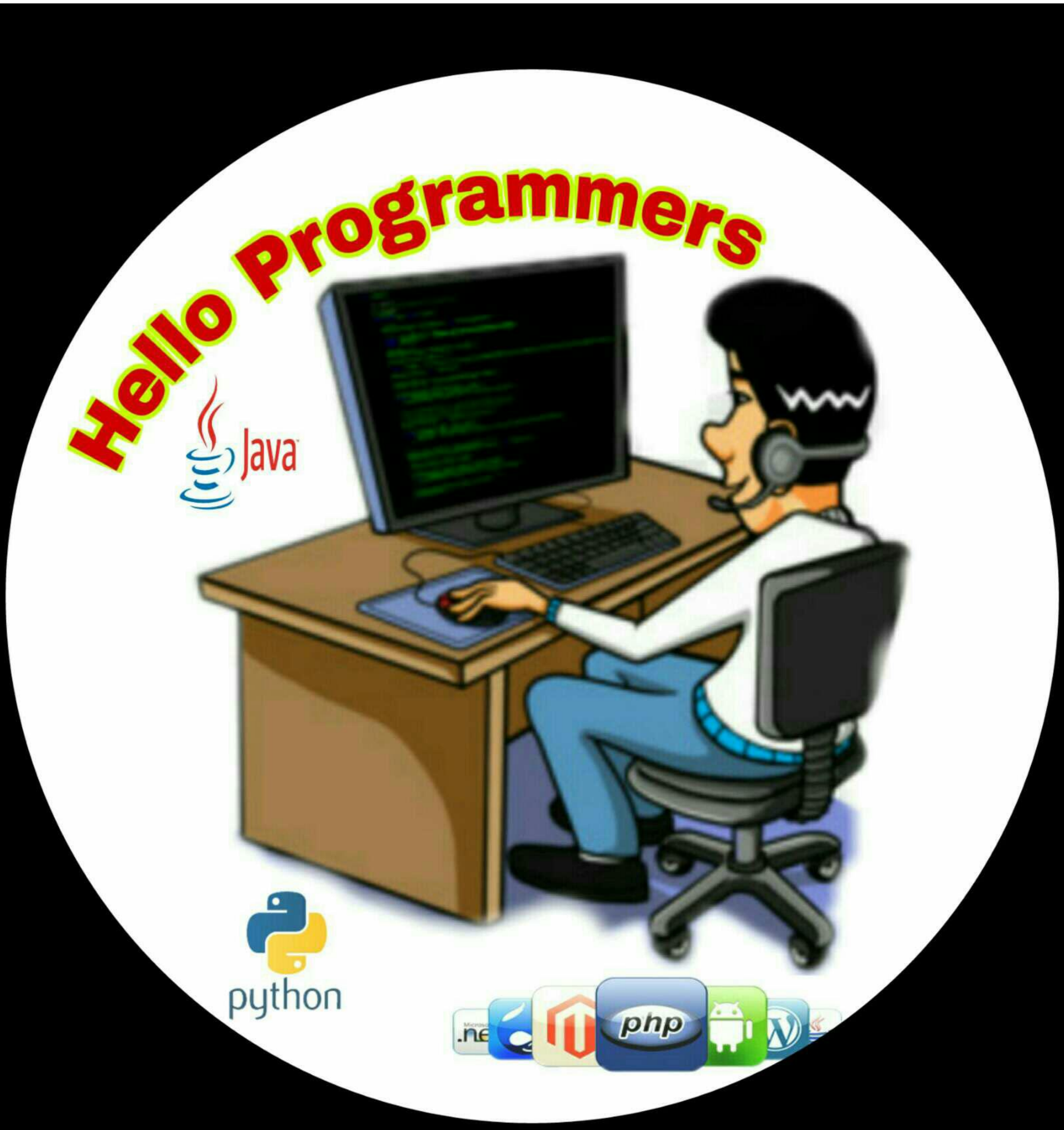

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Marks: 60 | Pass Marks: 24

Physics | Duration: 3 Hours

Attempt any TWO questions. [10x2 = 20]

		Descriptions
Long Question	[10]	>> Unit 5, 6 & 7
Long Question	[10]	>> Unit 1, 2
Long Question	[10]	>> Unit 3, 4

Attempt any 8 questions. [5x8 = 40]

Short Question	[5]	>> Unit 1, 2, 3
Short Question	[5]	>> Unit 4, 5
Short Question	[5]	>> Unit 6, 7
Numerical 1	[5]	>> Numerical: Unit 1
Numerical 2	[5]	>> Numerical: Unit 2
Numerical 3	[5]	>> Numerical: Unit 3
Numerical 4	[5]	>> Numerical: Unit 4
Numerical 5	[5]	>> Numerical: Unit 5
Numerical 6	[5]	>> Numerical: Unit 6,7

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Unit-1

Rotational Dynamics and Oscillatory Motion

Rotational Dynamics:

state of body
- Rest → Static state
- motion → dynamic state
  - change in position relative to time

Force
- change in position → Dyamic
  - translatory
  - Rotational
- change in shape, size → Deforming

Translatery → In which position changes with time in given dimension
- linear
- Curved

Rotational motion in which body changes position with time but remain same from a fixed position. A force that cause rotation is called rotational force. Such effect of force is called torque (τ) & it is the vector quantity.

Some terms in linear and rotational motion:

	linear	Rotation	Relation
- Displacement	— x	θ	$x = r\theta$
- Velocity	— v	$\omega = \left(\frac{d\theta}{dt}\right)$	$v = \omega r$
- acceleration	— a	$\alpha = \left(\frac{d\omega}{dt}\right)$	$a = \alpha r$
- force	— F	torque (τ)	$\tau = F \times d$
- Momentum	— $p = mv$	$L = I\omega$	$L = \pi p$

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– inertia	– m	I	$I = mr^2$
– Work	– $W = f \times h$	$W = \tau \times \theta$	
– Energy	– $\frac{1}{2} m v^2$	$\frac{1}{2} I \omega^2$.	

Torque and motion of inertia:

The rotational effect of force is torque. It rotates or tends to rotate a body about an axis when acts upon it. It is given by the cross product of $\perp^r$ distance from the axis of rotation with the force.

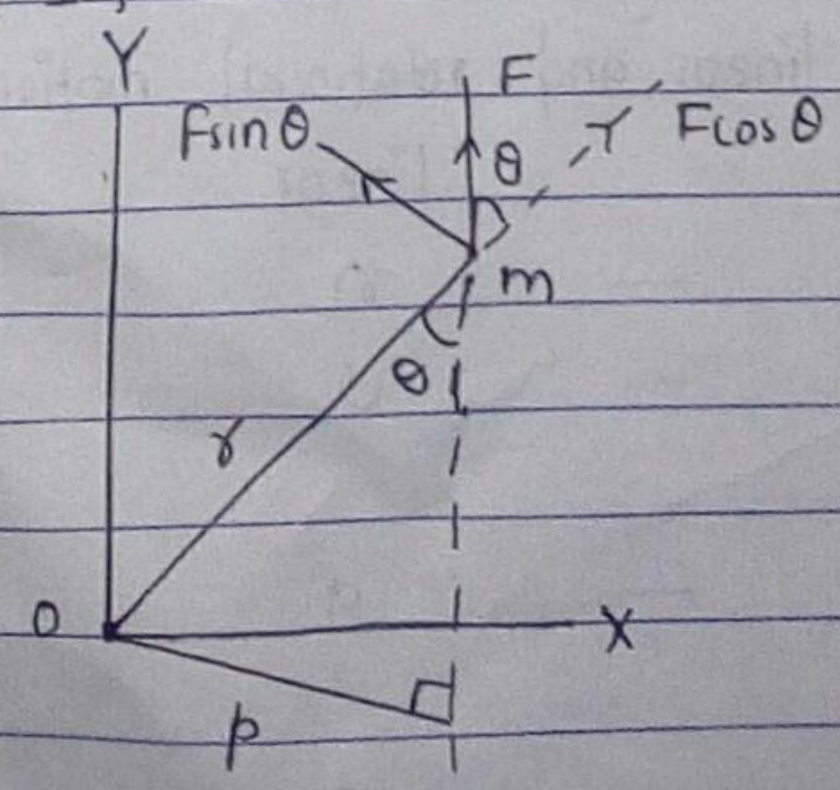
$\vec{\tau} = \vec{r} \times \vec{F}$; r is $\perp^r$ distance of line of action of force from axis of rotation.

In magnitude, $\tau = rF\sin\theta$.

Moment of inertia (I): It is inertia in rotation. It is an inability to change the state of motion in rotation. It is given by

$I = mr^2$ (unit = kgm^2)

Relation between τ & I;



$\sin\theta = \frac{p}{r}$

$p = r\sin\theta$

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let a force 'F' acts on a body of mass m lying at distance r from fixed position O. let θ be angle between r and line of action of force F.

Now, $F\sin\theta$ cause rotational motion

ie. $F\sin\theta = ma$

Now,

Torque, $\tau = r\sin\theta F$

$= rma$ ($a = r\alpha$, α being angular accn)

$= rmr\alpha$

$= mr^2\alpha$

$= I\alpha$

$\tau = I\alpha$

The relation between τ and I is $\tau = I\alpha$

Angular momentum (L): It is the moment of linear momentum. It is the product of linear momentum and distance.

$\vec{L} = \vec{r} \times \vec{p}$ ($\perp^r$ to r & p)

In magnitude, $L = rp\sin\theta$

$\Rightarrow L = p(r\sin\theta)$

Angular moment is conserved quantity

$L = r \times p$

$\Rightarrow \frac{dL}{dt} = \frac{d}{dt}(r \times p)$

$= \frac{dr}{dt} \times p + r \times \frac{dp}{dt}$ ($\because p = mv$)

$= v \times mv + r \times F$

$= m(v \times v) + \tau$

$= \tau$ .... (i)

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In case when a body rotates as well as translates then the K.E.

$$E = E_t + E_r$$
$$= \frac{1}{2}mv^2 + \frac{1}{2}I\omega^2.$$

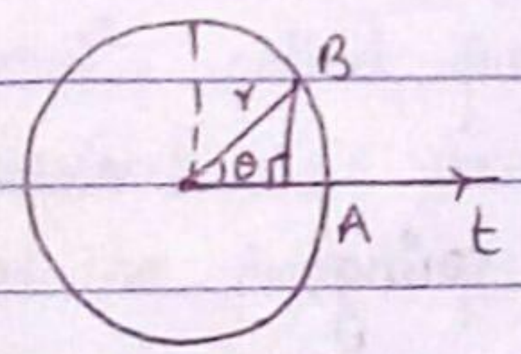
Oscillatory motion:

The motion of body is said to be an oscillatory motion if it repeats its position. If the repeatation takes place in equal time interval then the motion is said to be period motion. This motion is called simple harmonic motion if the acceleration is proportional but towards the mean position. This motion is under restoring force.

$$\text{i.e. } a \propto x$$
$$\Rightarrow a = -Kx.$$

Motion of simple pendulum is an example of SHM. It describe ordinary wave equation, $x = x_0 \sin \omega t$

where x_0 = amplitude.



$$\omega = \frac{\theta}{t}$$

$$\theta = \omega t$$

$$\sin\theta = \frac{x}{r}$$

$$x = r\,(= x_0) \sin \omega t$$

$$\frac{dx}{dt} = x_0 \omega \cos \omega t$$

$$\frac{d^2x^2}{dt^2} = -x_0 \omega^2 \sin \omega t$$
$$= -\omega^2 (x_0 \sin \omega t)$$

$$a = -\omega^2 x$$

$$a \propto x$$

$$\therefore K = \omega^2$$

where ω is called angular velocity

If $t = T$ (periodic) then

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$$\theta = 2\pi$$

$$\omega = \frac{2\pi}{T}$$

Variation of velocity:

$$x = x_0 \sin\omega t$$

$$\frac{dx}{dt} = v = \omega x_0 \cos\omega t$$

$$\Rightarrow v = \omega x_0 \sqrt{1-\sin^2\omega t}$$

$$= \omega x_0 \sqrt{1-\frac{x^2}{x_0^2}}$$

$$= \frac{x_0}{x_0}\sqrt{x_0^2-x^2}$$

$$= \omega\sqrt{x_0^2-x^2}$$

at $x = x_0$ (extreme position)

$v = 0$ (min)

at $x = 0$ $v = \omega x_0$ (max) {mean position}

so, the particle returns from the extreme position.

Mass spring system:

Spring load system (loaded spring)

A loaded spring obey motion under certain limit of applied load the motion becomes period, called SHM. The spring in such condition obey Hooke's law.

Hooke's law states that the elongation is directly proportional to the applied force. The internal resistive force that plays due to intermolecular force opposes the elongation. Till the internal force balance the external force the motion remains in the criteria of SHM within this condition.

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$$F_i = -F_q$$

For the resistive force, the form of Hooke's law is

$F = -kx$, -ve sign means the internal force tends to bring system in its original state. If m be the mass applied,

$ma = -kx$, a being accelerated (=g when placed vertically)

$$m\frac{dv}{dt} = -kx$$

$$m\frac{d^2x}{dt^2} = -kx$$

$$\frac{d^2x}{dt^2} = -\frac{k}{m}x \quad \ldots (i)$$

We have relation,

$$\frac{d^2x}{dt^2} = -\omega^2 x \quad \ldots (ii)$$

On compairing (i) & (ii)

$$\omega^2 = \frac{k}{m}$$

$\therefore k = m\omega^2$ called force constant & in case of load spring is spring constant. It's unit in Nm^{-1}.

It can be defined as the force that comes into play during unit deformation.

The angular velocity

$$\omega^2 = \frac{k}{m} \rightarrow \omega = \sqrt{k/m}$$

Hence ω depends upon force constant k.

Periodic time:

$$\omega = \frac{2\pi}{T}$$

$$\Rightarrow T = \frac{2\pi}{\omega} = 2\pi\sqrt{m/k}$$

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Equation of motion: $\frac{d^2x}{dt^2} = -\frac{K}{m}x$

$$\Rightarrow \frac{d^2x}{dt^2} + \frac{Kx}{m} = 0$$

$$\Rightarrow \frac{d^2x}{dt^2} + \omega^2 x = 0$$

Energy in SHM:

The energy of a body in SHM is sum of K.E & P.E.
for a body in SHM, it obey an equation given by

$$x = a\sin\omega t$$

$$\Rightarrow x = a\sin(\omega t + \phi)$$

ϕ → phase.

where x be displacement in time t having angular velocity ω.

$$\therefore K.E = \frac{1}{2}mv^2 = \frac{1}{2}m\left(\frac{dx}{dt}\right)^2 = \frac{1}{2}ma^2\omega^2\cos^2\omega t$$

$$= \frac{1}{2}m a^2\omega^2(1-\sin^2\omega t$$

$$= \frac{1}{2}ma^2\omega^2\left(1-\frac{x^2}{a^2}\right)$$

$$= \frac{1}{2}m\omega^2(a^2-x^2) \quad \ldots(i)$$

When $x=0$, $K.E \rightarrow max$, $\frac{1}{2}m\omega^2a^2$

when m being mass

when $x=a \Rightarrow K.E=0$ (Extreme position)

Hence, K.E is a function of displacement.

Now,

P.E = The workdone by restoring force at small displacement dx

$$dw = f\,dx$$

The total workdone, $P.E = \int_x^0 dw$

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$$= \int_x^0 F\,dx$$

$$= \int_x^0 -kx\,dx \qquad (\because F = -kx)$$

$$= -k\int_x^0 x\,dx$$

$$= -k\left[\frac{x^2}{2}\right]_x^0$$

$$= \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$$

$$= \frac{1}{2}m\omega^2a^2\sin^2\omega t \qquad \ldots (ii)$$

Total energy, $E = K.E + P.E$

$$= \frac{1}{2}m\omega^2a^2\cos^2\omega t + \frac{1}{2}m\omega^2a^2\sin^2\omega t$$

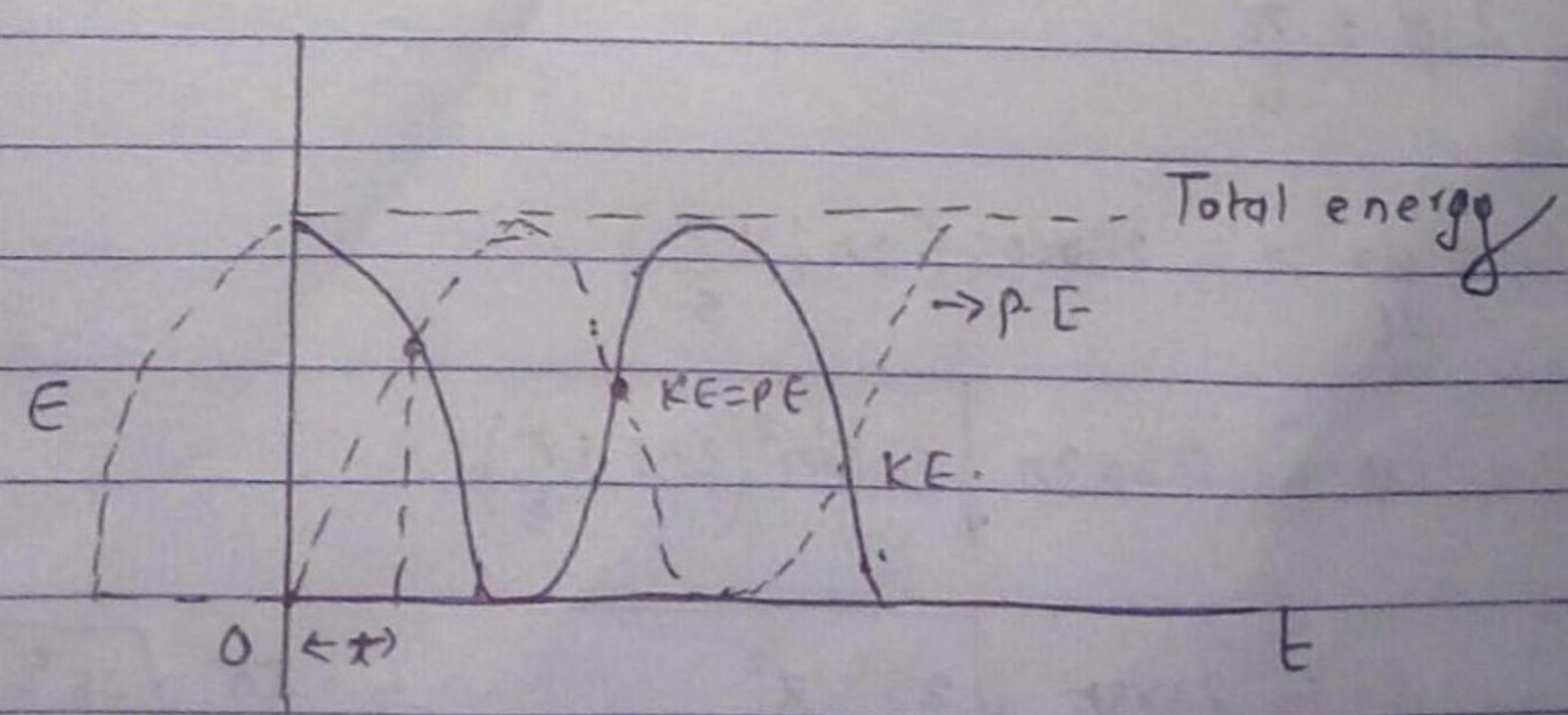
$$= \frac{1}{2}m\omega^2a^2 \qquad \ldots (iii)$$

If $x=0$, $PE=0$

Hence total energy $= K.E$ at $x=0$.

If $x=a$, $K.E=0$

Total energy $= P.E$



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An oscillatory motion of a body is represented by $x = A\cos(\omega t + \phi)$ where, x is displacement in time t, A is amplitude, ω angular frequency. Show that the motion is SH.

Soln

$$x = A\cos(\omega t + \phi)$$

$$\frac{dx}{dt} = -A\omega\sin(\omega t + \phi)$$

$$\frac{d^2t}{dt^2} = -A\omega^2\cos(\omega t + \phi)$$

$$a = -\omega^2 x$$

Hence, the motion is SH.

The position of particle undergoing oscillations is given by $x = 25\sin(3\pi t + \frac{\pi}{5})$, x is in cm and t is in sec. Find the frequency of motion, the amplitude of motion, max velocity, max. value of acceleration?

Soln. Given, $25\sin(3\pi t + \frac{\pi}{5})$

Compairing the given equation with $x = A\cos(\omega t + \phi)$

Here,

$$A = 25\text{ cm}$$

$$\omega = 3\pi$$

$$2\pi f = 3\pi$$

$$\Rightarrow f = \frac{3}{2}\text{ Hz}.$$

$$\& \ \phi = \frac{\pi}{5}$$

Now, $\frac{dx}{dt} = 25\cos(3\pi t + \frac{\pi}{5})$

$$v = 25\times 3\pi\sqrt{1 - \sin^2(3\pi t + \frac{\pi}{5})}$$

$$= \frac{25\times 3\pi}{25}\sqrt{25^2 - x^2} = 3\pi\sqrt{25^2 - x^2}$$

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where, $x = 0$ (mean position)

$v_{max} = 75\pi \, cms^{-1}$

$a = \frac{dv}{dt} = -25 \times 3\pi \times 3\pi \sin\left(3\pi t + \frac{\pi}{5}\right)$

$= -9\pi^2 x$

$a_{max} = 9\pi^2 x_{max}$

$= 9\pi^2 A$

$= 9\pi^2 \times 25 \, cm/s^2$

$= 225\pi^2 \, cms^{-2}$

✓ An oscillating block spring system has mechanical energy of 1.18 J, an amplitude 9.84 cm and max speed of $1.22 \, ms^{-1}$. Find the force constant K, mass of the block, frequency of the motion

Soln

Total energy, $1.18 J = K.E + P.E$

$= \frac{1}{2} m\omega^2 a^2$

Also,

$v = x\omega$

$v_{max} = a\omega$

$\omega = \frac{1.22 \times 100}{9.84}$

$\therefore m = \frac{2 \times 1.18}{\omega^2 a^2}$

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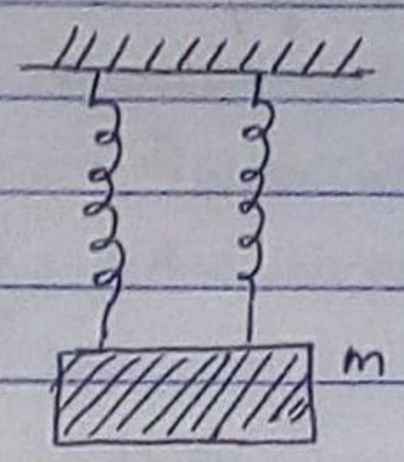
Two strings of force constant K_1 & K_2 are attached to mass m & joined to fixed supports as shown in fig. Show that the frequency of oscillation of mass m is $f = \frac{1}{2\pi}\sqrt{\frac{K_1+K_2}{m}}$.



Soln: Force by mass 'm', $F = mg = ma$
which divides into both of springs
$F = F_1 + F_2$, where F_1 & F_2 be forces on the separate spring.

Now,

$F = -K_1 l + (-K_2 l)$,

$\Rightarrow F = -l(K_1 + K_2)$

$\Rightarrow ma = -(K_1+K_2)l$

$\Rightarrow a = -\frac{(K_1+K_2)l}{m}$

$\Rightarrow \omega^2 = \frac{K_1+K_2}{m}$ $\quad (\because a = -\omega^2 l)$

$\Rightarrow \omega = \sqrt{\frac{K_1+K_2}{m}}$

$\Rightarrow f = \frac{1}{2\pi}\sqrt{\frac{K_1+K_2}{m}}$ □

If the springs are connected as shown in the figure, then find the frequency of motion..

$F_1 = F_1 = F_2$, where F_1 & F_2 be forces on same spring.

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Since, $F_1 = -k_1 l_1 = F$

$\Rightarrow l_1 = \frac{-F}{k_1}$

& $F_2 = -k_2 l_2 = F$

$\Rightarrow l_2 = \frac{-F}{k_2}$

$\therefore$ net elongation $= l_1 + l_2$

$\Rightarrow l = -F\left(\frac{1}{k_1} + \frac{1}{k_2}\right)$

$\Rightarrow F = \frac{-l}{(1/k_1 + 1/k_2)}$

$\Rightarrow ma = -\frac{l}{(1/k_1 + 1/k_2)}$

$\Rightarrow \omega^2 = \frac{1}{m\left(\frac{1}{k_1} + \frac{1}{k_2}\right)}$ $\quad (\because a = -\omega^2 l)$

$\Rightarrow f = \frac{1}{2\pi}\sqrt{\frac{k_1 k_2}{m(k_1+k_2)}}$ □

A rotating wheel
Moment of inertia $0.5\,kgm^2$ rotates with speed of $2\,revs^{-1}$.
The wheel stops by a friction. If the torque $0.4\,Nm$, How long does it take to stop.

Soln

$I = 0.5\,kgm^2$

$\tau = 0.4\,Nm.$, $f = 2\,revs^{-1}$

$t = ?$

$\tau = I\alpha$

$\Rightarrow \tau = I\left(\frac{\omega_i - \omega_f}{t}\right)$

$\Rightarrow \tau = \frac{I\omega_0}{t}$

$\Rightarrow t = I \cdot 2\pi f / \tau = \underline{15.71\,s}$

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A body of mass 100gm is suspended from a spring of negligible mass and is found to be stretched by 1cm. What is the force constant of spring? Also find period of oscillation.

Sol/n

$M = 100gm$

$l = 1cm$

$K = ?$

$T = ?$

$F = Nma$, $100 \times 1000 = -K \cdot 1$.

$\Rightarrow K = 100000$. dyne cm^{-1}.

$$\omega^2 = \frac{K}{m}$$

$$\Rightarrow \omega = \sqrt{\frac{K}{m}}$$

$$\Rightarrow \frac{2\pi}{T} = \sqrt{\frac{K}{m}}$$

$$\Rightarrow T = 2\pi\sqrt{\frac{m}{K}}$$

$$= 2$$

The equation of SHM of a body is in the form $x = a\cos\omega t + b\sin\omega t$. If $a = 3cm$, $b = 4cm$ & $\omega = 2$ rad s^{-1}. Determine the period, amplitude, max. velocity & max. acc. of the motion.

Sol/n

$2\pi f = 2$

$\Rightarrow T = \pi$

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Unit-2
Electric and Magnetic field

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Electric Charge.

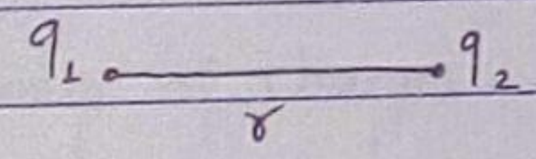
Charge is a fundamental property of matter. Every material contain charge. It has its own specific characters. They are:

1. It is a scalar quantity
2. It is of two types: +ve & negative charge.
3. It is a quantized character
4. They exert mutal force of attraction or repultion.

c.g.s unit of charge. stat. columb (or esu).

$$1C = 3\times10^{9} \text{ stat. c.}$$

Coulomb law: It states that there acts a force of attraction or repulsion between two electrical charges which is directly proportional to the product of charges & inversely proportional to the square of radius between two charges.



$$F \propto q_1 \cdot q_2 \quad \cdots (i)$$

$$F \propto \frac{1}{r^2} \quad \cdots (ii)$$

$$\therefore F \propto \frac{q_1 \cdot q_2}{r^2}$$

$$\Rightarrow F = K\frac{q_1 \cdot q_2}{r^2}$$ is the magnitude of force.

where K is the proportionality constant & depends upon the medium between two charges.

For air (or voccum)

$$K = \frac{1}{4\pi\varepsilon_0} = 9\times10^{9}\ Nm^2C^{-2} \text{ (S.I)}$$

$$= 1 \text{ (in c.g.s)}$$

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for any other medium, $K = \frac{1}{4\pi\varepsilon}$

$\therefore F \propto \frac{q_1 q_2}{r^2}$

ie. $F = K \frac{q_1 q_2}{r^2}$

ie. $F = \frac{1}{4\pi\varepsilon_0} \frac{q_1 q_2}{r^2}$

Permitivity - ability to provide permission for activity.

F is repulsive for similar charge.

Relative permitivity : $E_r = \frac{\varepsilon}{\varepsilon_0}$ - permitivity of a medium relative to the air. It is also called dielectric constant (k).

$K = \varepsilon_r = \frac{\varepsilon}{\varepsilon_0}$

ie. $\varepsilon = K \varepsilon_0$

K is different for different med. for water $K = 80$.

Electric field intensity:
It is the force on a unit positive charge placed at a position inside the field.

$E = \frac{F}{q_0} = \frac{F}{Q}$ unit: NC^{-1}, vector quantity.

and has direction along the force

In vector, $\vec{F} = \frac{1}{4\pi\varepsilon_0} \frac{q_1 q_2}{r^2} \hat{r}$ ie. $\vec{F} = \frac{1}{4\pi\varepsilon_0} \frac{q_1 q_2}{r^3} \vec{r}$.

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Hence, $\vec{E} = \frac{\vec{F}}{q} = \frac{1}{4\pi\varepsilon_0} \frac{q}{r^2} \hat{r}$.

ie. $\vec{E} = \frac{1}{4\pi\varepsilon_0} \frac{q}{r^3} \vec{r}$

E is towards negative charge & away from positive charge.

Line of force: It is the imaginary path followed by unit positive charge inside the field of a source.

Factors affecting E:

- Depends upon q => $E \propto q$.
- Depends upon r => $E \propto \frac{1}{r^2}$
- Depends upon permitivity => $E \propto \frac{1}{\varepsilon}$

E due to group of charges:

The total intensity is a vector sum of individual intensities called principle of superposition. The resultant intensity is given by,

$$\vec{E} = \vec{E}_1 + \vec{E}_2 + \vec{E}_3 + \cdots + \vec{E}_n.$$

The magnitude & direction can be obtained according as theire line of actions

- If all act along the same direction, the magnitude of resultant is algebric sum.
- If they act oppositely, the magnitude of the resultant is difference between their magnitude & direction along the greater one.
- If they act at an angle them parallelogram law is used.

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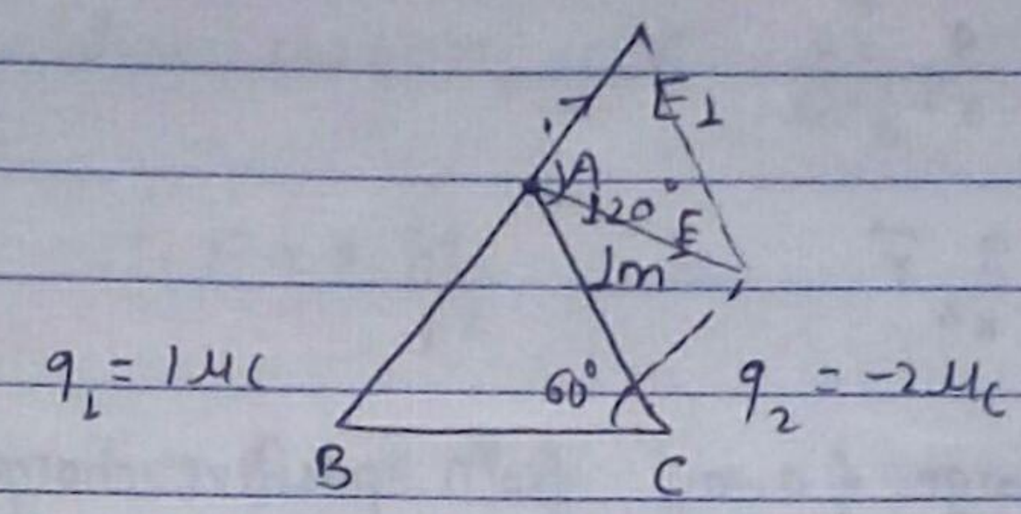

$E_A = ?$

$$E_1 = \frac{1}{4\pi\varepsilon_0}\frac{q_1}{(AB)^2} = \frac{9\times10^9\times1\times10^{-6}}{1^2} = 9\times10^3\ NC^{-1}\ (A)$$

$$E_2 = \frac{9\times10^9\times2\times10^{-6}}{1^2} = 9\times2\times10^3\ NC^{-1}\ (\text{towards } C)$$

Mag. of the E,

$$E = \sqrt{E_1^2+E_2^2+2E_1E_2\cdot\cos\theta}$$
$$= 9\times10^3\sqrt{1+4+4\cos120^\circ}$$
$$= 9\times10^3\sqrt{5+4(-1/2)}$$
$$= 9\times\sqrt{3}\times10^3\ NC^{-1}$$

For direction, $\tan\alpha = \dfrac{E_1\sin\alpha}{E_2+E_1\cos\alpha}$

$$= \frac{9\times10^3\times\sqrt{3}/2}{2\times9\times10^3+9\times10^3(-1/2)}$$

$$= \frac{9\times\sqrt{3}/2}{27/2} = \frac{1}{\sqrt{3}}$$

$\therefore \alpha = 30^\circ.$

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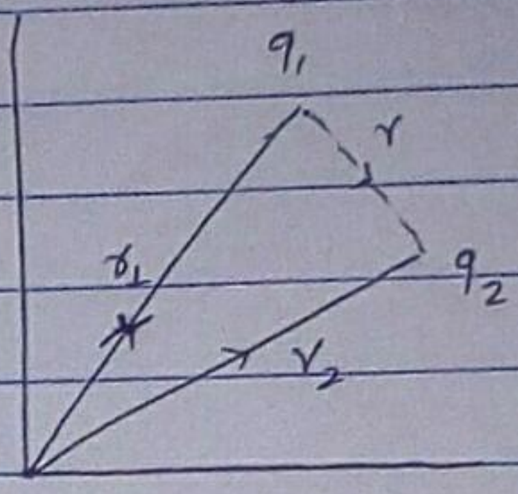
In position co-ordinate form:

$$\vec{F} = \frac{1}{4\pi\varepsilon_0} \frac{q_1 q_2}{r^2} \hat{r}$$

$$= \frac{1}{4\pi\varepsilon_0} \frac{q_1 q_2}{r^3} \vec{r}$$

$$= \frac{1}{4\pi\varepsilon_0} \frac{q_1 q_2}{|\vec{r}_2 - \vec{r}_1|^3} \vec{r}_2 - \vec{r}_1$$



$$\vec{E} = \frac{1}{4\pi\varepsilon_0} \frac{q(\vec{r}_2 - \vec{r}_1)}{|\vec{r}_2 - \vec{r}_1|^3}$$

for potential, $V = \frac{1}{4\pi\varepsilon_0} \frac{q}{r}$

$$= \frac{1}{4\pi\varepsilon_0} \frac{q_1}{|\vec{r}_2 - \vec{r}_1|}$$ is potential due to q_1 on q_2.

Superposition of potential:

The total potential due to group of charges at a position is the algebric sum of their individual potentials.

ie $V = V_1 + V_2 + V_2 + \cdots + V_n$

$$= \sum_{i=1}^{n} V_i.$$

$$= \sum_{i=1}^{n} \frac{1}{4\pi\varepsilon_0} \frac{q_i}{r_i}$$

$$= \frac{1}{4\pi\varepsilon_0} \sum_{i=1}^{n} \left(\frac{q}{r}\right)_i.$$

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Magnetic field:

The area around a pole or magnet inside which its effect can be realized is called magnetic field.

Magnet:

A material having properties:

1. Attractive or repulsive.
2. Directive.
3. Inductive.

Force in magnetism:

$$F = \frac{k m_1 m_2}{r^2}$$ (may be attractive or repulsive)

where, m = pole strength.

k (depends uponds the medium) $= \mu_0 / 4\pi$ =

Also, for air, $F = \frac{\mu_0}{4\pi} \frac{m_1 m_2}{r^2}$ called coblomb force.

where, μ_0 = permeability of air $= 4\pi \times 10^{-7}\ WebA^{-1}m^{-1}$ (Hm^{-1})

In vector form,

$$\vec{F} = \frac{\mu_0}{4\pi} \frac{m_1 m_2 (\vec{r}_2 - \vec{r}_1)}{|\vec{r}_2 - \vec{r}_1|^3}$$

for another medium,

$$k = \frac{\mu}{4\pi}$$

Permeability: It is a propety that provides permission for activities between any two magnetic poles.

$$\mu_r = \frac{\mu}{\mu_0}$$

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Magnetic field intensity (B):

It is the force due to magnet (or magnetic pole) on a unit pole (N-pole).

It is given as, $B = \frac{F}{m}$

$\Rightarrow NA^{-1}m^{-1}$

$\Rightarrow web/m^2$

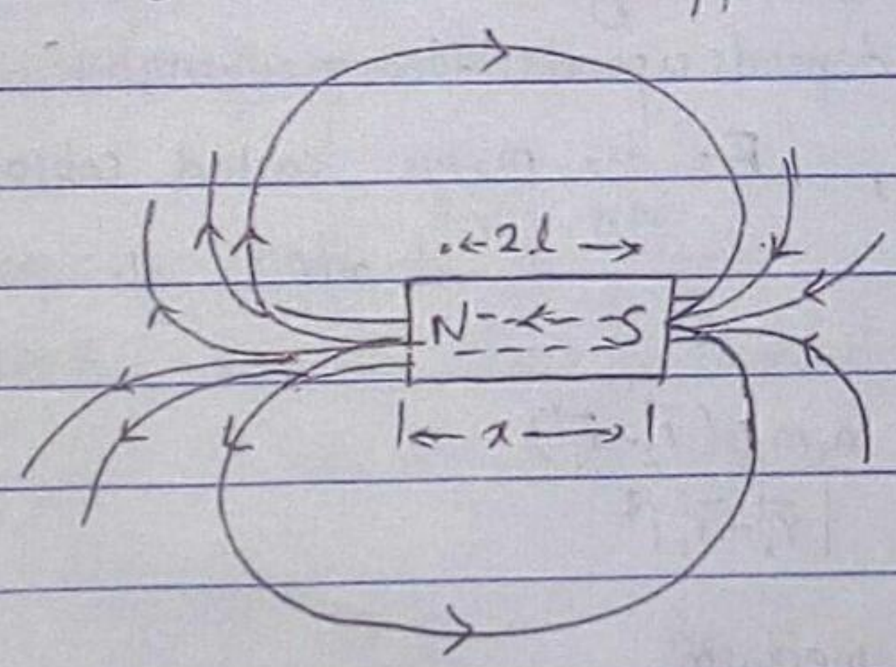
web/m^2 = Tesla (T) (unit of pole strength A.m)

in c.g.s → Gauss

$\vec{B} = \frac{\vec{F}}{m}$. It is a vector quantity.

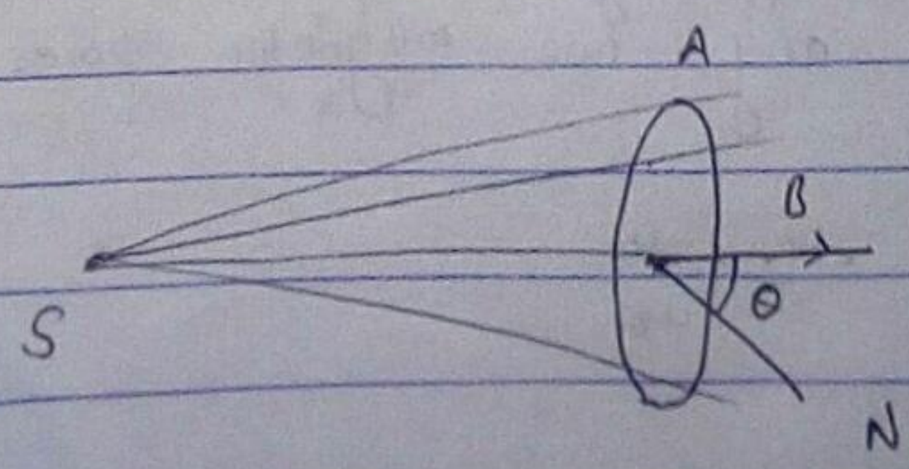
Hence, has line of action.

$2l = x \times 0.85$ (or effective length)



Magentic flux (ϕ):

The total number of lines of force passing normally through unit area.



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Intensity along the normal,

$$B_N = B\cos\theta$$

The intensity is flux per unit area.

$$B_N = \frac{\phi}{A}$$

$$B\cos\theta = \frac{\phi}{A}$$

$$\Rightarrow \phi = B\cos A$$

$$\phi = \vec{B}\cdot\vec{A}$$

When Area $\perp^r$ to B

$$\cos\theta = \cos 0 = 1$$

$$\therefore \phi = BA$$ (maximum flux linkage)

If A is along B.

$$\cos\theta = \cos 90^\circ = 0.$$

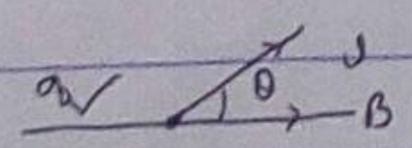
$$\therefore \phi = 0.$$

$\phi = \int \vec{B}\cdot d\vec{A}$ calculus form of flux linkage.

Force on moving charge.

A magnetic field exert force on a moving charge. This force is $\vec{F_m} = \vec{F_B} = q(\vec{v}\times\vec{B})$ (in vector form)

$F_m = F_B = qvB\sin\theta\,\hat{n}$ (scalar form) called lorentz f



If $\theta = 90$ $\quad$ If $\theta = 180^\circ$

$F_m = max.$ $\quad$ $F_m = min.$

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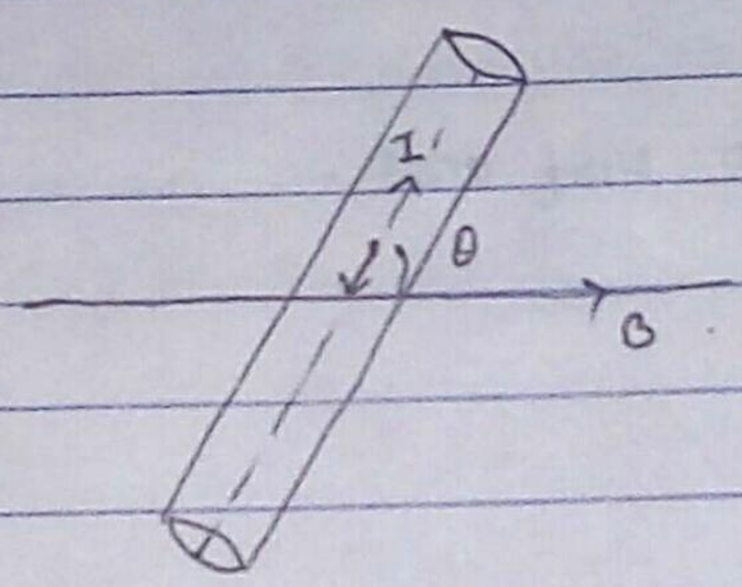
Force due to B on current carrying conductor.



Force by field,

$$F = qvB\sin\theta \quad \text{(lorentz force)}.$$

$$\because v_d = \frac{l}{t} = \frac{lI}{q} \qquad \text{Also, } I = \frac{q}{t} \Rightarrow t = \frac{q}{I}$$

$$\therefore F = q \cdot \frac{lI}{q} B\sin\theta$$

$$= BIl\sin\theta.$$

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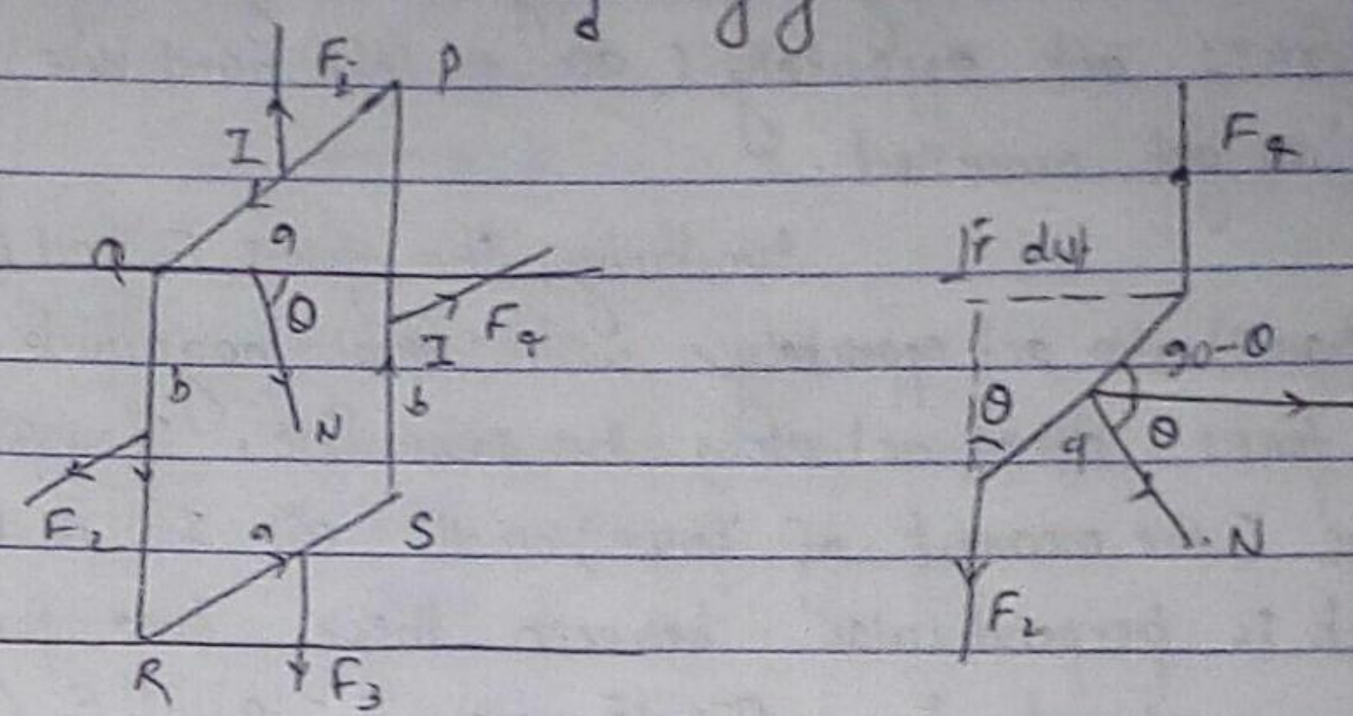
Torque due to B on a currenty carrying coil:



$F_1 = F_3$

$F = F_2 = F_4 = BIL\sin\theta = BIb.$

Now,

$\vec{\tau} = \vec{d} \times \vec{F}$

$= d\sin\theta F$

In magnitude.

$\tau = a\sin\theta \cdot F$

$= aBIb\sin\theta.$

$= BIA\sin\theta.$

A current carrying closed loop when placed in a magnetic field experience torque. Consider a rectangular coil PQRS carrying current I. Let the coil be placed in the magnetic field of uniform intensity B. Let A & B be the lengths of adjacent sides of the coil. Let θ be the angle made by the magnetic field with the normal of the plane of coil. Each sides of the coil behaves as current carrying conductors placed in a magnetic field.

So, the magnetic field exert force on them. Acc. to the theory force on segment PQ and RS will have equal magnitudes. If these forces are F_1 & F_3 (as shown in the figure), they have equal magnitudes. being with equal length & carry equal current

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as well as making equal angle to magnetic field. Since the two forces act oppositely (acc. to left hand rule) along the same line so get cancelled.

Similarly, the forces F_2 and F_4 (as shown in the figure) also act oppositely with equal magnitude BIb. These two forces donot act along the same line. Therefore, they produce torque (the moment of force) on the coil. If d be the distance which is perpendicular between these two forces, the torque produced is $\tau = dF$ i.e. $\tau = a\sin\theta F$ (from fig 2)

i.e. $\tau = aBIb\sin\theta$

$= BIA\sin\theta$.

If the coil has N turns (loop), total torque will be

$\tau = NBIA\sin\theta$.

This is the expression for torque. This relation shows that torque due to magnetic field on a current carrying closed loop depends upon the angle θ.

Special cases:

1. w/ $\theta = 0$, $\sin\theta = 0$

   ie. $\tau = 0$ (min. value)

2. When $\theta = 90^\circ$, $\sin 90^\circ = 1$.

   ie. $\tau = BINA$ (max. value)

Magnetic moment: A current carrying coil (or loop) when placed pole in a magnetic field experience magnetic moment. It is the tendency of rotation of the specimen about an axis. For a (Coil) loop carrying current having area A, the dipole moment is given by $\mu = M = IA$.

