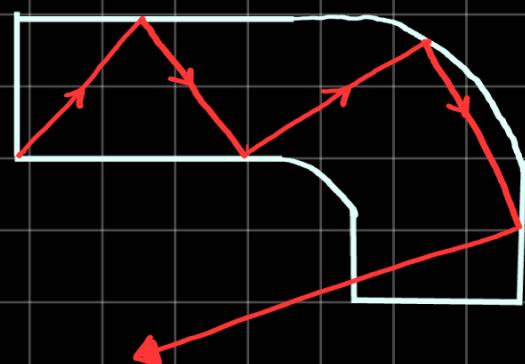
Microbending

microbending is commonly caused by poor cable design.



Macrobending

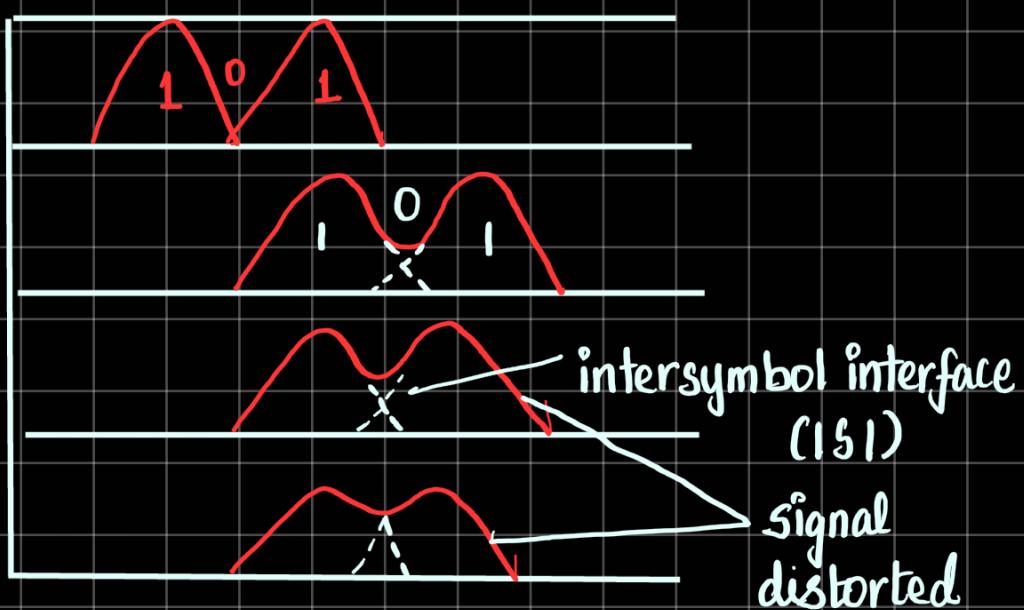
macrobending is commonly caused by poor installation or handling.



• Dispersion:

- ↳ Dispersion of the transmitted optical signals causes distortion for analog as well as digital transmission.
- ↳ Dispersions mechanisms causes broadening of transmitted light pulses as they travel along the channel

Hence, the number of optical pulses which may be transmitted is restricted by the amount of dispersion per unit length. The pulse broadening increases linearly with fiber length & thus the bandwidth is inversely proportional to distance.



• Intramodal (chromatic) dispersion:

Optical light sources do not emit just a single frequency but a band of frequencies. Hence, there may be a propagation delay differences b/w the different spectral components of the transmitted signal. This causes broadening of each mode and hence intramodal dispersion.

The delay differences can be caused by:

Material dispersion

waveguide dispersion

dispersive properties
of the waveguide
material

Guidance factors within the
fiber structure

- Intermodal dispersion

↳ When numerous waveguide modes are propagating, they all travel with different velocities.

Parts of the wave arrive at the output before other parts, spreading out the waveform.

It is independent of source linewidth & doesn't occur in a single mode fiber.

- Multimodal step-index fiber

Paths taken by the axial & the extreme meridional ray in a perfect multimode step index fiber.



T_{\min} → minimum delay time {axial ray}

T_{\max} → maximum delay time {meridional ray}

$$T_{\min} = \frac{\text{distance}}{c} = \frac{L}{c} \Rightarrow T_{\min} = \frac{Ln_1}{c}$$

$$T_{\max} = \frac{\left(\frac{L}{\cos \theta}\right)}{\left(\frac{C}{n_1}\right)} \Rightarrow T_{\max} = \frac{Ln_1}{C \cos \theta}$$

$$\delta T_s = T_{\max} - T_{\min} = \frac{Ln_1^2 \Delta}{C n_2} \approx \frac{Ln_1 \Delta}{C}$$

$$\Rightarrow \delta T_s = \frac{L(NA)^2}{2n_1 C}$$

LASER LED Incandescent Lamp

source should
be linear

Light output should be
highly directional

optical source is the
most active part of an
OFC system.

Converts electrical
energy to optical
energy

emit light wavelength
where fiber has low

very narrow
spectral linewidth

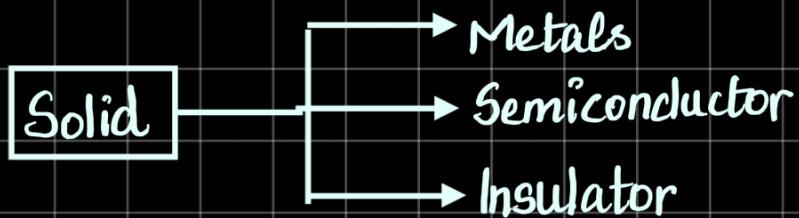
loss

Optoelectronic Devices

Module - 7

for a solid crystal, each energy band contain atleast N levels which can filled with electrons $\rightarrow N \sim 10^{22}/\text{cm}^3$
The distance between two bands is $\sim 10^{-22}\text{ eV} \rightarrow \text{Continuum}$

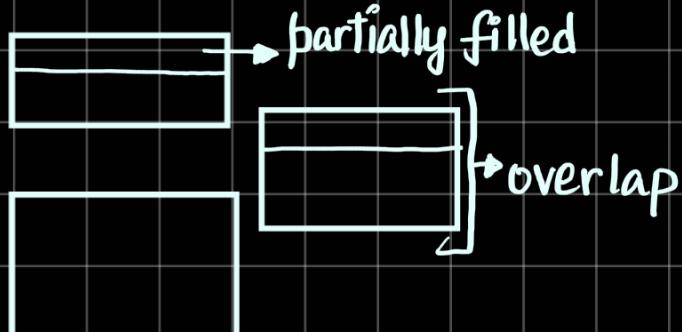
Based on bands being filled, solids can be classified as:



for electron to experience accⁿ in an applied \vec{E} field, there must be allowed empty states available for the electrons

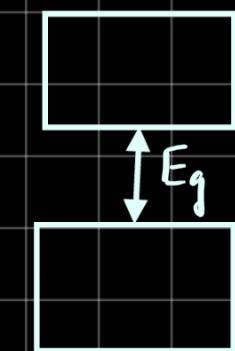
in metals, the bands are either partially filled or they overlap

Insulators & semiconductors have completed filled bands, but the difference is that the no. of electrons can be increased greatly in a semiconductor.