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since, $\tau = BINA\sin\theta$

$\therefore \tau = BN(IA)\sin\theta$

$= BN\mu \sin\theta$

$\vec{\tau} = N|\vec{B}||\vec{\mu}|\sin\theta\ \hat{n}$

$\vec{\tau} = N(\vec{\mu} \times \vec{B})$

This is a relation between torque & dipole moment.

Work done by force:

A magnetic field produce torque on a current carrying coil. Hence, torque produce angular displacement. So, work is said to be done by the torque. If τ be the torque & $d\theta$ is small angular displacement, the workdone,

$dw = \tau d\theta$

Total, $w = \int dw$

$= \int \tau d\theta$.

$\because \tau = \mu B \sin\theta$ for one coil.

$\therefore w = \int \mu B \sin\theta d\theta$.

$= \mu B \int \sin\theta d\theta$

$= -\mu B \cos\theta$. $- \mu B \cos\theta$.

$w = -\vec{\mu}.\vec{B}. = E$

This is the expression for workdone and depends upons angle θ betn μ & B.

* ($10^{183} + 1.458 \times 10^{227}$). – No. of things.

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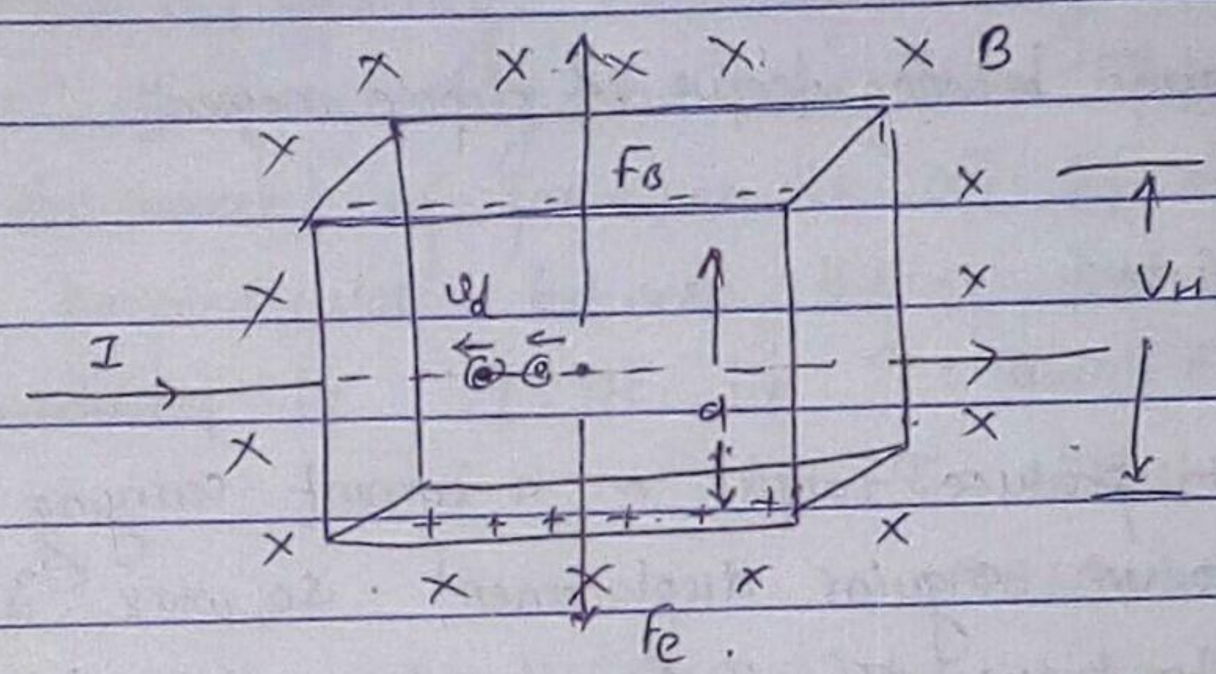
"May the force be with you" – star wars.

Hall effect:

A phenomenon of generation potential difference in a current carrying specimen, when placed perpendicular in a magnetic field is known as Hall effect.



Consider, a metallic specimen carrying current I is placed in a magnetic field of intensity B perpendicularly. When the current flows through the specimen the electrons drift in the direction opposite to the direction of current. The magnetic field exert force on these drifting electrons. Therefore, such electrons get displaced along the direction of force along magnetic field which is ⊥r to the drift velocity. As a result, there occurs separation of negative charges along the direction of force due to magnetic field and positive charge is in the opposite direction. As a result, a p.d. is produced in the direction ⊥r to both the magnetic field and the current. This p.d. is called Hall voltage.

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If E_H be generated electric field intensity in specimen (also called Hall field) then, $F_B = eE_H = Bev_d = Fe$.

where, B - magnetic field intensity
v_d - drift velocity

ie. $E_H = Bv_d$

If d be the width of specimen and J be current density,

$$\frac{V_H}{d} = \frac{BJ}{ne}$$

$$\Rightarrow \frac{V_H}{dBJ} = \frac{1}{ne} = R_H \text{ called Hall coefficient}$$

For N-type semiconducting specimen this coefficient I is negative and for p-type specimen it is +ve.

Mobility The mobility is defined by, $\mu = \frac{v_d}{E_H}$

$$= \frac{J\,d}{ne\,V_H}$$

$$\mu = \frac{Jd}{V_H} R_H$$

Also, $\mu = \frac{J}{neE_H}$ $(\because J = \sigma E_H)$

$$\Rightarrow \mu = \frac{\sigma E_H}{neE_H}$$

$$\Rightarrow \mu = \frac{\sigma}{ne} = \sigma R_H$$; σ being the conductivity

Hall resistance:

$$\frac{V_H}{I} = \frac{BJd}{neI}$$

$$\Rightarrow \frac{V_H}{I} = \frac{BJd}{neI} = r_H.$$

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"Electromagnetic waves"

These waves which have both time varying electric and magnetic fields. The amplitude and phase of electric and magnetic field change periodically. Both the electric & magnetic field act $\perp^r$ly such that they exert force along the two opposite direction upon a body. Their propagation is $\perp^r$ to both the fields. If the electric field acts along x-axis & magnetic field along the z-axis then, the propagation of the electromagnetic wave is along x-axis. They obey period motion and hence are represented by equation of SHM. For the electric field at time t the equation is $\vec{E} = E_0 \sin(\omega t - kx)\hat{i}$

Similarly, the magnetic field is given as, $\vec{B} = B_0 \sin(\omega t - kx)\hat{i}$, $k = \frac{2\pi}{\lambda}$.

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Unit-3

Fundamentals of Atomic Theory:

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Bohr's theory:

1. $\frac{mv^2}{r} = \frac{1}{4\pi\varepsilon_0}\frac{ze^2}{r^2}$

2. The angular momentum of an electron revolving around the nucleous is integral multiple of $\frac{h}{2\pi}$.

ie. $mvr = n\hbar = n\frac{h}{2\pi}$.

This is called Bohr's quantization condition.

$n = 1, 2, 3, 4, ---$

Here, 'n' is principle quantization number and it's values are $n = 1, 2, 3, 4, ---$.

This means angular momentum of electron is discrete and quantized.

Also, $2\pi r = n\lambda$

$= \frac{nh}{mv}$

$= \frac{nh}{p}$.

This means circumference orbit is the integral multiple of wavelength.

3. The stationary orbit has certain energy and electron moving in stationary orbit doesnot absorb or emit energy. An electron emits or absorbs energy when it jump's from one energy level to another energy level.

When an electron jumps from higher energy level to lower energy level it emit energy in the form of electromagnetic radiation. Similarly, when electron jumps from lower energy level

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to higher energy level it absorb energy in the level it absorb energy in the form of radiation.

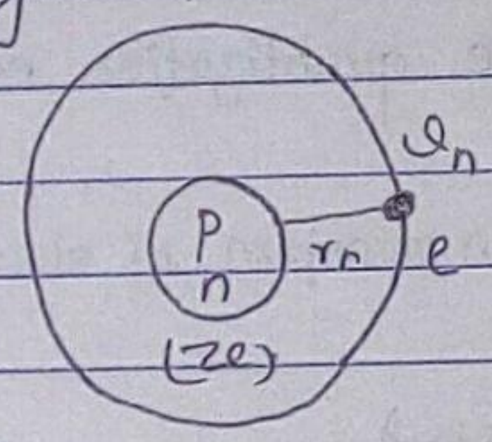
$\therefore E_f - E_i$ = energy of em wave

$E_f - E_i = h\nu$ (when $E_f > E_i$)

$\nu = \frac{E_f - E_i}{h}$ This is Bohr's frequency relation.

Here 'ν' is the frequency of em. wave (radiation).

Bohr's theory of hydrogen atom:



Suppose an electron of mass 'm', charge of magnitude e revolving around the nucleus in the circumference of radius 'r_n' with velocity 'v_n'

For stable orbit,

Centripetal force = electrostatic force between nucleus and electron.

$$\frac{m v_n^2}{r_n} = \frac{1}{4\pi\varepsilon_0} \frac{Ze^2}{r_n^2}$$

$$\Rightarrow r_n = \frac{Ze^2}{4\pi\varepsilon_0 m v_n^2} \quad \text{.... (i)}$$

From Bohr's quantization condition,

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$$m v_n r_n = \frac{nh}{2\pi}$$

$$\Rightarrow V_n = \frac{nh}{2\pi m r_n} \quad \ldots (ii)$$

Using (i) & (ii),

$$r_n = \frac{ze^2}{4\pi\varepsilon_0 m\left(\frac{n^2h^2}{4\pi^2 m^2 r_n^2}\right)}$$

$$\Rightarrow r_n = \frac{ze^2 4\pi^2 m^2 r_n^2}{4\pi\varepsilon_0 m n^2 h^2}$$

$$\Rightarrow r_n = \frac{\varepsilon_0 n^2 h^2}{z\pi m e^2} \quad \ldots (iii)$$

$$\Rightarrow r_n = \frac{h^2}{z}\left[\frac{8.85\times10^{-12}(6.62\times10^{-34})^2}{3.14\times9.1\times10^{-31}(1.6\times10^{-19})^2}\right]$$

$$= \frac{n^2}{z}(0.53\times10^{-10})\,m$$

$$\therefore r_n = \frac{n^2}{z}\,0.53\,\mathring{A}.$$

ie. $r_n \propto n^2$

Radius of orbit $r_1 = \frac{0.53\,\mathring{A}}{z}$

$$\therefore r_2 = \frac{4\times0.53\,\mathring{A}}{z}$$

$$r_3 = \frac{9\times0.53\,\mathring{A}}{z}.$$

$\therefore r_1 < r_2 < r_3$

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e.g. $r_n \propto \frac{1}{Z}$

$Z_H < Z_{He}$

$\boxed{r_H > r_{He}}$

For H-atom $Z = 1$.

Note: If $n=0$, $r_n = 0$. This means the electron lies inside nucleus which is impossible. Thus, we cannot take the value $n=0$.

Velocity of electron:

From Bohr's quantization condition,

$$m v_n r_n = \frac{nh}{2\pi}$$

$$v_n = \frac{nh}{2\pi m r_n} \quad \ldots \text{(iv)}$$

Here,

$$v_n = \frac{10^{-34}}{10^{-31} \times 10^{-10}}$$

$$v_n \simeq 10^{-7} ms^{-1}.$$

Thus, the velocity of electron in the orbit is very high compairable to the velocity of light.

Using 'r_n'

$$v_n = \frac{nh}{2\pi m \left(\frac{\varepsilon_0 n^2 h^2}{2\pi m e^2}\right)} \qquad v_n = \frac{Ze^2}{2\varepsilon_0 nh} \quad \ldots \text{(v)}$$

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$$v_n \propto Z$$
$$v_n \propto \frac{1}{n}$$

Frequency of electron:

The numbers of the revolutions completed by electron in one second is called frequency.

$$f = \frac{1}{T} = \frac{1}{2\pi/\omega} = \frac{\omega}{2\pi}$$

But, $v_n = \omega r_n$

$$\omega = \frac{v_n}{r_n}$$

$$f = \frac{v_n}{2\pi r_n} = \frac{\frac{Ze^2}{2\varepsilon_0 nh}}{2\pi\left(\frac{\varepsilon_0 n^2 h^2}{Z\pi me^2}\right)}$$

$$\therefore f = \frac{Z^2 me^4}{4\varepsilon_0^2 n^3 h^3} \quad \ldots (vi)$$

Energy: An electron is revolving around the nucleus with certain velocity. It has certain K.E.

$$K.E = \frac{1}{2} m v_n^2 = \frac{1}{2} m \left[\frac{1}{4\pi\varepsilon_0} \frac{Ze^2}{nh}\right]^2$$

$$= \frac{1}{8} \frac{mZ^2e^4}{\varepsilon_0^2 n^2 h^2}.$$

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The attractive force between nucleus and electron is the source of potential energy. Actually potential energy is the amount of workdone in bringing electron from ∞ to an orbit.

$$dW = F \cdot dr$$

$$W = \int_{\infty}^{r} F \cdot dr.$$

$$P.E = \int_{\infty}^{r} F dr.$$

$$= \int_{\infty}^{r} \frac{1}{4\pi\varepsilon_0} \frac{ze^2}{r^2} dr$$

$$= \frac{1}{4\pi\varepsilon_0} ze^2 \int_{\infty}^{r} r^{-2} dr$$

$$= \frac{ze^2}{4\pi\varepsilon_0} \left[\frac{r^{-2+1}}{-2+1} \right]_{\infty}^{r}$$

$$= \frac{-ze^2}{4\pi\varepsilon_0} \left[-\frac{1}{r} \right]_{\infty}^{r}$$

$$= \frac{-ze^2}{4\pi\varepsilon_0 r} - \left(\frac{-ze^2}{4\pi\varepsilon_0 \infty} \right)$$

$$= \frac{-ze^2}{4\pi\varepsilon_0 r}.$$

For n^{th} orbith:

$$P.E = \frac{-ze^2}{4\pi\varepsilon_0 r_n}$$

$$P.E = \frac{-ze^2}{4\pi\varepsilon_0} \left(\frac{z\pi me^2}{\varepsilon_0 n^2 h^2} \right)$$

$$= \frac{mz^2e^4}{4\varepsilon_0^2 n^2 h^2}$$

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Now,

Total energy of electron = P.E + K.E

$$= \frac{1}{8}\frac{mz^2e^4}{\varepsilon_0^2 n^2 h^2} + \left(\frac{-mz^2e^4}{4\varepsilon_0^2 n^2 h^2}\right)$$

$$= \frac{1}{4}\frac{mz^2e^4}{\varepsilon_0^2 n^2 h^2}\left(\frac{1}{2}-1\right)$$

$$E_n = \frac{-mz^2e^4}{8\varepsilon_0^2 n^2 h^2} \quad \cdots\cdots (i)$$

$$= \frac{-z^2}{n^2}\left[\frac{-9.1\times10^{-31}\times(1.6\times10^{-19})^4}{(8.85\times10^{-12})^2\times(6.62\times10^{-34})^2}\right]$$

$$= (-13.6\,eV)\frac{z^2}{n^2} \quad \cdots\cdots (ii)$$

For H-atom, $z = 1$

$$E_n = \frac{-13.6\,eV}{n^2}$$

For $n=1$, $E_1 = -13.6\,eV$

for $n=2$, $E_2 = \frac{-13.6}{4}\,eV = -3.4\,eV$.

for $n=\infty$, $E_\infty = 0$.

Here,

$$(E_3-E_2) \neq (E_2-E_1) \neq (E_4-E_3)$$

This indicates that energy levels of hydrogen atom are discrete and spacing between energy levels are not equal.

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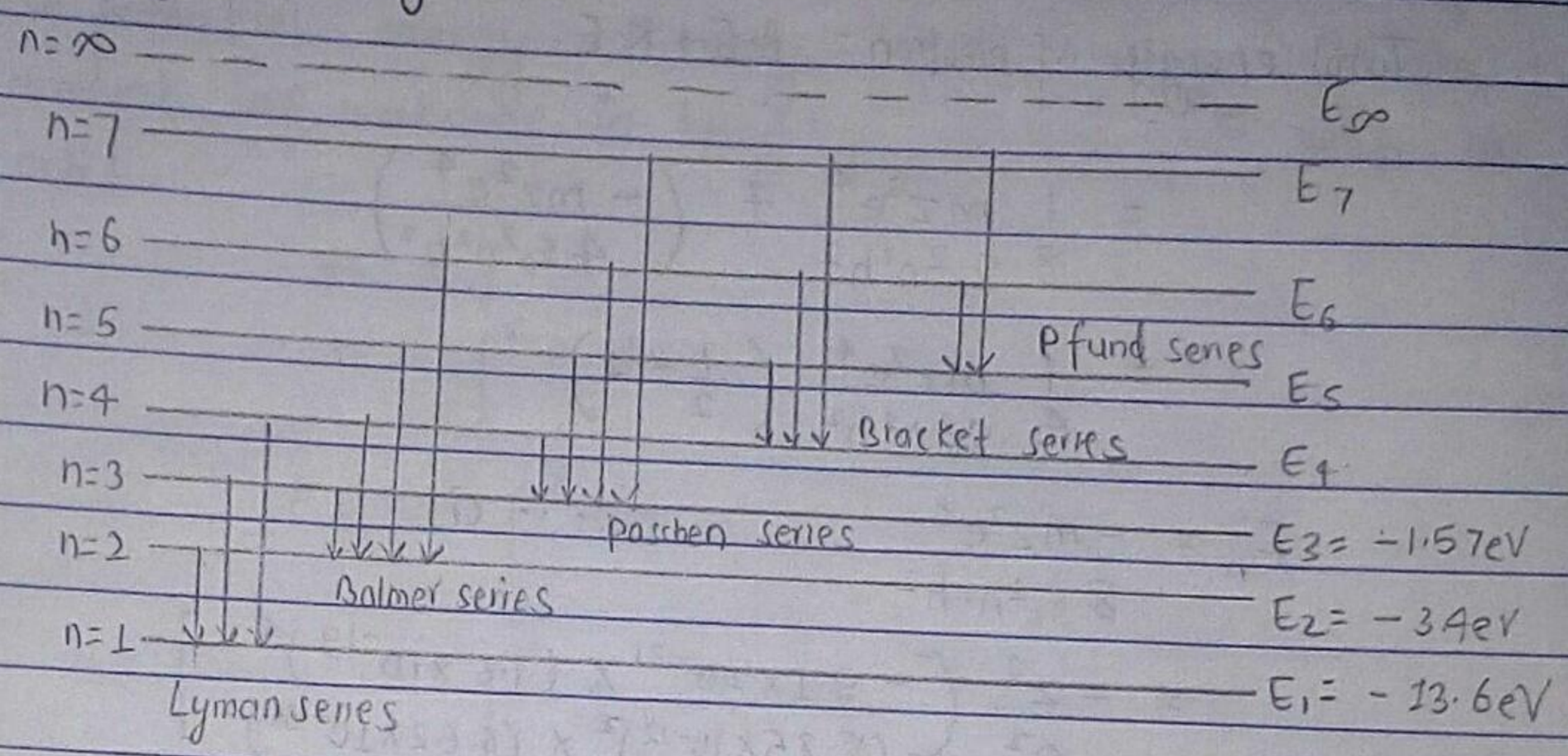
Energy level diagram:



A diagram in which horizontal lines represent the value of energy, vertical lines with arrow indicates electron from one level to another level is known as energy level diagram. The energy level diagram are not equally spaced. Whenever an electron jumps from higher energy state to lower state, the difference between the two state to lower state, the difference between the two state appears the radiation of coration frequency and wavelength called spectral line.

Suppose the translational of electron from higher energy $(E_n)_2$ to lower energy level $(E_n)_1$.

Now from Bohr's frequency condition,

$$(E_n)_2 - (E_n)_1 = h\nu$$

$$h\nu = -\frac{me^4z^2}{8\varepsilon_0^2 n_2^2 h^2} - \left(-\frac{me^4z^2}{8\varepsilon_0^2 n_1^2 h^2}\right)$$

$$\nu = \frac{me^4z^2}{8\varepsilon_0^2 h^3}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \quad \ldots (i)$$

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Eqn (i) gives the frequency of radiation when an electron jumps from n_2 level to n_1 level.

But

$$\nu = \frac{c}{\lambda}$$

$$\Rightarrow \frac{c}{\lambda} = \frac{me^4 z^2}{8\varepsilon_0^2 h^3}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$\Rightarrow \frac{1}{\lambda} = \frac{me^4 z^2}{8\varepsilon_0^2 h^2 c}\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

$$\Rightarrow \frac{1}{\lambda} = Rz^2\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \quad \cdots (ii)$$

Here, $1/\lambda$ is the wave number & it represents the number of the wave generating per unit length. Its unit is per meter.

Here, $R = \frac{me^4}{8\varepsilon_0^2 h^3 c}$

$$= \frac{9.1\times10^{-31} \times (1.6\times10^{-19})^4}{8\times(8.85\times10^{-12})^2 \times (6.62\times10^{-34})^3 \times 3\times10^8}$$

$= 1.097\times10^7 m^{-1}$ which is Redberg constant.

a lymen series

The series of spectral line which is originated due to transition of electron from high energy level ($n_2 = 2, 3, 4, \ldots$) to ground state $n_1 = 1$ is known as lymen series. It lies in UV region.

For lymen series (for hydrogen)

$z = 1$

$$\frac{1}{\lambda} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \quad (n_1 = 1)$$

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For longest wavelength, energy separation must be lowest

$$\therefore \frac{1}{\lambda_{longest}} = R\left(\frac{1}{1^2} - \frac{1}{2^2}\right)$$

$$= R \times \frac{3}{4} = \frac{3R}{4}$$

$$\Rightarrow \lambda_{longest} = \frac{4}{3 \times 1.097 \times 10^7}$$

$$= 1.21 \times 10^{-7} m$$

$$= 1210 \text{ Å}.$$

For shortest wavelength of lymen series (series limit)

$$\therefore \frac{1}{\lambda_{shortest}} = R\left(\frac{1}{1^2} - \frac{1}{\infty}\right)$$

$$\lambda_{smallest} = \frac{1}{R} = \frac{1}{1.097 \times 10^7} = 911 \text{ Å}.$$

Calculate the wavelength difference between shortest and longest wavelength of lymen series.

$$\lambda_{longest} - \lambda_{shortest} = \frac{4}{3R} - \frac{1}{R}$$

$$= \frac{1}{3R} = \frac{1}{3R}$$

6. Balmer series: The series of spectral line which is originated due to transition of electron from higher energy level $n_2 = 3, 4, 5, \ldots \infty$ to first excited state $n_1 = 2$ is called Balmer series. It lies in visible region.

The first line of Balmer series is called H_α line

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For H_α line, $n_1 = 2, n_2 = 3$

$$\frac{1}{\lambda_{H_\alpha}} = R1^2 \left(\frac{1}{4} - \frac{1}{9}\right)$$

$$= \frac{5R}{36}$$

$$\Rightarrow \lambda_{H_\alpha} = \frac{36}{5R} = \frac{36}{5 \times 1.097 \times 10^7} = 6.56 \times 10^{-7} m = 6560 \mathring{A}.$$

This is the longest wavelength of Balmer series.

The second, third, fourth lines of Balmer series are called H_β, H_γ, H_δ, respectively

For H_β, $n_1 = 2, n_2 = 4$
For H_γ, $n_1 = 3, n_2 = 5$
For shortest wavelength, $n_1 = 2, n_2 = \infty$

c. Paschen series: The series of spectral line which is originated due to the transition of electron from higher energy level $n_2 = 4, 5, 6, \ldots \infty$ to the second excited state $n_1 = 3$ is known as Paschen series.

For first line $n_1 = 3, n_2 = 4$

$$\frac{1}{\lambda} = R\left(\frac{1}{9} - \frac{1}{16}\right)$$

$$= \frac{R \times 7}{9 \times 16} = \frac{7R}{144}$$

$$\Rightarrow \lambda = \frac{144}{7R} = 26250 \mathring{A}.$$

It lies in the infra rayed region.

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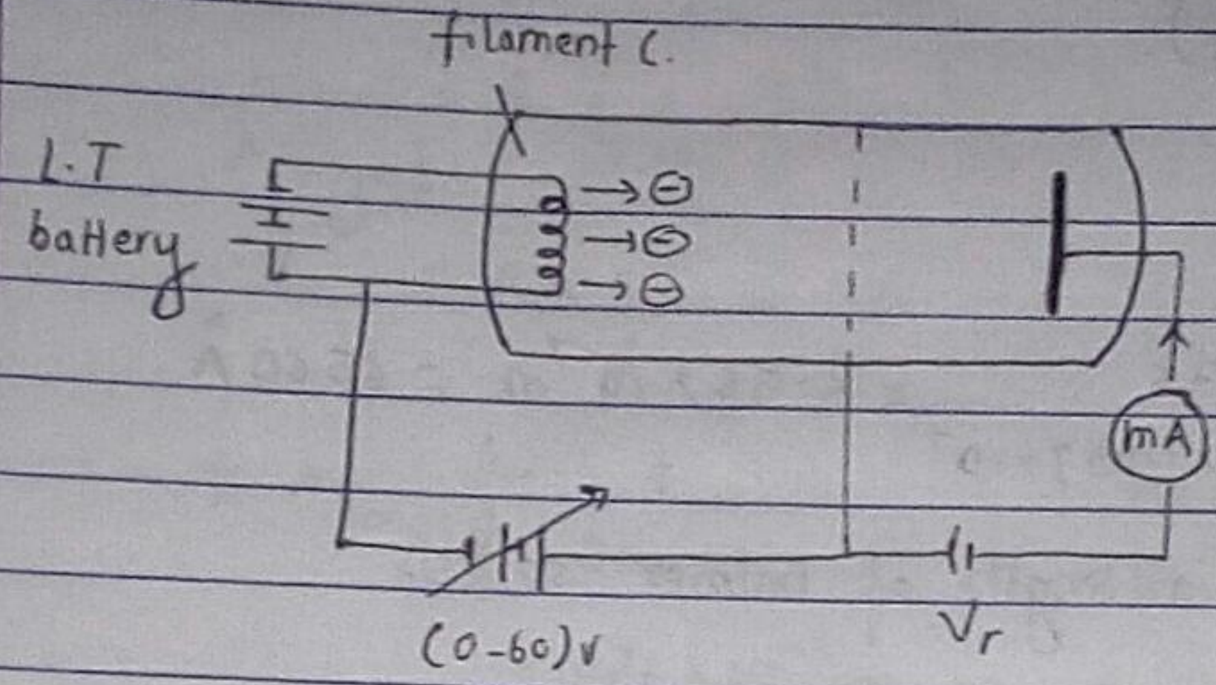
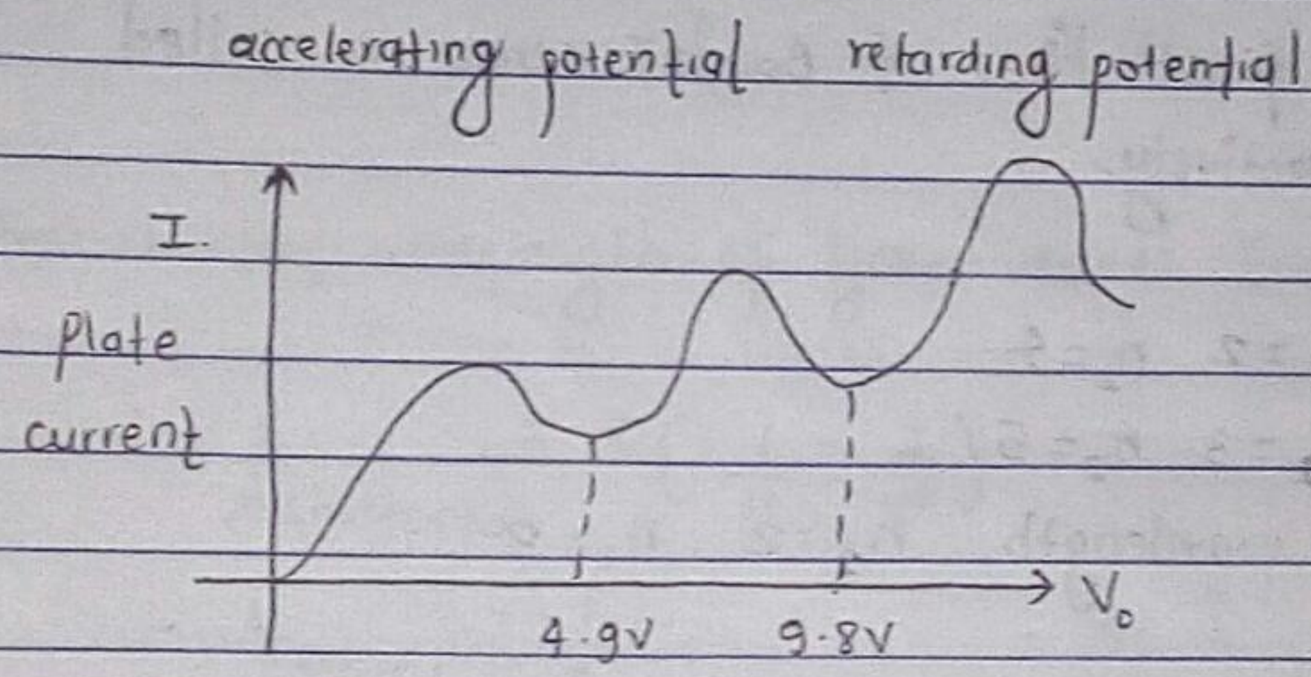
Frank- Hertz experiment:





Bohr predicted the correct electromagnetic spectrum for hydrogen by postulating total angular momentum condition

$L = mvr = n\hbar$. Frank- Hertz determine the existance of discrete energy level for Hg atom by the method of excitation of atom by collision, it requires very high retarding potential.

Experimental arrangement: It consists of filament f connected to low tension battery. The electrons are emitted thermo-ionically from filament and they are accelerated between filament grid. The accelerated electron reach to collector plates and give current called plate current measured by mA. The plate current depend's on the no.'s of electrons

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collected at collector. A small retarding potential $V_r = 0.5V$ is connected grid and collector plate to stop the low energy electrons.

Explaination: The graph between accelerating potential and plate current is as shown in graph above. Initially as accelerating potential (V_0) increases, plate current gradually increases and becomes maximum due to increase in speed of electron. At 4.9V, the current becomes minimum. Again, when potential increases, current increases becomes maximum and dips to minimum at 9.8V.

The minimum current at 4.9V is due to inelastic collision between electron and Hg atom. During collision electron losses K.E and Hg atoms gains energy and gets excited. Such low energy electron cannot reach to the plate and current becomes minimum. Similarly, the minimum current at 9.8V is due to inelastic collision between two Hg atoms.

Due to collision of electron with Hg atoms, Hg atoms will be excited and return to G.S by emission of photons of wavelength 2356 Å. The energy of such photon.

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

$$= \frac{6.62 \times 10^{-34} \times 3 \times 10^{8}}{2536 \times 10^{-10}}$$

$$= 4.9 eV$$

This experimental gives the existence for the discrete energy level of Hydrogen.

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De-Broglie's Hypothesis: The phenomenons of interference, diffraction, polarization of light can be explained on basis of wave theory of light. These phenomenon show that light posses wave nature.

However in certain phenomenon photoelatric effect, compton effect, black body radiation can be explained on the basis of quantum theory. Acc. to this theory, light behaves like particle.

Thus, we can say that light posses dual nature.

De-Broglie suggested that particle such as electron, proton should also posses dual nature like radiation. These waves associated with moving particle called matter waves or pilot waves.

To show the wave particle dualism, De-Broglie used Plank's theory of quantum radiation and Einstein's theory of relative.

Acc. to Plank's theory of quantum radiation, the energy of photon, $E = hf, = \frac{hc}{\lambda}$ .... (i)

where, λ = wavelength of em radiation.

From Einstein's mass-energy relation, energy of photon

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

from (i) & (ii)

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

$$\lambda = \frac{h}{mc} = \frac{h}{p} \quad \text{.... (iii)}$$

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where $p = mc$ is momentum of photon.

According to De-Broglie's, the wavelength of wave associated with a moving particle having momentum $p = mv$ is given by

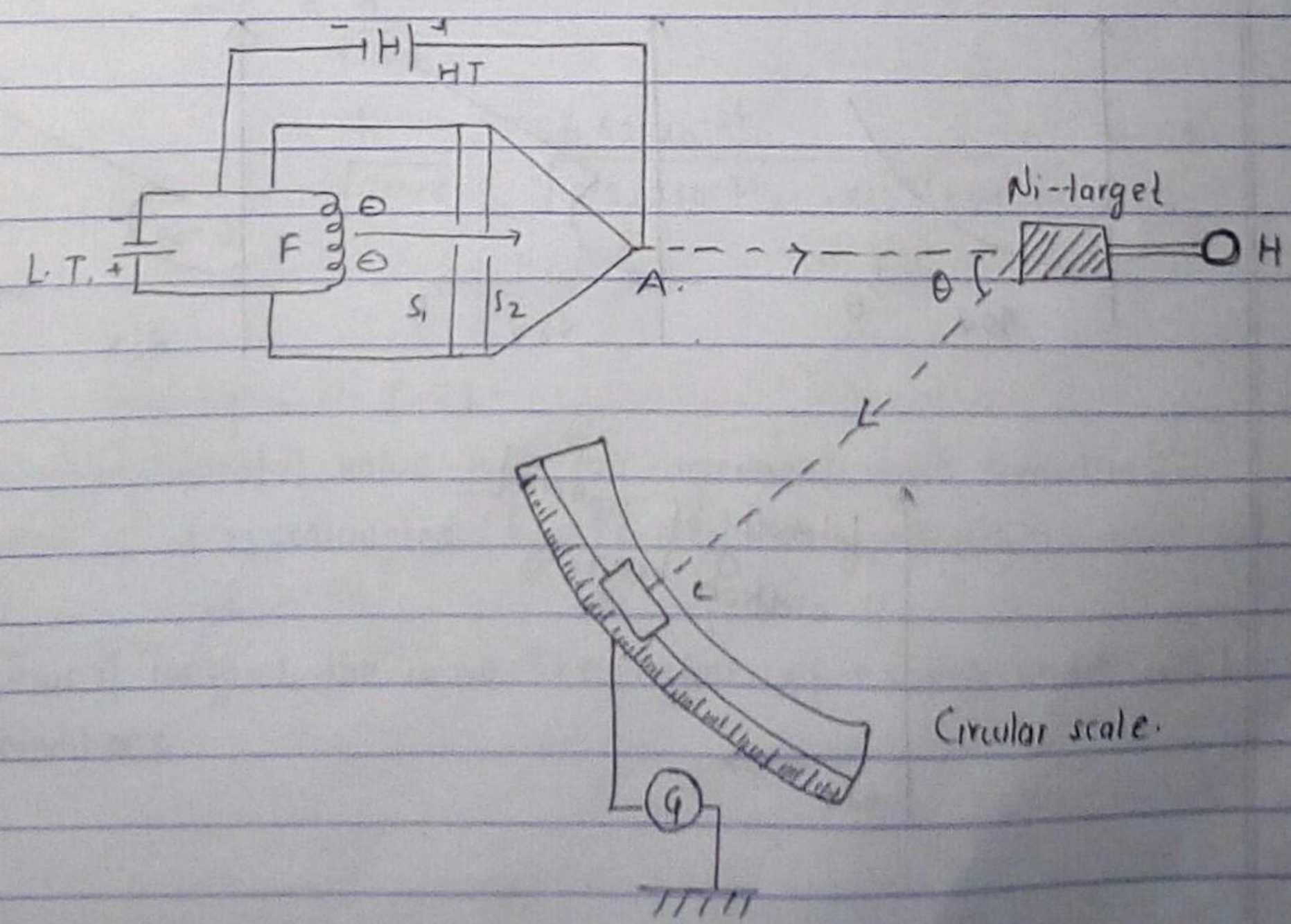
$$\lambda = \frac{h}{mv}.$$

clearly, if $v = 0$, $\lambda = \infty$

Thus, the matter particle will have a wavelength associated with it only if it is motion.

Experimental verification of De-Broglie's hypothesis
(Experimental study of matter wave).
or Davisson & Germer experiment.

Davisson and Germer performed an exp. to demonstrate the wave nature of electron.



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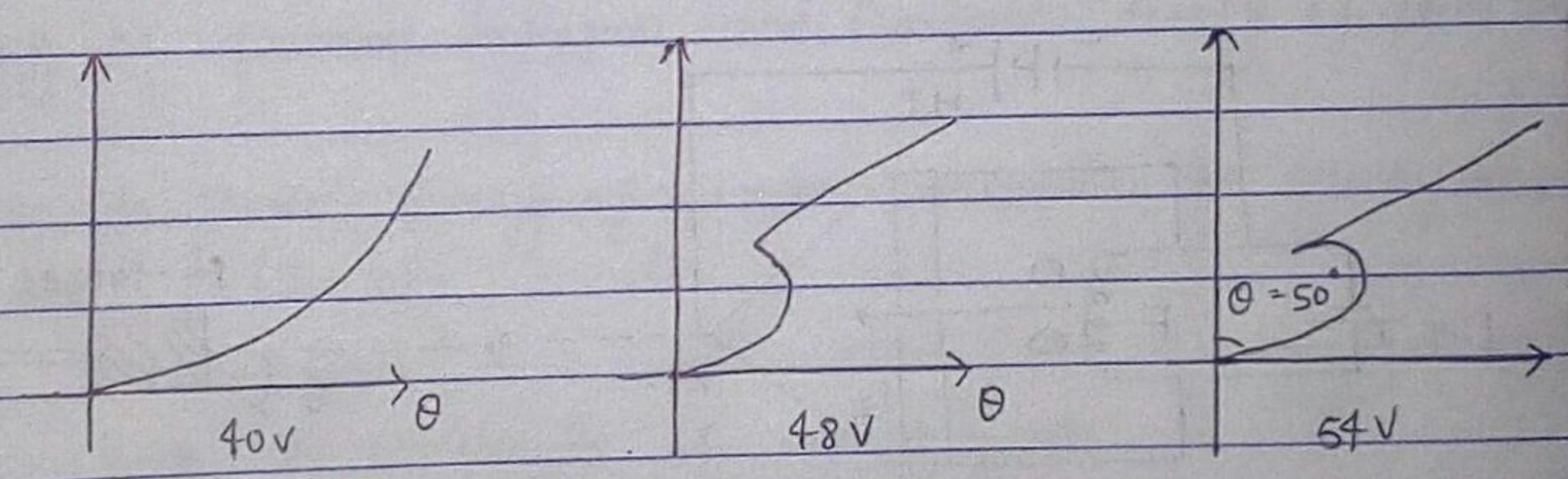
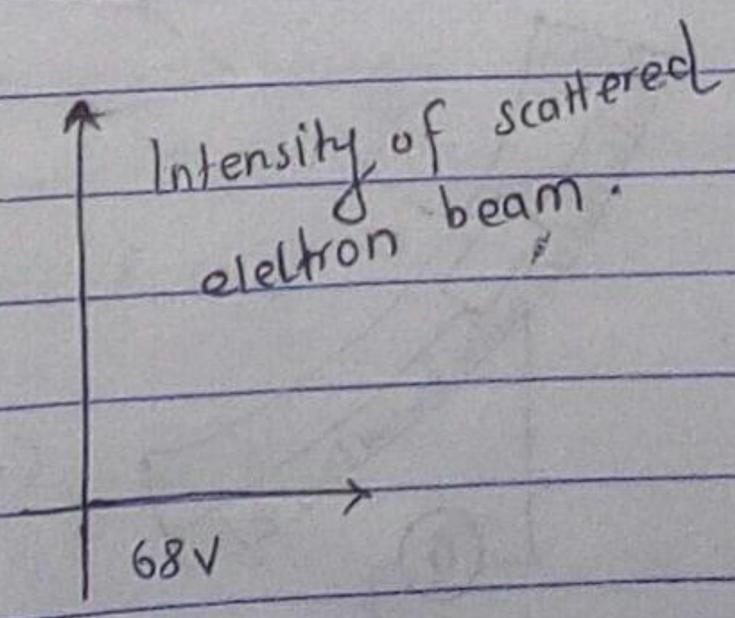
Experimental arrangement: It consists of tungsten filament F heated by L.T battery and it emits electron thermoionically. A system of slits S_1 & S_2 are used to make fine beam of electrons. and they are accelerated towards anode A by H.T battery. The electron beam is incident on single crystal of Nickel N which can be rotated by handle H. The scattered electrons are collector current which is measured by sensitive galvanometer G. A retarding potential V_r is applied between the walls of the collector so, that electrons having lesser energy are stopped.

The beam of the electrons fall normally on the crystal and collector current is measured for different positions. Actually collector current measures the intensity of scattered electron beam. The intensity of scattered beam with colatitude angle or different accelerating potential are noted and curves are drawn.





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From the curves, it was observed that a smooth curve is obtained at 40V. On increasing accelerating potential, a distinct hump appears on curve and it becomes prominent at 54V at angle of 50°. But at higher voltage, hump decreases and disappears about 68V. Maximum current or hump at 54V is due to constructive interference of scattered electron waves.

For plane diffraction grading,

$$d\sin\theta = n\lambda$$

where, d = interplanner spacing in crystal for Ni-crystal,

$$d = 2.15\ \text{Å}$$

and for first order maxima, n=1,

$$\therefore \lambda = 1.65\ \text{Å} \quad \ldots (i)$$

Also from De-Broglie's hypothesis,

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

$$= \frac{h}{\sqrt{2meV}} = \frac{6.62\times10^{-34}}{\sqrt{2.91\times10^{-31}\times1.6\times10^{-19}\times54}} \quad (\because V=54)$$

$$= 1.66\ \text{Å} \quad \ldots (ii)$$

From eqn's (i) & (ii)
the experimental value is in fair agreement with theoritical value of λ as calculated by De-Broglie's hypothesis.

Thus, it confirms the wave like nature of electron under suitable conditions.

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De-Broglie's relations in different cases :

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

a. If the electron of charge e and mass m is accelerated by potential V.

$$(K.E)_f - (K.E)_i = \text{workdone}$$

$$\Rightarrow \frac{1}{2}mv^2 - \frac{1}{2}mu^2 = qV$$

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

$$\Rightarrow v = \sqrt{\frac{2eV}{m}}$$

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

b. In terms of K.E (E)

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

$$\Rightarrow E = \frac{p^2}{2m}$$

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

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

c. In thermal equilibrium av. K.E of molecules (E):

$$E = \frac{3}{2}K_\beta T.$$

K_β = Boltzmann constant
$= 1.38 \times 10^{-23}\ JK^{-1}$

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

$$= \frac{h}{\sqrt{2m\,3/2\,K_\beta T}} = \frac{h}{\sqrt{3mK_\beta T}}$$; T = Absolute temperature

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Uncertainity principle : Acc. to classical mechanics, a moving particle has definite momentum and definite position in the space. so, they both can be measured accurately at any instant.

But in quantum mechanics, the particle is described by wave packet may be anywhere ie. position is uncertain. Also as the wave packet has different wavelengths momentum will also be uncertain.

It is impossible to specify precisely and simultaneously the value of both the members of physical variables that describe the behaviour of atomic system. Such pairs are called cannonical conjugate variable.

If Δx and Δp are uncertainities in determining position and momentum of particle then,

$$\Delta x \cdot \Delta p \geq \hbar \quad \text{where } \hbar = \frac{h}{2\pi}$$

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

If Δx is small, Δp is large and vice versa. ie. if one quantity is measured accurately the other quantity becomes less accurate. This relation is universal & hold for all cannonically conjugate variable like angle & angular momentum, energy and time, etc.

$$\Delta \theta \cdot \Delta L \geq \hbar$$

$$\Delta E \cdot \Delta t \geq \hbar$$

$\Delta \theta$ = uncertainity in angle.

ΔL = uncertainity in angular momentum.

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Applications of uncertainity principle:

a. Non-existance of electron inside nucleus:

Radius of the nucleus = 10^{-14} m
If electron exists inside nucleus, it can be anywhere within the diameter of nucleus

$$d = 2r = 2\times10^{-14}\,m.$$

This is the max. uncertainity in position.

$$\therefore \Delta x = 2\times10^{-14}\,m.$$

Now,

from uncertainity principle

$$\Delta x \cdot \Delta p \geq \hbar$$

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

$$\Rightarrow \Delta p = \frac{h}{2\pi \times 2\times10^{-14}}$$

$$= \frac{6.62\times10^{-34}}{4\pi\times10^{-14}} = 5.278\times10^{-21}\,kg\,ms^{-1}.$$

This is the min. uncertainity in momentum.

Now, let $\Delta p = p$

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

$$= \frac{(5.278\times10^{-21})^2}{2.91\times10^{-13}}$$

$$= 1.5834\times10^{-13}\,J$$

$$= 9.89\times10^{6}\,eV$$

$$= 9.89\,meV.$$

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Hence, if electron exists inside nucleus, it must have the energy about 9.89 meV.

But, max. K.E of electron (β-particle) emitted from radioactive nuclei can have 4 meV

Thus, the free electron cannot be present within the nucleus.

b. Size of hydrogen atom (Bohr's radius)

The total energy for hydrogen atom,

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

$$= \frac{p^2}{2m} + \left(\frac{-e^2}{4\pi\varepsilon_0 r}\right) \quad \cdots (i)$$

But from uncertainity principle,

$$\Delta x \cdot \Delta p = \hbar$$

$$\Delta r \cdot \Delta p = \hbar$$

$$r \cdot \Delta p = \hbar$$

$$p = \frac{\hbar}{r} \quad \cdots (ii)$$

$$\therefore E = \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\varepsilon_0 r} \quad \cdots (iii)$$

The G.S. energy must be minimum. so we can use condition of minima, ie. $\frac{dE}{dr} = 0$.

$$\Rightarrow \frac{d}{dr}\left[\frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\varepsilon_0 r}\right] = 0$$

$$\Rightarrow \frac{d}{dr}\frac{\hbar^2}{2mr^2} - \frac{d}{dr}\frac{e^2}{4\pi\varepsilon_0 r} = 0$$

$$\Rightarrow \frac{\hbar^2}{2m}\frac{d}{dr}\frac{1}{r^2} - \frac{e^2}{4\pi\varepsilon_0}\frac{d}{dr}\frac{1}{r} = 0 \Rightarrow \frac{-2\hbar^2}{2mr^3} + \frac{e^2}{4\pi\varepsilon_0 r^2} = 0$$

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$$\Rightarrow \frac{e^2}{4\pi\varepsilon_0 r^2} = \frac{2\hbar^2}{2mr^3}$$

$$\Rightarrow r = \frac{4\pi\varepsilon_0\hbar^2}{me^2} \quad \cdots (iv)$$ gives the radius of Bohr's 1st orbit

c. Energy of hydrogen in ground state.

The total energy of atom,

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

$$= \frac{p^2}{2m} - \frac{e^2}{4\pi\varepsilon_0 r} \quad \cdots (i)$$

Using uncertainity principle,

$$\Delta r . \Delta p = \hbar$$

$$\Rightarrow r . p = \hbar$$

$$\Rightarrow p = \frac{\hbar}{r} \quad \cdots (ii)$$

from (i) & (ii)

$$E = \frac{\hbar^2}{2mr^2} - \frac{e^2}{4\pi\varepsilon_0 r}$$

$$= \frac{h^2}{8m\pi^2 r^2} - \frac{e^2}{4\pi\varepsilon_0 r}$$

$$= \frac{1}{r}\left[\frac{h^2}{8\pi^2 m r} - \frac{e^2}{4\pi\varepsilon_0}\right]$$

Using (v),

$$E = \frac{\pi m e^2}{\varepsilon_0 h^2}\left[\frac{\pi m e^2 h^2}{8\pi^2 m \varepsilon_0 h^2} - \frac{e^2}{4\pi\varepsilon_0}\right]$$

$$= \frac{\pi m e^2}{\varepsilon_0 h^2}\left[\frac{e^2}{8\pi\varepsilon_0} - \frac{e^2}{4\pi\varepsilon_0}\right]$$

$$= \frac{\pi m e^4}{4\pi\varepsilon_0^2 h^2}\left(\frac{1}{2} - 1\right) = \frac{-me^4}{8\varepsilon_0^2 h^2} \quad \cdots (iii)$$

This equation gives the ground state energy of hydrogen atom.