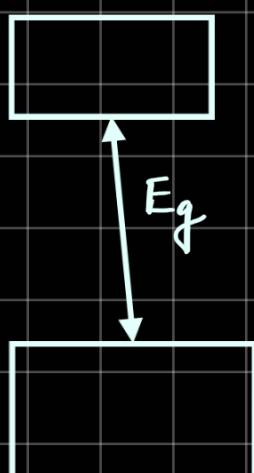


Metals

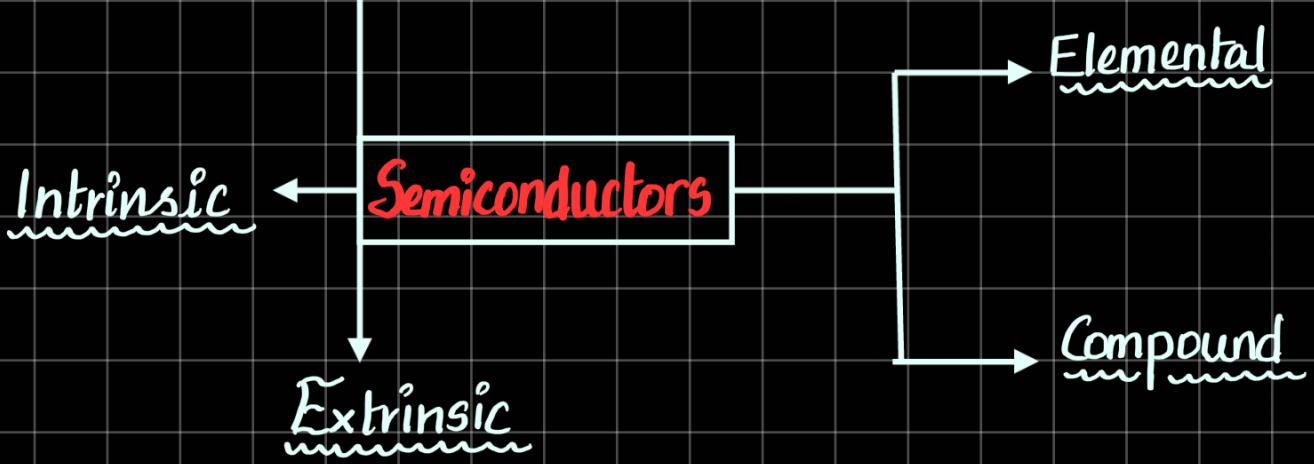
Pure
imp.



Semiconductors



Insulators



Bonds and Bands :

- ↳ Material properties of solids are strongly dependant on the arrangement of atoms : **Atomic Bonding**
- ↳ There are two forces that act on the solids :-

Attractive forces → **holds the atoms together**

Repulsive forces → **Resists the force of compression**

The force of attraction **decreases as the distance of separation(r) increases.**

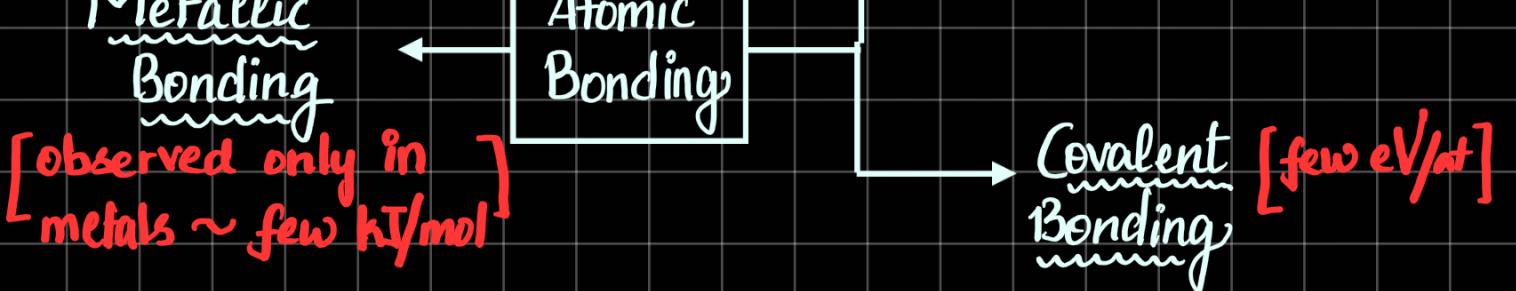
Repulsive forces are generally of **shorter range** to attractive forces

Atomic Bonding :-

attractive forces in solids are primarily **electrostatic** in nature & repulsive forces are of **quantum mechanical** origin

Solids are **stable** as the attractive & repulsive forces **exactly balance each other.**

Ionic Bonding [**strongest**]
~ **5eV/atom**



We use the Fauling equation to find %.age of ionic character

$$\% = \left\{ 1 - \exp \frac{(x_A - x_B)^2}{4} \right\} \times 100$$

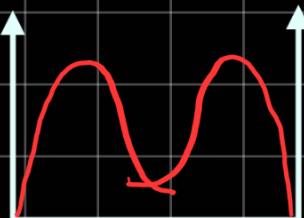
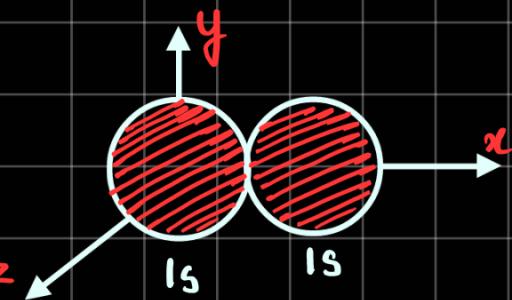
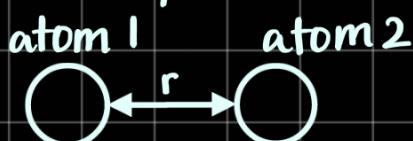
↳ Energy Band formation

When two atoms are brought together, various interactions take place and at a particular distance, attractive & repulsive forces exactly balance each other.

In this process, important changes occur to the energy level configuration in accordance to Pauli Exclusion Principle.

As the atoms come closer, the electronic wavefunctions begin to overlap. Hence, there will be Energy Level Splitting of discrete energy levels, in pairs.

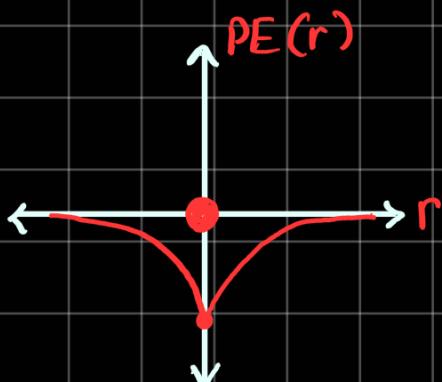
energy levels associated with the higher quantum no. & farthest from the nucleus will be affected first and begin overlap.



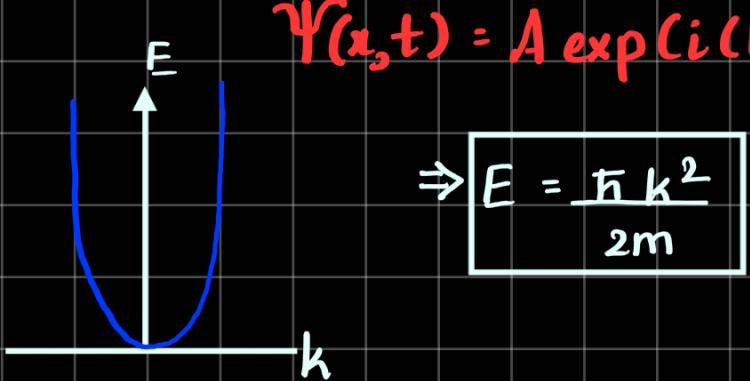
10^{20} energy states are equidistant & they are at a distance of 10^{-20} eV from each other.

↳ Energy Band Diagram

Potential energy (PE) of an electron across an isolated atom



Relation between E & k for a free electron :



$$\Psi(x, t) = A \exp(i(kx - \omega t))$$

$$\Rightarrow E = \frac{\hbar k^2}{2m}$$

- Direct Gap Semiconductor

The electrons & holes have the same value of crystal momentum

energy maximum of VB occurs at the same crystal momentum value as energy minimum of CB