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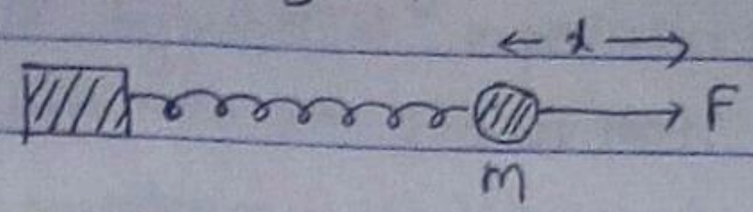
d. Ground state energy of linear harmonic oscillator (zero point energy)



Suppose a particle of mass m executing SHM along x-axis

$\therefore F \propto x$

$F = -kx$

Now, $dW = -Fx\,dx$

$W = -\int F\,dx = -\int_0^x -kx\,dx$

$P.E = W = \frac{kx^2}{2} = \frac{1}{2}m\omega^2x^2$

Also, $K.E = \frac{1}{2}m\omega^2 = \frac{p^2}{2m}$

From uncertainity principle,

$\Delta x \cdot \Delta p = \frac{\hbar}{2}$

$\Rightarrow \Delta p = \frac{\hbar}{2\Delta x}$

$\Rightarrow p = \frac{\hbar}{2x}$

$\therefore K.E = \frac{p^2}{2m} = \frac{\hbar^2}{4x^2 \cdot 2m}$

Now, $E = K.E + P.E$

$= \frac{\hbar^2}{8x^2m} + \frac{1}{2}m\omega^2x^2 \quad \ldots (i)$

$\therefore$ G.S. energy is the min. energy. so, for minima,

$\frac{dE}{dx} = 0$

$\Rightarrow \frac{d}{dx}\left(\frac{\hbar^2}{8mx^2} + \frac{1}{2}m\omega^2x^2\right) = 0$

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$$\Rightarrow \frac{-\hbar^2}{4mx^3} + m\omega^2 x = 0$$

$$\Rightarrow m\omega^2 x = \frac{\hbar^2}{4mx^3}$$

$$\Rightarrow x^4 = \frac{\hbar}{4m^2\omega^2}$$

$$\Rightarrow x^2 = \frac{\hbar}{2m\omega} \quad \ldots (ii)$$

Now, from eqn (i)

$$E = \frac{2\hbar\omega}{8} + \frac{1}{4}\hbar\omega$$

$$\therefore E = \frac{\hbar\omega}{2} \quad \ldots (iii)$$

This equation gives the zero point energy of harmonic oscillator.

Physical origin of uncertainity principle.

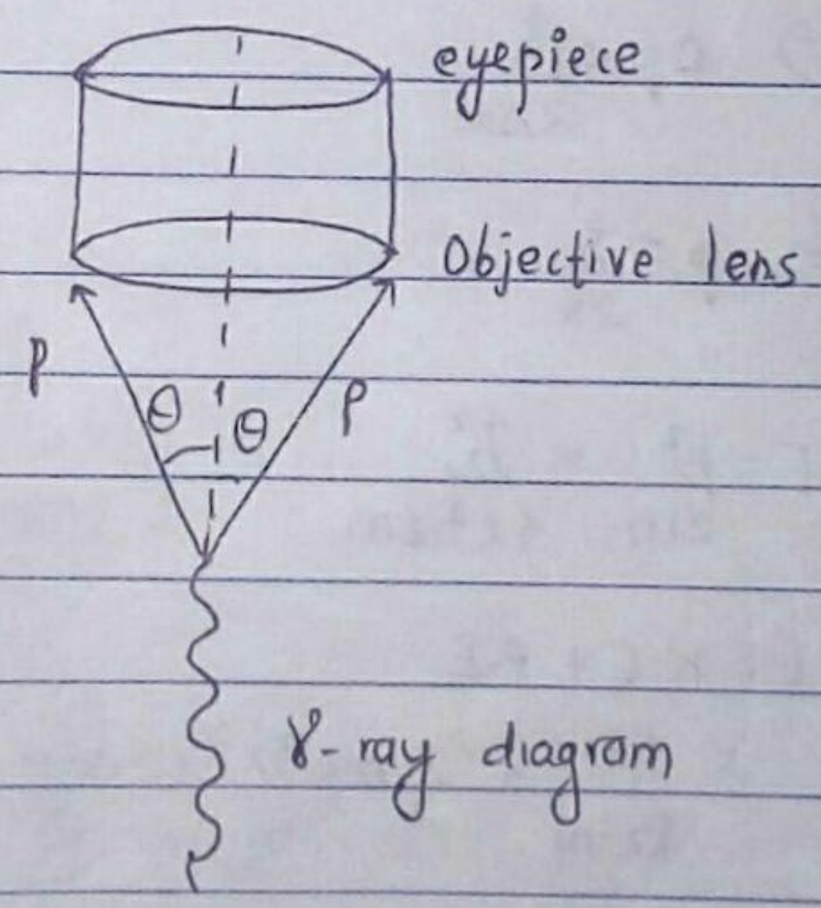

Fig: looking at an electron with a hypothetical γ-ray microscope in Bohr's gedanken experiment.

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Heisenberg's uncertainity relation can be illustrated by considering a simple hypothetical experiment. suppose we have to determine the position of $e^{\ominus}$ and we look the electron with a hypothetical γ-ray microscope. let the electron be illuminated by γ-ray photon of very short wavelength and scattered radiations are observed by γ-ray microscope.

From wave-optics the resolving power of microscope,

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

From fig, any photon scattered by electron within angle 2θ will be focused by microscope lenses and detected by eye.

The x-component of the momentum of photon and components are $p\sin\theta$ along positive x-axis and $-p\sin\theta$ along -ve x-axis.

$\therefore$ Uncertainity (change in momentum) of photon along x-direction.

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

$\therefore$ Δp_x for photon $=$ Δp_x for electron $= \frac{2h}{\lambda}\sin\theta \quad \ldots (iii)$

From (i) & (iii),

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

$$\Delta x \cdot \Delta p_x = 2h \quad \ldots (iv)$$

Eq^n (iv) is very close agreement with ultimate limit set by uncertainity relation. Hence, this experiment shows the validity of Heisenberg's uncertainity principle.

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Black body radiation:

The body which neither reflects nor transmits the heat radiations falling on it but absorbs all the incident radiations, appears to be black is called black body.

When the black body is placed in an isothermal enclosur. It will emit the radiations. such heat radiations are called black body radiation.

A perfectly black body is an ideal concept. There is no known surface which can be regarded as perfectly black. Lamp black or platinum black are nearest approach to black body.

For experimental purposes, a perfectly black body consists of hollow sphere whose inner surface is coated with black pigments and a small hole on its surface. The heat radiation entering through the hole suffers multiple reflection in the inner surface and finally it is completely absorbed. Thus, the small hole acts a perfectly black body.

Character of a spectrum of a black body:

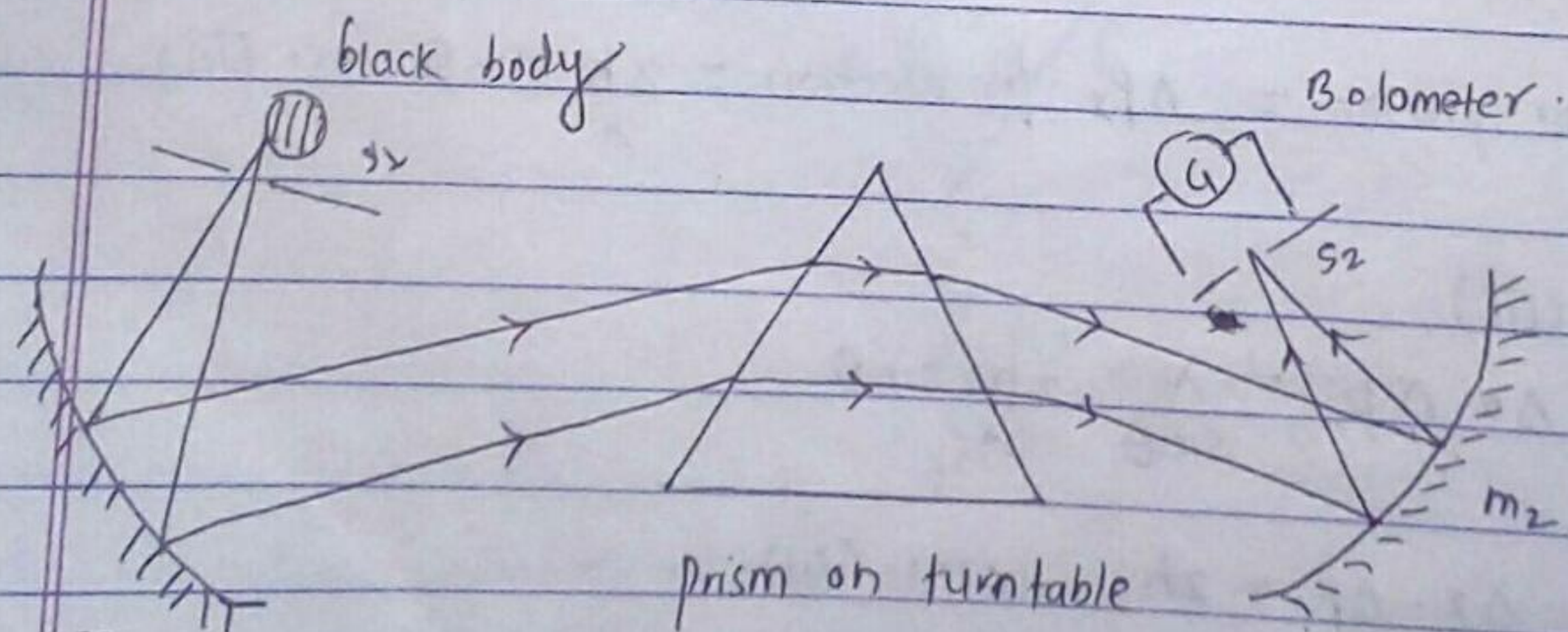

fig. lummer & Pringsheim experiment

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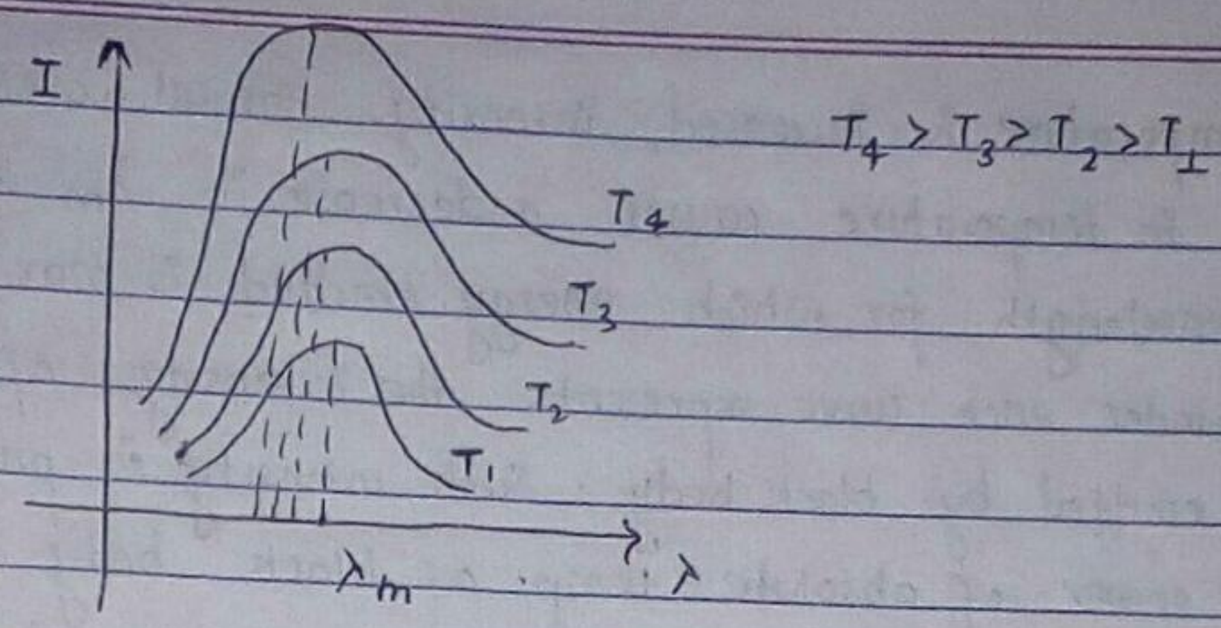

Lummer and Pringsheim investigated distribution of the energy of black body radiation at different temperatures.

An electrically heated chamber with small apperture is taken as black body. The radiations from the black body are passed through the slit S_1 and fall on concave mirror m_1. After reflected from m_1, the parallel beam of radiation fall on rocksalt prism which is placed on the turntable of spectrometer. Finally, the radiations are passed to concave mirror m_2 and reflected radiations from m_2 are incident on bolometer placed behind the slit S_2. The galvanometer deflects when the heat radiations fall on bolometer and deflection of galvanometer is proportional to the intensity of heat radiation. The radiations of different wavelength are incident on bolometer by rotating turntable of spectrometer and crossponding deflection are measured.

The graph between intensity and wavelength has the following main features:

a. The distribution of intensity $I = E/A \times t$ is not uniform for black body.
b. The intensity of radiation increases with wavelength, becomes max at particular wavelength and on further increasing wavelength intensity decreases.

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c. If the temperature is increased, intensity for all wavelengths increases.
d. An increases in temperature causes a decrease in λ_m where λ_m is wavelength for which energy emitted is maximum.
e. The area under each curve represents the intensity of heat radiation emitted by black body. Such intensity is proportional to fourth power of absolute temp. of black body.

ie. $I \propto T^4$

i.e. $I = \sigma T^4$ is the stephen's law.

Also, heat current, $\frac{E}{t} = \sigma A T^4$. ; $\sigma = 5.67 \times 10^{-8}\ W m^{-2} K^{-4}$.

Plank's radiation law:

In order to explain the distribution of energy in the spectrum of black body, Max Planck put forward the quantum theory of radiation.

Assumptions:

- According to this law, the black body radiation chamber is filled up not only with radiation but also with the simple harmonic oscillators of molecular dimensions which cannot have any value of energies and having the energies as,

$$E_n = nh\nu$$

where, h = planks constant
ν = frequency of oscillator
E = Energy of oscillator.
$n = 0, 1, 2, 3, 4, ---$.

Here, $h\nu$ is the basic unit of energy and is called quantum of energy. Thus, the total energy of oscillator is quantized.

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$E_3 = 3h\nu$

$E_2 = 2h\nu$

$E_1 = h\nu$

$E_0 = 0$

- The oscillator in a state cannot emit or absorb energy. The oscillator is said to be in stationary state. But when the oscillator jumps from one state to another, emission or absorption of energy takes place.

If the oscillator jumps from higher energy state of quantum number and lower state quantum number n_1, the energy is emitted.

$$\therefore E_2 - E_1 = 2h\nu - h\nu$$
$$= h\nu.$$

Similarly, if the oscillator jumps from lower energy state to higher energy state, energy is absorbed.

- The average energy of plank's oscillator is given by,

$$\bar{E} \text{ or } E_{av} = \frac{h\nu}{(e^{h\nu/K_BT} - 1)}$$

- The energy density (E/V) within the frequency range $\nu \to \nu + d\nu$ is the product of number density of oscillator (N/V) in the frequency range $\nu + d\nu$ and av. energy of oscillator.

$\therefore$ Energy density = no. density × av. energy of harmonic oscillator.

$$E_\nu d\nu = \frac{8\pi\nu^2 d\nu}{c^3} \times \frac{h\nu}{(e^{h\nu/K_BT} - 1)}.$$

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$$E_\nu d\nu = \frac{8\pi h \nu^3 d\nu}{c^3\left(e^{h\nu/k_BT} - 1\right)} \quad \cdots (i)$$

But, $\nu = \frac{c}{\lambda}$

Differentiating w.r.t λ

$$d\nu = d\frac{c}{\lambda}$$

$$= -\frac{c}{\lambda^2} d\lambda$$

In magnitude, $d\nu = \frac{c}{\lambda^2} d\lambda$

from (i).

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

$$= \frac{8\pi hc}{\lambda^5} \frac{d\lambda}{\left(e^{hc/\lambda k_BT} - 1\right)} \quad \cdots (ii).$$

(In terms of wavelength.)

Eqn's (i) & (ii) are called planck's radiation law.

✓ Find the energy of neutron in eV whose De broglie's wavelength is 1 Å (Given $m_n = 1.64 \times 10^{-27}$ kg, $h = 6.62 \times 10^{-34}$ Js^{-1})

Soln:

$E = ?$

$\lambda = 1Å = 10^{-10}$ m.

$p = h/\lambda$

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

$E = \frac{h^2}{2m\lambda^2} = ___$.

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✓ The electron is confined to an infinite potential well of width 0.1 nm. Determine the uncertainity in momentum & K.E.

The max. uncertainity in position will be width of potential well.

$$\Delta x \cdot \Delta p = \hbar$$

$$\Rightarrow \Delta p = \frac{\hbar}{\Delta x}$$

$$\Rightarrow \Delta p = ___.$$

$$\Delta E = \frac{\Delta p^2}{2m}$$

$$= ___.$$

Matter waves and uncertainity principle :

The spatial propagation of a particle can be represented by a simple sinusodial function as $A \sin z(kx - \omega t)$. This wave has following properties:

a. The amplitude A is same at all points in the space
b. It has ~~diffe~~ defined wavelength, $\lambda = \frac{2\pi}{K}$.

c. It has well-defined frequency, $f = \frac{\omega}{2\pi}$.

d. It travels with the velocity, $v = f \times \lambda = \frac{\omega}{K}$.

For an unlocalized wave, the amplitude of wave is same at all values of x and particle can be found with equal probability at any point in the space.

$\therefore \Delta x \rightarrow \infty$.

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But for well defined λ, the momentum $p = \frac{h}{\lambda}$ is also well defined

$\therefore \Delta p \to 0$. Thus, for unlocalized wave, $\Delta x \to \infty$ & $\Delta p \to 0$ which is in agreement with uncertainity principle.

The velocity of wave $v = f \times \lambda = \frac{E}{p}$

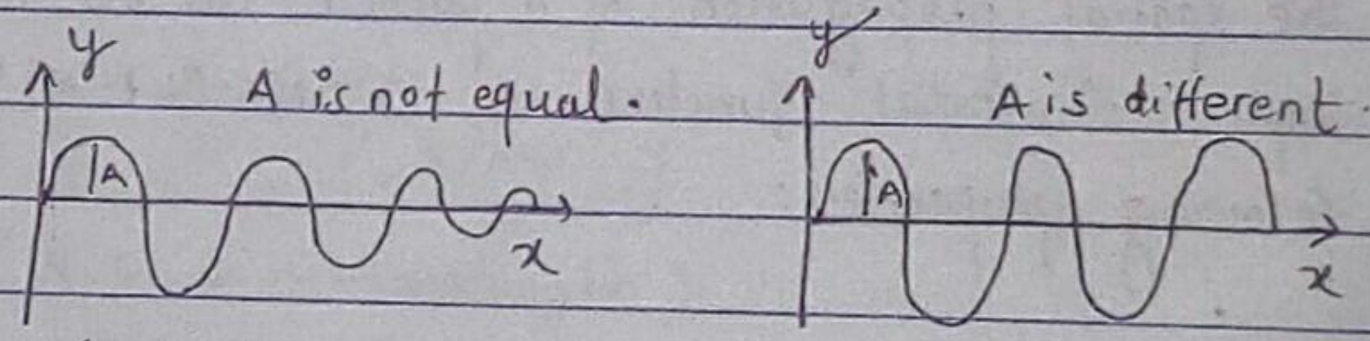
For a particle, $E = \frac{1}{2} m v_{par}^2$, $p = m v_{par}$

$$v_{wave} = \frac{\frac{1}{2} m v_{particle}^2}{m v_{particle}}$$

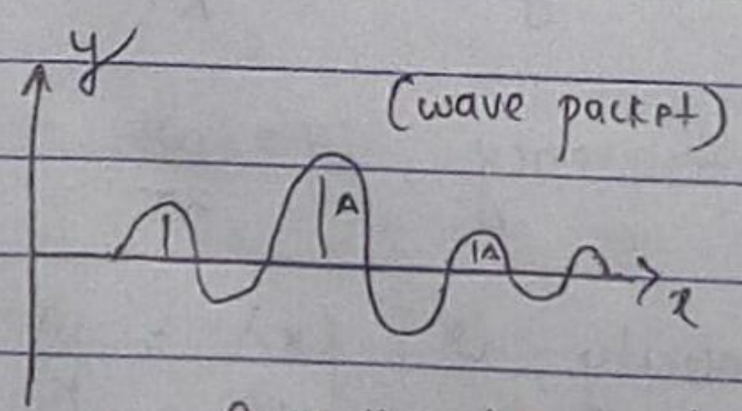
$$= v_{par}/2$$

Thus, v_{wave} is not as the $v_{particle}$ for unlocalized wave.

This result is not acceptable for partially localized particle.



localized wave. unlocalized wave



Partially localized wave

To describe a partially localized wave we use the concept of wave packet. The wave packet is obtained by mixing infinetly large no. of sinusodial wave having slightly diff. wavelength and frequency.

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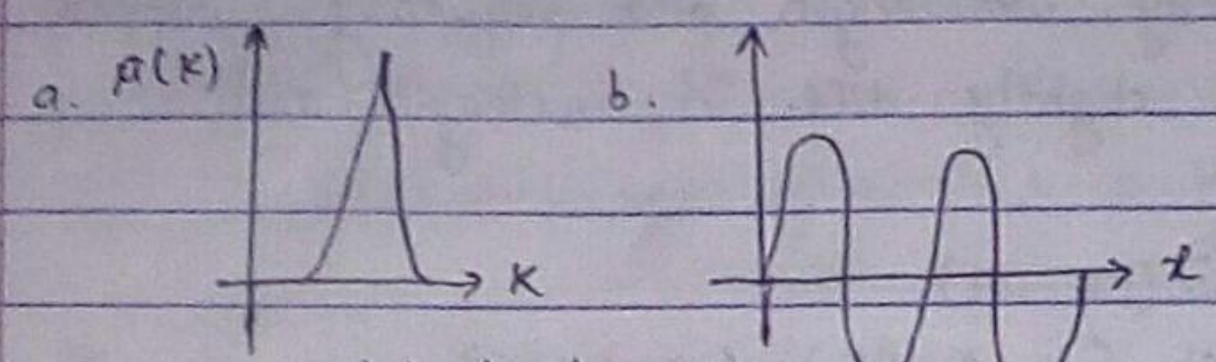
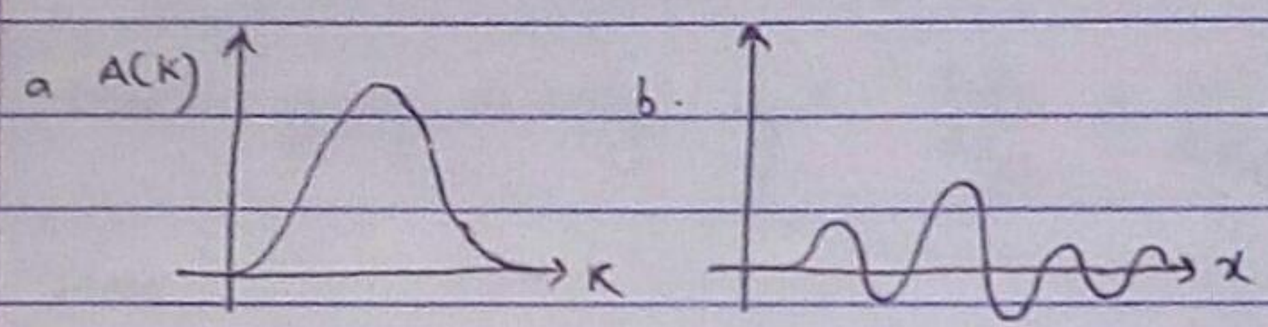
Comparision of unlocalized and partially localized wave:



1. Unlocalized wave.



2. Partially localized wave.

In fig 1 a. ψ contains only one k so, only one defined wavelength and a defined momentum ie. $\Delta p \to 0$.
For this, the amplitude of the wave must be same at all point in the space and particle is completely unlocalized.

In fig 2a ψ contains a range of k with different waves. The wave packet doesnot have definited wavelength and undefined momentum $\therefore \Delta p \to \infty$. For this, the particle must be localized in a narrow region.

Group velocity:

The particles of the matter can be regarded to consist of a group of waves or wave packets. Each component wave propagates with different velocity called phase velocity. Π

The group velocity is the velocity with which definite phase of amp. of resultant wave moves.

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Wave packect have the group of the wave each with slightly different velocity, wavelength and frequency. Suppose, two waves which are slightly diff. in wavelength and frequency.

$$\psi_1 = A\sin(Kx - \omega t)$$
$$\psi_2 = A\sin\left[x(K+\Delta K) - (\omega+\Delta\omega)t\right]$$

When, $\Delta K << K$
$\Delta\omega << \omega$.

Now, the resulting wave is,

$$\psi = \psi_1 + \psi_2$$
$$= A\sin(Kx-\omega t) + A\sin\left[(K+\Delta K)x - (\omega+\Delta\omega)t\right]$$

$$\Rightarrow \psi = A\,2\sin\left[\frac{(Kx-\omega t)+(K+\Delta K)x-(\omega+\Delta\omega)t}{2}\right]\cos\left[\frac{(Kx-\omega t)-(K+\Delta K)x+(\omega+\Delta\omega t)}{2}\right]$$

$$\Rightarrow \psi = 2A\sin\left[\frac{2Kx-2\omega t+\Delta Kx-\Delta\omega t}{2}\right]\cos\left[\frac{-\Delta Kx+\Delta\omega t}{2}\right]$$

$\because \Delta K << K$, $\Delta\omega << \omega$ so, they can be neglected in first term.

$$\therefore \psi = 2A\sin\left[\frac{2Kx-2\omega t}{2}\right]\cos\left(\frac{\Delta Kx-\Delta\omega t}{2}\right)$$

$$= 2A\cos\left(\frac{\Delta Kx-\Delta\omega t}{2}\right)\sin(Kx-\omega t) \quad \ldots (i)$$

Compairing the wave function ψ of eq^n (i) with wave function ψ_1,

the amplitude $(A') = 2A\cos\left(\frac{\Delta Kx-\Delta\omega t}{2}\right)$

$$\therefore \psi = A'\sin(Kx-\omega t).$$

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The velocity of diff. components of wave packet is called phase velocity or wave velocity.

$\therefore$ phase velocity $v_p = f \times \lambda = \frac{\omega}{2\pi} \times \frac{2\pi}{K} = \frac{\omega}{K}$ .... (ii)

The velocity of the wave packet as a whole is called group velocity.

Now, group velocity $v_g = \frac{\Delta\omega/2}{\Delta K/2} = \frac{\Delta\omega}{\Delta K} = \frac{d\omega}{dK}$ .... (iii)

Here,

$$E = hf = \frac{h}{2\pi} \cdot 2\pi f = \hbar\omega,$$

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

From eqn (iii),

$$v_g = \frac{d(\hbar\omega)}{d(\hbar K)}$$

$$= \frac{dE}{dp} \quad \text{.... (iv)}$$

and from eqn (ii),

$$v_p = \frac{\omega}{K} = \frac{\hbar\omega}{\hbar K} = \frac{E}{p} \quad \text{.... (v)}$$

But: $E = \frac{p^2}{2m}$

$$v_g = \frac{d}{dp}\left(\frac{p^2}{2m}\right)$$

$$= \frac{1}{2m} \times 2p = \frac{p}{m} \qquad v_g = v$$

Thus, group velocity is equal to particle velocity. This means.

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wave packet moves with particle.

Uncertainity in the position of particle is equal to De-Broglie's wavelength of the particle. Calculate the uncertainity in the velocity of the particle in terms of the velocity of De-Broglie's wave associated with the particle.

Given,

$$\Delta x = \lambda$$

$$\Delta v = ?$$

Now,

$$\Delta x \cdot \Delta p = \hbar$$

$$\Delta x \cdot m \Delta v = \hbar$$

$$\Delta x = \frac{\hbar}{m \Delta v} \quad \ldots (i)$$

Acc. to question,

$$\Delta x = \lambda = \frac{h}{P} = \frac{h}{mv}$$

$$\Delta x = \frac{h}{mv} \quad \ldots (ii)$$

from eqn (i) & (ii)

$$\frac{h}{2\pi m \Delta v} = \frac{h}{mv}$$

$$\Rightarrow \Delta v = \frac{v}{2\pi}.$$

This shows that uncertainity in velocity is $\frac{1}{2\pi} \times v$.

The small particle of mass 10^{-6} g moves along x-axis, its speed is uncertain by $10^{-6} ms^{-1}$,

a. What is uncertainity in x-coordinate of the particle?

b. Repeat the calculation for electron assuming that the uncertainity in its velocity is also $10^{-6} ms^{-1}$.

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versus.

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a. $m = 10^{-6} g = 10^{-9} kg$

$\Delta v = 10^{-6} ms^{-1}$.

$\Delta x = ?$

$\Delta x \cdot \Delta p = \hbar$

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

$= \frac{6.62 \times 10^{-32}}{2\pi \times 10^{-9} \times 10^{-6}}$

$\therefore \Delta x = 1.05 \times 10^{-19} m$.

b. $m_e = 9.1 \times 10^{-31} kg$

$\Delta v = 10^{-6} ms^{-1}$

$\Delta x = \frac{\hbar}{m_e \cdot \Delta p} = \frac{h}{2\pi m_e \Delta p} =$ ____.

✓ The ground state and first excited state energies of atoms are $-4.3 eV$ & $-2.7 eV$ respectively. If we use potassium vapour in Frank-Hertz exp. at what voltages would we see drop in the plot of current vs voltage.

Solⁿ

$E_1 = -4.3 eV$

$E_2 = -2.7 eV$

Energy difference $= E_2 - E_1$

$= 1.6 eV$.

This energy is called excitation energy

Excitation energy = e × excitation potential.

$\Rightarrow E.P = \frac{E.E}{e} = \frac{1.6 eV}{e} = 1.6 V$.

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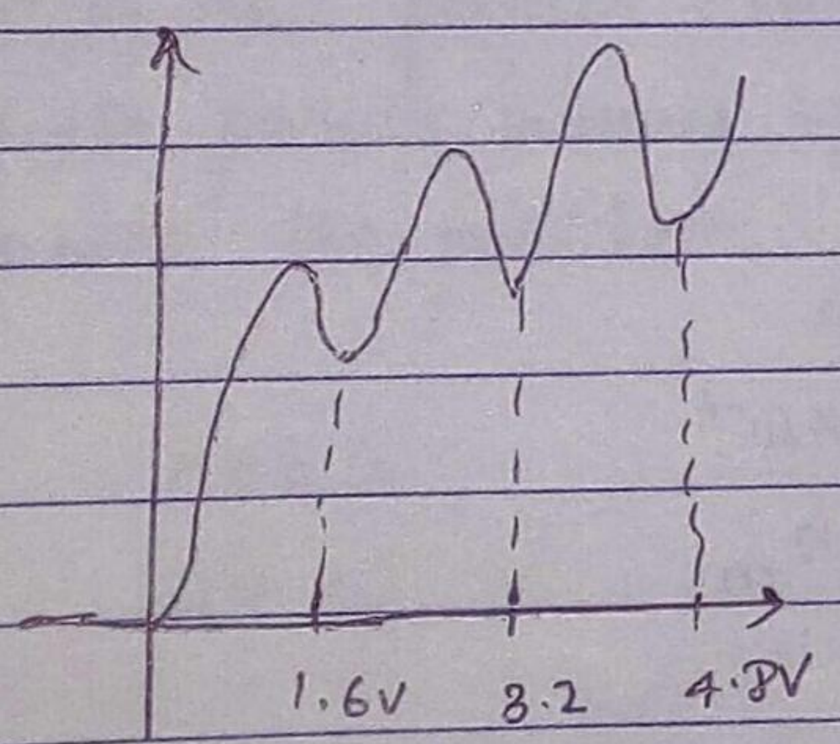
The another drops are seen in current vs voltage curve at 1.6V, 3.2V, 4.8V, 6.4V, ...



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Unit-4

Methods of Quantum Mechanics:-

"Quantum Mechanics."

Quantum Mechanics is a brahchof physics which helps to interpret the physical principles mathematically. The quantum mechanics deals the principles of physical phenomena of a microscopic particle. Since, classical mechanics fail to explain many physical phenomenal like photoelectric effect, comptun effect, diffraction, hydrogen spectrum in hydrogen atom etc. Therefore, a new branch called quantum mechanics came in existance. This ~~phenomena~~ branch successfully provides mathematical terms together with physical principle of such specific phenomenal governed by microscopic particles. To explain such principles a fundamental function called wave function is taken into consideration.

Wave function:

It is a fundamental function which relates the position of a quantum mechanical particle at an instant. Generally, the function is denoted by symbol 'ψ'. It is a function of position and time. The wave function is a sum of real and imaginary states of a particle. It means a wave function can be separated into two parts- real and imaginary. In general, cos function is used for the real part and sin function for the imaginary part. For a wave function $\psi(x,t)$. A complex function is given as $\psi^*(x,t)$. called complex conjugate in 1D. Wave function is 3D, is given as

$\psi(r,t)$, where $r = x\hat{i} + y\hat{j} + z\hat{k}$

and $\hat{i}, \hat{j}$ & $\hat{k}$ are unit vectors along respective axes.

For a free particle, the wave function is given by

$\psi(x,t) = Ae^{i(kx-\omega t)}$, where x is the position at time t for a particle moving along +ve x-axis with angular vel. ω.

& k is called propagatn constant.

Significance of ψ:

The wave function has different significances. They are:

1. It determines the position of particle at any instant t.
2. If the wave function is operated by schoginder wave equation, it gives values of energy and crosspponding momentum.
3. A wave function multiplied by its complex conjugate over a given volume gives probability of finding particle within that volume.

The total probability is given by $p = \int_{-\infty}^{\infty} \psi\psi^* dv = 1$.

It means a particle exist within the given space.

Characteristic of wave function ψ:

- A wave function is finite function.
- It is single valued - It is continuous function.

Operators:

Operator is that which when operates upon a wave function transform it from one space to another. Some of operaters - momentum, energy, position operators etc.

let $\psi = Ae^{i(kx-\omega t)} = Ae^{-i(\omega t-kx)}$ .... (i) is a wave function for a free particle. where, $k = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{p}{\hbar} \Rightarrow p = \hbar k$.

and $\omega = 2\pi f = 2\pi \frac{E}{h} = \frac{E}{\hbar} \Rightarrow E = \hbar\omega$.

$\therefore \psi = Ae^{-i/\hbar(Et-px)}$ .... (ii)

d. w.r.t time (t).

$$\frac{d\psi}{dt} = \frac{d}{dt}\left(Ae^{-i/\hbar(Et-px)}\right) = A - \frac{iE}{\hbar} e^{-i/\hbar(Et-px)}$$

$$= \frac{-iE}{\hbar}\left[Ae^{-i/\hbar(Et-Px)}\right]$$

$$\Rightarrow \frac{d\psi}{dt} = \frac{-iE}{\hbar}\psi$$

Comparing both sides.

$$\frac{d}{dt} = \frac{-iE}{\hbar}$$

$$\Rightarrow E = -\frac{\hbar}{i}\frac{d}{dt}$$

and in 3D,

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

$$= \frac{-\hbar \times i}{i \times i}\frac{\partial}{\partial t}$$

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

Energy operator when operates upon a wave function gives the crossponding value of energy called energy Eigen value.

Momentum operator.

let $\psi = Ae^{-i/\hbar(Et-Px)}$. be a free particle wave function.

d.w.r.t x.

$$\frac{d\psi}{dx} = +A\frac{i}{\hbar}p\,e^{-i/\hbar(Et-Px)}$$

$$= \frac{i}{\hbar}p\psi$$

Compairing,

$$\Rightarrow \frac{d}{dx} = \frac{i}{\hbar}p \Rightarrow p = \frac{\hbar}{i}\frac{d}{dx}$$

$$\Rightarrow p = -i\hbar\frac{d}{dx}.$$

In 3D, $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ is momentum op.

Expectation value (Av. value): The expectation value of the parameter of quantum mechanical particle is the av. value of its measurement within the given space. The expectation values are obtained by finding av. values of the given parameter associated with the quantum mechanical partical.

$$\bar{E} = \langle E \rangle$$

$$= \frac{\int_{-\infty}^{-\infty} \psi^* \hat{E} \psi(x,t)\, dx}{\int_{-\infty}^{+\infty} \psi^* \psi\, dx}.$$

$$= \int_{-\infty}^{\infty} \psi^* E \psi\, dx$$

$$= \int_{-\infty}^{\infty} \psi^* i\hbar \frac{\partial}{\partial t} \psi\, dx$$

$$= i\hbar \frac{\partial}{\partial t} \int_{-\infty}^{\infty} \psi^* \psi\, dx$$

$$= i\hbar \frac{\partial}{\partial t} 1$$

$$= E.$$

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Average value of momentum:

The average value of momentum is given by,

$$\bar{p} = \langle p \rangle = \frac{\int_{-\infty}^{\infty} \psi^* \hat{p} \psi \, dx}{\int_{-\infty}^{\infty} \psi^* \psi \, dx} = \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi \, dx \times \frac{1}{\int_{-\infty}^{\infty} \psi^* \psi \, dx}$$

$$= -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial}{\partial x} \psi \, dx \times \frac{1}{\int_{-\infty}^{\infty} \psi^* \psi \, dx}$$

$$= -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{i}{\hbar} p \psi \, dx \times \frac{1}{\int_{-\infty}^{\infty} \psi^* \psi \, dx}$$

$$= -i\hbar \frac{i}{\hbar} p$$

ie. $\langle p \rangle = p$.

Hence, expectation value of momentum is itself momentum.

$$\therefore \langle p \rangle = \hbar k$$
$$\langle E \rangle = E = \hbar \omega.$$

Schrodinger wave equation:

It is a 2nd degree differential wave equation. Schrodinger wave equation is a relation for the wave function of a quantum mechanical particle with its energy when acted by a force.

For a free particle, wave function can be expressed as $\psi = A e^{\frac{-i}{\hbar}(Et - px)}$. which is the sum of both real and imaginary parts.

Differentiating w.r.t t,

$$\frac{\partial \psi}{dt} = A\left(\frac{-i}{\hbar}\right) E e^{-\frac{i}{\hbar}(Et - px)} = \frac{-i}{\hbar} E \psi.$$

$$\Rightarrow E\psi = -\frac{\hbar}{i} \frac{\partial \psi}{dt} \Rightarrow E\psi = i\hbar \frac{\partial \psi}{\partial t}.$$

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Again

differentiating wrt x.

$$\Rightarrow \frac{\partial \psi}{\partial x} = \frac{\partial^2 \psi}{\partial x^2} = \left(\frac{ip}{\hbar}\right)^2 \psi$$

$$= -\frac{p^2}{\hbar^2} \psi \quad \ldots (iii)$$

The total energy of particle,

$$E = KE + PE.$$

$$= \frac{1}{2}\frac{p^2}{m} + V_{(x)} \quad \ldots (iv)$$

Now, operating with this value (E) on wave function,

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

$$\Rightarrow E\psi = \frac{1}{2m} p^2 \psi + V\psi$$

$$\Rightarrow i\hbar \frac{\partial \psi}{\partial t} = -\frac{1}{2m}\hbar^2 \frac{\partial^2 \psi}{\partial x^2} + V\psi.$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t}(\psi) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right]\psi \quad \ldots (v)$$

Eqn (v) is schrodinger time dependent wave equation.

where,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V = \hat{H} \text{ called Hemiltonian operator.}$$

and $i\hbar \frac{\partial}{\partial t} = \hat{E}$ Energy operator.

ie. $\hat{H}\psi = \hat{E}\psi$.

$\Rightarrow H\psi = E\psi$. E = Eigen value.

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Schrodinger time independent equation.
The equation of motion of a particle whose energy doesnot depend upon the time.

Let $\psi = Ae^{-\frac{i}{\hbar}(Et - Px)}$ — (i) be a free particle wave equation.

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

again $$\frac{\partial^2 \psi}{\partial x^2} = \frac{i}{\hbar} p \frac{\partial \psi}{\partial x} = \left(\frac{ip}{\hbar}\right)^2 \psi.$$

$$\Rightarrow p^2 \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} \quad \ldots (ii)$$

Total energy of particle, $E = KE + PE = \frac{p^2}{2m} + V$.
Operating on the wave function ψ.

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

$$E\psi = \frac{1}{2m} p^2 \psi + V\psi$$

$$= \frac{1}{2m}\left(-\hbar^2 \frac{\partial^2 \psi}{\partial x^2}\right) + V\psi$$

$$\Rightarrow \frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + (E - V)\psi = 0.$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \quad \ldots (iii)$$ is 1D Schrodinger time independent wave equation.

In 1-D, $\frac{\partial}{\partial x} \rightarrow \frac{d}{dx}$

In 3-D, $\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi + \frac{2m}{\hbar^2}(E - V_{(x)})\psi = 0$; $\nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$

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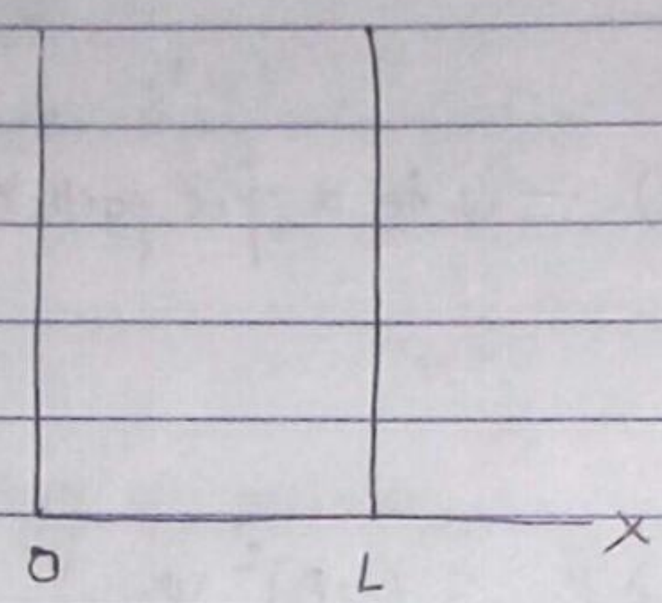
Application:

Particle in box (potential well)



Let us consider a potential well having potential

$V=0$ for $0 < x < L$ Inside

& $V=\infty$ for $x>L$ & $x<0$ } outside.

A particle is confined in the potential well.

The time independent wave equation for particle in the well (box). is

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

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}E\psi = 0 \quad (\because V=0) \quad \ldots (i)$$

for 1D, $\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \ldots (ii)$

where, $k^2 = \frac{2m}{\hbar^2}E$.

eqn (ii) is a 2nd degree diff. wave eqn whose solution can be given as,

$$\psi = A\cos kx + B\sin kx \quad \ldots (iii).$$

where A & B are the coefficient and can be known using boundary condition. at $x=0$, $\psi=0$

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$\therefore \quad 0 = A.$

$\therefore \psi = B\sin kx \quad \ldots (iv)$

At other boundary

$x = L \; ; \; \psi = 0.$

Then, eqn (iv) becomes $0 = B\sin kL$

$\Rightarrow \sin kL = 0.$

$\Rightarrow \sin kL = \sin n\pi.$

$\Rightarrow kL = n\pi$

$\Rightarrow k = \frac{n\pi}{L}. \quad \ldots (v).$

$\Rightarrow k^2 = \frac{n^2\pi^2}{L^2}$

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

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

$= \frac{n^2h^2}{8mL^2} \quad \ldots (vi)$

which depends upon n, $n = 0, 1, 2, 3 \ldots$

Hence, energy is quantized.

$\therefore \psi = B\sin\left(\frac{n\pi}{L}\right)x. \quad \ldots (vii).$

Using normalization condition,

$\int_0^L \psi^* \psi \, dx = 1. \quad \Rightarrow B = \sqrt{\frac{2}{L}}.$

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

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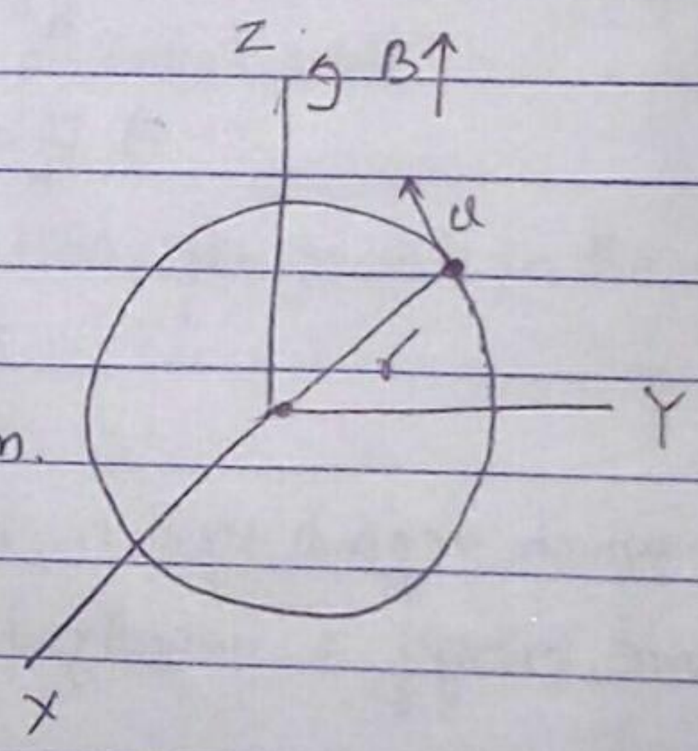
Zeeman effect:

The phenomenon of splitting of a spectral line into more lines due to the effect of magnetic field is called zeeman effect. If a spectral line splits into 2 or 3 lines the phenomenon is called normal zeeman effect. If a line splits into more lines, the phenomenon is called anomolus zeeman effect. Normal zeeman effect occurs on applying high value of the field while anamoulus effect occurs during the application of low field. The normal effect can be explained by both the classical & Quantum theories, but the anamolus effect can be explained with the help of Quantum theories only. The normal effect considers only the orbital motion of electrons but the theories for anamolus effect consider both the orbital as well as spin ~~method~~ motion of electron.

Theory:



Consider an electron moving around the nucleus of an atom. let u be the velocity of the electron having mass m in an orbit of radius r. let a magnetic field of intensity B is applied along the vertical direction. The electron obeys rotational motion about the field which is also known as precessional motion. Due to this phenomena the electron acquires dipole moment & hence an additional energy. The dipole moment due to orbital motion is given as

$$\mu = iA$$

A - area enclosed, i - current

$$= \frac{e}{T}\pi r^2$$

T - period.

$\Delta m_l = 0, \pm 1.$ $\nu = \frac{c}{\lambda} \Rightarrow \Delta\nu = c\left(-\frac{1}{\lambda^2}\right)\Delta\lambda.$

$\nu = \nu_0 + \frac{eB}{4\pi m}\Delta m_l.$

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Zeeman shift

- Change in λ of spectral line due to B.

$\mu = \frac{e\pi r^2}{T}$ ... (i)

If ω be angular velocity,

$$\omega = \frac{2\pi}{T}$$

$$\therefore \mu = \frac{e\pi r^2 \omega}{2\pi} = \frac{mr^2\omega}{2m}$$

$$= \frac{e}{2m} L, \quad L = \text{angular momentum} = mr^2\omega \quad \ldots (ii)$$

$\because L = \frac{h}{2\pi} l$, l being orbital quantum number.

$$\therefore \mu = \frac{eh}{4\pi m} l \quad \ldots (iii)$$

Due to this fact, the system gain addition energy which is given by

$$\Delta E = \vec{\mu} \cdot \vec{B}$$
$$= \mu B \cos\theta$$
$$= \frac{eh}{4\pi m} B l \cos\theta$$

$\therefore \Delta E = \frac{eh}{4\pi m} B m_l \quad \ldots (v)$, $m_l = l\cos\theta$ be magnetic orbital quantum number.

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Stern and Gerlach experiment.

Stern and Gerlach exp is an experimental evidence for the existence of atomic dipole moment and electronic spin. This experiment governs the quantization of spin and space. This exp is based on the behavior of variable magnetic field (non-uniform B) upon a dipole on moving through it (principle). The non-uniform B exert transitory effect on the dipole along the direction of its variable.

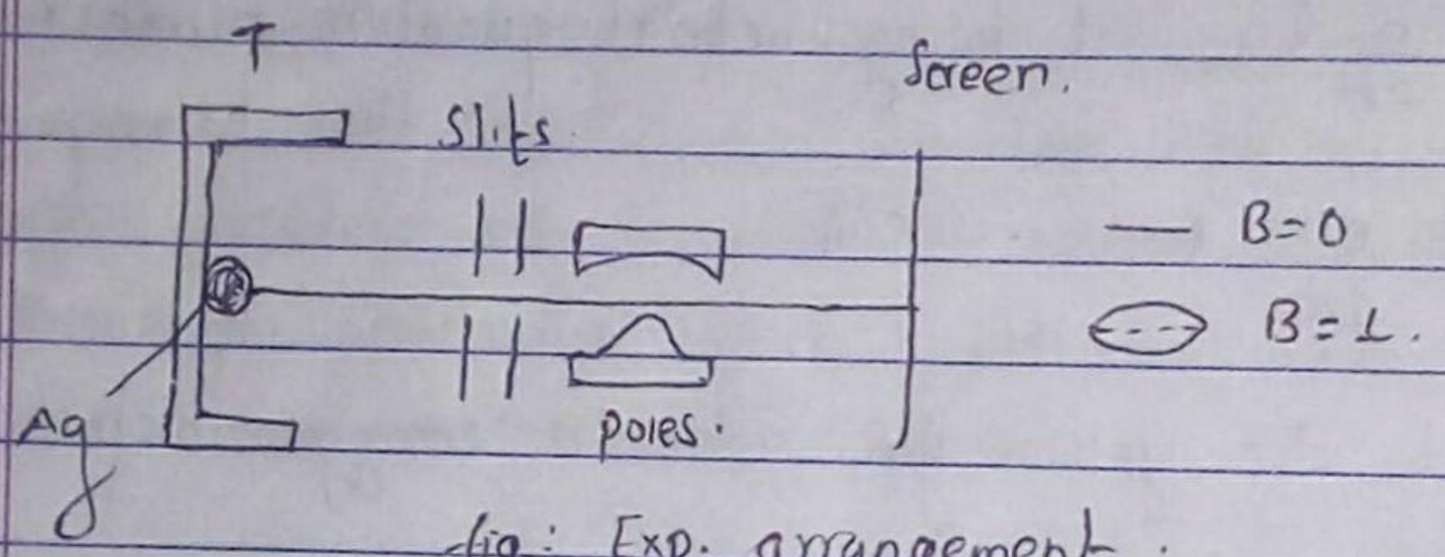

fig: Exp. arrangement.

Experimental arrangement:

It consists a region of non-uniform magnetic field. Such region is adjusted with the help of pole of electro magnets having cavity on either pole & sharp edge on the other. A stream of atoms is allowed to move through this region. For the stream of atoms silver element is heated in a furnace. A screen is introduced infront of the magnetic poles.

Theory:

Consider a stream of atoms (behave atomic dipole) move through region of non-uniform B. let variation in B is $\perp^r$ to to stream of particles. Experimentally, there occurs a fine line (sketch) on the screen introduced infront of the magnetic poles, when the field is zero. when the field is applied then

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the lining splits into to lines of equal intensity. The two lines get displaced along the direction of variation of the field (direction of field gradiant) : $dB \times 1/dz$. let $\frac{dB}{dz}$ is the field gradiant along the vertical (z-axis). The ~~force on~~ translatory force on a dipole can be written as,

$$F_z = \vec{\mu_l} \cdot \frac{\vec{dB}}{dz}$$

$$F_z = \mu_z \frac{dB}{dz} \cos\theta$$

$$= \frac{e}{4\pi m} l \cos\theta \frac{dB}{dz}$$

$$= \frac{eh}{4\pi m} \frac{dB}{dz} m_l \quad \cdots (i).$$

This force produce acceleration along the direction of variation in B. As a resut, the dipole get displaced from its original position. Therefore, the displacement of line appears on the screen. from the eqn of motion, the displacement can be known.

Using relation, $s = ut + \frac{1}{2}at^2$.

$$D = 0 + \frac{1}{2}at^2$$

$$\Rightarrow D = \frac{1}{2}\frac{F_z}{m}\frac{l^2}{v^2} \quad \cdots (ii)$$

where, $F_z = ma$ & $t = \frac{l}{v}$, l = length of field region
v = vel. of stream of atoms by which it enters into the field region.

Significances:

- Stern-Gerlach experiment provides following significances.

1. In the absence of B, a fine linear sketch occurs on the screen. This indidates the existence of dipole (atomic dipole) and hence, the dipole moment.
2. In the presence of B, the splitting of line into two lines suggests the existence of two values of spin. One along the field direction and the other along opposite direction.
3. The equal intensity of both the lines suggests that the space and spin associated with the electrons are quantized.

Schrodinger wave equation for Hydrogen atom.

Hydrogen atom has a single orbiting electron around the nucleus having single proton. The nucleus exert electrostatic potential on an electron. given by,

$$V(r) = \frac{+e(-e)}{4\pi\varepsilon_0 r}, \quad r = \text{radius of } e. \quad \ldots (ii)$$

The time independent wave equation,

$$H\psi = E\psi \quad \ldots (ii) \qquad H = \text{Hamiltorian operator},$$

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V, \quad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Now, eqn (ii) becomes,

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi$$

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

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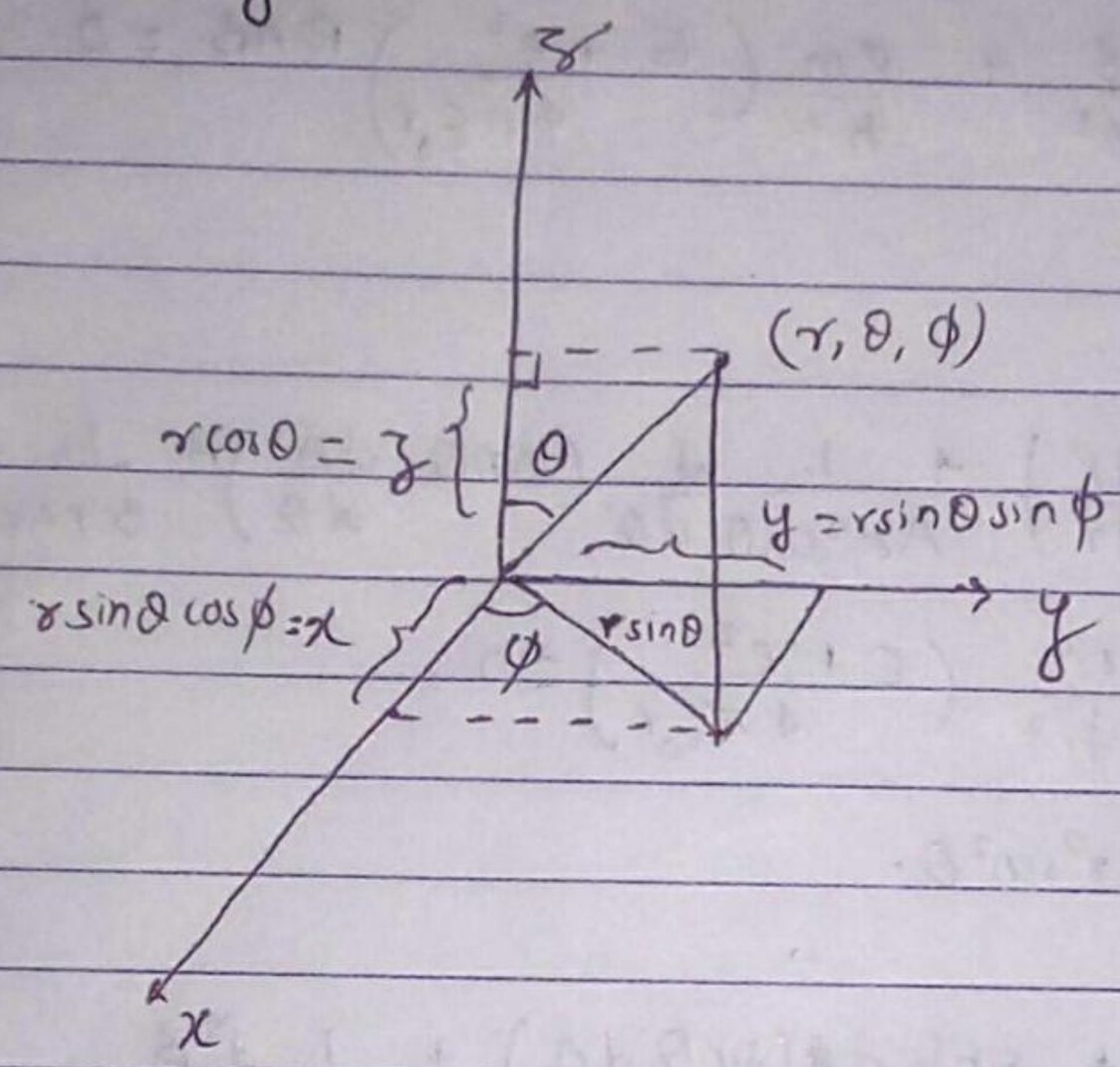
$$\Rightarrow \quad \nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad \ldots (iii)$$

is the form of time independent equation in cartesian coordinate system.



Then This can be reduced in polar form. If $r, \theta, \& \phi$ be the polar coordinates as shown in figure. Then the cartesian product can be written as,

$$\left.\begin{aligned} z &= r\cos\theta \\ y &= r\sin\theta\sin\phi \\ x &= r\sin\theta\cos\phi \end{aligned}\right\} \quad \ldots (iv)$$

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

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}$$

$$+ \frac{2m}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right)\psi = 0 \quad \ldots (v).$$

which is complex differential equation.

The wave function can be reduced in the independent variables

$$\psi(r,\theta,\phi) = R(r)\,A(\theta)\,B(\phi) \quad \ldots (vi)$$

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Eqn (v) can be written as,

$$\frac{A(\theta)B\phi}{r^2}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{RB}{r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dA}{d\theta}\right)$$

$$+ \frac{RA}{r^2\sin^2\theta}\frac{d^2B}{d\phi^2} + \frac{2m}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right)RAB = 0$$

diving by RAB

$$\frac{1}{Rr^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{1}{Ar^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dA}{d\theta}\right) + \frac{1}{Br^2\sin^2\theta}\frac{d^2B}{d\phi^2}$$

$$+ \frac{2m}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right) = 0.$$

Multiplying by $r^2\sin^2\theta$.

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{\sin\theta}{A}\frac{d}{d\theta}\left(\sin\theta\frac{dA}{d\theta}\right) + \frac{1}{B}\frac{d^2B}{d\phi^2}$$

$$+ \frac{2mr^2\sin^2\theta}{\hbar^2}\left(E + \frac{e^2}{4\pi\varepsilon_0 r}\right) = 0. \quad \ldots \text{(vii)}$$

$$\left(-\frac{1}{B}\frac{d^2B}{d\phi^2} = m_l^2 = k\right).$$

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Unit-5

Fundamentals of solid state physics:

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Solid state physics : The branch of physics which deals with the properties of solid particular crystals and behaviour of electrons in solids.

Crystalline solid : A substance is said to be crystalline if the arrangement of atom, ions, molecules of matter inside it is regular and periodic.

Properties :

- Crystal has long range order in its structure & hence has fixed shape & size.
- They have sharp melting point.
- The crystalline structure is low entropy state due to the ordered structure.
- The crystal is an isotropic for the measurement ie. it has diff. properties like tensile stress, electrical conductivity, thermal conductivity along different direction (direction dependent property)

e.g. NaCl structure, diamond structure, etc.

Crystal lattice (space lattice):

The regular and periodic arrangement of geometrical points in netlike structure is called crystal lattice or space lattice. It is the mathematical illustrate or geometrical visualization only.

Basis :

The group of atoms, ions or molecules which are identical in composition and orientation is called basis. When basis is placed on the lattice points of the space lattice, it generates the crystal structure.

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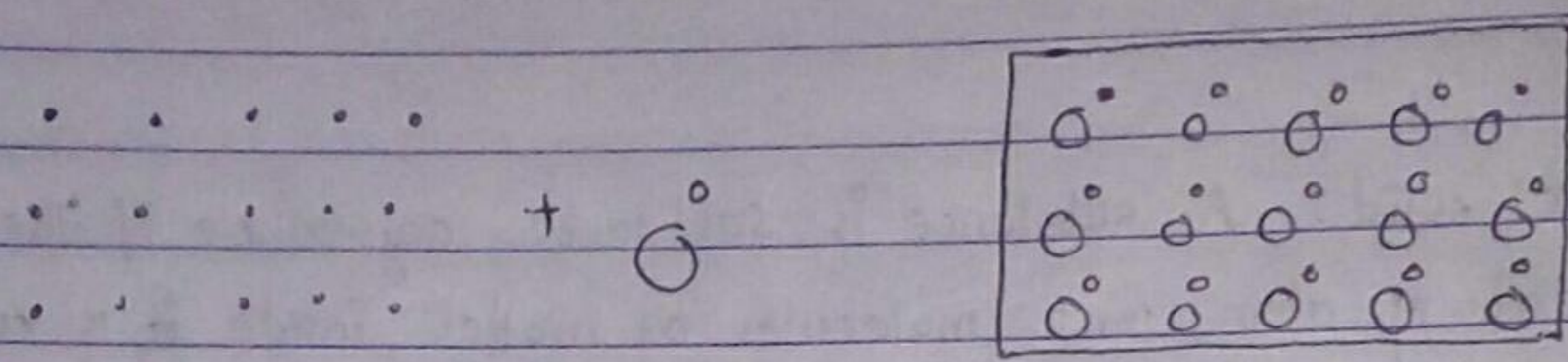
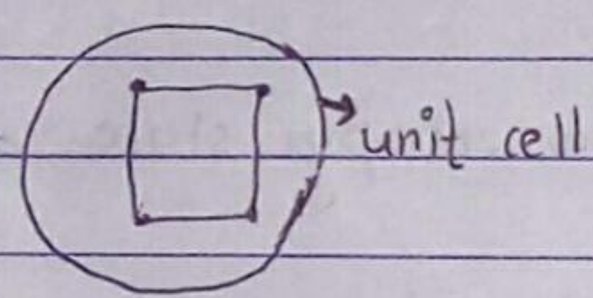
The crystal structure is a physical concept.



Space lattice + Basis. ⟶ Crystal structure.

Unit cell:

The building block of the space lattice is called unit cell. It is the small group of lattice points.



Types of unit cell:

1. Primitive unit cell
2. Non-primitive unit cell.

Unit cells can be classified into two types on the basis of arrangement of atom.

1. Primitive unit cell:

The unit cell which contains lattice points at corners only is called primitive unit cell. The axes a, b, c which are parallel x, y, z are called lattice constant or lattice vectors. The angle between them are called interfacial angle. In fig α, β, γ are the interfacial angles.

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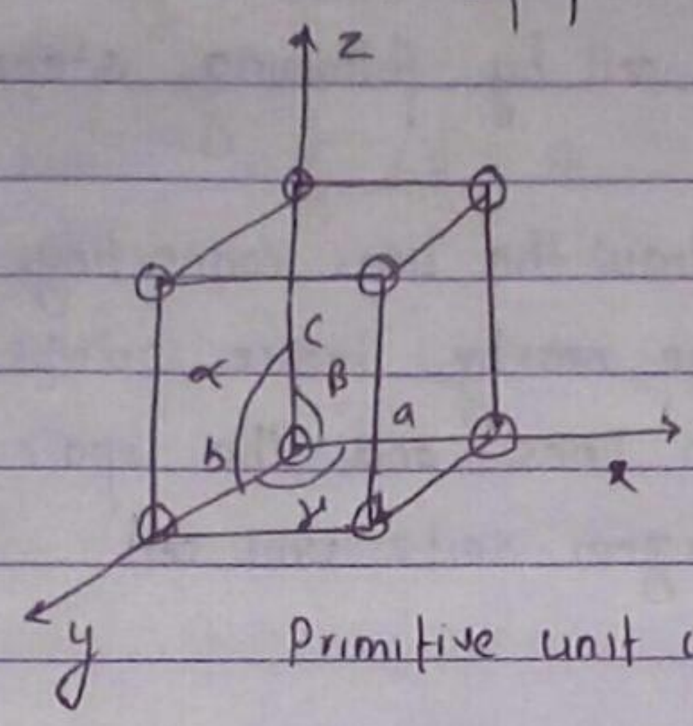
In 3D, minimum volume of primitive unit is, $V = \vec{a} \cdot |\vec{b} \times \vec{c}|$.



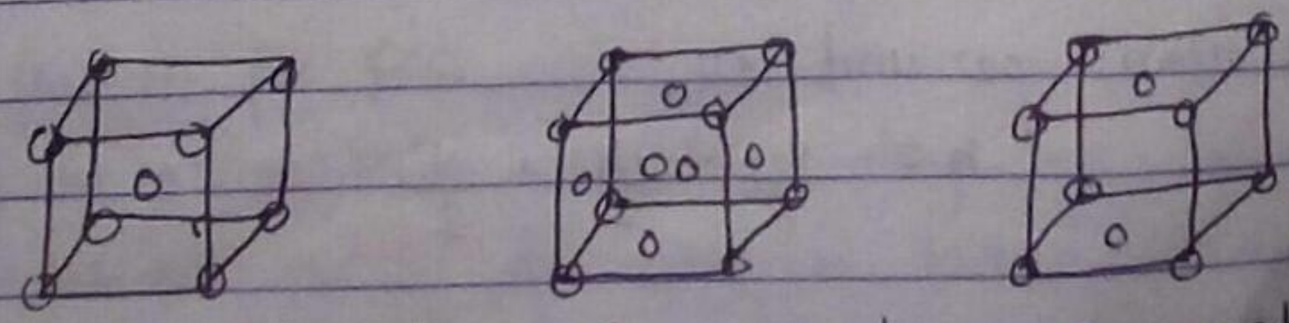
Primitive unit cell.

2. Non-primitive unit cell:
The unit cell which contains the lattice point at the corners as well as other location both inside & surface of the cell is called non primitive unit cell. There are three types of non-primitive unit cell:

a. Body centered cell:
The non-primitive unit cell in which lattice point lie at its corners as well as lattice point at its body center is called body centered cell.

b. Face centered cell:
It is non-primitive unit cell in which lattice point lie at its corners as well as center of each face.

c. Base centered (end) cell:
It is the non-primitive unit cell in which lattice point lie at its corners as well as one of the pair of the lattice at its opposite faces.



Body centered cell. Face centered. c. Base centered cell.

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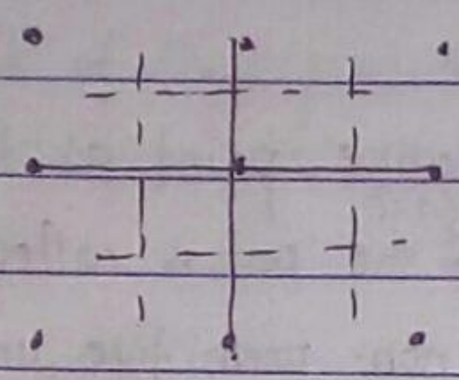
Wigner Seitz unit cell:

Wigner Seitz draw a unit cell by following steps:

1. Choose a reference point and draw the lines connecting given lattice point to all the nearby lattice points.
2. Draw the $\perp^r$ bisectors of each lines and the space closed by such normal planes is called Wigner seitz unit cell.



Wigner sertz unit cell.

Numbers of atom per unit cell.

The atom lying at the corner of the cubic unit cell is shared among 8 unit cells. Therefore, it contributes $\frac{1}{8}^{th}$ of an atom to the unit cell.

An atom lying ~~int~~ the face of unit cell is equally shared between two unit cells and theorefore, it contributes $\frac{1}{2}^{th}$ of an atom to the unit cell.

An atom lying completely within the unit cell belong wholy to that cell.

$\therefore$ No's of atoms per unit cell,

$$n = \frac{N_c}{8} + \frac{N_f}{2} + \frac{N_i}{1}.$$

N_c = No's of corner atoms ; N_f = No.'s of face atoms & N_i = No's of inner atoms

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For scc, $n = \frac{8}{8} + \frac{0}{2} + 0 = 1$; scc - simple cubic crystal.

For fcc, $n = \frac{8}{8} + \frac{6}{2} + 0 = 4$; fcc - face centered cubic crystal.

for bcc, $n = \frac{8}{8} + \frac{0}{2} + 1 = 2$; bcc - Body centered cubic crystal.

Atomic radius:

It is assumed that all the atoms in the crystal have same size and are touching each other. Thus, the atomic radius is half of the distance between the center of two neighbouring atoms.

Packing fraction (p.f)

Atomic packing fraction is defined as the ratio of the vol. of atoms occupying the unit cell to the vol. of unit cell relating to the structure of crystal. It's also called packing efficiency.

$$p.f. = \frac{\text{Vol. of atoms inside unit cells}}{\text{Volume of unit cell}} = \frac{\text{no. of atoms per unit cell} \times \text{vol. of each atom}}{\text{Vol. of unit cell}}$$

ie. $p.f = \frac{n.v}{V}$

In percentage, (% p.f) $= \frac{nv}{V} \times 100\%$.

It gives the ideo about the closeness of the atom inside unit cell.
e.g. If p.f is 52%, it means 52% of unit cell is packed by the atoms and 48% is empty.

A. Packing fraction for scc.

For scc, the atoms touch each other along the cube edge. If r is the atomic radius & a is ~~rad~~ lattice constant, then

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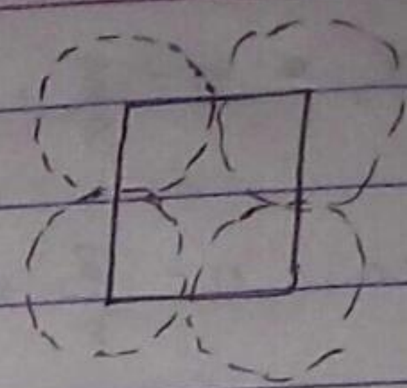


$a = 2r$

$\Rightarrow r = a/2$

Vol. of an atom $(v) = \frac{4}{3}\pi r^3 = \frac{4}{3}\pi\left(\frac{a}{2}\right)^3$

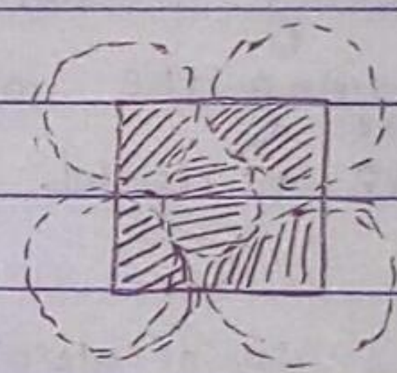
Vol. of cubic unit cell $(V) = a^3$

No's of atoms per unit cell $(n) = 1$.

$$\text{p.f for scc} = \frac{nv}{V} = \frac{\frac{4}{3}\pi\left(\frac{a}{2}\right)^3}{a^3}$$

$$= \frac{\pi}{6} = 0.54.$$

B. Packing fraction for fcc:



In fcc, the atoms touch each other along the diagonal of faces.

From fig,

$$a^2 + a^2 = (r + 2r + r)^2$$

$$\Rightarrow 2a^2 = 16r^2$$

$$\Rightarrow r = \frac{2a^2}{16}$$

$$\Rightarrow r = \frac{a}{2\sqrt{2}}$$

Volume of an atom $v = \frac{4}{3}\pi r^3 = \frac{4}{3}\pi\left(\frac{a}{2\sqrt{2}}\right)^3 = \frac{\pi a^3}{12\sqrt{2}}$

Volume of unit cell $V = a^3$

No's of atom per unit cell $(n) = 4$.

$$\therefore \text{p.f for fcc} = \frac{nv}{V} = \frac{4 \cdot \pi a^3}{a^3 \times 12\sqrt{2}} = 0.74.$$

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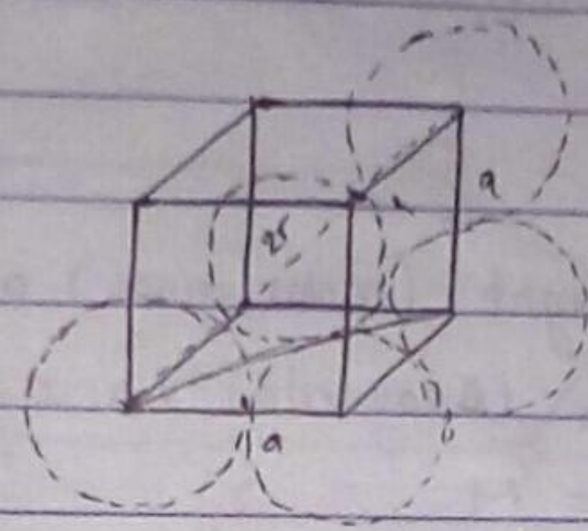
c. p.f for bcc.



In bcc, the atoms touch each other along the diagonal of cube.
From fig;

$$(a\sqrt{2})^2 + a^2 = (r+2r+r)^2$$

$$\Rightarrow 2a^2 + a^2 = 16r^2$$

$$\Rightarrow 3a^2 = 16r^2$$

$$\Rightarrow r = \frac{\sqrt{3}}{4}a.$$

Volume of atom $v = \frac{4}{3}\pi r^3 = \frac{4}{3}\pi\left(\frac{\sqrt{3}}{4}a\right)^3$

$$= \frac{4}{3}\pi \cdot \frac{3\sqrt{3}\cdot a^3}{64}$$

$$= \frac{\sqrt{3}\,a^3\pi}{16}.$$

Volume of unit cell $V = a^3$.
no's of atom per unit cell $(n) = 2$.

$$\therefore \text{p.f for bcc} = \frac{nv}{V} = \frac{2.\sqrt{3}a^3\pi}{16.a^3} = \frac{\sqrt{3}\pi}{8} = 0.68 = 68\%.$$

Fundamental types of lattice:

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Relation between density of material and lattice constant in a cubic lattice :

Let M be the molecular weight (molar mass) of cubic crystal.
One of crystal contains N_A (Avogardos no. of molecules)

$\therefore$ mass of N_A molecules $= M$

mass of 1 molecule $= \frac{M}{N_A}$

$\because$ unit cell contains n molecules

$\therefore$ mass of n molecule $= \frac{nM}{N_A} = m$

If ρ be the density of cubic crystal, then

$$\rho = \frac{\text{total mass}}{\text{total vol.}} = \frac{m}{V}$$

$$\Rightarrow \rho = \frac{nM}{VN_A} \quad \ldots \quad (i)$$

for cubic crystal,

$$V = a^3$$

$$\therefore \rho = \frac{nM}{a^3 \cdot N_A}$$

$$\Rightarrow a^3 = \frac{nM}{\rho N_A}$$

$$\Rightarrow a = \left(\frac{nM}{\rho N_A}\right)^{1/3} \quad \ldots (ii) \quad ; n = 1$$

Eqn (ii) gives the relation between ρ & a.

eg. Find lattice parameter of sc crystal if material has molecular wt. 58.74 gm & density $2.17\ g\,cc^{-1}$.

Sol^n

$M = 58.74$ gm

$\rho = 2.17\ g\,cc^{-1}$ & $n = 1$

$a =$ ___ .

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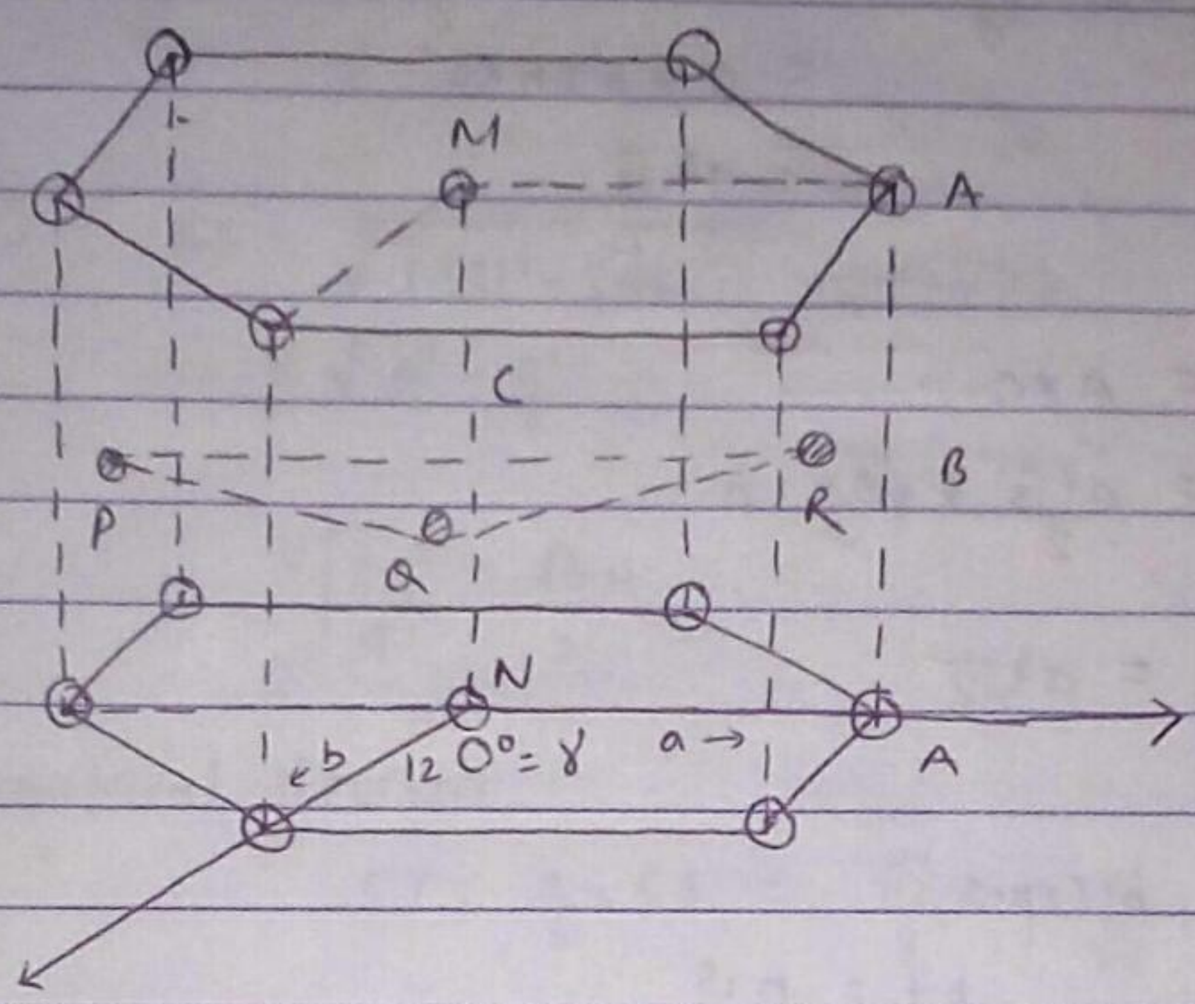
Hexagonal closed packed structure (h.c.p.s)



In h.c.p.s, layer A has six atoms with each atom surrounded by six atoms. B can be placed on the top of A such that atoms of layer B occupy the alterthate vallies formed by atoms of layer A. Third layer is on the top of B layer in such a way that atom of B layer exactly overlaps atoms of layer A.

For h.c.p.s, $a = b \neq c$

$\alpha = \beta \neq \gamma$; $\alpha = \beta = 90^\circ$ & $\gamma = 120^\circ$. Also, $\frac{c}{a} = \sqrt{\frac{8}{3}}$.

Packing fraction for h.c.p.s. :

The conventional unit cell of h.c.p.s is a hexagonal cell and three such cells form a h.c.p.s unit.

No. of atoms per unit cell (n) = 2.

∵ atoms touch each other,

$\therefore r = \frac{a}{2}$

Vol. of atom $v = \frac{4}{3}\pi r^3 = \frac{4}{3}\pi \frac{a^3}{8} = \frac{a^3\pi}{3}$

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The base of the hexagonal cell is parallelogram with $A = B$

$\therefore$ Ar. of parallelogram = base × height

$$= a \times b \sin 60^\circ$$

$$= a^2 \frac{\sqrt{3}}{2}$$

Vol. of unit cell $V = A \times C$

$$= \frac{a^2\sqrt{3}}{2} \times \sqrt{8/3} \cdot a.$$

$$= a^3\sqrt{2}$$

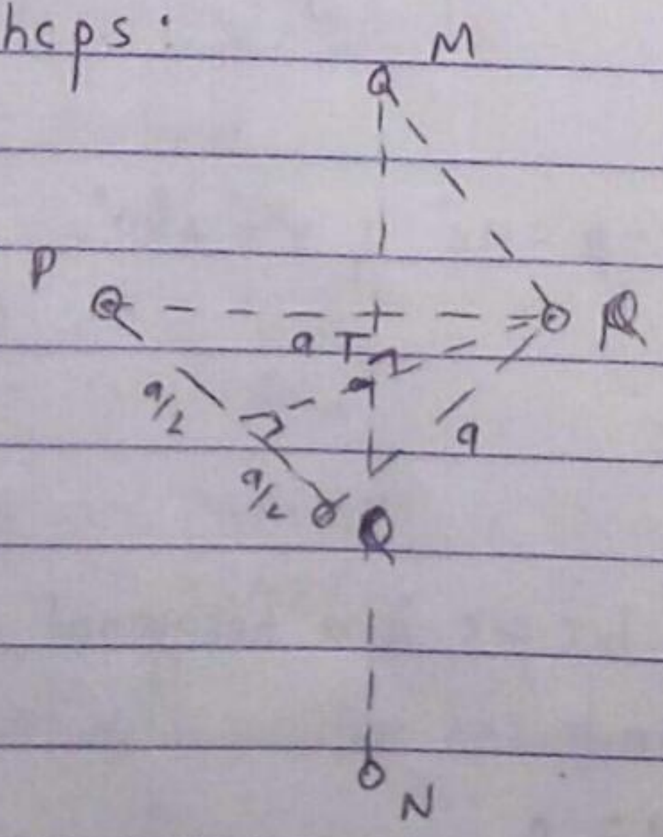
$\therefore$ p.f for h.c.p.s,

$$p.f = \frac{n v}{V}$$

$$= \frac{2 \cdot 4/3 \, a^3/8}{a^3\sqrt{2}}$$

$$= \frac{\pi}{3\sqrt{2}} = 0.74 = 74\%$$

c/a ratio in hcps:



Suppose, p, q P, Q, & R be the centers of adjacent atoms in middle plain forming equilateral triangle with side length a let M & N be center of adjacent atom in the plain immediately above and below PQR.

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MN passes through the centroid T of ΔPQR and $\perp^r$ to the plane of triangle.

From fig,

$$RS = \sqrt{(QR)^2 - (QS)^2}$$
$$= \sqrt{a^2 - \frac{a^2}{4}}$$
$$= \sqrt{\frac{3a^2}{4}} = \frac{\sqrt{3}}{2} a$$

from geometrical theorem,

$$RT = \frac{2}{3} \times R.S = \frac{\sqrt{3}}{3} a = \frac{a}{\sqrt{3}}$$

from ΔMTR,

$$MT = \sqrt{(MR)^2 - (RT)^2}$$
$$= \sqrt{a^2 - \left(\frac{a}{\sqrt{3}}\right)^2} = \sqrt{\frac{2}{3}} \cdot a.$$

$$C = MN = 2 \times MT = 2 \times \sqrt{\frac{2}{3}} a$$

$$\Rightarrow \frac{c}{a} = \sqrt{\frac{8}{3}} \quad \square$$

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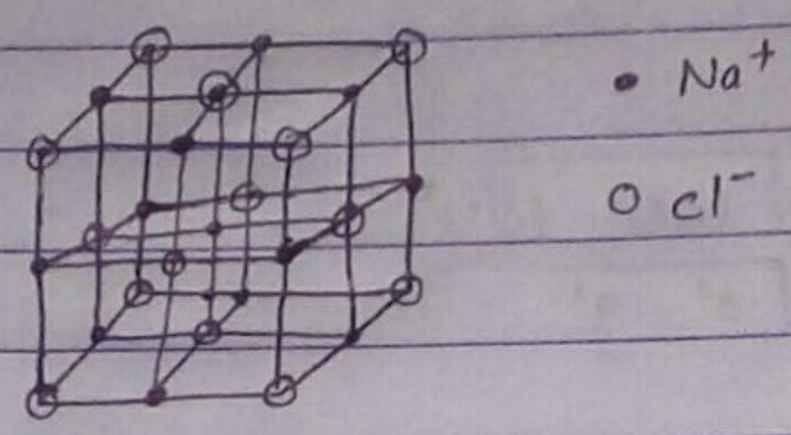
Sodium chloride structure :

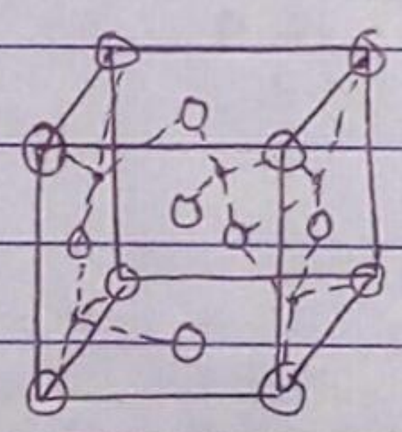


The unit cell of NaCl is face centered cubic crystal and it contains 4 NaCl molecules. Thus, there are four Na^+ and 4 Cl^- ions per unit cell. In the crystal each ion is surrounded by six nearest neighbours of opposite charge.

∴ Co-ordination no. for cation & anion is six.

The basis of this structure has 1 Na^+ and 1 Cl^- ion

Diamond structure :



Diamond is extremely attractive material with low electrical conductivity & high thermal conductivity. In diamond structure each carbon bonds to four other carbons & these bonds are totally covalent.

Diamond has fcc structure in common. It contains 4 atoms at the tetrahedral void position in fcc arrangement of C-atom. As covalent bonding has directional nature so, the structure is very loose.

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Crystal bonding:

The ability to hold the atoms or molecules or ions together is called crystal bonding / chemical bonding.

Types

1. Ionic bonding:

- This type of bonding is due to gain or loss of electron between atoms of different elements.
- Ionic compounds are composed of both metallic & non-metallic elements among which metallic elements give up their valance electron to non-metallic electron to achieve stable electronic configuration.
- Due to formation of -ve & +ve charges their exist an attractive electrostatic force.
- This type of bonding is non-directional (direction independent) ie. magnitude of bond is equal in all direction around an ion.
- Bonding energy is high & melting point is high.
- They are soluble in liquid like water.
- e.g. NaCl, CaO, $MgCl_2$, K_2O, etc.

2. Covalent bonding:

- This type of bonding is formed by sharing of electrons between neighbouring atoms thereby by acquiring the stable electronic configuration.
- The no.'s of covalent bonds possible for a particular atom is determined by the no.'s of valence electrons.
- If N' be the no. of valence electrons, then no. of covalent bond.

$$N = 8 - N'.$$

e.g. for carbon,

$$N' = 4$$

$$\therefore N = 8 - 4 = 4 \text{ bonds.}$$

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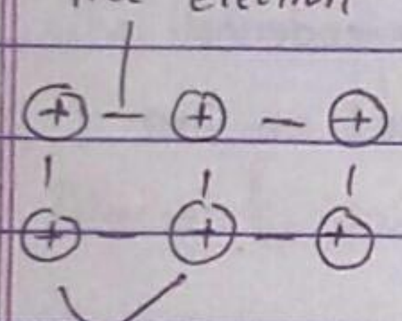
- The covalent bond is a strong directional. This means it is between two specific atoms in a particular direction. Thus, the covalently bonded crystal cannot pack together in a densed manner. (loose)

- The covalent bonds may be v. strong as in diamond having m.p. > 3500°C. and may be vary ~~with~~ as in Bismith. having m.p - 270°C

- They are insoluble in water but soluble in ether like solvent.
e.g H_2, SH_4, GaAs (S.C), SiC, diamond etc.

3. Metallic bonding :- In metals having 1, 2 or 3 valence electrons are not strongly bound to the nucleus. They are free to move throughout the entire metal. so, such electrons forms electronic cloud & atomic nuclei forms the positively charged ion cores known as kernels. The free electron acts as glue to hold such kernels and such bonding is called metallic bonding.



- This type of bonding is non-directional.
- This bonding may be weak or strong.
e.g. Bondings in metals & their alloys.

4. Vander Waal's bonding (Molecular bonding).

- In an atom, electronic cloud is symmetric around the +vely charged nucleus. All the atoms are experiencing the vibrational motion & hence structure is distorted. Such distrotions forms electric dipoles which are weakly attracted such bonding is called Vander waal's bonding.

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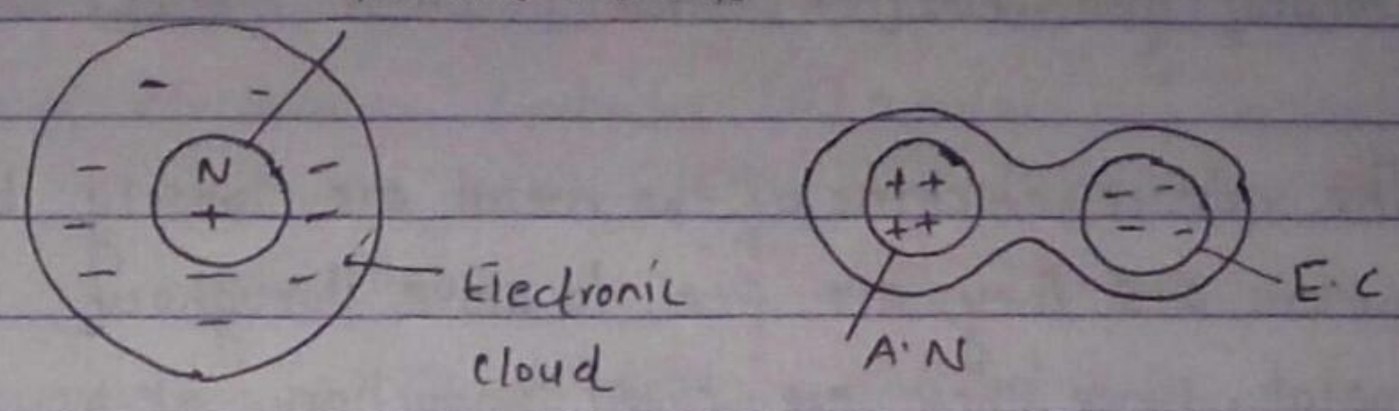


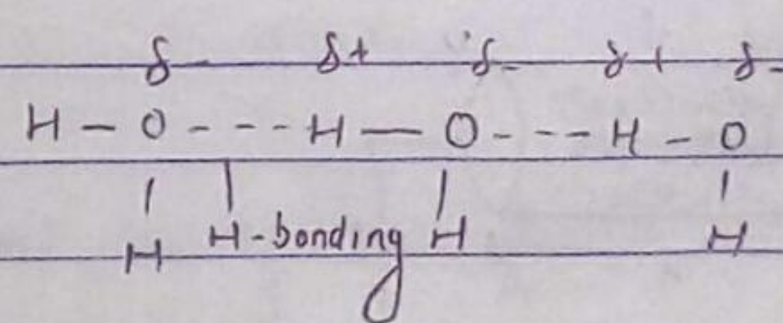
Symmetric. Electric dipole.

- This type of bonding exist only at v. low temperature (lesser than R.T.)
- These compounds have v. low bonding energy & v. low m.p.

5. Hydrogen bonding:

- H-atom forms bonding with highly. E.N atom as F, O, C, etc. called H-bonding.
- These bonding have low bonding energy & low m.p.
- The H-bonding is stronger than vander waal bonding but weaker than ionic & covalent bonding.

e.g. H_2O, HF, etc.



Free electron model (FEM)

Electron gas:

Metal consists of large numbers of weakly bonded free electrons. There is no interaction between electrons & hence P.E is zero.

Thus, all energy $E = K.E + P.E$

ie. $E = K.E.$ (free)

The behaviour of conduction electron is similar to molecules of ideal gas. Thus the system of such free & non-intracting electrons is E.G.

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✓ Classical free electron model (Drude model)

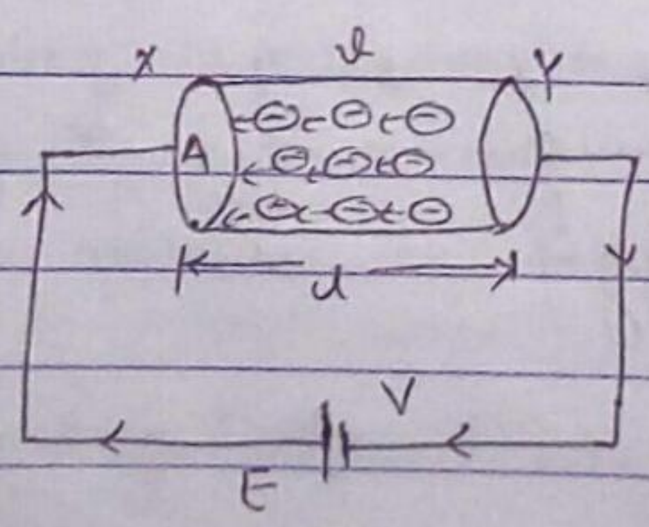
- The valence electrons of the metal are loosely bound to the nucleus and they are free to move throughout the volume of metal. Hence, they are called conduction electron.

- There is no interaction between electrons and hence, P.E = 0. Thus, total energy is in the form of K.E only.

- In absence of electric field, the electrons are in random motion. But when electric field is applied, free electrons drift in the direction opposite to electric field and they produce electric current.

- This model treats free electrons as classical particles and they obey Maxwell - Boltzmann statistics.

✓ Ohm's law



Suppose a metallic XY of length l and cross sectional area A. Let V be the p.d across the ends of the conductor.

The electric field due to p.d, $E = \frac{V}{l}$ .... (i)

The volume of conductor, Vol. of conductor $= A \cdot l$

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If n be the no's of electrons per unit volume (no. density),

Total no. of electrons in conductor $(N) = n\,Vol.$

$$= n(A \times l) \quad \ldots (ii)$$

If q be the charge passing through the cross sectional area A in time t,

$$q = Ne$$

$$= nAle \quad \ldots (iii)$$

Also, drift velocity $v = \frac{l}{t}$

$$\Rightarrow l = v \times t \quad \ldots (iv)$$

Using (iv) in (iii),

$$q = nA(vt)e \quad \ldots (v)$$

Now,

$$I = \frac{q}{t} = \frac{nA(vt)e}{t}$$

$$= ven A. \quad \ldots (vi)$$

Also,

Current density $(J) = \frac{I}{A} = ven. \quad \ldots (vii)$

Suppose electron of mass 'm' and charge $-e$ is placed electric field E.

Electric force on electron, $F = eE \quad \ldots (viii)$

Also, from Newton's second law of motion,

$$F = ma \quad \ldots (ix)$$

from (viii) & (ix)

$$ma = eE$$

$$\Rightarrow a = \frac{eE}{m}$$

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$$\Rightarrow \frac{dv}{dt} = \frac{eE}{m}$$

$$\Rightarrow dv = \frac{eE}{m} \cdot dt \quad \ldots (x)$$

Integrating eqn (x).

$$\int_0^v dv = \frac{eE}{m} \int_0^\tau dt$$

$$\Rightarrow v = \frac{eEt}{m} \quad \ldots (xi)$$

τ = relaxation time or collision time.

Now,

from (xi) & (vii),

$$J = \left(\frac{eE\tau}{m}\right) ne$$

$$= \left(\frac{ne^2\tau}{m}\right) E \quad \ldots (xii)$$

Comparing with Ohm's law, $J = \sigma E \quad \ldots (xiii)$

$$\sigma = \frac{ne^2\tau}{m}.$$

where σ is the electrical conductivity of conductor.
Thus, ohm's law was successfully explained by clasical free electron model.

Note: $V = IR$

$$\Rightarrow V = \frac{I\rho l}{A}$$

$$\Rightarrow \frac{V}{l} = \frac{I}{A}\frac{1}{\sigma}$$

$$\Rightarrow E = J\sigma^{-1} \Rightarrow J = \sigma E.$$

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Electrical Conductivity:

The ability of the conductor to conduct electric current is called electrical conductivity.