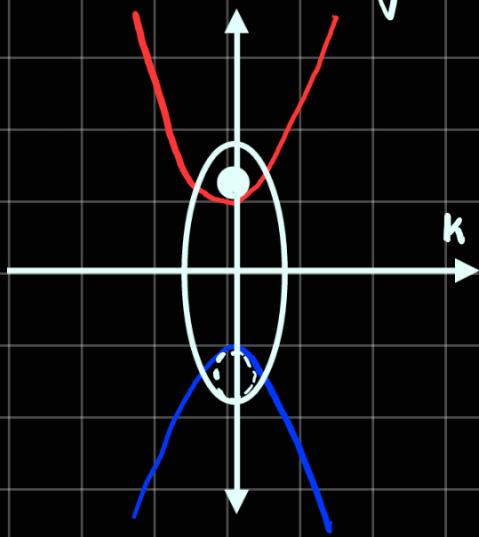
- Indirect Gap Semiconductors

VB maximum & CB minimum occur at different crystal momenta

The momentum of the electron must occur for e-h recombination to occur

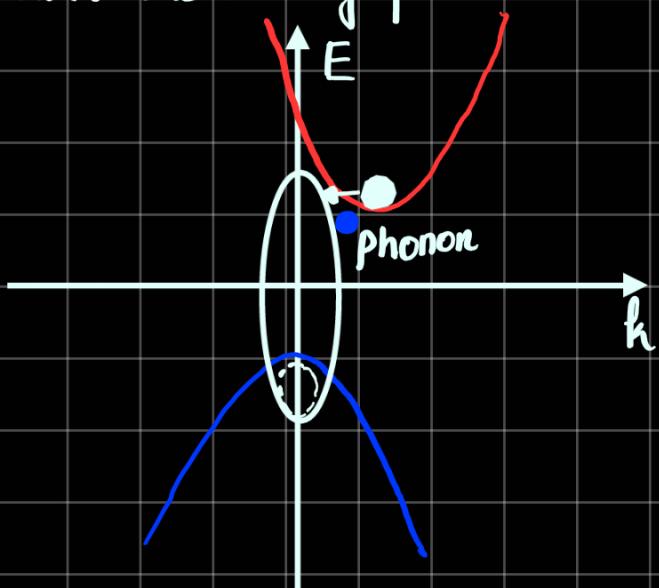
as energy minimum of CB

when e-h recombination occurs, the momentum of the electron remains const. & the energy corresponding to band gap energy is emitted due to light.

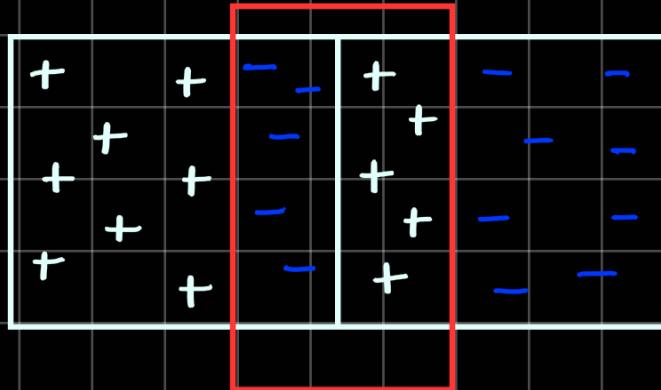


The momentum conservation requires the emission of a third particle called phonon

Therefore, the recombination of direct gap is relatively lesser than indirect gap.