From Newton's second law of motion,

$$F = \frac{d\vec{p}}{dt} = \frac{d(m\vec{v})}{dt} = m\frac{d\vec{v}}{dt} \quad \dots (i)$$

Also, wave machanics,

$$F = \frac{d(\hbar\vec{k})}{dt} = \hbar\frac{d\vec{k}}{dt} \quad \dots (ii)$$

The force on electron due to electric field,

$$F = -e\vec{E} \quad \dots (iii)$$

from eqn's (i), (ii) & (iii),

$$m\frac{d\vec{v}}{dt} = \hbar\frac{d\vec{k}}{dt} = -e\vec{E}. \quad \dots (iv)$$

from eqn (iv),

$$\hbar\frac{d\vec{k}}{dt} = m\frac{d\vec{v}}{dt} = -e\vec{E}$$

$$\Rightarrow m\frac{d\vec{v}}{dt} = -e\vec{E} = \hbar\frac{d\vec{k}}{dt}$$

integrating,

$$\Rightarrow \int d\vec{k} = \frac{-e\vec{E}}{\hbar}\int dt$$

$$\Rightarrow \int_{k(0)}^{k(\tau)} = \frac{-e\vec{E}}{\hbar}\int_0^{\tau} dt$$

$$\Rightarrow k(\tau) - k(0) = \frac{-e\vec{E}}{\hbar}\tau$$

$$\Rightarrow \delta k = \frac{-e\vec{E}}{\hbar}\tau \quad \Rightarrow \delta\vec{v} = \frac{-e\tau\vec{E}}{m} \quad \dots (iv)$$

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Now,

$$J = \frac{I}{A} = nev$$

$$\vec{J} = n(-e)\vec{v}$$

$$\vec{J} = n(-e)\left(\frac{-e\vec{E}\tau}{m}\right) = \left(\frac{ne^2\tau}{m}\right)\vec{E}$$

Comparing eqn (vii) with Ohm's law,

$$\therefore \sigma = \frac{ne^2\tau}{m} \quad \cdots \text{(viii)}$$

Eqn (viii) gives the electrical conductivity of conductor.

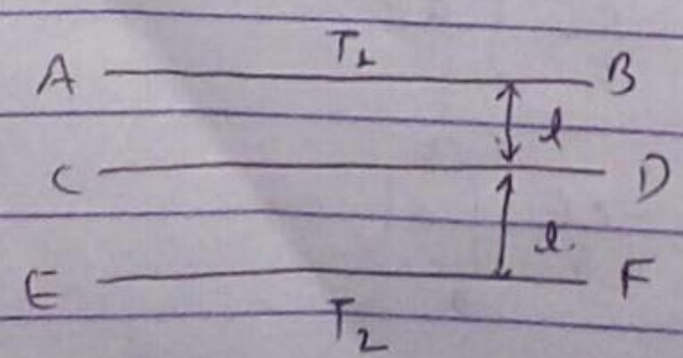
Thermal conductivity

The ability of the conductor to conduct heat through it is called thermal conductivity.

The heat energy transmited per unit area per unit time Q',

$$Q' = \frac{Q}{A \times t} = K\left(\frac{dT}{dl}\right) \quad \cdots \text{(i)}$$

$$\left[Q = \frac{KAt(dT)}{dl}\right]; \text{ K thermal conductivity.}$$



Let A, B, C, D, E & F are the three planes in which plane CD is at a distance l (mean free path). from planes AB & EF. Also, T_1 & T_2 ($T_1 > T_2$) are the temperatures of AB & EF respectively.

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c - heat capacity
s - sp. " " g

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Let n be the no's of the electrons per unit volume & v be the velocity of each electron. Then nos of the electron per unit area per unit time crossing the plane CD.

$$N' = \frac{nv}{6} \qquad \left(\frac{N}{V} \times \frac{l}{t} = \frac{N}{A \times l} \times \frac{l}{t} = \frac{N}{A \times t} = N'\right) \quad nv;$$

Now,

heat carried by electrons downward across the plane CD per unit area per unit time from plane AB,

$$Q_1' = N' c T_1$$
$$= \frac{nv}{6} c T_1 \quad \ldots (ii)$$

Also, heat energy carried by electrons upward across the plane CD per unit area per unit time from EF.

$$Q_2' = N' c T_2 \quad \ldots (iii)$$

Now, net heat energy carried by electrons downward across the plane CD per unit area per unit time.

$$\phi' = Q_1' - Q_2'$$
$$= \frac{nv}{6} c (T_1 - T_2) \quad \ldots (iv)$$

Now, from fig temperatur gradient;

$$\frac{dT}{dl} = \frac{T_1 - T_2}{(l+l)}$$

$$\Rightarrow T_1 - T_2 = 2l \frac{dT}{dl} \quad \ldots (v)$$

Using (v) in (iv)

$$\phi' = \frac{nv}{6} c \, 2l \left(\frac{dT}{dl}\right) \quad \ldots (vi)$$

$$= K \left(dT/dl\right) \quad \ldots (vii)$$

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Compairing eq^n (vi) with (i),

$$k = \frac{n v c l}{3} \quad \ldots (vii)$$

for $n = 1$, $k = \frac{c v l}{3}$ $\quad \ldots (viii)$

where $C = \frac{\pi^2}{2} n k_B \left(\frac{T}{T_f}\right)$ $\quad \ldots (ix)$

$T_f \leftarrow$ fermi temp.

~~But~~ heat capacity of electron; where T_f is fermi temp.

and fermi energy, $E_f = k_B T_f$

also $E_f = \frac{1}{2} m v_f^2$; v_f - fermi velocity

Also, fermi velocity $v_f = \frac{l}{\tau}$

Now, from eq^n (viii), using (ix)

$$K = \frac{\pi^2}{2} n k_B \left(\frac{T}{T_f}\right) \times \frac{1}{3} \times v_f (v_f \times \tau)$$

$$= \frac{\pi^2}{6} n k_B \left(\frac{T}{E_f / k_B}\right) v_f^2 \tau$$

$$= \frac{\pi^2}{6} n k_B^2 \left(\frac{T}{E_f}\right) v_f^2 \tau$$

$$\therefore K = \frac{\pi^2}{6} n k_B^2 \left(\frac{2T}{m v_f^2}\right) v_f^2 \tau$$

$$= \frac{\pi^2}{3} \frac{n k_B^2}{m} T \tau \quad \ldots (xi)$$

It gives thermal conductivity of solid.

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$k_B = 1.38 \times 10^{-23}$.

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CFE model.
(Classical free electron)

Wiedmann - Frantz law:

The thermal conductivity of solid.

$$K = \frac{\pi^2}{3} \frac{n k_B^2}{m} T\tau \quad \cdots (i)$$

Also,

electrical conductivity,

$$\sigma = \frac{ne^2\tau}{m} \quad \cdots (ii)$$

Now, ratio of K & σ,

$$\frac{K}{\sigma} = \frac{\pi^2}{3} \frac{n k_B^2}{m} T\tau \times \frac{m}{ne^2\tau}$$

$$= \left[\frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2\right] T$$

$$\therefore \frac{K}{\sigma} = lT \quad \cdots (iii)$$

where, $l = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$

$= 2.458 \times 10^{-8}$ watt ΩK^{-2}. is lorentz unit.

ie. $\frac{K}{\sigma} \propto T$.

Thus, for metal the ratio of thermal conductivity to electrical conductivity is directly proportional to the absolute temperature.

Failure of CFET:

EFET fails to explain sp. heat capacity at low temperature, temperature dependence of electrical conductivity etc.

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Success of CFET.

It is successful in explaining Ohm's law, electrical & thermal conductivity, Wiedmann-Franz law, etc.

Quantum free electron theory (Sommer feld model)

Sommer feld modified CFET in two important ways:

- The electrons are to be treated quantum mechanically. Thus, energy of electrons must be quantized (discrete energies)
- The electron must obey Pauli's exclusion principle i.e. no two electrons having same quantum number can lie in a same state.
- Besides these asumptions:

i. The valence electrons are free to move throughout the solid.
ii. There is no interaction between electron & ion core.
$\therefore P.E = 0$ So, $E = K.E$.

Fermi level and fermi energy:

The top most ~~fill~~ energy level at absolute zero is called fermi level and energy of that level is called fermi energy. It is denoted by E_f.

At absolute zero (0K) fermi energy E_f is equal to chemical potential.

i.e. $E_f = \mu$.

Suppose, there are 11 electrons in an atom. These electrons can lie in 6th energy level and 6th energy level is partially filled. Thus, energy level with $n > 6$ are completely empty & $n < 6$ are completely

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filled. Thus, fermi level $n = 61$ and energy of this level is called fermi energy.

The distribution function,

$$f(E) = \frac{1}{e^{\left(\frac{E-\mu}{k_B T}\right)} + 1}$$

$$= \frac{1}{e^{(E-E_f)\times\frac{1}{k_B T}} + 1}$$

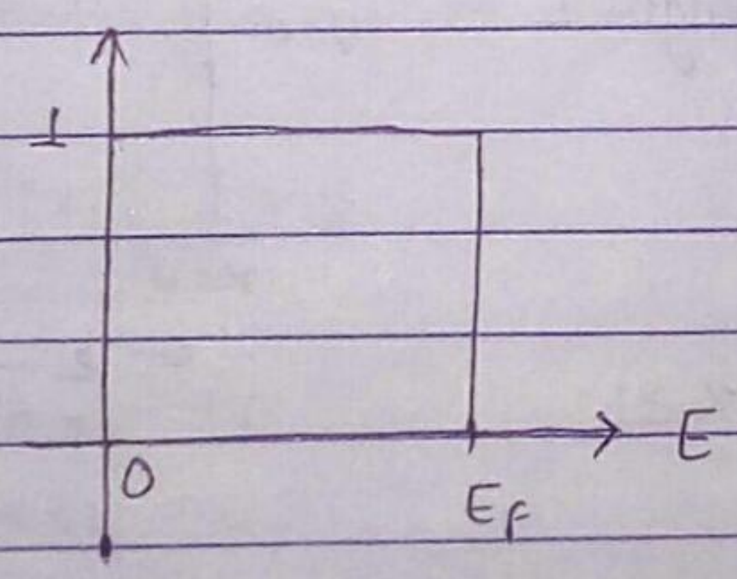
Actually, this function measure the probability.

$f(E) = 0, \quad E > E_f$

$f(E) = 1, \quad E < E_f$

$f(E) = 1 \quad E = E_f$

$F(E)$ vs E graph.



The function has step nature

Note:

→ Schrodinger wave equation:

$$(-\hbar^2 \nabla^2 + V)\psi = E\psi$$

$\Rightarrow H\psi = E\psi \quad ; \quad H = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right), \quad \psi =$ wave function.

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

In 1D,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V\right)\psi = E\psi$$

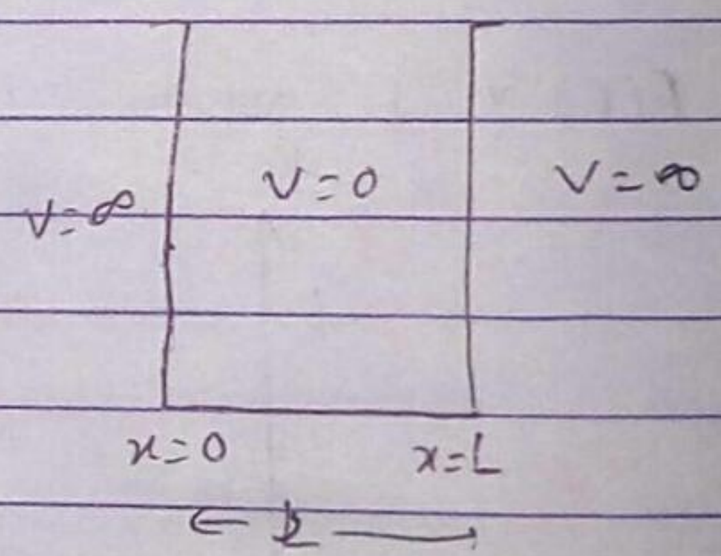
$$\Rightarrow \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = (E-V)\psi$$

$$\Rightarrow \frac{d^2\psi}{dx^2} = \frac{-2m}{\hbar^2}(E-V)\psi$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E-V]\psi = 0.$$

Free electron gas in 1D - box.

Suppose an electron of mass m is confined in 1D box of length L.



The potential is given by,

$V(x) = 0$ for $0 < x < L$

$V(x) = \infty$ for $x \leq 0$, $x \geq L$

SWE (Schrodinger Wave Equation) in 1D,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\cdot[E-V]\psi = 0 \quad \ldots (i)$$

For region $0 < x < L$, $V = 0$

$\therefore$ from eqn (i),

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0.$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + k^2\psi = 0 \; ; \quad k^2 = \frac{2mE}{\hbar^2}.$$

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Solution of eqn (ii) is of the type

$$\psi(x) = A \sin kx + B \cos kx \quad \dots (iii)$$

where, A & B are arbitary constants.

Using boundry condition, at $x=0$,

$$[\psi(x)]_{x=0} = 0$$ (The wave function ψ vanishes at boundry)

$\Rightarrow A \sin k \times 0 + B \cos k \times 0 = 0$

$\Rightarrow B \times 1 = 0$

$\Rightarrow B = 0 \quad \dots (iv)$

Using (iv) in (iii),

$$\psi(x) = A \sin kx \quad \dots (v)$$

Also, using boundry condition at $x = L$

$$[\psi(x)]_{x=L} = 0$$

$\Rightarrow A \sin kL = 0$

$\Rightarrow \sin kL = 0$

$\Rightarrow \sin kL = \sin n\pi \quad ; n = 1, 2, 3, 4 \dots$

$\Rightarrow kL = n\pi$

$\Rightarrow k = \frac{n\pi}{L} \quad \dots (v)$

$$\psi(x) = A \sin \left(\frac{n\pi}{L}\right) x \quad \dots (vii)$$

Using normalization condition:

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

$$\int_0^L \left[A^* \sin\left(\frac{n\pi x}{L}\right)\right] A \sin\left(\frac{n\pi x}{L}\right) dx = 1$$

$$A^* A = |A|^2 = A^2$$

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

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

$$\Rightarrow A^2 \int_0^L \left[1 - \cos\frac{2n\pi x}{L} \times \frac{1}{2}\right] dx = 1.$$

$$\Rightarrow \cos^2 x - \sin^2 x = \cos 2x$$

$$\Rightarrow -2\sin^2 x = \cos 2x$$

$$(\sin^2 x = -\cos x$$

$$\Rightarrow \frac{A^2}{2} \int_0^L \left(1 - \cos\frac{2n\pi x}{L}\right) dx = 1.$$

$$\Rightarrow \frac{A^2}{2}\left[[x]_0^L - \left[\sin\frac{2n\pi x}{L} \times \frac{L}{2n\pi}\right]_0^L\right] = 1.$$

$$\Rightarrow \frac{A^2}{2}\left[L - \frac{L}{2n\pi}\left\{\sin\frac{2n\pi L}{L} - \sin\frac{2n\pi \cdot 0}{L}\right\}\right] = 1.$$

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

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

$$\Rightarrow A = \sqrt{\frac{2}{L}} \quad \ldots (viii)$$

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Using (viii) in (vii)

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

for $n=0$, $\psi_0(x) = 0$

$n=1$, $\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right).$

$\vdots$

for n^{th}, $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right).$

Also from equation (ii)

$$K^2 = \frac{2mE}{\hbar^2}$$

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

$$\frac{\hbar^2 K^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

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

Using eqn (vi)

$$\Rightarrow E_n = \frac{n^2\pi^2\hbar^2}{2m} = \frac{n^2h^2}{8mL^2} \quad \cdots (ix)$$

$$= \frac{h(h/2\pi)^2}{2mL^2}$$

$E_0 = 0$

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

Thus, the energy level of electron are not equally spaced.

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Fermi energy of density of state in 3D.

Schrodinger wave equation in 3D,

$$H\psi(r) = E\psi(r) \quad \ldots (i)$$

where $H = K.E + P.E$

$$= \frac{p^2}{2m} + V$$

$$= \frac{(i\hbar\nabla)^2}{2m} + V$$

$$= \frac{-\hbar^2\nabla^2}{2m} + V$$

$$\therefore \left(\frac{-\hbar\nabla^2}{2m} + V\right)\psi(r) = E\psi(r)$$

$$\Rightarrow \frac{-\hbar^2\nabla^2}{2m}\psi(r) + V\psi(r) = E\psi(r)$$

$$\Rightarrow \frac{-\hbar^2\nabla^2}{2m}\psi(r) = (E-V)\psi(r)$$

$$\Rightarrow \nabla^2\psi(r) = \frac{-2m}{\hbar^2}(E-V)\psi(r)$$

$$\Rightarrow \nabla^2\psi(r) + \frac{2m}{\hbar^2}(E-V)\psi(r) = 0 \quad \ldots (ii)$$

$$\Rightarrow \nabla^2\psi(r) + k^2\psi(r) = 0 \quad \ldots (iii)$$

$$\Rightarrow k^2 = \frac{2m}{\hbar^2}(E-V)$$

for free particle, $V=0$

$$\Rightarrow k^2 = \frac{2m}{\hbar^2}E \quad \ldots (iv)$$

Sol^n of eq^n of (iii) is of the form.

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$$\psi(r) = Ae^{i\vec{k}\cdot\vec{r}} \quad \ldots (v)$$

where $\vec{k}\cdot\vec{r} = (\hat{i}k_x + \hat{j}k_y + \hat{k}k_z)\cdot(\hat{i}x + \hat{j}y + \hat{k}z)$

$= xk_x + yk_y + zk_z$

Using normalization condition,

$$\int_0^V \psi^*(r)\,\psi(r)\,dV = 1$$

$$\Rightarrow \int_0^V \left[A^* e^{-i\vec{k}\cdot\vec{r}}\right]\left[Ae^{i\vec{k}\cdot\vec{r}}\right] dV = 1$$

$$\Rightarrow \int_0^V A^2\,dV = 1$$

$$\Rightarrow A^2 \int_0^V dV = 1$$

$$\Rightarrow A^2 V = 1$$

$$\Rightarrow A^2 = \frac{1}{V}$$

$$\Rightarrow A = \frac{1}{\sqrt{V}} \quad \ldots (vi)$$

Using (vi) in (v),

$$\psi(r) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}, \quad V = \text{Vol. of cube.}$$

for ideal crystal, the wave function satisfies the condition.

$$\psi(r) = \psi(x,y,z) = \psi(x+L, y+z)$$

$$\Rightarrow \frac{1}{\sqrt{V}} e^{i(xk_x + yk_y + zk_z)} = \frac{1}{\sqrt{V}} e^{i[(x+L)k_x + yk_y + zk_z]}$$

$$\Rightarrow e^{i(xk_x + yk_y + zk_y)} = e^{iLk_x} \cdot e^{i(xk_x + yk_y + zk_y)}$$

$$\Rightarrow 1 = e^{iLk_x}$$

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$$\Rightarrow e^{ik_xL} = e^{\pm i2n\pi}$$

$e^{ix} = \cos x + i\sin x$.

$e^{i(2n\pi)} = \cos(2n\pi) + i\sin(2n\pi)$
$= (-1)^{2n} = 1$.

$$\Rightarrow ik_xL = \pm i2n\pi$$

$$\Rightarrow k_x = \pm\frac{2\pi n}{L} \quad \ldots (vii)$$

$$\therefore k_x = \pm\frac{2\pi n}{L}, \; k_x = 0, \; \pm\frac{2\pi}{L}, \; \pm\frac{4\pi}{L}, \ldots \pm\frac{n\pi}{L}$$

Similarly,

$$k_y = \pm\frac{2\pi n}{L}$$

$$\& \; k_z = \pm\frac{2\pi n}{L}$$

In 3D,

$$\vec{k} = \hat{i}k_x + \hat{j}k_y + \hat{k}k_z$$

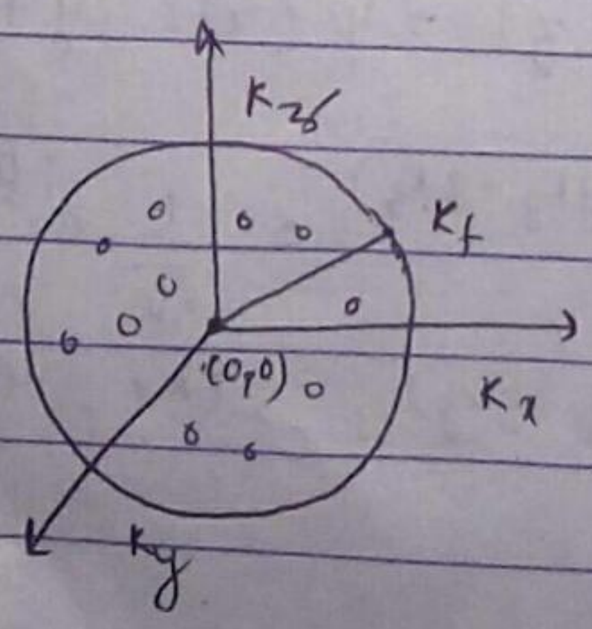
Now,

$$k^2 = \vec{k}\cdot\vec{k} = (\hat{i}k_x + \hat{j}k_y + \hat{k}k_z)\cdot(\hat{i}k_x + \hat{j}k_y + \hat{k}k_z)$$
$$= k_x^2 + k_y^2 + k_z^2 \quad \ldots (viii)$$

from (iv),

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

$$\Rightarrow E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2). \quad \ldots (ix)$$



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The electrons can be represented by points inside the fermi sphere
The energy of the surface of this sphere is called fermi energy
If k_f is the fermi radius, then

$$k_f^2 = k_x^2 + k_y^2 + k_z^2 \quad \ldots\ldots (x)$$

Using (x) in (ix),

$$E_f = \frac{\hbar^2}{2m} k_f^2 \quad \ldots\ldots (xi)$$

Eqn (xi) gives the fermi energy in 3D.

Total numbers of orbital inside fermi sphere 'n' = $2 \times \frac{\text{Vol. of k-sphere (fermi s)}}{\text{Vol. of an element}}$

where 2 is introduced for spin up and spin down.

Volume of k-sphere = $\frac{4}{3}\pi k_f^3$.

Volume of element = $k_x \cdot k_y \cdot k_z$

$$= k_x^3$$

$$= \left(\frac{2\pi}{L}\right)^3$$

$$\therefore N = 2 \times \frac{4/3\,\pi k_f^3}{(2\pi/L)^3}$$

$$= \frac{L^3}{3\pi^2} k_f^3$$

$$= \frac{V}{3\pi^2} k_f^3 \quad \ldots\ldots (xii)$$

where, $V = L^3$.

from eqn (xii),

$$k_f^3 = 3\pi^2 \frac{N}{V} \Rightarrow k_f = \left(3\pi^2 \frac{N}{V}\right)^{1/3}$$

$$\Rightarrow k_f^2 = \left(3\pi^2 \frac{N}{V}\right)^{2/3} \quad \ldots (xiii)$$

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from (xiii) in (xi),

$$E_f = \frac{\hbar^2}{2m}\left(3\pi^2 \frac{N}{V}\right)^{2/3} \quad \ldots (xiv)$$

where, $\frac{N}{V} = n$ (number density).

Density of state (DOS)

It is defined as the total numbers of electronic states per unit energy range. i.e.

$$D(E) = \frac{dN}{dE}$$

for fermi level,

$$D(E_f) = \frac{dN}{dE_f} \quad \ldots (xv)$$

from eqn (xii),

$$N = \frac{V}{3\pi^2} k_f^3 \qquad \left[\text{from (xi), } k_f = \frac{\hbar^2 k_f^2}{2m}\right]$$

$$= \frac{V}{3\pi^2}\left(k_f^2\right)^{3/2}$$

$$= \frac{V}{3\pi^2}\left(\frac{2mE_f}{\hbar^2}\right)^{3/2} \quad \ldots (xvi)$$

using (xvi) in (xv),

$$D(E_f) = \frac{d}{dE_f}\left[\frac{V}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_f^{3/2}\right].$$

$$= \frac{V}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{d}{dE_f} E_f^{3/2}.$$

$$= \frac{V}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{3}{2} E_f^{1/2}.$$

$$= \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_f^{1/2}. \quad \ldots (xvii)$$

Also, $D(E) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} \quad \ldots (xviii)$.

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Thus, density of state in 3D is directly proportional to square root energy.

ie. $D(E) \propto \sqrt{E}$.

Density of state in 2D.

In 2D, electrons are confined inside a fermi circle of radius K_f.

No. of orbitals $(N) = 2 \times \frac{\text{Ar. of fermi circle}}{\text{Ar. of element}}$.

Now, $N = 2 \times \frac{\pi K_f^2}{(2\pi/L)^2}$

$= \frac{2L^2 K_f^2}{4\pi^2}$

$= \frac{A}{2\pi}\left(\frac{2m E_f}{\hbar^2}\right)$ .... (i)

$\left[E_f = \frac{\hbar^2 K_f^2}{2m} \quad K_f^2 = \frac{2m E_f}{\hbar^2} \right]$

Again, DOS in 2D,

$D(E_f) = \frac{dN}{dE_f}$

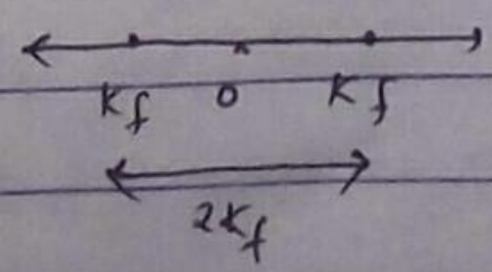
$= \frac{A}{2\pi} \frac{2m}{\hbar^2} \frac{dE_f}{dE_f}$.

$= \frac{A}{2\pi} \frac{2m}{\hbar^2}$ ... (ii)

Thus, DOS in 2D is independent of energy.

fermi energy :

DOS in 1D:



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In 1D, the electrons lie across a fermi line.

Now, No. of orbitals $N = 2 \times \frac{\text{length of fermi line}}{\text{length of element}}$

$$= 2 \times \frac{2k_f}{2\pi/L}$$

$$= 4 \cdot \frac{2L}{\pi} k_f$$

$$= \frac{2L}{\pi}\left(\frac{2mE_f}{\hbar^2}\right)^{1/2} \quad \ldots (i)$$

Again,

DOS in 1D,

$$D(E_f) = \frac{dN}{dE_f}$$

$$= \frac{2L}{\pi}\left(\frac{2m}{\hbar^2}\right)^{1/2} \frac{d}{dE_f} E_f^{1/2}$$

$$= \frac{L}{\pi}\left(\frac{2m}{\hbar^2}\right)^{1/2} \frac{1}{\sqrt{E_f}}$$

Also, $D(k_f) \propto \frac{1}{\sqrt{E_f}}$.

Thus, DOS in 1D is inversely proportional to square root of energy.

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Energy bands in solid:

In solid, there are a large numbers of interacting atoms and large numbers of energy level which are very close to each other. The large numbers of such energy levels in a small range forms the band called energy band. There are nos of energy band in solid. The important bands are:

1. Valence band (V.B)

Elecectron in valence shell of atoms form a band called a valence band. Those valence electrons which cannot get sufficient energy from external field lie in valence band. The valence band may be completely filled (inert gas) or partially filled (metals, semi-conductor) but can never be empty.

2. Conduction band (CB).

In metal, the valence electrons are loosely bound to the nucleus and some electrons may leave the valence band even at room temperature. These electrons form a band called conduction band & these electrons can conduct current in solid. These electrons can gain energy from external electric field. Cond^n B can never be completely field.

3. Forbidden band (F.B):

The separation between V.B & C.B is called forbidden band. No electrons can stay in this gap. To push the electron from VB to CB, the energy equal to band gap must be supplied.

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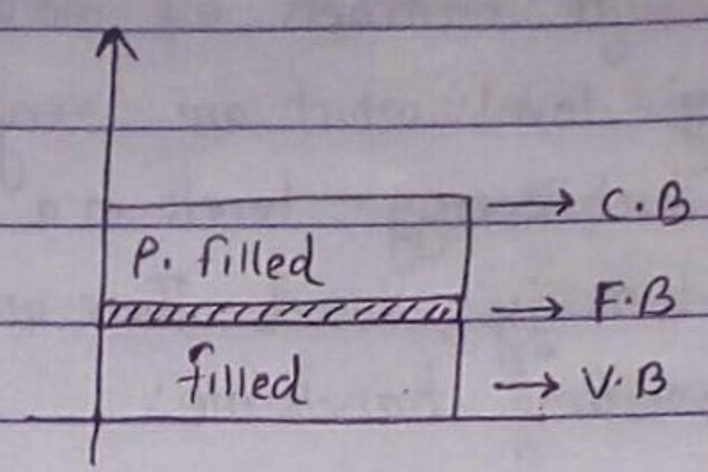
Classification of solid:

1. Conductor:



- VB and CB are overlapped.
- There is no F.B energy gap.
- Electron can jump from VB to C.B.
- When electric field is applied, electron move to the direction opp. to electric field and current flows.
- Electrical conductivity very high but it decrease with increase in temperature ((T↑, R↑)(σ↑, σ↓))
- Resistance increases with temperature so, $\alpha = \frac{R_2 - R_1}{R_1(T_2 - T_1)}$ = +ve. (temperature coeff. of resistance)

e.g iron, copper, Ag, etc.

2. Insulator:
- VB is completely filled and C.V is completely empty.
- Very large band gap (Approx. 15eV) between VB and CB.
- Electrons can jump easily from VB to CB although the external electric field is applied.
- Electrical conductivity is very small & negligible
- Resistance is nearly independent of temperature i.e. $\alpha \approx 0$.

eg. glass, paper, wood, ceramics, gases, diamond, etc.

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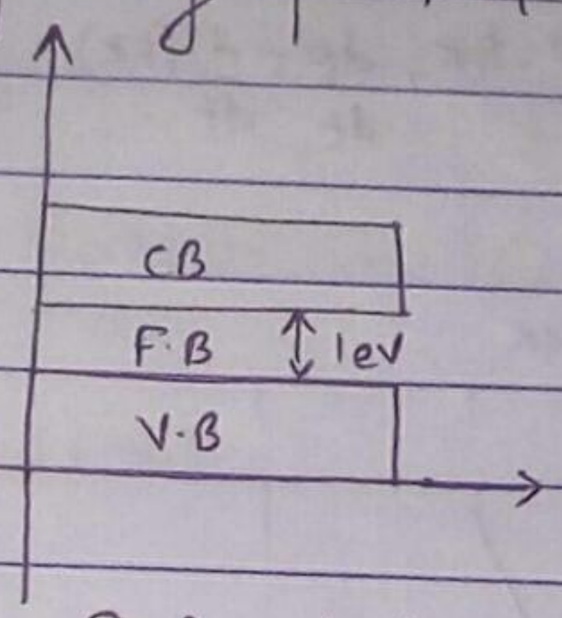
3 Semi conductor:

- They have four valence electrons.
- VB and CB are partially filled at room temperature.



Semi conductor.

- The band gap is of the order of 1eV.
- Electrical conductivity lies between conductor & insulator.
- It behaves as conductor at high temperature and insulator at low temperature.
- Temperature coefficent of resistance is negative ie. ($\alpha = -ve$) resistance decreases with increasing temperature.

$$\alpha = \frac{(R_2 - R_1)}{R_1 (T_2 - T_1)}$$

$\theta_2 > \theta_1$ $\theta_2 - \theta_1 =$ positive.

$R_2 < R_1$ $R_2 - R_1 = -ve$

$\alpha = -ve$

eg. Silicon, germinium, graphite etc.

Effective mass:

According to FET, the electron in crystal are completely free and they have certain mass.

But according to band theory the electrons in crystal are not completely free. But interact by periodic potential of crystal. Thus, the motion of electron differ due to the interaction This altered value of mass is called effective mass.

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The velocity of electron (v) = Gr. vel. of wave packet. $v = v_g = \frac{d\omega}{dK}$ .... (i)

* Remembering

$E = hf = \left(\frac{h}{2\pi}\right) 2\pi f = \hbar\omega$

$\Rightarrow \omega = \frac{E}{\hbar}$ .... (ii)

$v_g = \frac{d}{dK}\left(\frac{E}{\hbar}\right) = \frac{1}{\hbar}\frac{dE}{dK}$ .... (iii)

differentiating eqn (iii)

$\frac{dv_g}{dt} = \frac{d}{dt}\left(\frac{1}{\hbar}\frac{dE}{dK}\right)$ (iv)

$\frac{dv_g}{dt} = a = \left(\frac{1}{\hbar^2}\frac{d^2E}{dK^2}\right)\left(\hbar\frac{dK}{dt}\right)$

$p = \hbar K$, $\frac{dp}{dt} = \frac{d}{dt}(\hbar K)$

$F = \hbar\frac{dK}{dt}$ .... (v)

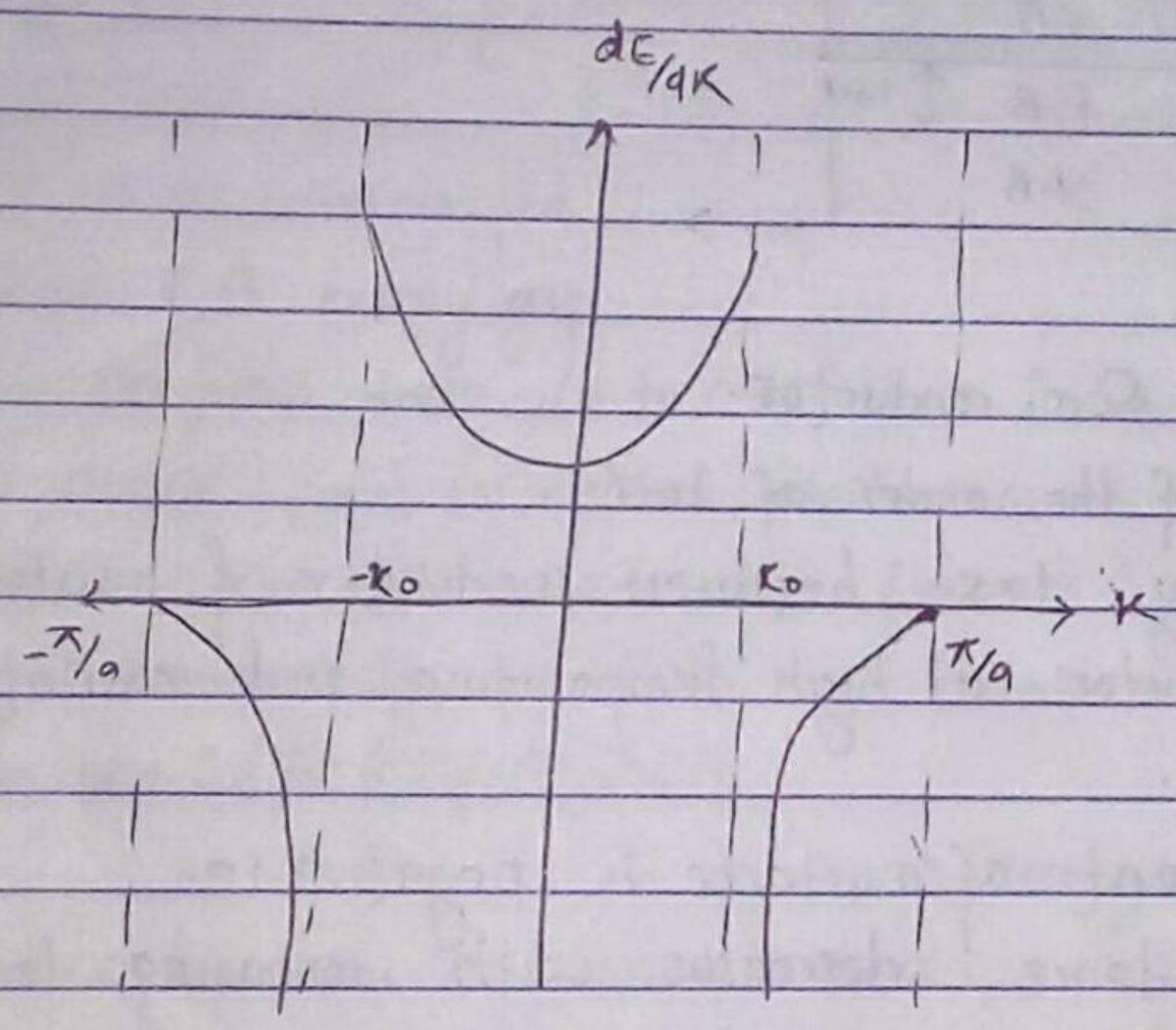
$a = \left(\frac{1}{\hbar^2}\frac{d^2E}{dK^2}\right)F$

$\Rightarrow a = \frac{1}{m^*}F$

where, $\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2E}{dK^2}$ ... (vi)

$\Rightarrow F = m^* a$

is effective mass.



In equation (vii), $\frac{d^2E}{dK^2}$ gives the slope of $\frac{dE}{dK}$ vs K.

For $K = -K_0$ to K_0, the slope is +ve i.e. $\frac{d^2E}{dK^2}$ is +ve.

and hence m^* is +ve.

Also, for $K = -\pi/a$ to $-K_0$ and $K = K_0$ to π/a, the slope is -ve ie.
$\frac{d^2E}{dK^2}$ is -ve and hence m^* is -ve.

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Bloch theorem:

In 1D, SWE for an electron moving in the constant potential V_0 is

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E-V_0)\psi(x) = 0.$$

$$\Rightarrow \frac{d^2}{dx}\psi(x) + K^2\psi(x) = 0. \quad \ldots (i)$$

where, $K^2 = \frac{2m}{\hbar^2}(E-V_0)$

The solution of equation (i) is of the form,

$$\psi(x) = e^{\pm iKx} \quad \ldots (ii)$$

But for an electron moving in 1D periodic potential, $V(x) = V(x+a)$.

The SWE is

$$\frac{d^2}{dx^2}\psi(x+a) + \frac{2m}{\hbar^2}(E - V(x+a)\psi(x+a) = 0.$$

$$\Rightarrow \frac{d^2}{dx^2}\psi(x) + \frac{2m}{\hbar^2}(E-V(x))\psi(x) = 0 \quad \ldots (iii)$$

Bloch theorem is concerned with the solution of eqn (iii) which are of the type of equation (ii) modulated by a function $u_k(x)$ which is also periodic.

$\therefore$ Soln of eqn (iii) is of the form,

$$\psi(x) \; u_k(x)\, e^{-ikx} \quad \ldots (iv)$$

where $u_k(x)$ is periodic, $u_k(x) = u_k(x+a) \quad \ldots (v)$.

The solution of type of eqn (iv) are called Bloch function.

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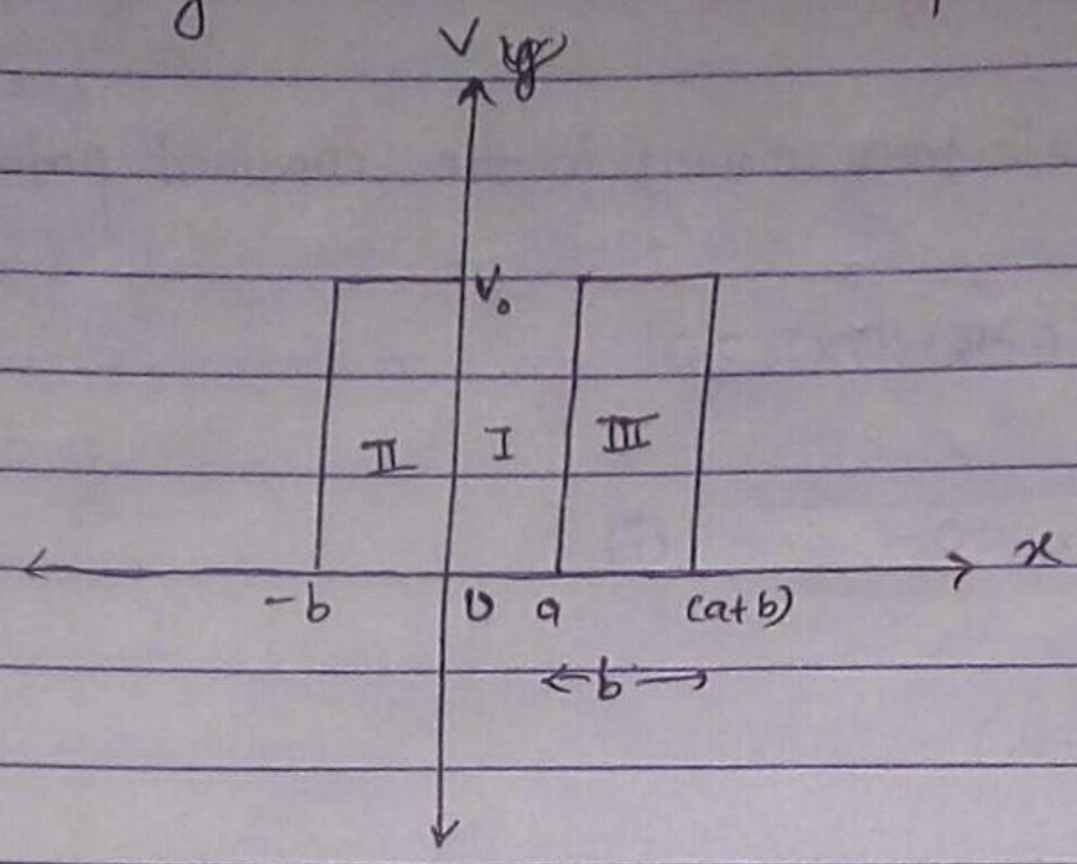
Kronig - Penny model. (Behaviour of electron in periodic potential)



The kronig-Penny model describes the behaviour of electron in the periodic potential. It consists of the regularly spaced potential wells and barriers

The potential experienced by electron due to ion core is given by,

$$V(x) = 0 \quad , \quad 0 < x < a$$
$$V(x) = V_0 , \quad -b \le x \le 0$$
$$a \le x \le (a+b)$$

Now, the SWE in 1D,

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi(x) = 0$$

Using this in region I $(0<x<a)$

$$\frac{d^2\psi_1(x)}{dx^2} + \frac{2m}{\hbar^2}(E-0)\psi_1(x) = 0.$$

$$\Rightarrow d^2\psi_1(x) + \frac{2m}{\hbar^2}\alpha^2\psi_1(x) = 0 \quad \ldots (i)$$

where $\alpha^2 = \frac{2m}{\hbar^2}(E-0)$

Soln. of eqn (i) is of the form, $\psi_1(x) = Ae^{\pm i\alpha x} + Be^{-i\alpha x} \quad \ldots (ii)$

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In the region II $(-b \le x \le 0)$, $V = V_0 > E$

Now, using SWE in this region,

$$\frac{d^2\psi_2(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\,\psi_2(x) = 0$$

$$\frac{d^2\psi_2(x)}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\,\psi_2(x) = 0$$

$$\frac{d^2\psi_2(x)}{dx^2} - \beta^2\,\psi_2(x) = 0 \quad \ldots (iii)$$

where, $\beta^2 = \frac{2m}{\hbar^2}(V_0 - E)$

The solⁿ of eqⁿ (iii) is of the type,

$$\psi_2(x) = A_2 e^{\beta x} + B_2 e^{-\beta x} \quad \ldots (iv).$$

In region III $(a \le x \le (a+b))$, $V = V_0$

Since potential is periodic, the solution in the region III can $\psi_3(x)$ be written by using Bloch function.

$$\therefore \psi_3(x) = \psi_2(x)\, e^{\pm iK(a+b)} \quad [a+b, \text{separation betⁿ reg II \& III}]$$

$$= \left(A_2 e^{\beta x} + B_2 e^{-\beta x}\right) e^{iK(a+b)} \quad \ldots (v)$$

Applying the boundary condition for region I & II at $x = 0$,

$$\psi_1(x)\big|_{x=0} = \psi_2(x)\big|_{x=0}$$

$$\Rightarrow \left(Ae^{i\alpha x} + Be^{-i\alpha x}\right)_{x=0} = \left(A_2 e^{\beta x} + B_2 e^{-\beta x}\right)_{x=0}$$

$$\Rightarrow A + B = A_2 + B_2 \quad \ldots (vi) \qquad A_2 = C,\ B_2 = D.$$

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Also,

$$\left[\frac{d}{dx}\psi_1(x)\right]_{x=0} = \left[\frac{d}{dx}\psi_2(x)\right]_{x=0}$$

$$\Rightarrow \left[\frac{d}{dx}\left(Ae^{i\alpha x} + Be^{-i\alpha x}\right)\right]_{x=0} = \left[\frac{d}{dx}\, Ce^{\beta x} + De^{-\beta x}\right]_{x=0}$$

$$\Rightarrow \left(i\alpha Ae^{i\alpha x} - i\alpha Be^{-i\alpha x}\right)_{x=0} = \left(\beta Ce^{\beta x} - \beta De^{-\beta x}\right)_{x=0}$$

$$\Rightarrow i\alpha(A - B) = \beta(C - D) \qquad \ldots\ (vii)$$

Also, applying boundary condition for boundary between region I & III,

$$\psi_1(x)\Big|_{x=a} = \psi_3(x)\Big|_{x=-b}$$

$$\Rightarrow \left(Ae^{+i\alpha x} + Be^{-i\alpha x}\right)_{x=a} = \left[\left(Ce^{\beta x} + De^{-\beta x}\right) e^{ik(a+b)}\right]_{x=-b}$$

$$\Rightarrow Ae^{+i\alpha a} + Be^{-i\alpha a} = \left(Ce^{-\beta b} + De^{\beta b}\right)e^{ik(a+b)} \qquad \ldots\ (viii)$$

Also,

$$\left[\frac{d}{dx}\psi_1(x)\right]_{x=a} = \left[\frac{d}{dx}\psi_3(x)\right]_{x=-b}$$

$$\Rightarrow \left(i\alpha Ae^{i\alpha x} - i\alpha Be^{-i\alpha x}\right)_{x=a} = \left[\left(\beta Ce^{\beta x} - \beta De^{-\beta x}\right)e^{ik(a+b)}\right]_{x=-b}$$

$$\Rightarrow i\alpha Ae^{i\alpha a} - i\alpha Be^{-i\alpha a} = \left(\beta Ce^{-\beta b} - \beta De^{\beta b}\right)e^{ik(a+b)} \qquad \ldots\ (ix)$$

Equations vi, vii, viii, & ix are the four homogeneous eq^n.s with four unknowns. The non-trivial solution of these equations is possible only when the determinant of the coefficient vanishes.

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$$\begin{vmatrix} 1 & 1 & -1 & -1 \\ i\alpha & -i\alpha & -\beta & \beta \\ e^{i\alpha a} & e^{-i\alpha a} & -e^{-\beta b}\cdot e^{ik(a+b)} & -\beta e^{\beta b} e^{ik(a+b)} \\ i\alpha e^{i\alpha a} & -i\alpha e^{-i\alpha a} & -\beta e^{-\beta b}\cdot e^{ik(a+b)} & \beta e^{\beta b}\cdot e^{ik(a+b)} \end{vmatrix} = 0$$

On solving,

$$\left(\frac{\beta^2-\alpha^2}{2\alpha\beta}\right)\sinh\beta b \sin\alpha a + \cosh\beta b \cos\alpha a = \cos k(a+b)$$

for $\beta \gg \alpha$, & $b \to 0$.

$$\beta^2 - \alpha^2 \approx \beta^2$$
$$\sinh\beta b \approx \beta b$$
$$\cosh\beta b \approx 1.$$

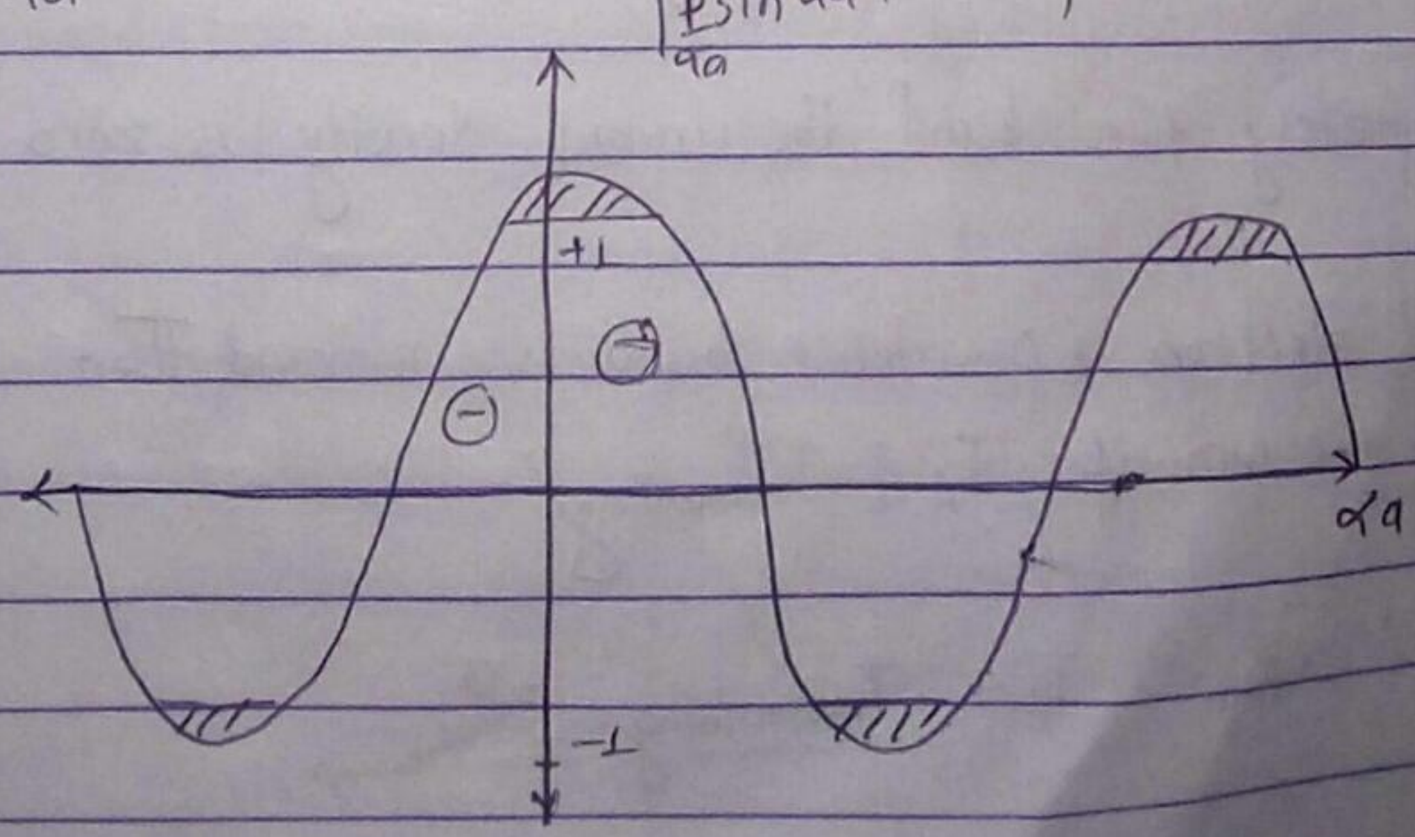
ie. $\frac{\beta^2}{2\alpha\beta}\beta b \sin\alpha a + \cos\alpha a = \cos ka.$

$$\Rightarrow \frac{\beta^2}{2a\alpha} ab \sin\alpha a + \cos\alpha a = \cos ka.$$

$$\Rightarrow \frac{P}{\alpha a}\sin\alpha a + \cos\alpha a = \cos ka \quad \dots \quad (x)$$

where, $P = \frac{\beta^2 ab}{2}$.

Graph of $\frac{P}{\alpha a}\sin\alpha a + \cos\alpha a = \cos ka$



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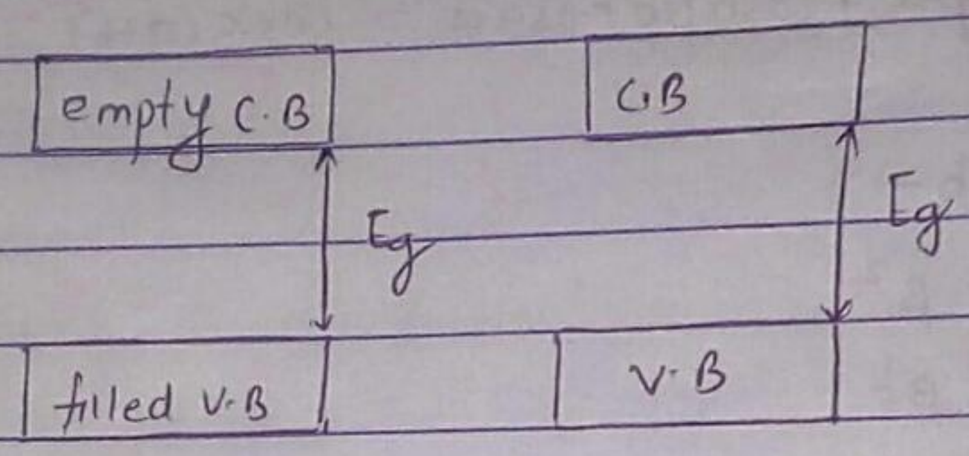
The wave solutions are possible only for the region where the value of $\left|\frac{P}{\alpha a}\sin\alpha a + \cos\alpha a\right|$ lies between -1 to $+1$. But, at other regions, there is no possible wave function. Thus, the energy spectrum of electron consists of allowed energy regions separated by forbidden energy region.

Holes:



a. fig - at absolute zero (0K) b. fig - at $T > 0K$

At absolute zero (0K), semiconductor has completely filled valance band, completely empty band. The VB and CB are separated by energy gap E_g and hence semiconductor behaves as insulator

But, when temperature is increased ($T > 0K$). The electrons in VB are excited to conduction band and there will be missing of electron in V.B. The empty state in VB is called hole. and it behaves as mobile positive charge.

For completely filled band, the current density is zero ie. $J_{full} = 0 \ldots (i)$

Suppose i^{th} electron of valence band is removed. Then current density is the sum of J_i & $J_{remaining}$

$$\therefore J_{full} = J_i + J_{remaining} = 0$$

$$\Rightarrow J_i = -J_{remaining} \ldots (ii)$$

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If v_i the drift velocity of ith electron,

$$J_i = -ev_i \quad (J = ven \text{ for } n=1) \quad \ldots (iii)$$

But the acceleration of ith electron,

$$a_i = \frac{v_i}{\tau_i}$$

$$\Rightarrow v_i = a_i \tau_i \quad \ldots (iv) \qquad \tau_i = \text{relaxation time.}$$

Using (iv) in (iii),

$$J_i = -e a_i \tau_i \quad \ldots (v)$$

Also, $J_{remaining} = e a_i \tau_i \quad \ldots (vi)$

Thus, current density due to remaining electrons after i^{th} electron is removed is equivalent to that of single i^{th} electron

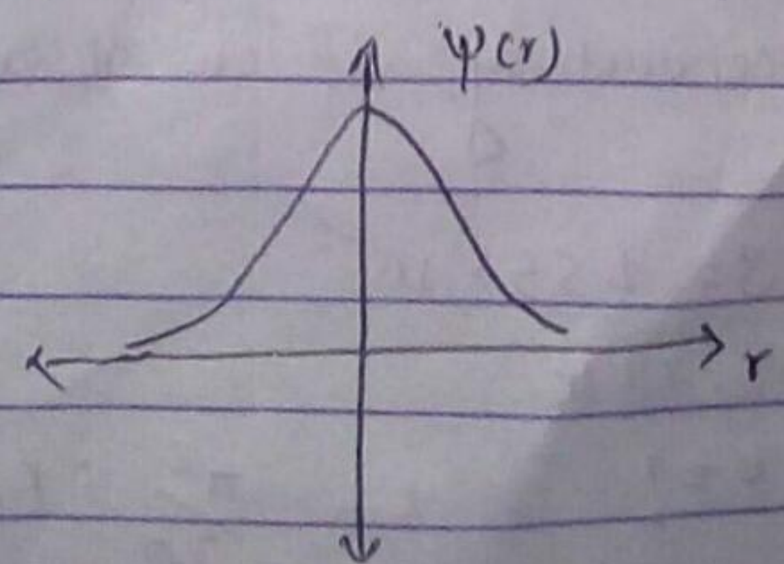
Tight binding approximation :

The TBA is used to calculate the electronic band structure using wave functions. This approximation holds good for inner electrons of atoms but not for conduction electrons.

The ground state wave function of hydrogen atom,

$$\psi(r) = e^{-r/a_0}, \quad a_0 = \text{Bohr's radius} = \frac{\varepsilon_0 n^2 h^2}{\pi m e^2}.$$

From this wave function it is clear that ψ decreases exponentially with r.



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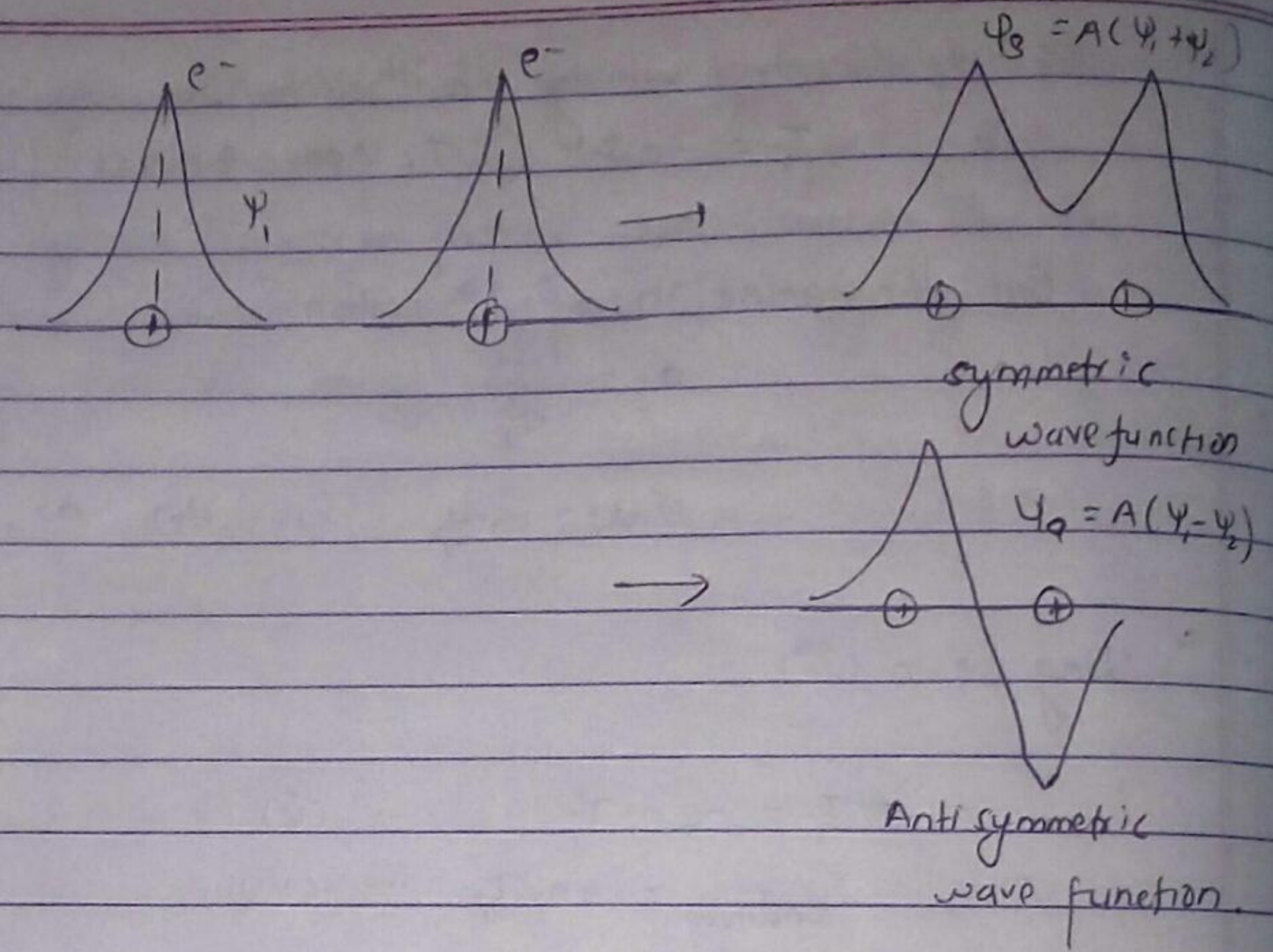

Remarks

T.B.A.

When two hydrogen atoms approach each other, their wave functions overlap. They may form symmetric wave function if they are in phase and form antisymmetric wave function if they are out of phase.

$\psi_S = A(\psi_1 + \psi_2)$, is the symmetric wave function.

Also, $\psi_A = A(\psi_1 - \psi_2)$, is the antisymmetric wave function.

But,

$|\psi_S^2|$ and $|\psi_A^2|$ represents the probability associated with symmetric and antisymmetric wave function.

When atoms are brought together, the energy levels are formed for each atoms and hence, energy band is formed.

Resistivity of copper at 273K is 1.55×10^{-6} Ωm. Estimate the electronic thermal conductivity of Cu at same temperature.

Soln

$\rho = 1.55 \times 10^{-6}$.

$T = 273K$

$\sigma = \frac{ne^2\tau}{m}$

f. $k = ?$

$k = \frac{\pi^2}{3m} n k_B^2 T \tau$.

$\frac{1}{\rho} = \sigma$

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Copper has phase standard cubic structure with one atom basis. The density of copper is $8.96\ gm\,cc^{-1}$. and its at. weight is $63.5\ gm\,mole^{-1}$. What is the length of unit cube of the structure?

Soln Here,

density of copper (ρ) $= 8.96 \times 10^3\ kg\ m^{-3}$

at. weight (M) $= 63.5 \times 10^{-3}\ kg$, $a = ?$

Now,

for f.c.c.,

$n = 4$.

$$V = \frac{nM}{\rho N_A} = \frac{4 \times 63.5 \times 10^{-3}}{8.9 \times 10^3 \times 6.023 \times 10^{23}} = ___$$

$V = a^3$

$\Rightarrow a = (V)^{1/3}$

$= ___$.

The electrical conductivity of copper at room temperature is $5.89 \times 10^7\ \Omega^{-1} m^{-1}$. The fermi energy of copper is 6.95 eV. and carrier density $8.4 \times 10^{28}\ e^{-s} m^{-3}$. Calculate mean free path of electrons.

Soln Here,

$\sigma = 5.89 \times 10^7\ \Omega^{-1} m^{-1}$.

$E_f = 6.95\ eV$.

$= 6.95 \times 1.6 \times 10^{-19}\ J$.

$n = 8.4 \times 10^{28}\ e^{-s}/m^3$.

mean free path of electrons $= ?$

The mean free path of electrons $(l) = v_f \tau$

Now,

$$v_f = \left(\frac{2E_f}{m}\right)^{1/2} = ___$$

$$\tau = \frac{\sigma m}{ne^2} = ___$$

$\therefore l = v_f \tau$. $= ___$

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The density of alumunium is $2.70\ gmcc^{-1}$ and molecular wt. is $26.98\ gm\,mole^{-1}$. Calculate the fermi energy. What is the effective mass of electron in alumunium if experimental value of fermie energy is 12eV. (Al. is trivalent).

Soln Here,

$$\rho = 2.70\ gmcc^{-1} = 2.70\times10^{3}\ kgm^{-3}$$
$$M = 26.98\ gm\,mol^{-1} = 26.98\times10^{-3}\ kgmol^{-1}$$

$$\rho = \frac{NM}{VN_A}$$

$$\Rightarrow \frac{N}{V} = \frac{\rho N_A}{M}$$

$$\Rightarrow n = ____\ atm/m^3$$
$$= ____\ \times 3\ e^{\ominus}/m^3$$

$$V = \frac{\rho}{M} = ____$$

$$\therefore E_f = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

$$= ____\ J.$$

Now,

$$m^* = ?$$

Here, $m^* = \dfrac{\hbar^2 (3\pi^2 n)^{2/3}}{2E_f}$.

$$= ____.$$

If the fermi energy of metal is 12eV; what is the crosspondng classical temperature.

Soln

$$E_f = 12eV$$
$$T_f = ? = E_f/k_B.\ K.$$

Unit-6
Semiconductor and Semiconductor devices

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Semi-Conductor.

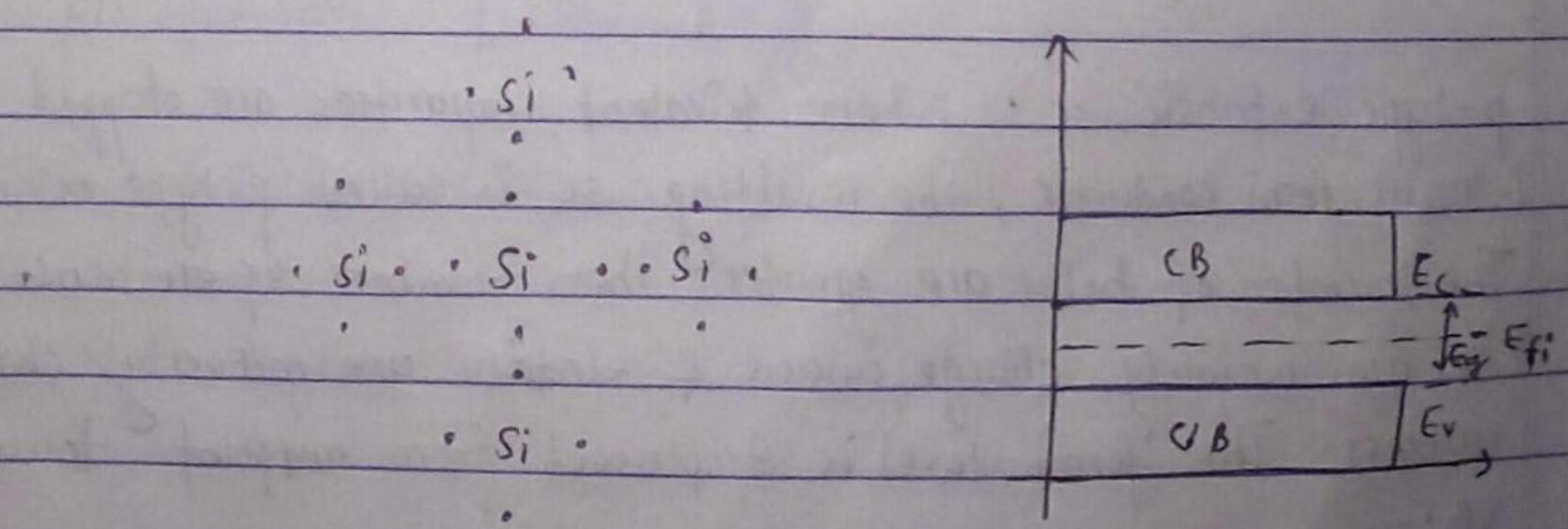
The material whose electrical conductivity lies between conductor and insulator is called semi-conductor. For semi conductor the forbidden energy gap between VB & CB is less than ~~free~~ 3eV.
for silicon - 1.1eV, ge - 0.7eV.

At absolute zero, no conduction is possible and it behaves as insulator. But, when temperature is increased some of the valence electrons are excited to the conduction band which causes the electric conduction. As the electrons leave the VB, there will be the missing of electron in VB called hole. Such holes also contribute to the electric conduction. Thus, the conductivity of semi conductor increases with temperature.

Types of semi-conductor:

The conductivity of semi conductor can be increased by adding certain impurities. Based on these impurities concentration semi conductor are classified into two types:

1. Intrinsic semiconductor:
It is the pure form of semi conductor. It has equal numbers of electrons & holes and fermi level lies in between VB & CB



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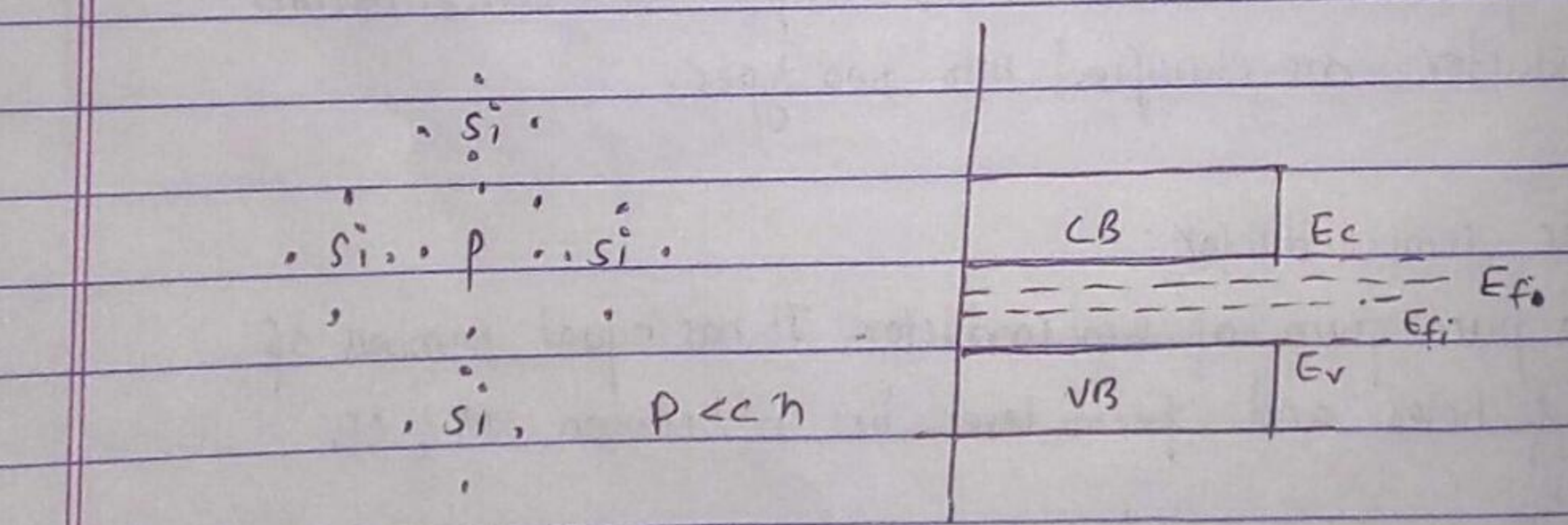
The fermi level lies at middle betn VB & CB. Therefore, $E_{f_i} = \frac{E_c + E_v}{2}$

2. Extrinsic semiconductor: When an ~~Extrinsic~~ Intrinsic SC dopped with atom of trivalent or pentavalent impurities the resulting SC is called Extrinsic semiconductor. The fermi level is displaced in extrinsic SC.

Types of extrinsic SC:

a. n-type extrinsic SC: When pentavalent impurities are dopped to intrinsic semi conductor, the resulting SC is called n-type extrinsic SC. The no's of electrons are greater than numbers of hole in this type of SC. The electrons are majority and holes are minority charge carrier. The fermi level is displaced from mid point towards CB.



b. p-type extrinsic SC: When trivalent impurities are dopped to intrinsic semi conductor, the resulting SC is called p-type extrinsic SC. The numbers of holes are greater than numbers of electrons. The holes are majority charge carriers & electrons are minority charge carriers. The fermi level is displaced from midpoint towards VB.

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" Density of state $D(E) = \frac{dn}{dE}$ "

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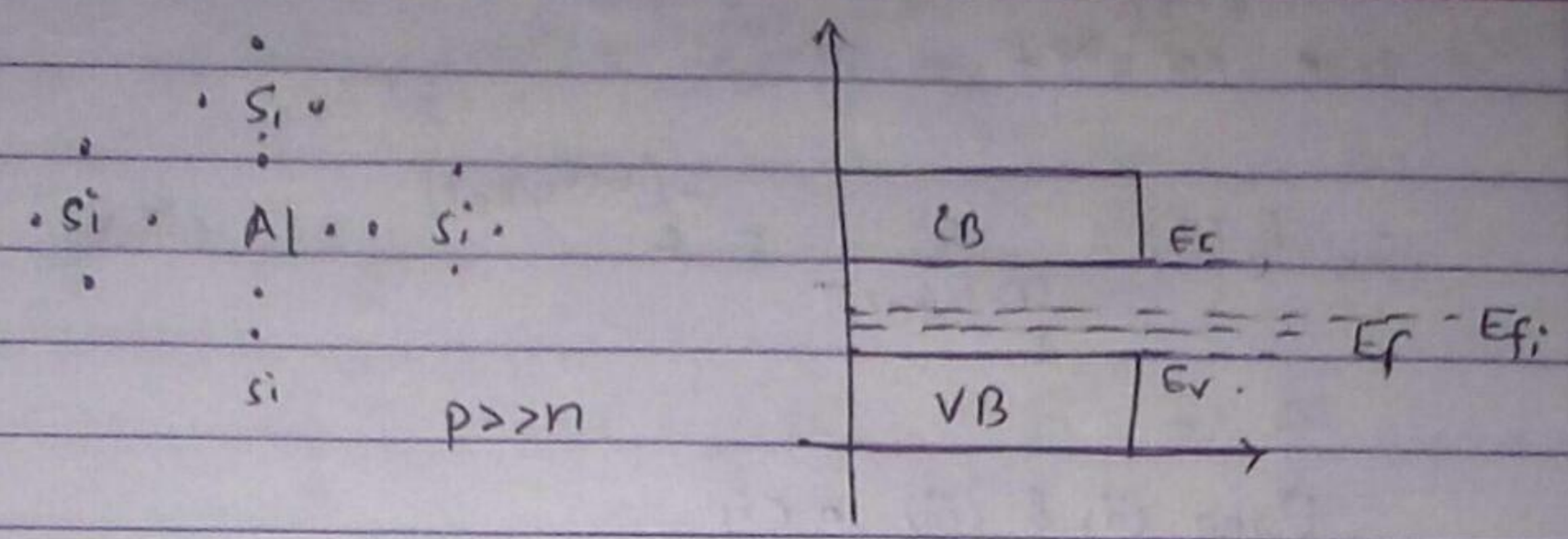

Statics of holes and electrons:

The concentration (number) of electron and holes in CB and VB of semiconductor are called statics of electrons and holes resp. These are also called carrier concentration.

Carrier concentration in intrinsic SC.

a. Electron concentration (n): The concentration of electrons in CB

$$n = \int D_e(E)\, f_e(E)\, dE \quad \dots (i)$$

where, $D_e(E) = \frac{V}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}(E - E_c)^{1/2}$

for $V=1$, $D_e(E) = \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}(E-E_c)^{1/2}$ ... (ii) is density of electron in 3D.

Also, FD function, $f_e(E) = \frac{1}{e^{\left(\frac{E-\mu}{k_BT}\right)}+1}$

But, at $T = 0K$, $\mu = E_f$

$$\therefore f_e(E) = \frac{1}{e^{\left(\frac{E-E_f}{k_BT}\right)}+1}$$

If $E - E_f \gg k_BT$

$$\frac{E-E_f}{k_BT} \to \infty$$

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$$e^{\frac{E-E_f}{K_BT}} >> 1$$

$$\therefore f_e(E) = \frac{1}{e^{(E-E_f/K_BT)}} = e^{-(E-E_f/K_BT)} \quad \ldots (iii)$$

Using (ii) & (iii) in (i)

$$n = \int_{E_c}^{\infty} \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2}(E-E_c)^{1/2} \times e^{-\left(\frac{E-E_f}{K_BT}\right)} dE$$

$$= \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} \int_{E_c}^{\infty} (E-E_c)^{1/2} \times e^{-\left(\frac{E-E_f}{K_BT}\right)} dE$$

$$= \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} \int_{E_c}^{\infty} (E-E_c)^{1/2} \times e^{-\left(\frac{E-E_c+E_c-E_f}{K_BT}\right)} dE$$

$$= \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} \int_{E_c}^{\infty} (E-E_c)^{1/2} \times e^{-\left(\frac{E-E_c}{K_BT}\right)} \cdot e^{-\left(\frac{E_c-E_f}{K_BT}\right)} dE$$

$$= \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} e^{-\frac{(E_c-E_f)}{K_BT}} \int_{E_c}^{\infty} (E-E_c)^{1/2} e^{-\left(\frac{E-E_c}{K_BT}\right)} dE.$$

put $\frac{E-E_c}{K_BT} = x$.

$$\Rightarrow \frac{E}{K_BT} - \frac{E_c}{K_BT} = x$$

$$\Rightarrow \frac{dE}{K_BT} = dx$$

$$\Rightarrow dE = K_BT\,dx$$

When, $E = E_c$, $x = 0$

$E = \infty$, $x = \infty$

$$\therefore n = \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} e^{-\left(\frac{E_c-E_f}{K_BT}\right)} \int_0^{\infty} (K_BT \cdot x)^{1/2} e^{-x} K_BT\,dx.$$

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gamma function $\int_0^\infty e^{-x} x^n dx = \Gamma(n+1)$

$= n\Gamma(n)$.

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$$= \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} e^{-\left(\frac{E_c-E_f}{k_BT}\right)} (k_BT)^{3/2} \int_0^\infty e^{-x} x^{1/2} \quad \ldots (iv)$$

Using gamma integral,

$$\int_0^\infty e^{-x} x^{1/2} dx = \frac{1}{2}\Gamma\tfrac{1}{2} = \frac{1}{2}\sqrt{\pi} = \frac{\sqrt{\pi}}{2} \quad \ldots (v)$$

$$\therefore n = \frac{1}{2\pi^2}\left(\frac{2m_e}{\hbar^2}\right)^{3/2} e^{-\left(\frac{E_c-E_f}{k_BT}\right)} \cdot (k_BT)^{3/2} \cdot \frac{\sqrt{\pi}}{2}.$$

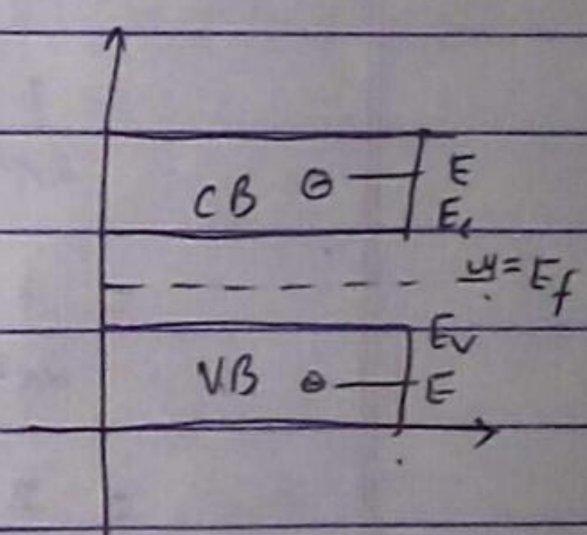
$$= \frac{1}{4\pi^{3/2}}\left(\frac{2m_e k_BT}{\hbar^2}\right)^{3/2} e^{-\left(\frac{E_c-E_f}{k_BT}\right)}$$

$$= 2\left(\frac{m_e k_BT}{2\pi\hbar^2}\right)^{3/2} e^{-\left(\frac{E_c-E_f}{k_BT}\right)}.$$

$$n = N_c e^{-(E_c-E_f)/k_BT} \quad \ldots (vi)$$

where $N_c = 2\left(\frac{m_e k_BT}{2\pi\hbar^2}\right)^{3/2}$.

eqn (vi) gives carrier concentration for electron



b. Carrier concentration of holes:

The carrier concentration of holes in VB is

$$p = \int_{-\infty}^{E_v} f_h(E) D_h(E) dE \quad \text{where } D_h(E) = \frac{V}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2}(E_v-E)^{1/2}$$

$$\Rightarrow p = \int_{-\infty}^{E_v} e^{\frac{E-E_f}{k_BT}} \cdot \frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2}(E_v-E)^{1/2} dE \quad \& \quad f_h(E) = 1 - \frac{1}{e^{\left(\frac{E-\mu}{k_BT}\right)}+1}$$

$$= \frac{e^{\frac{E-\mu}{k_BT}}}{e^{\frac{(E-\mu)}{k_BT}}+1}$$

$$\Rightarrow p = \frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2} \int_{-\infty}^{E_v} e^{\frac{E-E_f}{k_BT}} \cdot (E_v-E)^{1/2} dE.$$

$$\Rightarrow p = \frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2} \int_{-\infty}^{E_v} e^{\frac{E-E_v+E_v-E_f}{k_BT}} \cdot (E_v-E)^{1/2} dE$$

If $E-\mu \gg k_BT$ & $E-\mu$ is $-ve$.

$\therefore f_h(E) = e^{\frac{E-\mu}{k_BT}} / 0+1$

$$\Rightarrow p = \frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2} e^{-\frac{(E_f-E_v)}{k_BT}} \int_{-\infty}^{E_v} e^{-\frac{(E_v-E)}{k_BT}} (E_v-E)^{1/2} dE$$

ie. $f_h(E) = e^{\frac{E-\mu}{k_BT}}$ for abs. zero $\mu = E_f$.

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$\Rightarrow p =$

Let $\frac{E_v - E}{k_B T} = x$

$\Rightarrow E_v - E = k_B T x$

$\Rightarrow -dE = k_B T dx$.

If $E = -\infty$, $x = \infty$

If $E = E_v$, $x = 0$

Now, from eq^n (i)

$$p = \frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2} e^{-\frac{(E_f - E_v)}{k_B T}} \int_{\infty}^{0} e^{-x} (k_B T x)^{1/2} (-k_B T\, dx)$$

$$= \frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2} e^{-\frac{(E_f - E_v)}{k_B T}} \int_{0}^{\infty} e^{-x} (k_B T x)^{1/2} k_B T\, dx$$

$$= \frac{1}{2\pi^2}\left(\frac{2m_h}{\hbar^2}\right)^{3/2} e^{-\frac{(E_f - E_v)}{k_B T}} (k_B T)^{3/2} \int_{0}^{\infty} e^{-x} x^{1/2}\, dx$$

$$= \frac{1}{2\pi^2}\left(\frac{2m_h k_B T}{\hbar^2}\right)^{3/2} e^{-\frac{(E_f - E_v)}{k_B T}} \frac{1}{2}\sqrt{\pi} \quad \left(\because \text{using gamma integral}\right)$$

$$= 2\left(\frac{m_h k_B T}{2\pi\hbar^2}\right)^{3/2} e^{-\frac{(E_f - E_v)}{k_B T}}.$$

$$= N_v e^{-\frac{(E_f - E_v)}{k_B T}} \quad \text{where } N_v = 2\left(\frac{m_h k_B T}{2\pi\hbar^2}\right)^{3/2}$$

Intrinsic carrier density

The intrinsic carrier density can be obtained as,

$$n_i^2 = np$$

$$= N_c e^{-\frac{E_c + \mu}{k_B T}} \cdot N_v e^{-\frac{\mu + E_v}{k_B T}}$$

$$= N_c \cdot N_v e^{-\frac{E_c + \mu - \mu + E_v}{k_B T}}$$

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$$= N_c N_v \, e^{-\frac{(E_c - E_v)}{K_B T}}$$

$$n_i^2 = N_c N_v \, e^{-E_g/K_B T}, \quad E_g = E_c - E_v \text{ is band gap.}$$

$$n_i = \sqrt{N_c N_v} \cdot e^{\frac{-E_g}{2K_B T}} \quad \cdots (*).$$

Fermi level in intrinsic SC.

for intrinsic SC.

$$n = p$$

$$N_c \cdot e^{-\frac{(E_c - \mu)}{K_B T}} = N_v \cdot e^{-\frac{(\mu - E_v)}{K_B T}}$$

$$\Rightarrow 2\left(\frac{m_e K_B T}{2\pi \hbar^2}\right)^{3/2} e^{-\frac{(E_c - \mu)}{K_B T}} = 2\left(\frac{m_h K_B T}{2\pi \hbar^2}\right)^{3/2} e^{-\frac{(\mu - E_v)}{K_B T}}$$

$$\Rightarrow (m_e)^{3/2} \cdot e^{\frac{-E_c}{K_B T}} e^{\frac{\mu}{K_B T}} = (m_h)^{3/2} \cdot e^{-\mu/K_B T} \cdot e^{E_v/K_B T}$$

$$\Rightarrow e^{\frac{2\mu}{K_B T}} = \left(\frac{m_h}{m_e}\right)^{3/2} \cdot e^{\frac{E_c + E_v}{K_B T}}$$

Taking ln on both sides.

$$\Rightarrow \frac{2\mu}{K_B T} = \ln\left(\frac{m_h}{m_e}\right)^{3/2} + \frac{E_c + E_v}{K_B T}$$

$$\Rightarrow \frac{2\mu}{K_B T} = \frac{3}{2} \ln\left(\frac{m_h}{m_e}\right) + \frac{E_c + E_v}{K_B T}$$

$$\Rightarrow \mu = \frac{3}{4} K_B T \ln\left(\frac{m_h}{m_e}\right) + \frac{K_B T}{2}\left(\frac{E_c + E_v}{K_B T}\right)$$

$$\Rightarrow E_f = \frac{3}{4} K_B T \ln\left(\frac{m_h}{m_e}\right) + \frac{E_c + E_v}{2} \quad \cdots (i)$$

eqn (i) gives the fermi energy.

If $m_e = m_h$, $E_f = \frac{E_c + E_v}{2}$. $\cdots (ii)$

Thus, the fermi level lies exactly midway between VB and CB. if $m_e = m_h$.

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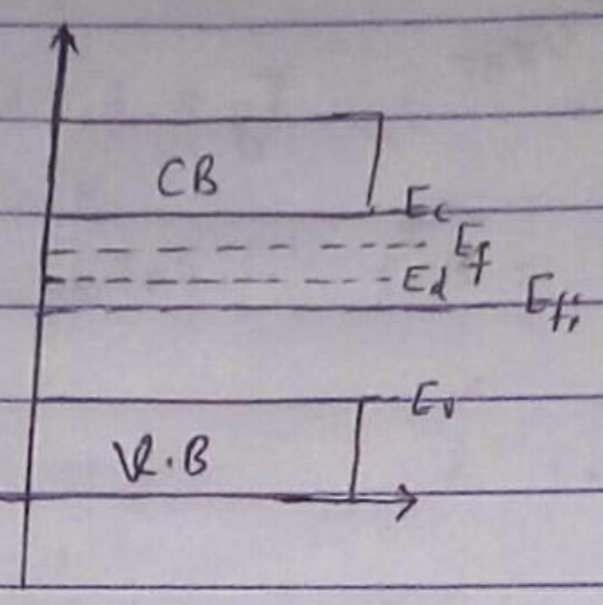
Carrier concentration of n-type sc.



The energy level diagram for n-type sc. is as shown in fig above. As the temperature is increased slightly, some of the donor atoms get ionizer. contribute electron to CB. Let N_d^+ be the ionized donor atoms out of donor atoms N_d having energ E_d. Also, some of the electrons from VB jump to CB creating holes in VB If p be the nos of holes in VB, there will be p electrons in CB.

$\therefore$ Total concentration of e^- in CB $(n) = p + N_d^+$ ....(i)

If the holes are very lesser than donor atoms,

$N_d^+ >> p$, p can be neglected

$\therefore n = N_d^+$ .... (ii), $n = N_c \cdot e^{-\frac{(E_c - \mu)}{K_B T}}$ ...(iii)

Now,

N_d = N_d^+ (ionized donor atoms) + unionized donor atoms.

$\Rightarrow N_d^+ = N_d -$ unionized donor atoms.

$\Rightarrow N_d^+ = N_d - N_d f(E_d)$

where, $f(E_d) = \frac{1}{e^{\frac{E_d - \mu}{K_B T}} + 1}$ i.e. probability for unionized atom to stay in E_d.

$\therefore N_d^+ = N_d [1 - f(E_d)]$

$= N_d \left[1 - \frac{1}{e^{\frac{E_d - \mu}{K_B T}} + 1} \right]$

$= N_d \frac{e^{\frac{E_d - \mu}{K_B T}}}{e^{(E_d - \mu)/K_B T} + 1}$.

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$N_d^+ = N_d$

$\because E_d - \mu = -ve,$

At, $T = 0\,K$ $\quad e^{\frac{E_d - \mu}{k_B \cdot 0}} = e^{-\infty} = 0$

ie. $N_d^+ = N_d\, e^{(E_d - \mu)/k_B T}$ .... (iv).

Using (iii) & (iv) in (ii)

$n = N_d^+$

$\Rightarrow N_c e^{-(E_c - \mu)/k_B T} = N_d e^{(E_d - \mu)/k_B T}$

$\Rightarrow \frac{N_c}{N_d} = e^{(E_d - \mu)/k_B T} \cdot e^{(E_c - \mu)/k_B T}$

$\Rightarrow \frac{N_c}{N_d} = e^{(E_d + E_c)/k_B T} \cdot e^{-2\mu/k_B T}.$

$\Rightarrow \frac{N_d}{N_c} = e^{-(E_d + E_c)/k_B T} \cdot e^{2\mu/k_B T}$

$\Rightarrow \ln\left(\frac{N_d}{N_c}\right) = -\frac{E_d + E_c}{k_B T} + \frac{2\mu}{k_B T}$

$\Rightarrow \frac{2\mu}{k_B T} = \ln\left(\frac{N_d}{N_c}\right) + \frac{E_d + E_c}{k_B T}$

$\Rightarrow E_f = \frac{k_B T}{2} \ln\left(\frac{N_d}{N_c}\right) + \frac{E_d + E_c}{2}$ .... (v)

Now from eqn (iii)

$n = N_c\, e^{\left[-E_c - k_B T \ln\left(\frac{N_d}{N_c}\right) - \frac{(E_d + E_d)}{2} \times \frac{1}{k_B T}\right]}$

$\therefore n = \sqrt{N_c N_v}\; e^{-E_g \times \frac{1}{2 k_B T}}$

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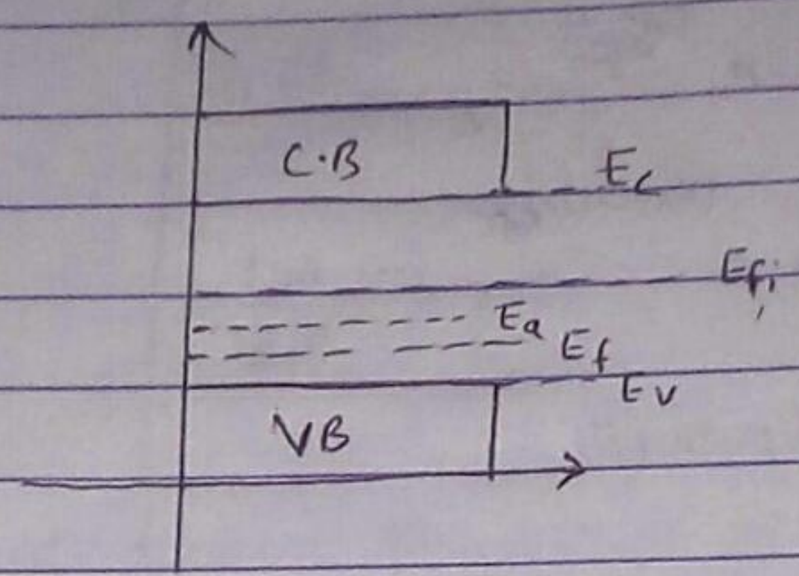
Carrier concentration of p-type SC.



The energy level diagram for p-type semiconductor is as shown in fig above.

Suppose N_a be the numbers of accepter impurity atoms having energy E_a. The holes in VB are generated by exciting electrons in CB and by accepting electrons.

$$\therefore p = n + N_a^- \quad \ldots (i)$$

where, n = no.s of electrons jumping from VB to CB.
N_a^- = no.s of ionized acceptor atoms.

If $n << N_a^-$, $p = N_a^-$ $\ldots (ii)$

But $p = N_v e^{-(E_v - E_v)/K_B T}$ $\ldots (iii)$

If $f(E_a)$ gives the probability to ionize to acceptor atoms, concentration of ionized acceptor atoms.

$$N_a^- = N_a f(E_a)$$

$$= N_a \cdot \frac{1}{e^{(E_a - E_f)/K_B T} + 1}$$

from fig. $E_a - E_f = 0$

$\therefore \frac{E_a - E_f}{K_B T}$ for $T \to 0$ is $-\infty$

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ie. $N_a^- = N_a e^{-(E_a - E_f)/k_B T}$ .... (iv)

Using eq's (iii) & (iv) in (ii),

$$p = N_a e^{-(E_a - E_f) \times \frac{1}{k_B T}}$$

$$\Rightarrow N_v e^{-(\mu - E_v)/k_B T} = N_a \cdot e^{-(E_a - E_f) \times \frac{1}{k_B T}}$$

$$\Rightarrow \frac{N_v}{N_a} = e^{-(E_a - E_f)\frac{1}{k_B T}} \cdot e^{(\mu - E_v)\frac{1}{k_B T}}$$

$$\Rightarrow \frac{N_v}{N_a} = e^{2E_f \times \frac{1}{k_B T}} e^{-(E_a + E_v)\frac{1}{k_B T}}$$

$$\Rightarrow \ln\left(\frac{N_v}{N_a}\right) = \frac{2E_f}{k_B T} - \frac{(E_a + E_v)}{k_B T}$$

$$\Rightarrow \frac{2E_f}{k_B T} = \ln\left(\frac{N_v}{N_a}\right) + \frac{E_a + E_v}{k_B T}$$

$$\Rightarrow E_f = \frac{k_B T}{2} \ln\left(\frac{N_v}{N_a}\right) + \frac{E_a + E_v}{2} \quad \text{.... (v).}$$

Now,

$$p = N_v e^{-\left\{\left[\frac{k_B T}{2} \ln\left(\frac{N_v}{N_a}\right) + \frac{E_a + E_v}{2}\right] - E_v\right\} \times \frac{1}{k_B T}}$$

On solving,

$$p = \sqrt{N_a N_v}\, e^{-\frac{E_g}{2k_B T}} \quad \text{.... (vi).}$$

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Mobility:

When electric field is applied to SC, the charge carriers ~~attend~~ a attain a certain velocity called drift velocity (v).

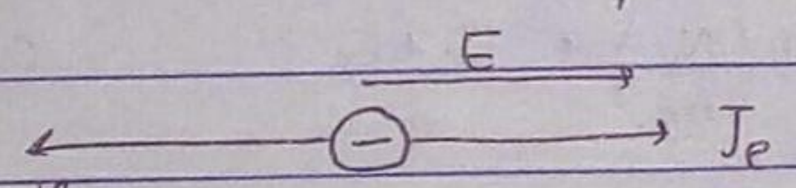
Drift velocity 'v' is directly proportional to electric field E

i.e. $v \propto E \Rightarrow v = \mu E$

$\Rightarrow \mu = \frac{v}{E}$ unit = $m^2 V^{-1} s^{-1}$

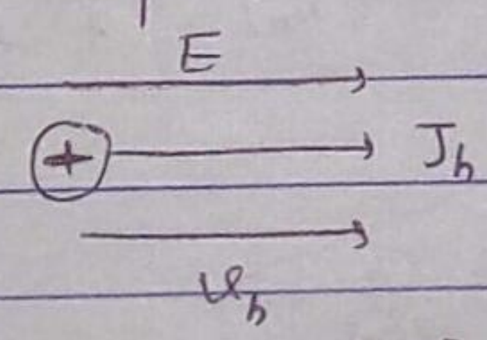
where, μ is the proportionality constant and is called mobility of charge carrier.

for electron, drift velocity v_e is in opposite to electric field E. But current density J_e is in the direction of electric field E.



Motion of e⁻ in E.

for hole, drift velocity v_h and current density J_e both are in the direction of electric field E.



Motion of h in E.

for electron, $\mu_e = \frac{|v_e|}{E}$, μ_e is mobility of electron.

for hole, $\mu_h = \frac{|v_h|}{E}$, μ_h is mobility of hole.

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Electric field in terms of mobility:

Current density $J = ven$

$J = ne(\mu E)$ .... (i)

Also, $J = \sigma E$ .... (ii), σ = electrical conductivity

from eqn (i) & (ii)

$\sigma = ne\mu$ ... (iii)

eqn (iii) gives the relation between electrical conductivity and mobility.

But for SC, the electrical conductivity is due to both electrons and holes

The electrical conductivity due to electrons $\sigma_e = ne\mu_e$

The electrical conductivity due to hole $\sigma_h = pe\mu_h$

$$\therefore \sigma = \sigma_e + \sigma_h$$
$$= ne\mu_e + pe\mu_h$$
$$= e(n\mu_e + p\mu_h) \quad \text{.... (iv)}$$

For intrinsic SC, $n = p = n_i$

$$\therefore \sigma = n_i e(\mu_e + \mu_h) \quad \text{.... (v)}$$

But, $n_i = \sqrt{N_c N_v}\, e^{-E_g/2k_BT}$

Using n_i in eqn (v),

$$\sigma = \sqrt{N_c N_v}\, e^{-E_g/2k_BT}\, e(\mu_e + \mu_h).$$
$$= \sqrt{N_c N_v}\, e(\mu_e + \mu_h)\, e^{-E_g/2k_BT} \quad \text{.... (vi)}$$

$\sigma = \sigma_0 e^{-E_g/2k_BT}$

where $\sigma_0 = \sqrt{N_c N_v}\, e(\mu_e + \mu_h)$ is a constant and is independent of temperature.