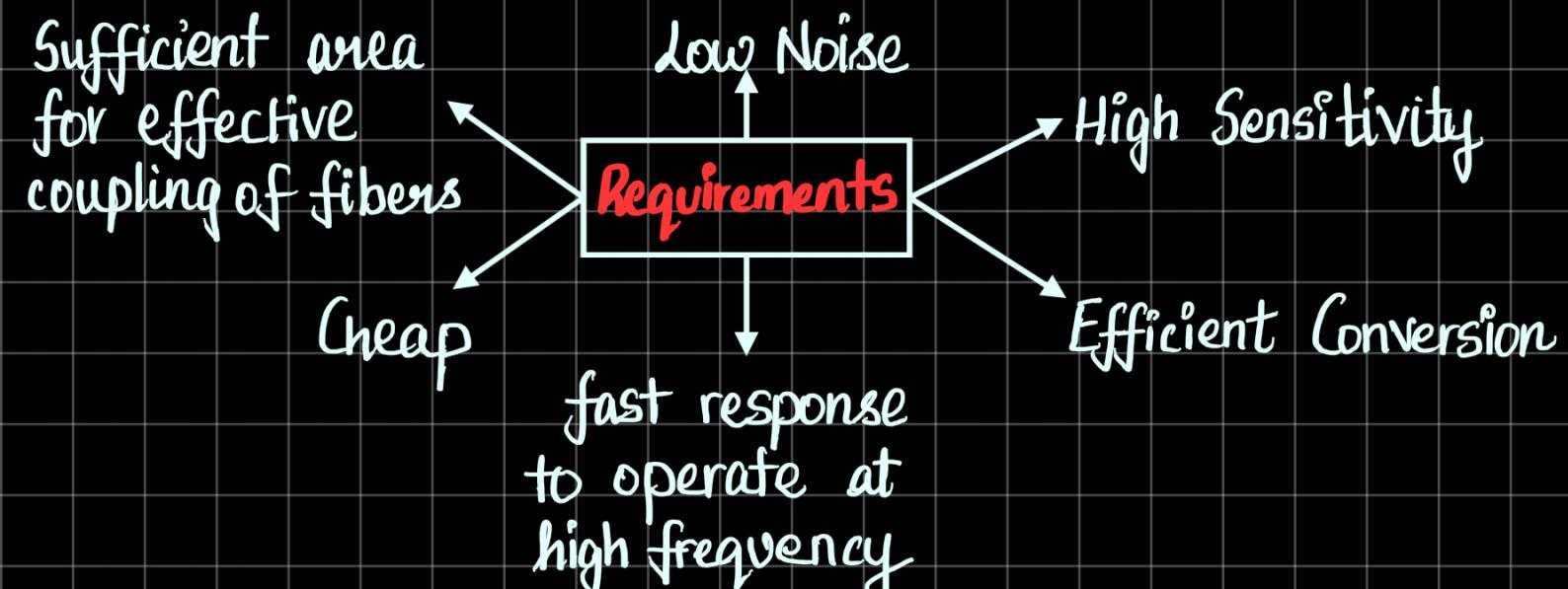
• P-N junction



Semiconductors n-type and p-type are brought together. The electrons and holes migrate the junction & a depletion region is formed. A potential difference is set across the depletion layer.

→ Photo-Detectors:

- Converts optical signal to electrical signal
- Made up of semiconductors to absorb photons & produce electrons/holes



→ Retentivity and Quantum efficiency

retentivity is the measure of conversion efficiency of a photodetector.

Current produced is linearly related to the no. of incident photon

$$I_p \propto P \text{ (input power)}$$

$$\boxed{\eta \text{ (retentivity)} = \frac{I_p}{P}}$$

↪ Photocurrent is equal to number of electrons times the charge per unit time

$$\text{(or.) } I_p = \frac{N_p e}{t}$$

↪ Light Energy is equal to the number of photons times the Energy of the photon (or) $P = \frac{N_p E_p}{t}$

$$\text{But } E_p = \frac{hc}{\lambda} \text{ and } P = \frac{N_p hc}{\lambda t}$$

$$R = \frac{I_p}{P} \Rightarrow R = \frac{N_e(e)}{t} \Rightarrow R = \left(\frac{N_e}{N_p} \right) \left(\frac{e\lambda}{hc} \right)$$

$\frac{N_p \ h c}{\lambda t}$

Quantum efficiency is the ratio of no. of electrons to the no. of photons. It shows the ability of a semiconductor to convert light to current.

$$\eta = \frac{N_e}{N_p}$$

Therefore, the relation between the retentivity and quantum efficiency is -:

$$R = \eta \left(\frac{e\lambda}{hc} \right)$$

- Reverse Biasing:
 - ↳ Depletion region is devoid of charge particles.
 - ↳ Width of the depletion region increases upon reverse bias which inturn increases the quantum efficiency
 - ↳ Helps eliminate dark current
 - ↳ The carriers produced due to photons are driven by the potential applied to generate photocurrent.

- P-I-N Photodiode
[Positive - Intrinsic - Negative]

- ↳ Intrinsic layer is the depletion region
 - ↳ High quantum efficiency exists when photons entering it produce charge carriers

carriers.

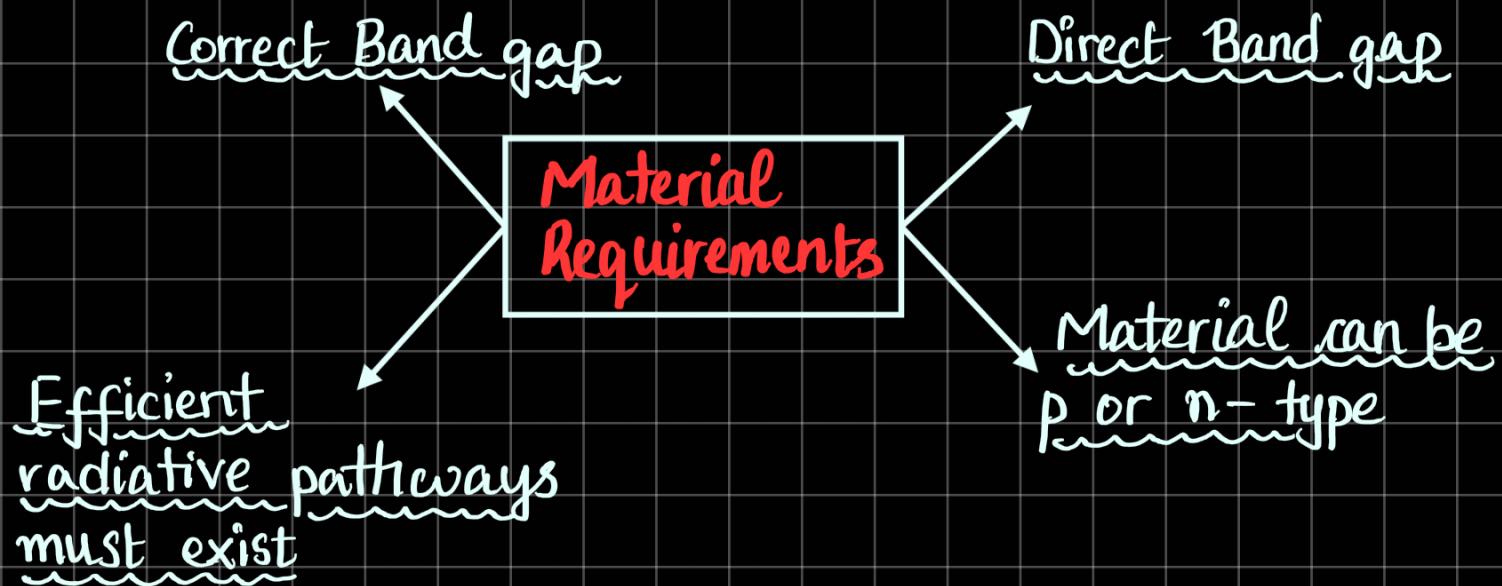
↳ As it is reverse biased, the carriers produced are driven by the terminals