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Taking ln on both sides,

$$\ln\sigma = \ln\sigma_0 - \frac{E_g}{2k_BT} \quad \ldots (vii)$$

Comparing eqn (viii) with $y = mx + C$,

$$y = \ln\sigma, \quad m = -\frac{E_g}{2k_B} \text{ (slope -ve)}, \quad x = \frac{1}{T}.$$

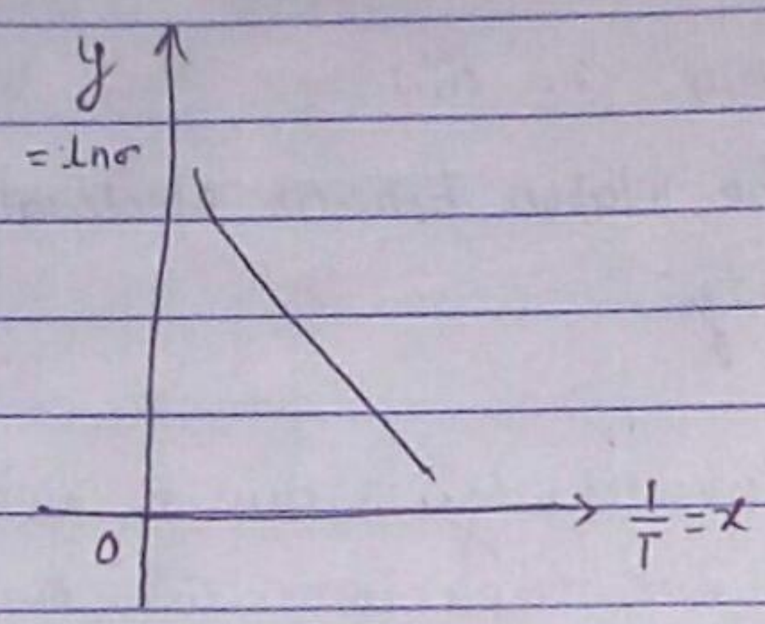
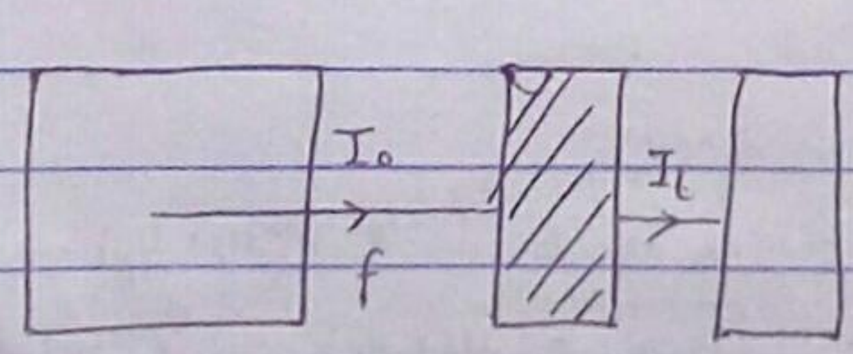


Photo conductivity:

When the semiconductor is illuminated by photons (em-radiation) of different energies, the SC absorbs photons and creates extra electrons. Due to these extra electrons, the electrical conductivity of SC is increased. This effect is called photoconductivity.



Suppose the monochromatich light from a monochromator incident on the thin slab of sc which absorbs the photons. The transmitted radiation is detected by the detector

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Suppose I_0, I_t and I_a be the intensities of incident, transmitted, and absorbed of radiation respectively. Then,

$$I_a = I_0 - I_t \quad \ldots (i)$$

Above, exp. is repeated for different wavelengths. For sc, it was observed that there is negligible absorption at higher wavelength.

At higher wavelength (low frequency),

$$E = \frac{hc}{\lambda} \text{ is lesser}$$

$$\therefore E < E_g \; ; \quad E_g = \text{Band gap betn. VB \& CB of sc.}$$

This energy cannot excit electron from VB to CB and hence there is no absorption of photons or radiations. But, at lesser.

But at lesser wavelength (high frequency),

$$E = \frac{hc}{\lambda} \text{ is greater.}$$

$$\therefore E \geq E_g \, ,$$

This energy can excit electron from VB to CB and hence results the absorption of photon.

The minimum frequency to cause photo conduction i.e. $f_{min} = \frac{E_g}{h}$. ($\because$ E_g is min. energy required for photocond.^{n})

Also,

At minimum frequency, wavelength is maximum.

$$E_g = \frac{hc}{\lambda_{max}}$$

$$\therefore \lambda_{max} = \frac{hc}{E_g}.$$

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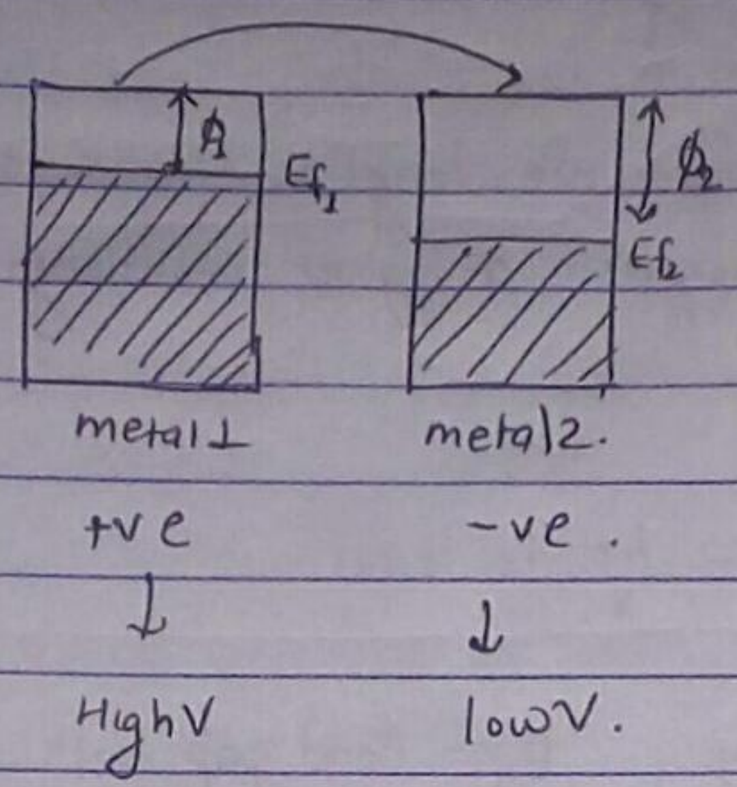
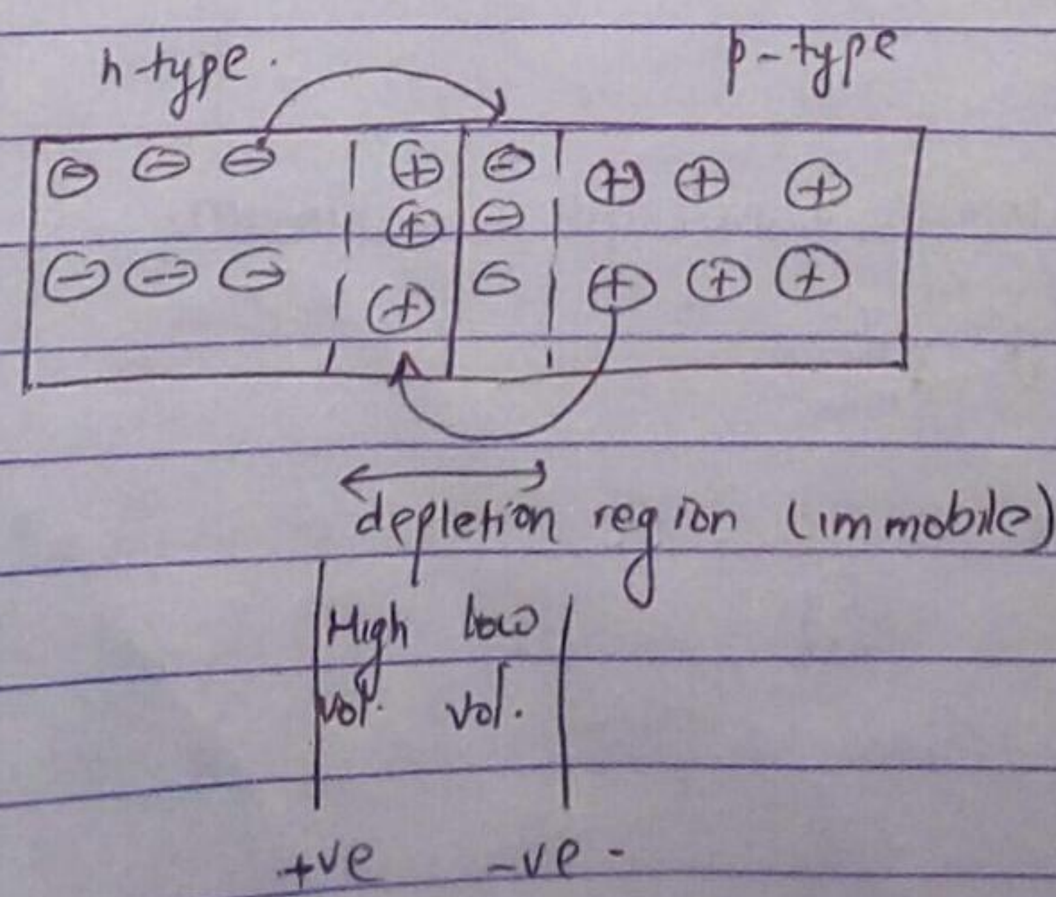
Metal-metal junction (contact potential)



Suppose the two metals of work functions ϕ_1 & ϕ_2 ($\phi_1 < \phi_2$). When they are placed in contact electrons will flow from the metal 1 of low work function to the metal 2 of high work function. This flow continues untill both metals have common fermi energy.

Due to flow of electron, metal 2 gains electrons and becomes negatively charged whereas metal 1 losses electrons and becomes +vely charged. Thus, metal 1 has higher potential than metal 2. This p.d. established across the junction when two metals are in contact is called contact potential. The contact potential (V_c) is due to difference in work function.

$$\therefore \phi_2 - \phi_1 = eV_c.$$



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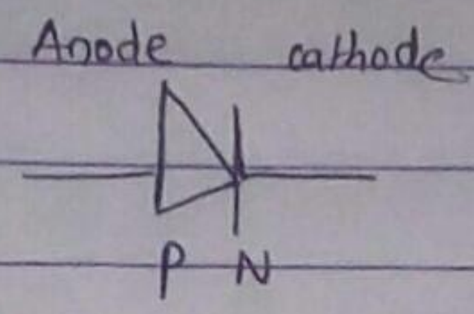
When p-type of semiconductor is joined to n-type of SC, a junction is formed between them called PN Junction and device so formed is called PN Junction diode.



PN Junction diode

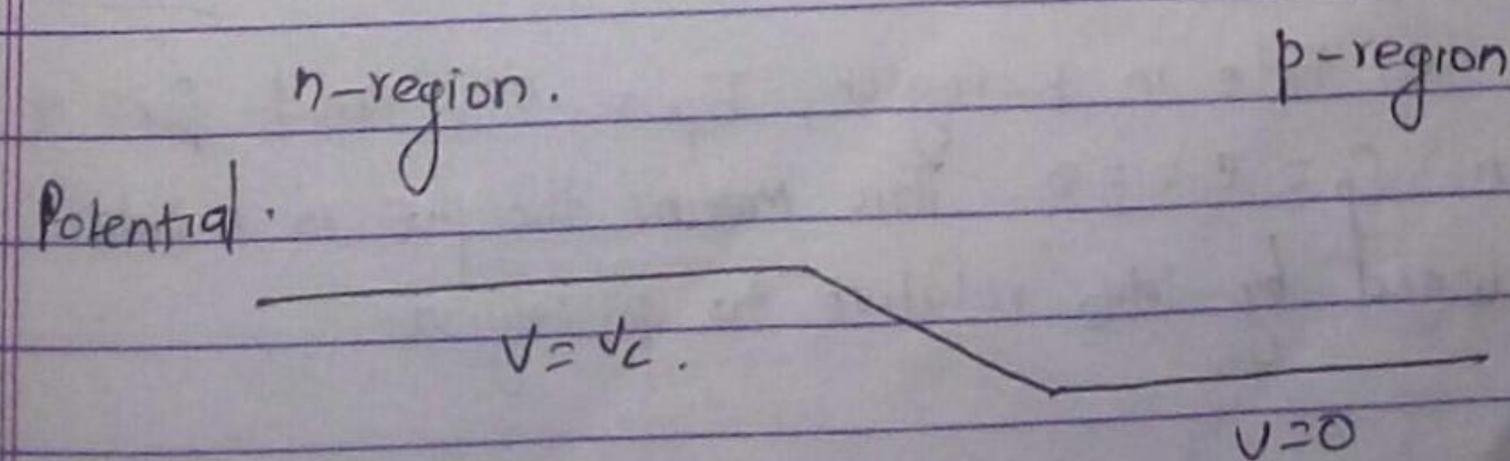
It has two terminals. The p-type region is called anode & N type region is called cathode.

Depletion region and barrier potential:

When n-type and p-type SC are joined, the electrons diffuse from n to p region and holes diffuse from p to N region. Due to diffusion negative ion is formed on P side and positive charge is formed in N region. These +ve and -ve charges are immobile and accumulate across the junction such layer at the junction is called defletion layer.

The p.d. developed across the junction due to accumulation of +ve and -ve ions is called barrier potential.

Band scheme for P-N junction diode:



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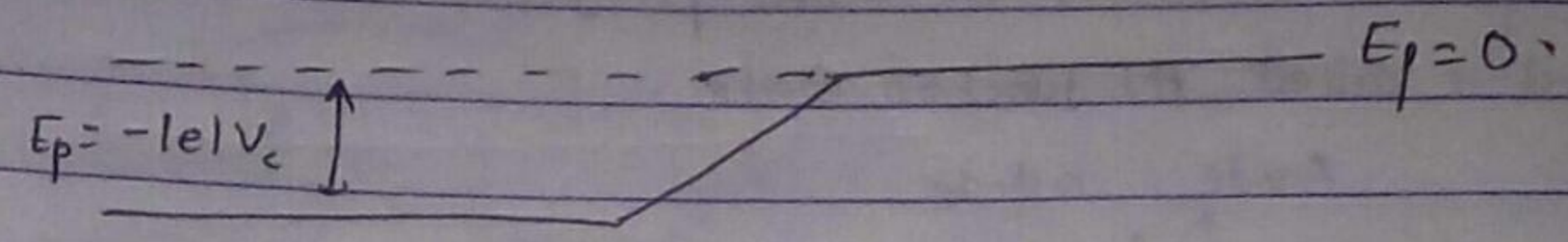
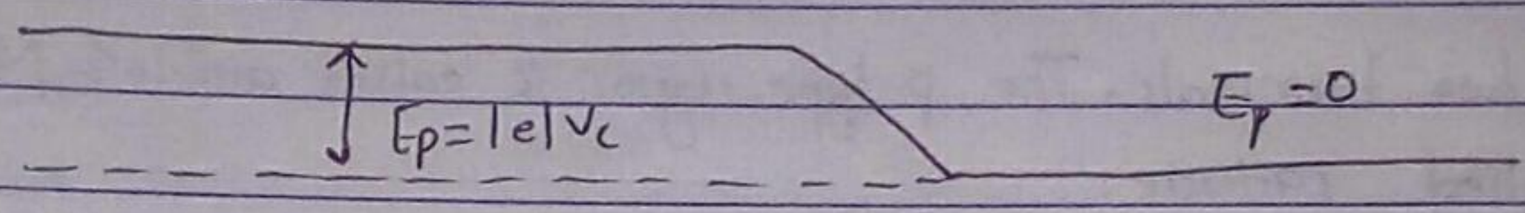
P.E of electron.



P.E of hole.



Due to diffusion of electron and holes across the junction, the N-side becomes +vely charged and is at higher potential V_c. Also, P side becomes negatively charged is at lesser potential. $V=0$. The potential energy of charge q when placed in potential V is

$$P.E = qV$$
$$E_p = qV.$$

for electron, $E_p = -|e|V.$

for hole, $E_p = |e|V.$

When electron is in n-region, $E_p = -|e|V_c$ and when electron is in p region, $E_p = -|e|V = 0$. This means p.E. of electron in p-side is shifted upward by eV_c ~~rel~~ relative.

Similarly, for hole in n-region, $E_p = eV_c$ and for hole in p-region $E_p = e.V = 0$. This means the p.E in n side is shifted ~~down~~ upward by $|e|V_c$ relative to p-region.

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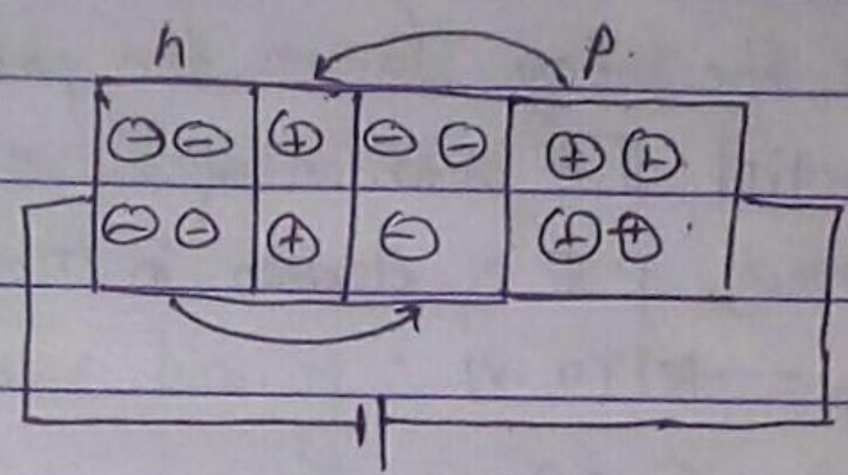
Biasing of pn junction diode:

When p-n junction diode is connected to the external source of battery, then it is called biasing.

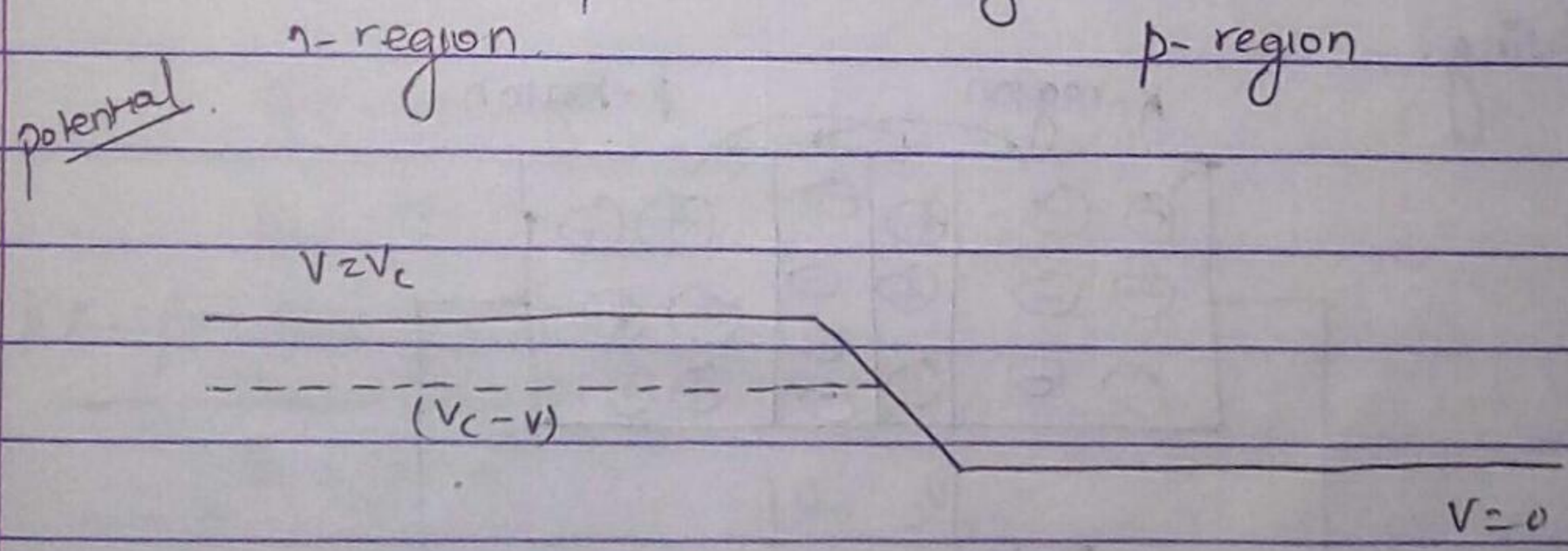
1. Forward biasing:



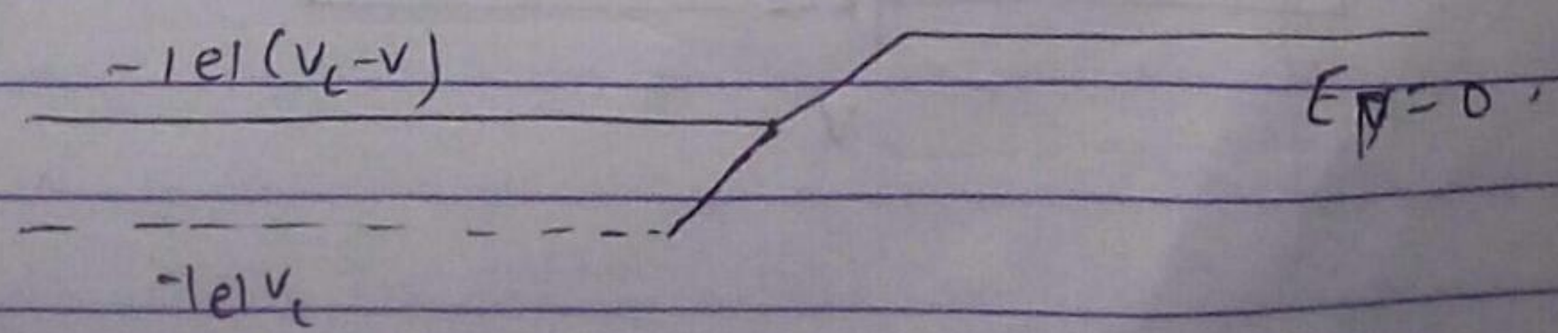
When p-side of junction diode is connected to +ve terminal of battery and n-side is connected to -ve terminal to battery, then it is called forward biasing. During forward biasing,

- The width of depletion layer decreases & diode has very low resistance.
- The flow of current due to majority charge carriers.
- The diode behaves as closed switch.

Band scheme for forward biasing.



P.E of electron:



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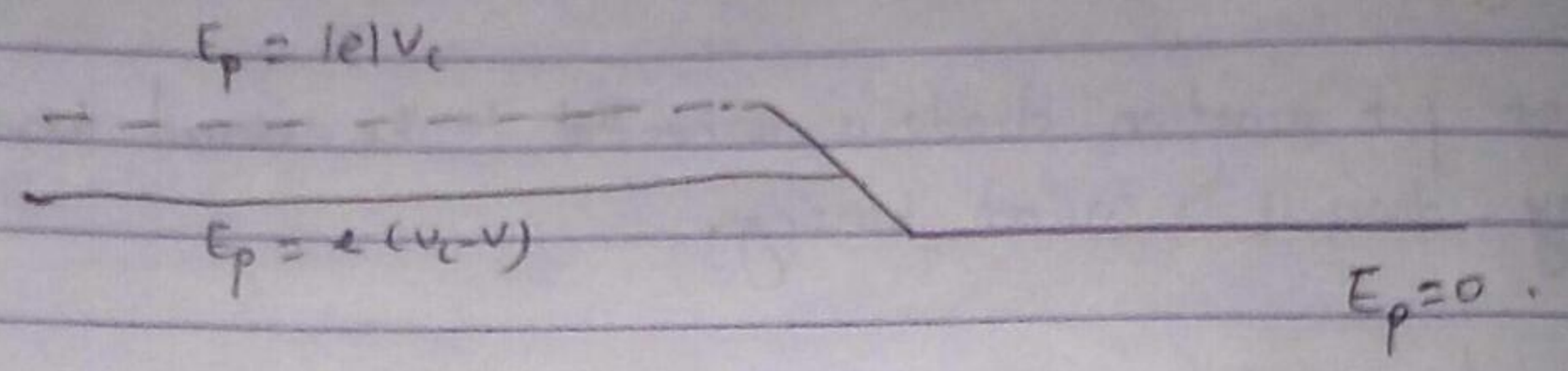
P.E for hole.



During forward biasing, the battery lowers the potential of n-side if V is the applied potential. The potential of n side V_c is now reduced to $V_c - V$. Now, P.E of electron in n-region.

$$E_p = -|e|(V_c - V)$$

and in p region, $E_p = 0$.

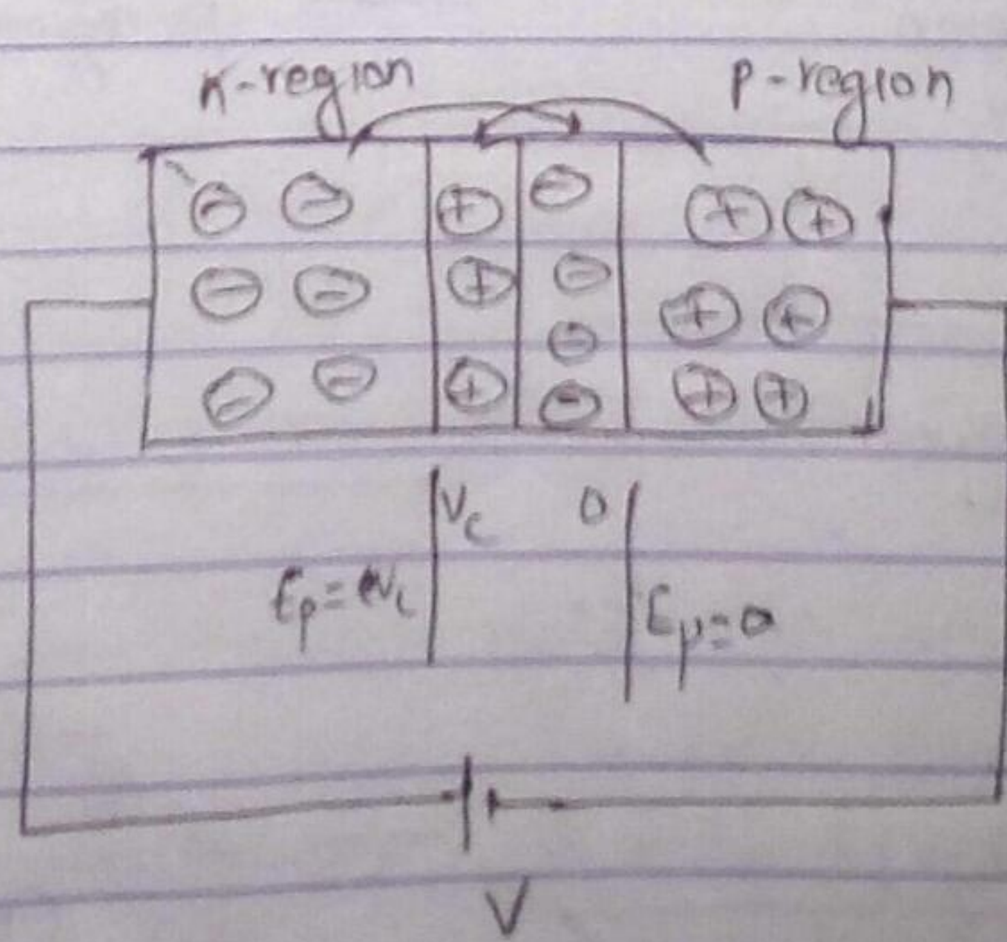
Also, P.E of hole in n-region,

$$E_p = |e|(V_c - V)$$

& in p-region, $E_p = 0$.

In diagram above, dotted lines represents the P.E before battery is connected and solid line represents the P.E after apply battery.

Reverse biasing.



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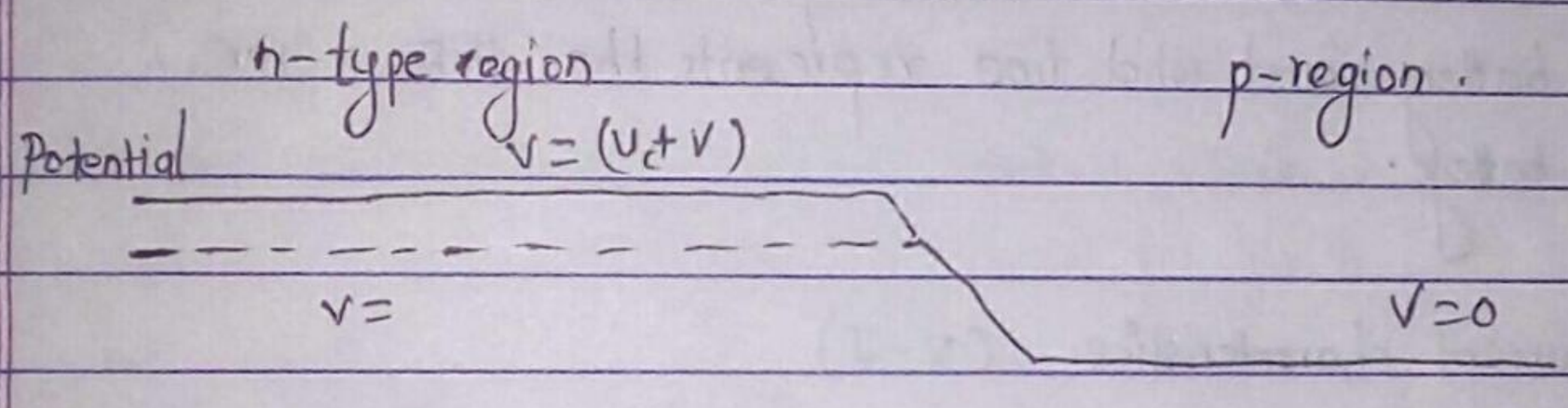
When +ve terminal of battery is connected to n-region and -ve terminal is connected to p-region of SC, the biasing is called reverse biasing.

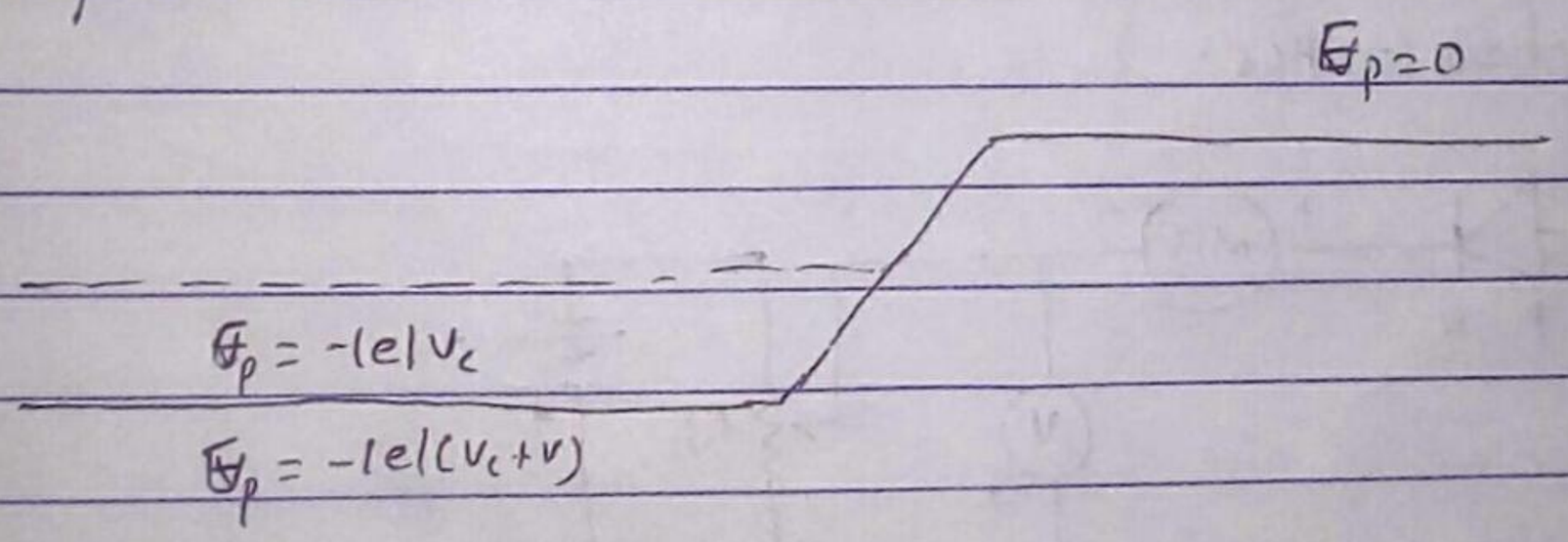
In reverse biasing,

- Width of depletion layer increasing
- The diode has very high resistance
- The flow of the current is due to minority charge carriers.
- Diode behaves as open switch.

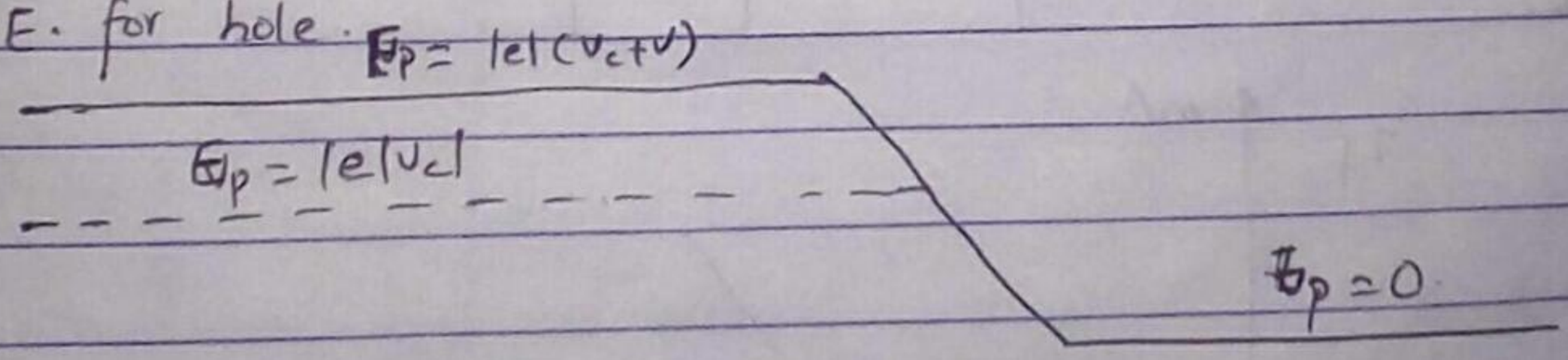
Band scheme for reverse biasing.



P.E. for electron.



P.E. for hole.



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In reverse biasing, the battery will raise the potential of n-side. If V is the applied potential & V_c is the potential of n-side, then new potential will be (V_c+V).

P.E of electron, $E_p = -|e|(V_c+V)$ (for n-region)

$E_p = 0$ (for p-region)

AND, P.E of hole,

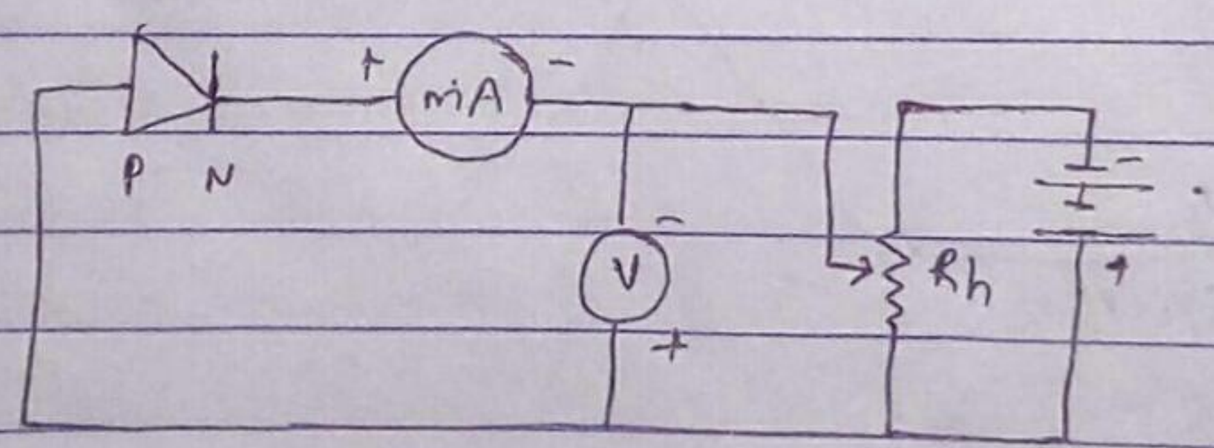
$E_p = |e|(V_c+V)$ (for n-region)

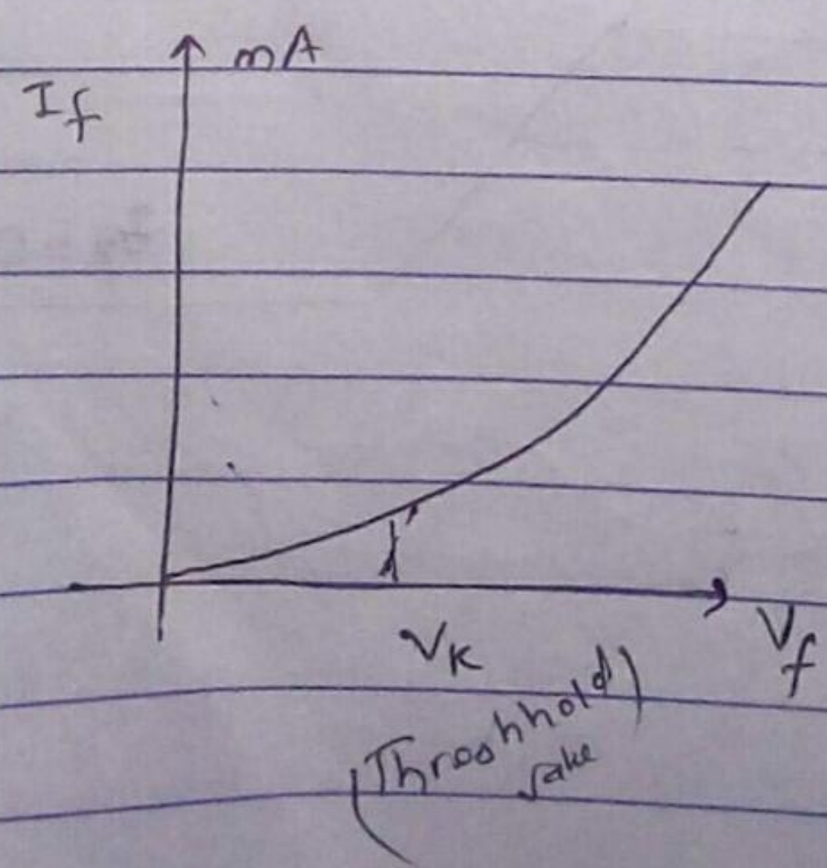
$E_p = 0$ (for p-region).

In diagram above, dotted lines represents the P.E before applying battery and solid line represents the P.E after applying battery.

Voltage current characteristics: (V-I) of P-N junction diode.

a. forward characteristics.





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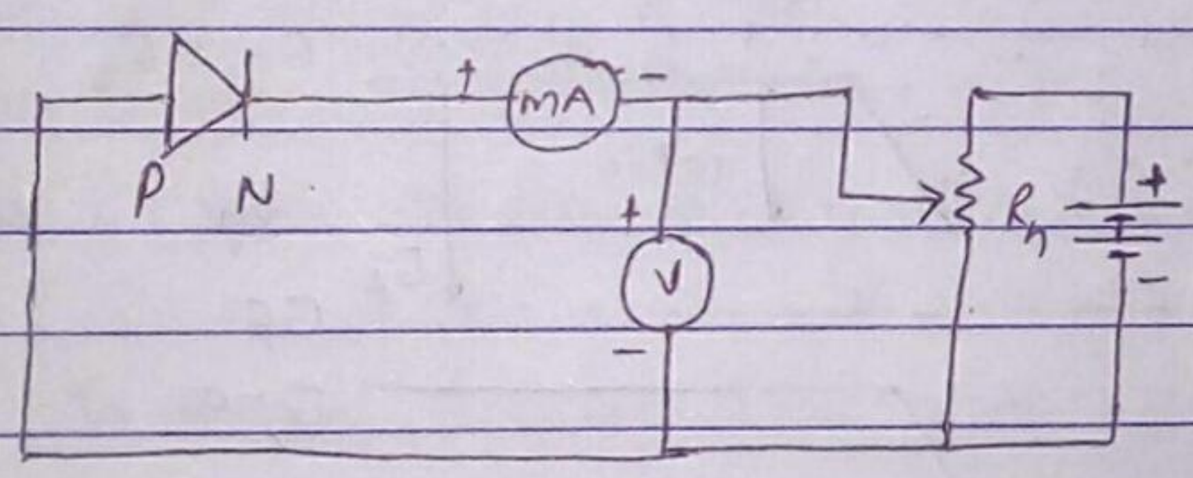
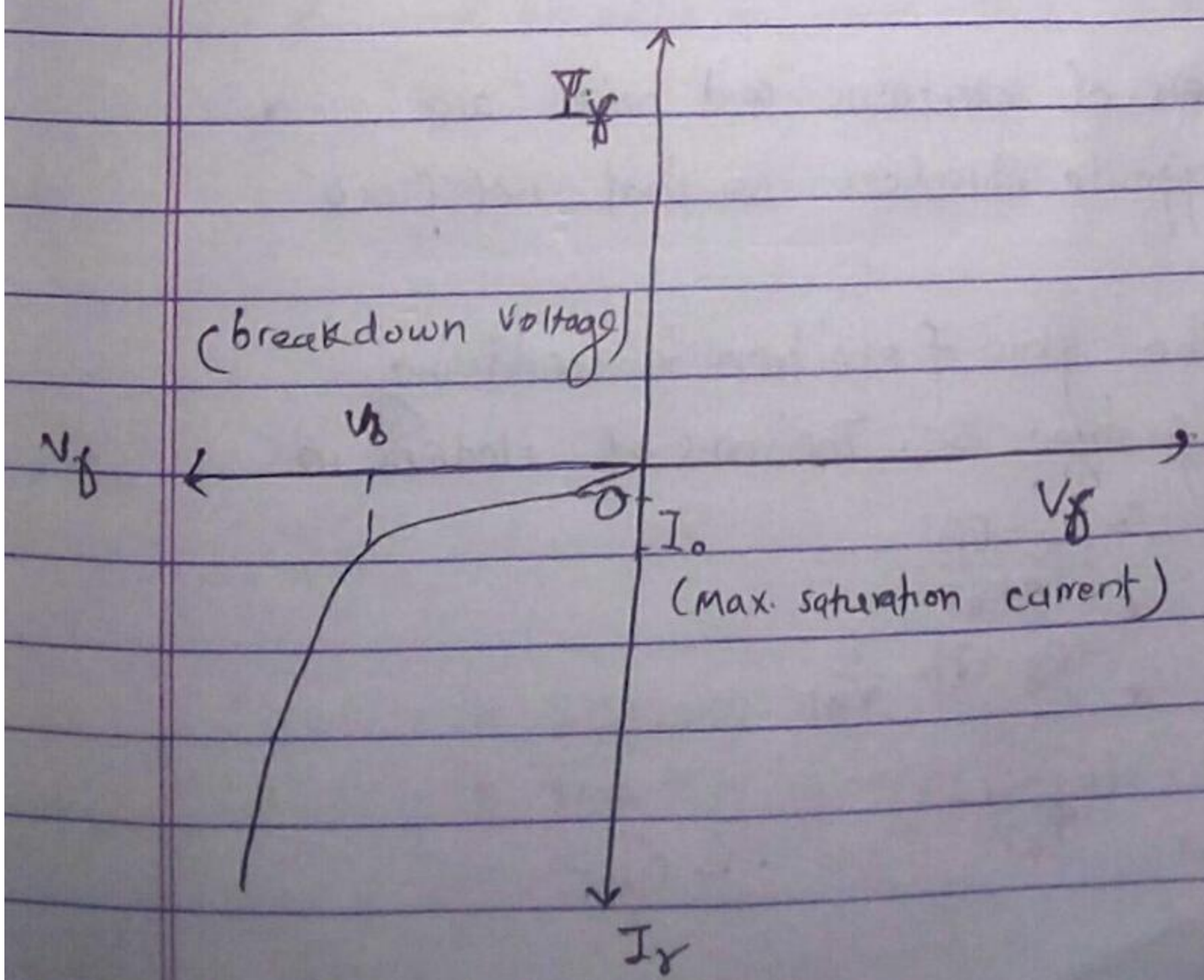
The circuit diagram for study forward characteristics of PN junction diode is as shown in figure. The forward voltage V_f is increased from 0 in equal ~~steps~~ state and crosponding current is measured by mA. The graph between V_f and I_f is called forward characteristics.

From graph,

- When $V_f = 0$, $I_f = 0$
- When V_f is increased, I_f begins to flow in the diode. But I_f increases rapidly when voltage is increased upto knee voltage V_K such voltage is also called threshold or cutin voltage.
- After V_K, the current is almost linear.

Reverse characteristics of PN junction diode





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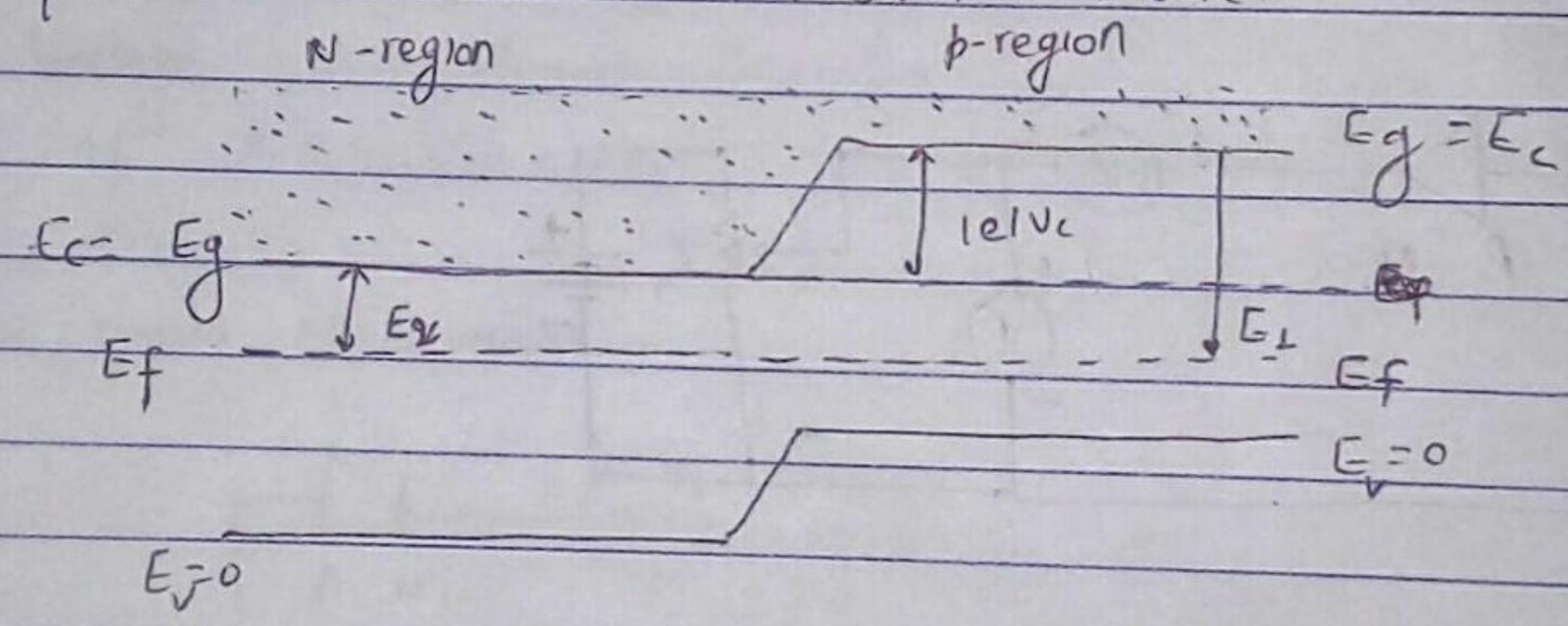
The circuit diagram to study the reverse characteristic of PN Junction diode is as shown in figure. The reverse voltage V_r is increased in small steps and corresponding current is recorded. The graph beth rev. voltage V_r and rev. current I_r is called reverse characteristics.

from graph, I

- If $V_r = 0$, $I_r = 0$.
- When V_r is increased, I_r also increases and reaches to max current I_0 called saturation current.
- When V_r is increased, beyond a value called breakdown voltage V_b the reverse current I_r increases sharply.