• Light Emitting Diode

A p-n junction diode in forward bias

Electroluminescence

Quantum of energy emitted is almost equal to band gap



↳ Electroluminescence:

- Luminescence means emission of radiation from a solid when supplied with energy
- Excitation due to an applied electric field is called Electroluminescence
- Injection: Generation of excess charge carriers
 - Barrier potential is reduced under forward bias
 - Majority charge carriers can easily cross the barriers while the other side is minority carriers
 - The minority carriers will diffuse & recombine with majority carriers and emit light → **Radiative recombination**

All created photons must leave

direct band gap

Efficient LED

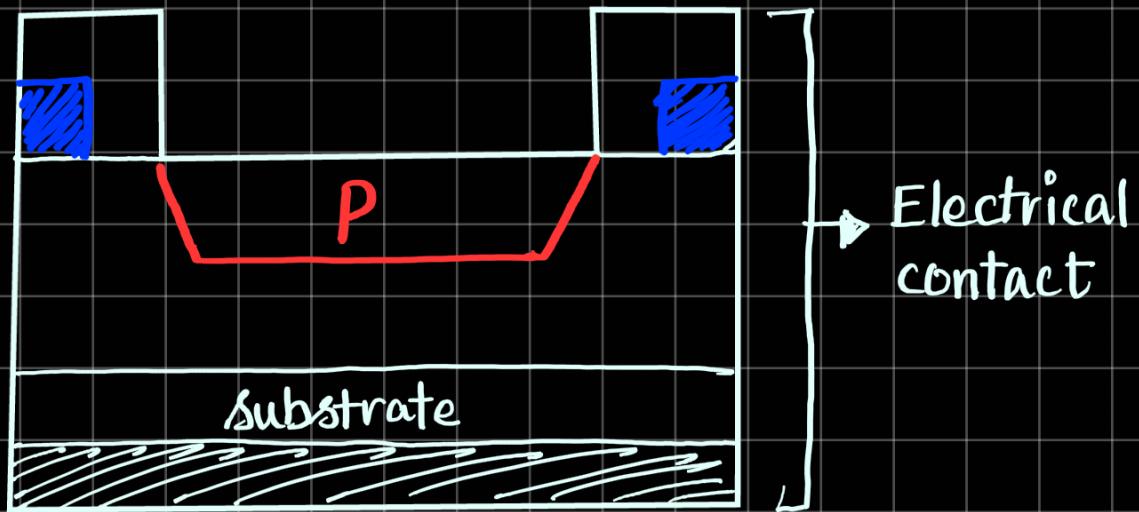
No readsorption

Needs a p-n junⁿ
(same materials
yet dif. dopants)

Recombination must occur

$$E_g = E_c - E_v$$

↳ Structure of LED



• LASER Diode:

↳ LASER → Light Amplification due to Stimulated Emission of Radiation
Intense Coherent Source

P-n junction diode under forward bias

High directionality and narrow linewidth

↳ LASER Amplifier