Current across P-N Junction diode

(a) Equilibrium current across P-N Junction diode.



At PN Junction, equal numbers of electrons and holes are continueously flowing in opposite direction so that net flow will be zero.

Considering the flow of electron in conducting band CB of both n- and p-type SC. The no.s of electrons in conduction band.

$$N_e = N_c \cdot e^{-\frac{(E_c - E_f)}{k_B T}}$$

$$= N_c \cdot e^{-(E_g - E_f) \times \frac{1}{k_B T}}$$

$$N_e \propto e^{-\frac{(E_g - E_f)}{k_B T}} \quad \ldots (i)$$

$-eV_c$

$-|e|V_c$.

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~~from~~ eq^n (i) gives free electron concentration for both n- and p-type SC.

for n-region,

$$E_c - E_f = E_2$$
$$\Rightarrow E_g - E_f = E_2$$

for p-region,

$$E_c - E_f = E_1$$
$$\Rightarrow E_g - E_f = E_1$$

Here $E_1 > E_2$,

$$\therefore E_1 = E_2 + |e| V_c \quad , \quad V_c = \text{contact potential.}$$

Now, current from P to N region,

$$I(P \to N) \propto N_e \quad , \quad N_e = \text{No.s of electron in p-region.}$$

ie. $I(P \to N) \propto e^{(-E_g - E_f) \times \frac{1}{K_B T}}$

ie. $I(P \to N) \propto e^{-E_1/K_B T}$

ie. $I(P \to N) = Ae^{-\frac{E_1}{K_B T}}$ .... (ii).

But, in n-side there are the large no. of electron in the conduction band. However, only the electrons having energy greater or equal to $|e|V_c$. will be able to move from n-region to p-region. Suppose $f(E \geq |e|V_c)$ is the fraction of electrons whose energy is greater than or equal to $|e|V_c$.

$\therefore$ The electron that will be able to move from N to P region,

$$N_e' = N_e f(E \geq |e|V_c)$$

Now, the current from N to P region, $I(N \to P) \propto N_e'$, N_e - no. of electron in N-region whose energy $\geq |e|V_c$.

ie. $I(N \to P) \propto N_e \cdot f(E \geq |e|V_c)$

ie. $I(N \to P) \propto e^{-\frac{E_2}{K_B T}} \cdot f(E \geq |e|V_c)$

ie. $I(N \to P) \propto A e^{-\frac{E_2}{K_B T}} f(E \geq |e|V_c)$. .... (iv).

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The fraction of ~~energy~~ electron having energy $< V_c$ is approximated by maxwell Boltzmann distribution.

$$f(E \geq |e| V_c) = e^{\frac{-|e| V_c}{K_B T}}$$

Now from equation (iv)

$$I(P \to N) = A e^{\frac{-E_2}{K_B T}} \cdot e^{\frac{-|e| V_c}{K_B T}}$$

$$= A e^{-\left[\frac{E_2 + |e| V_c}{K_B T}\right]}$$

$$= A e^{-\left[\frac{E_2}{K_B T}\right]} \quad \ldots (v)$$

Now from (ii) & (v),

$$I(P \to N) = I(N \to P) \quad \ldots (vi).$$

Thus, the flow of electron from N to P is equal to P to N. The net flow of current is zero. This is the condition of equilibrium current across PN Junction.

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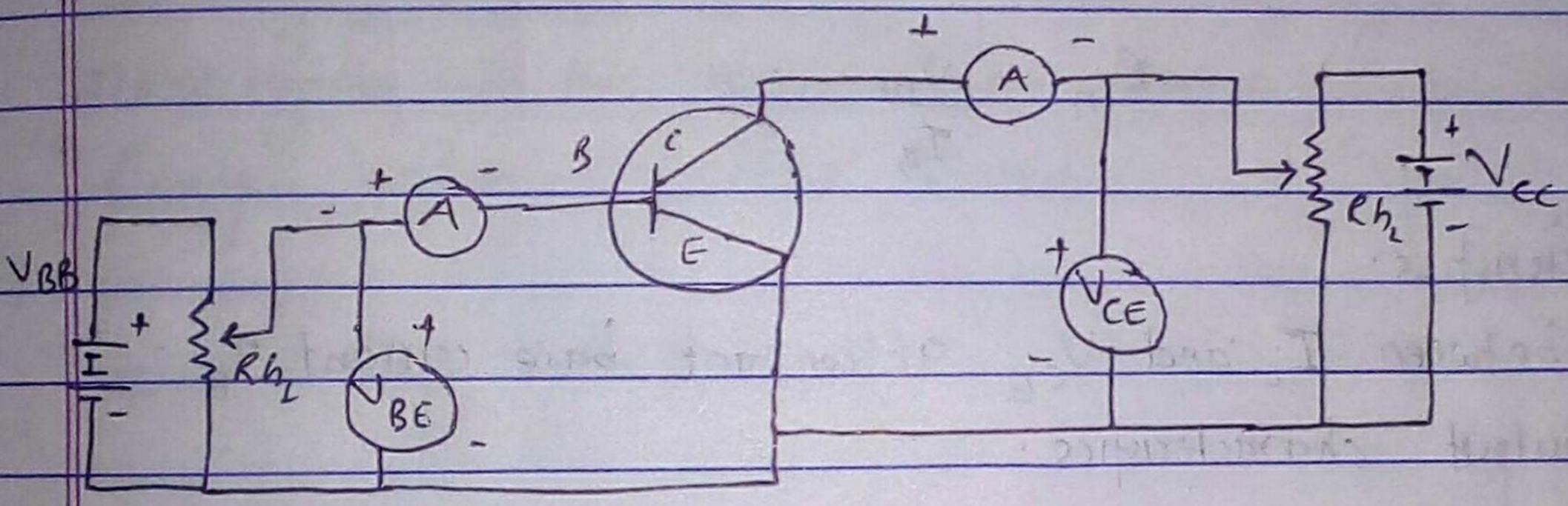
CE- characteristics



The graphical relation between current & V across transistor is called CE characteristics. The CE characteristics are studied as

a. Input characteristics: The graph between base current I_B and Base-emitter voltage V_{BE} at constant collect emitter voltage V_{CE} is called input characteristics.

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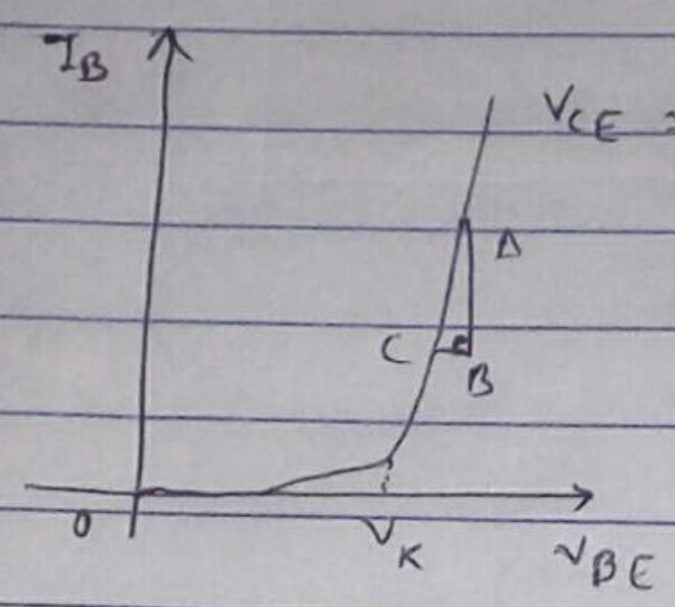
For this, V_{BE} is increased in small steps by rehostat Rh_1. and crossponding current I_B are measured keeping V_{CE} constant



From graph, as V_{BE} is increased from 0, I_B is approximately zero upto knee voltage V_K. when V_{BE} exceeds knee voltage, the base current I_B increases sharply.

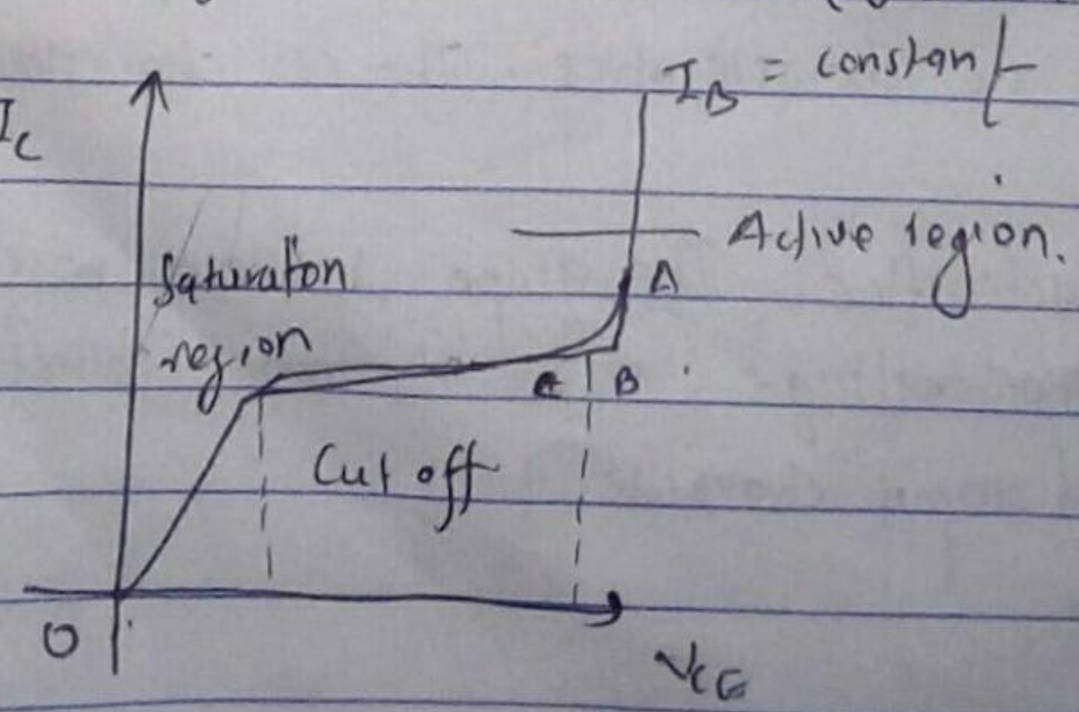
$$\text{Slope of curve} = \tan\theta = \frac{AB}{BC} = \frac{I_B}{V_{BE}}$$

$$R_{in} = \frac{V_{BE}}{I_B}.$$

6. Output ac charterisitics.

- The graph between I_c and V_{CE} at constant base current I_B is called output characteristics.

for this, V_{CE} is increased in small steps using rehostat Rh_2. and crossponding current I_c are measured at constant current I_B.



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As V_{CE} is increased from zero, I_C increases sharpbly & becomes maximum. This is called saturation. After saturation, I_C is constant is independent of V_{CE}. But, if V_{CE} is increased enough, breakdown takes place & I_C increases rapidly. There are three regions of transistor operation:

1. Cut-off region:
The region between I_B axis & V_{CE} axis is called cut off region. In this region, both junctions are reversed biased.

2. Saturation region:
The region between saturation line & I_C axis is called saturation region. In this region, both junctions are forward biased.

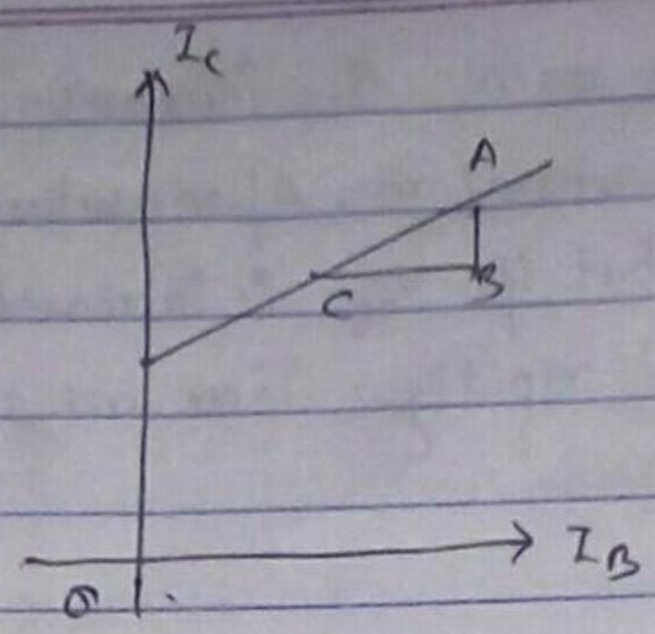
3. Active region:
The region between cut off & saturation region is called active region. In this region. Input junction is forward biased & output junction is reverse biased.

$$\text{Slope} = \tan\theta = \frac{I_C}{V_{CE}}$$

$$R_{out} = \frac{V_{CE}}{I_C}$$

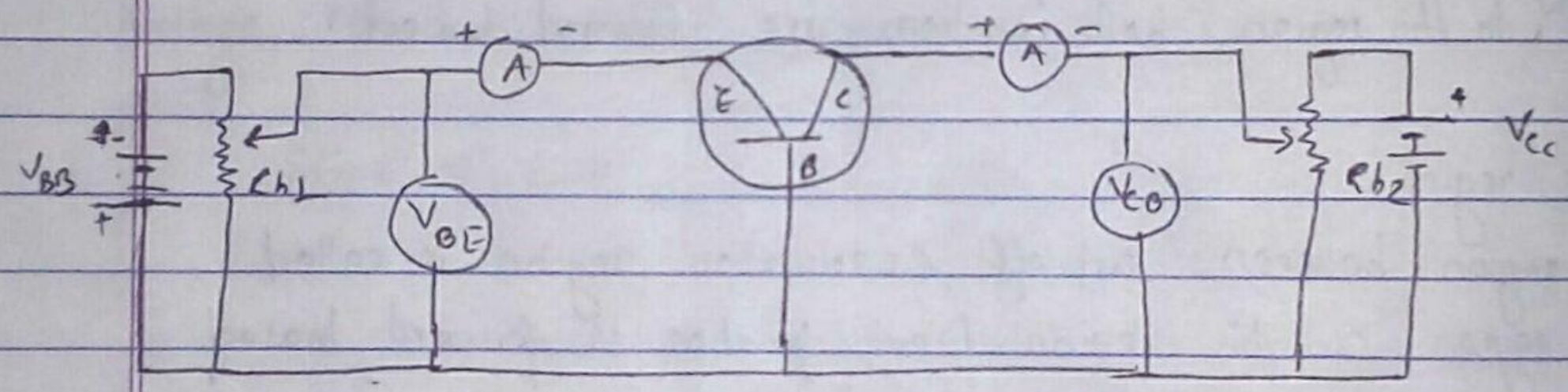
c. Current transfer characteristics:

The graph between I_C & I_B at constant V_{CE} is called current transfer characteristic. The graph is linear but not pass through 0. If even $I_B = 0$ & $I_C \neq 0$.
Such current is called leakage current. Slope of current gives the value of β.



$$\text{Slope} = \tan\theta = \frac{AB}{BC} = \frac{I_C}{I_B} = \beta.$$

CB - characteristics :

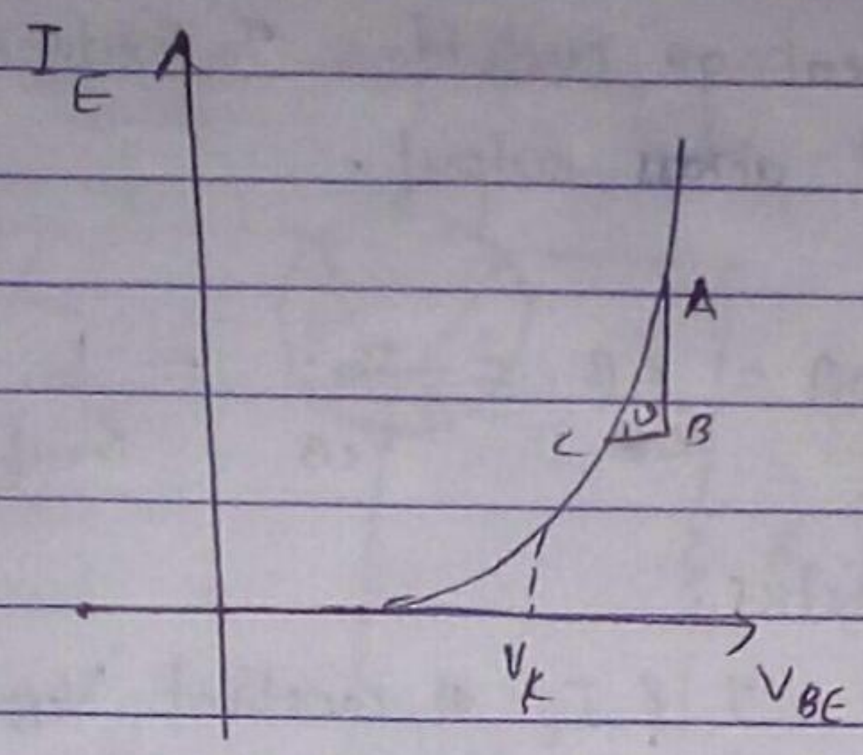


The circuit diagram to study CB characteristic is a shown in fig above. In input circuit, V_{BE} is the base emitter voltage, I_E is emitter current, R_{h1} controls V_{BE} & V_{BB} is the biasing voltage.

In output circuit, V_{CB} is collector - base voltage, I_C is collector (output) current, R_{h2} controls V_{CB} & V_{CC} is the biasing voltage.

Input characteristics:

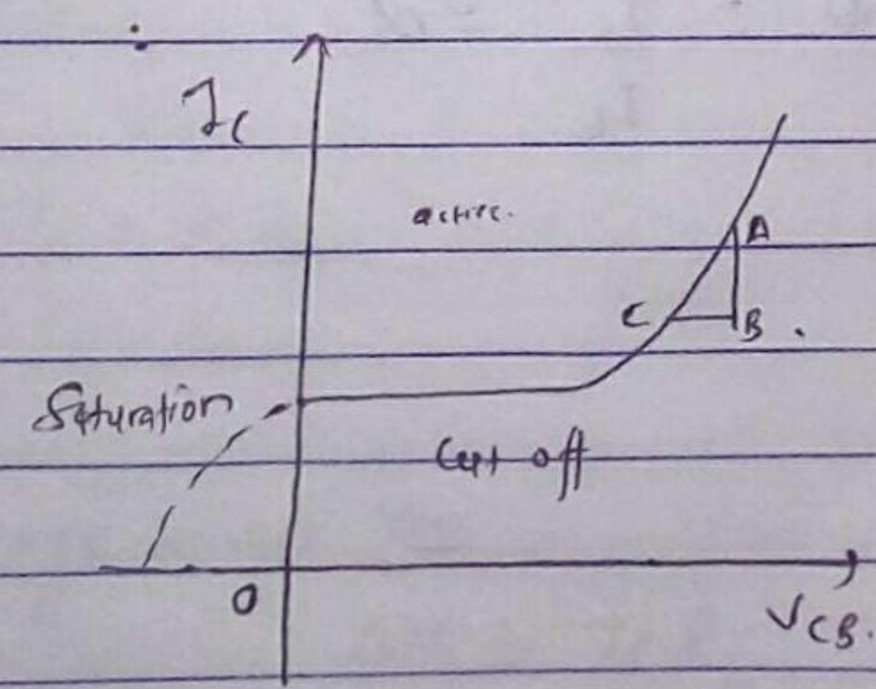
The graph between V_{BE} & I_E at constant V_{CB} is called input characteristics.



V_{BE} is increased in small steps by rehostat Rh1. & crosponding I_E are measured for constant V_{CB}. When $V_{BE}=0$, $I_E=0$. When V_{BE} is increased above the knee voltage, I_E increases sharply.

$$\text{Slope} = \tan\theta = \frac{AB}{CB} = \frac{1}{R_{in}} = \frac{I_E}{V_{BE}}.$$

b. Output characteristics: Graph betn V_{CB} & I_C at constant I_E is called output characteristics



V_{CB} is increased in small steps by Rh2 and crosponding I_C are measured at constant I_E.

From graph, I_C becomes constant and is independent of V_{CB}. When V_{CB} is increased from zero. If V_{CB} is increased further, breakdown takes place I_C increases sharply. But at $V_{CB}=0$.

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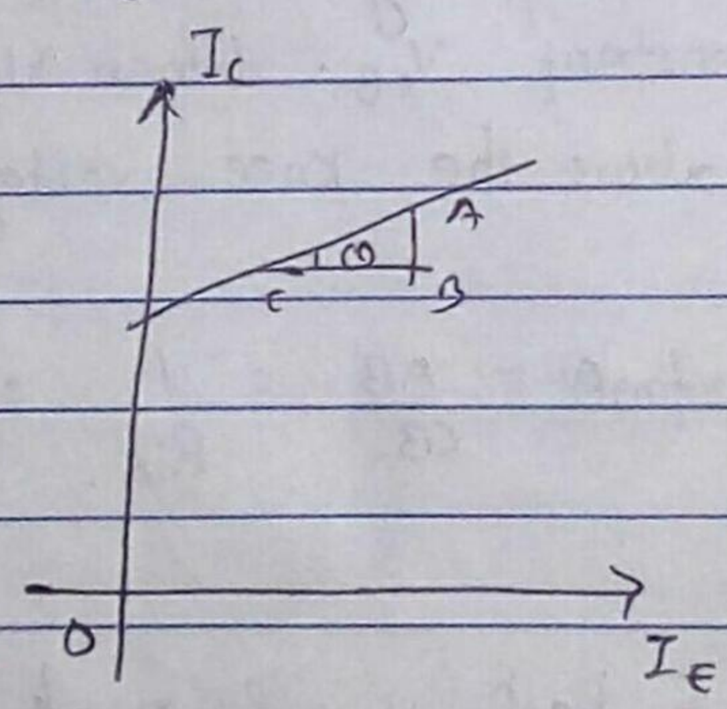
$I_c \neq 0$. This is called leakage current. To reduce $I_c = 0$ some voltage is to be applied across output.

$$\text{Slope} = \tan\theta = \frac{AB}{CB} = \frac{I_c}{V_{CB}} = \frac{1}{R_{out}}$$

c. Current transfer characteristics.

The graph between I_c & I_E at constant V_{CB} gives current transfer characteristics. If $I_c \neq 0$ even if $I_E = 0$. Such current is called leakage current



$$\text{Slope} = \tan\theta = \frac{I_c}{I_E} = \alpha$$

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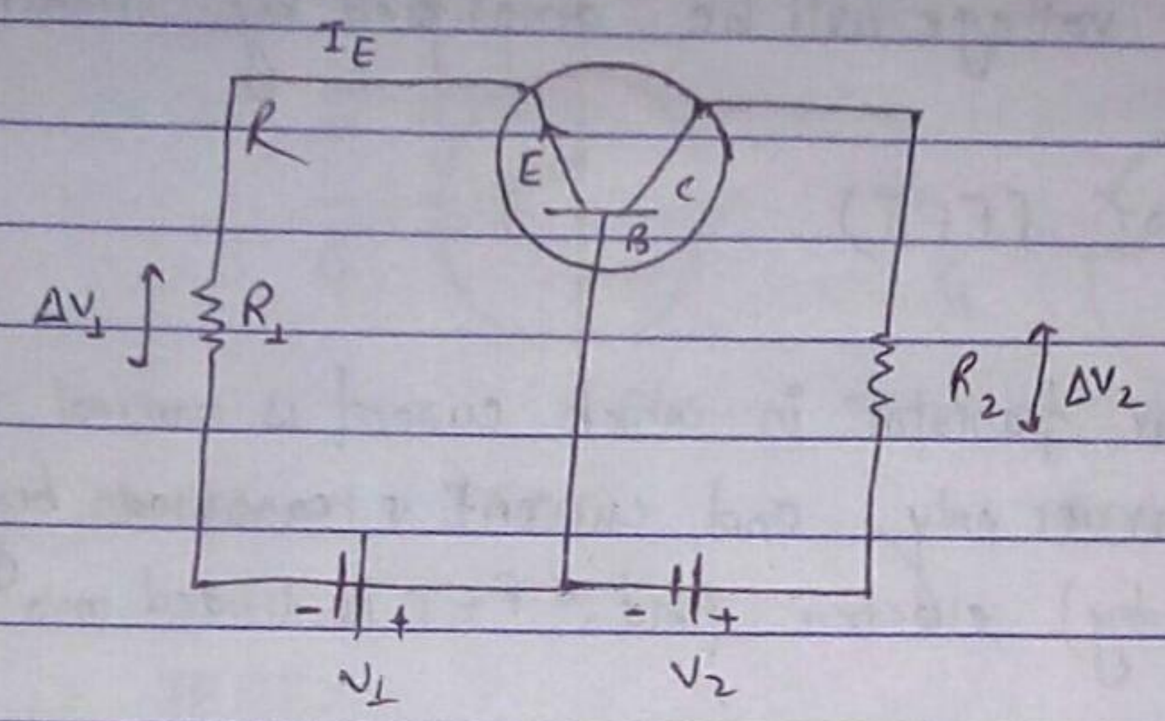
Transistor as voltage amplifier,



Suppose, resistance is R_1 & R_2 ($R_2 > R_1$) are connected in base emitter junction, C-B junction respectively. Let ΔV_1 & ΔV_2 be the voltages across R_1 & R_2 respectively.

Across input:

$$\Delta V_1 = I_E (R_1 + R)$$

$$I_E = \frac{\Delta V_1}{R_1 + R} \quad \ldots (i)$$, R = resistance of B-E junction.

Now, $\alpha = \frac{I_C}{I_E}$

$$\Rightarrow I_C = \alpha I_E = \alpha \frac{\Delta V_1}{R_1 + R} \quad \ldots (ii)$$

Across output:

voltage across R2,

$$\Delta V_2 = I_C R_2$$

$$= \frac{\alpha \Delta V_1}{(R_1 + R)} R_2.$$

for $\alpha = 1$,

$$\Delta V_2 = \frac{\Delta V_1}{R_1 + R} R.$$

Since $R_2 > R_1$ $\quad \frac{R_2}{R_1 + R} > 1$.

$\Delta V_2 > \Delta V_1$.

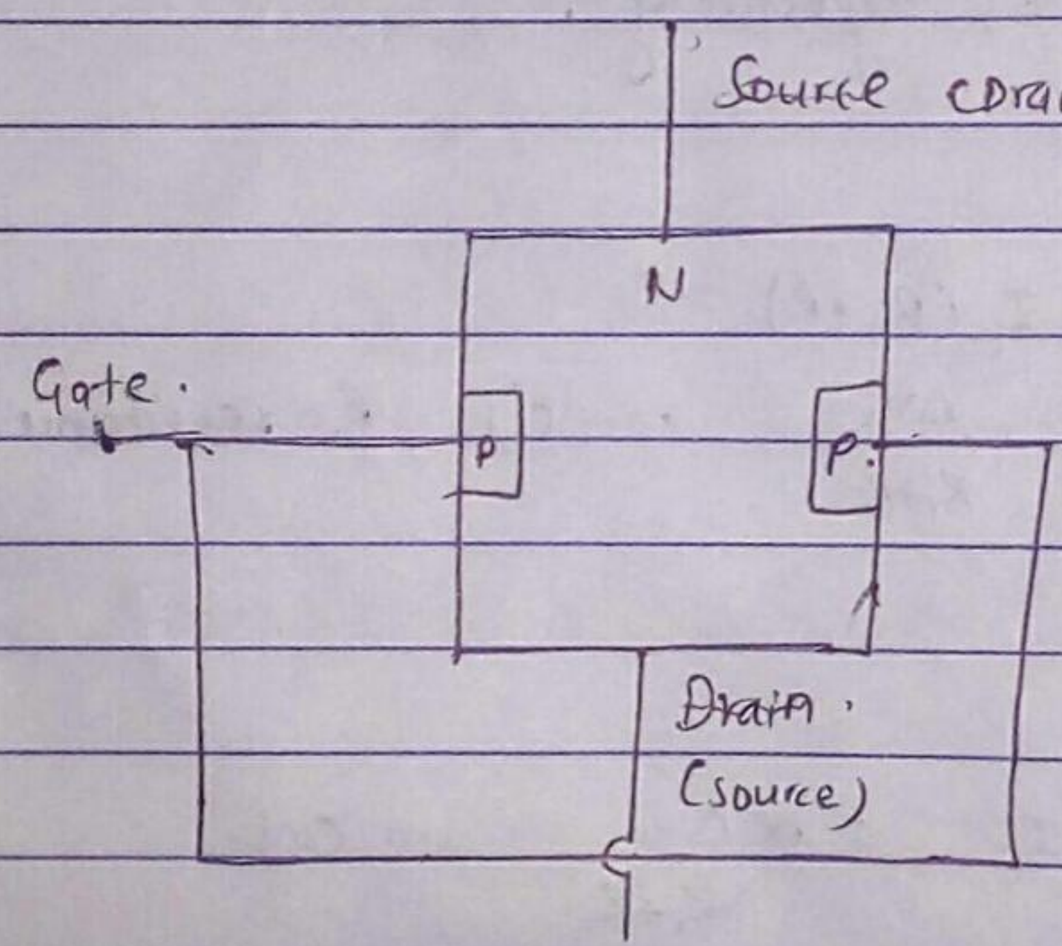
This means input voltage will be amplified by transistor.

Field effect transistor (FET)

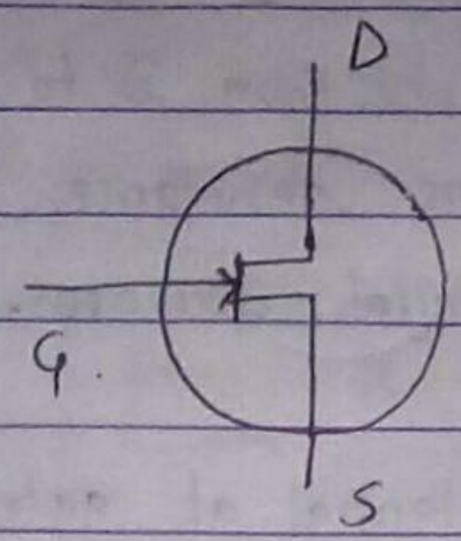
FET is the unipolar transistor in which current is carried by majority charge carrier only and current is controlled by external (effected by) electric field. FET is divided into two group:

1. JFET (Junction FET)
2. MOSFET (Metal oxide Semiconductor FET)

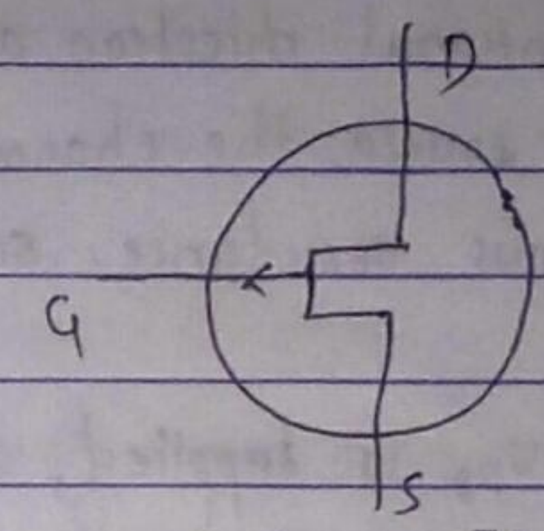
1. JFET.



JFET is the 3-terminal SC device. It consists of n- or p-type SC bar and two P or N type SCs fused on opposite side of the bar. The two PN junctions are formed. The area between two PN junction is called channel through which charge carriers can flow. The 2 PN-junctions are connected by single lid called gate terminal. The other two terminals are taken out from the ends of the bar called drain and source. The majority charge carrier enter the bar through source terminal and they leave the bar through drain terminal.

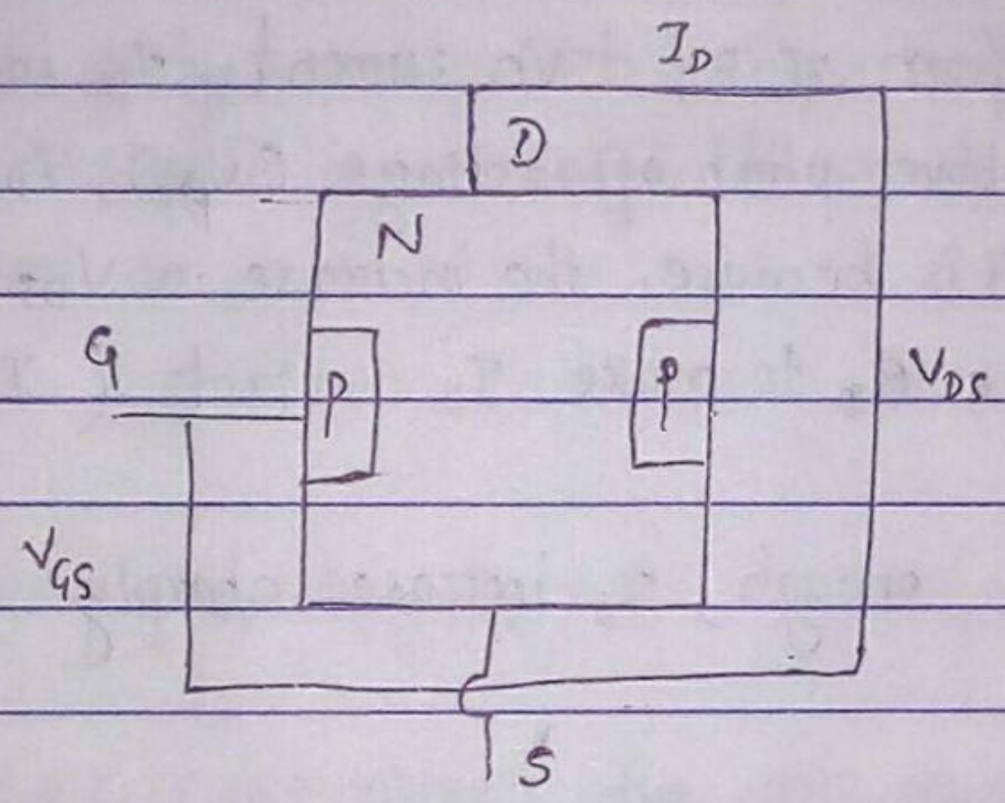


N-channel JFET.



P- channel JFET.

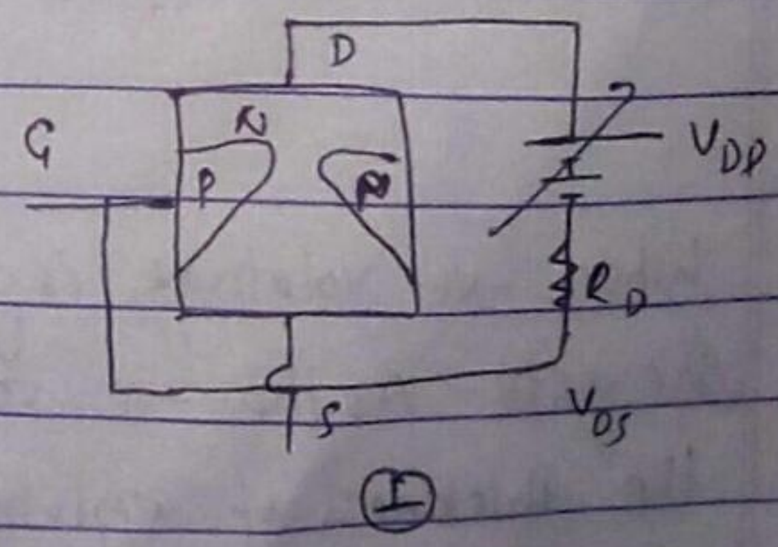
Working of JFET:



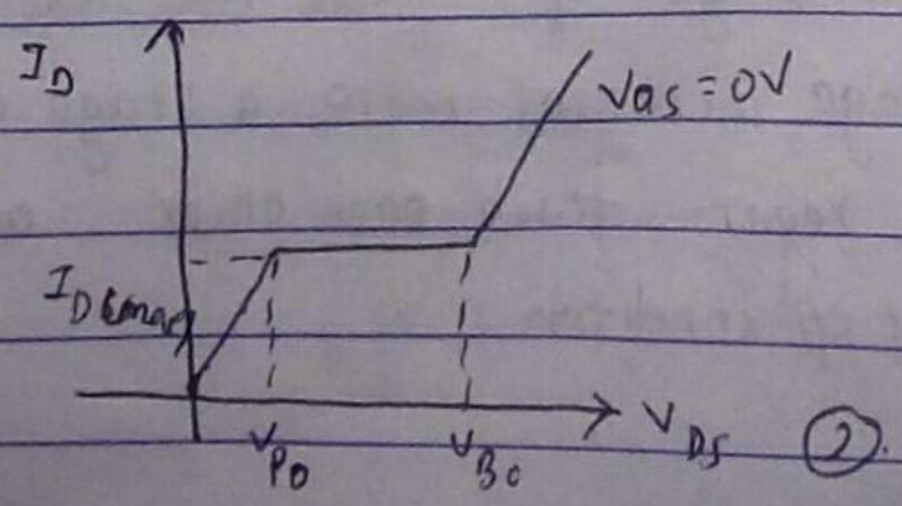
Consider a n- channel JFET. The working of JFET can be discussed as

a. $V_{GS} = 0$, $V_{DS} = 0$.

In this case, no current flows through the channel ie. $I_D = 0$. The depletion regions are of equal thickness and symmetrical as shown in fig a.



b. V_{GS} is increased, $V_{DS} = 0$.



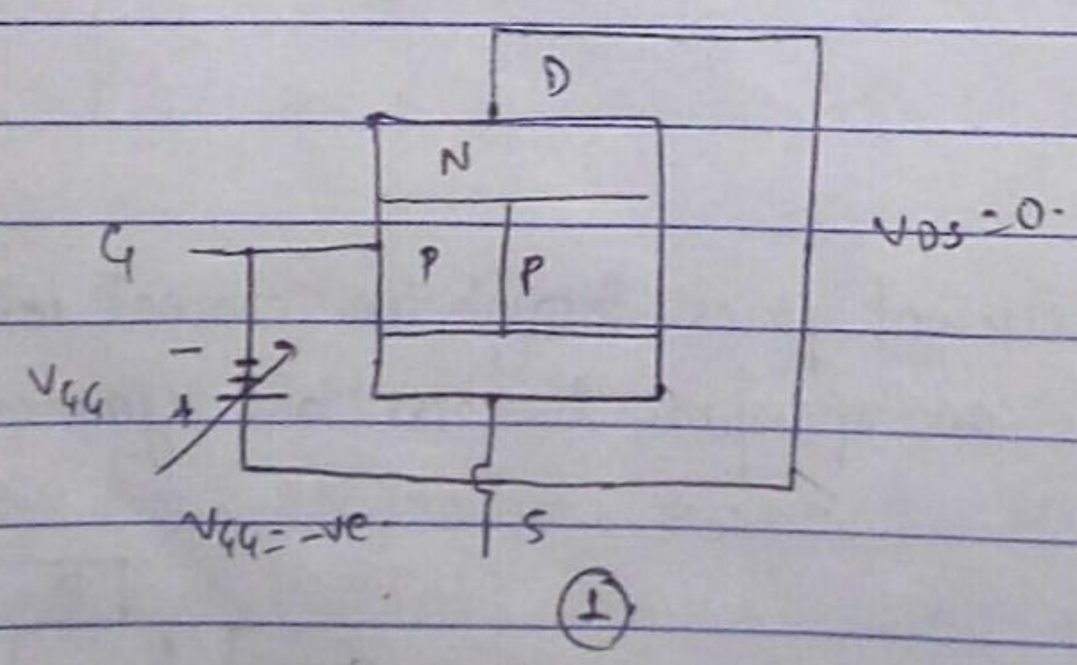
Suppose, a source V_{DD} is connected as shown in figure 2. The conventional direction of I is from D to S. as we go from drain to source, the channel offers resistance & some potential drops across resistance. So, potential decreases.

As V_{DD} is supplied, the potential at gate-drain region is greater that gate source region. Thus, the depletion region penetrate more in channel in G-D region than G-soure region

As V_{DS} is increased from zero, drain current I_D increases acc. to ohm's law. But, above pinch off voltage (V_{PO}), I_D becomes K. at the value $I_{D(max)}$. It is because, the increase in V_{DS} is neutralized by increase in resistance R_D to make I_D constant ($I_D = \frac{V_{DS}\uparrow}{R_D\uparrow}$).

But, if V_{DS} is increased enough, I_D increases sharply due to JFET breakdown.

c. When $V_{DS}=0$, V_{GS} = -ve.



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When -ve volatage is given to gate it increases the reverse bias of the gate. As the -ve voltage increases more, a stage comes at which the thickness of depletion region touch each other and cut offs of channel this is called cut off condition.

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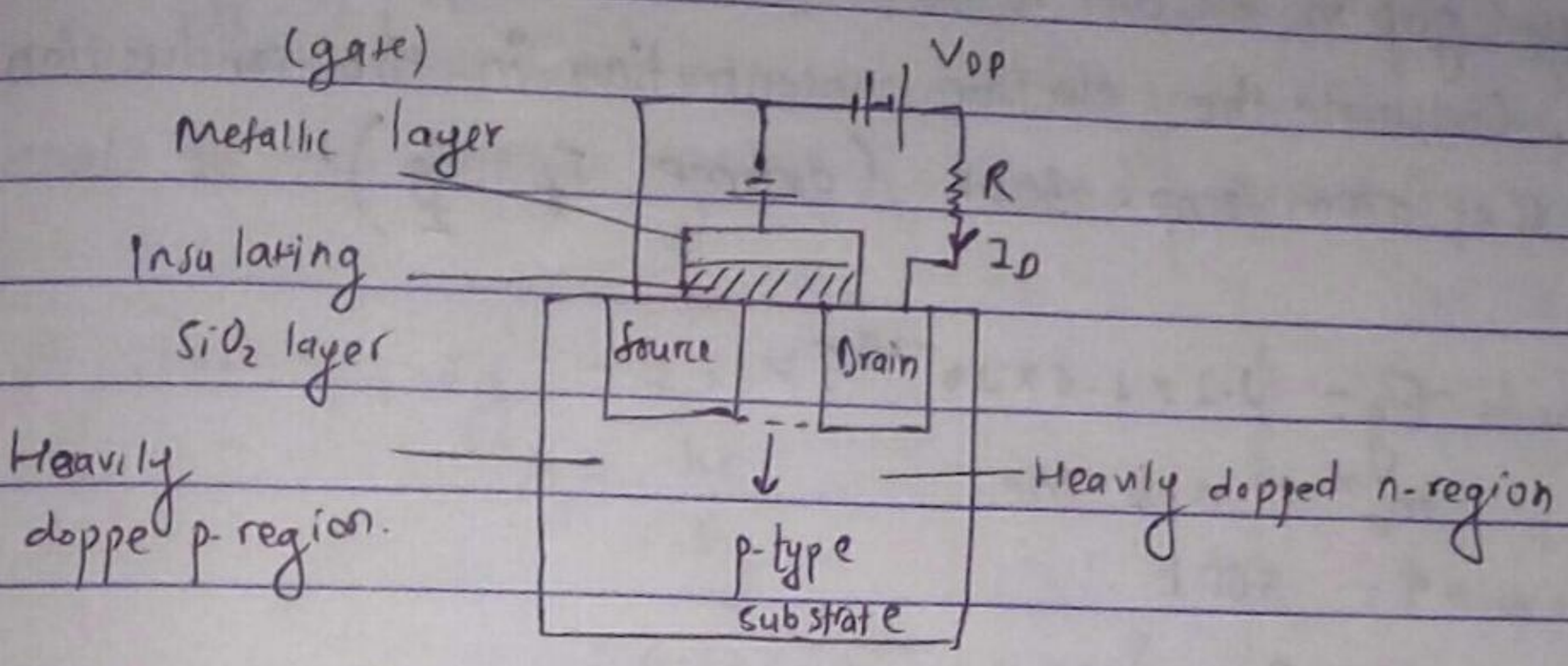
b. MOSFET.



The n-channel MOSFET consists of two heavily dopped n-regions diffused into p-type substrate. The two n-regions acts as source and drain. The metallic layer desposited on the insulating layer of SiO_2 behaves as gate.

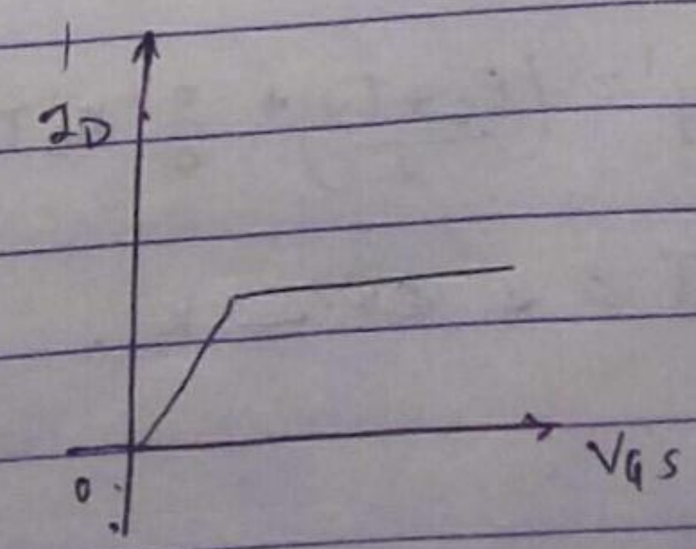
Working.

When $V_{GS} = 0$, $I_D = 0$ ie. no flow of current between D & S.

If $V_{GS} \neq 0$ (+ve value), the +ve terminal of the gate attracts the electrons from p-type substrate towards interface between SiO_2 and substrate so, a small layer of n-type is formed near to the interface which provides the channel for I_D to flow from drain to source when V_{GS} is applied.

When V_{GS} is increased more, the length of the depletion layer increases which increases the resistance of channel and current becomes constant.

$$I_D = \frac{V_{GS}}{R_D}.$$



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N. The energy gap in silicon is 1.1 eV. the av. effective mass is $0.31\ m_e$. Calculate the electron concentration in the conduction band of Si at room temp. 300K (assume $E_f = \frac{E_g}{2}$).

Soln

$E_g = 1.1 \times 1.6 \times 10^{-19}\ J$.

$m_e^* = 0.31\ m_e$.

$T = 300\ K$.

$n = ?$.

Now,

$$n = N_c\, e^{-\frac{E_c - E_f}{k_B T}}$$

$$= 2\left(\frac{m_e^* k_B T}{2\pi\hbar^2}\right)^{3/2} \cdot e^{-\frac{E_g - E_f}{k_B T}}$$

$$= 2\left(\frac{0.31 \times m_e \times 1.38 \times 10^{-23} \times 300}{2\pi \frac{h^2}{4\pi^2}}\right) \cdot e^{\frac{1.1 \times 1.6 \times 10^{-19} \times \frac{1}{2} \times \frac{1}{k_B \cdot 300}}}$$

$= ___\ Nm^{-3}$.

N. Suppose that the effective mass of hole in a material is 4 times that of electron. At what temperature would the fermi level be shifted by 10% from the middle of the ~~for~~ forbidden energy gap? ($E_g = 1eV$.)

Soln

$m_h = 4m_e$ $\quad E_f = \frac{E_g}{2} = 0.5\ eV$.

$T = ?$

Now,

$$E_f' = E_f + 10\%\ E_f.$$

Again, $$E_f' = \left(\frac{E_c + E_v}{2}\right) + \frac{3}{4} k_B T \ln\left(\frac{m_h^*}{m_e^*}\right)$$

$T = ___\ K$.

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N/ The energy gap in silicon is 1.1eV. whereas in diamond is 6eV. What conclusion can you draw about the two materials to the visible light ($\lambda_v = 4000\,\mathring{A} - 7000\,\mathring{A}$.).

Soln

for Si, $E_g = 1.1eV$.

$$\lambda_s = \frac{hc}{E_g}$$

$$= \frac{6.62\times10^{-34} \times 3\times10^{8}}{1.1}$$

$$= 11,290\,\mathring{A}.$$

$\lambda_{visible} = 4000\,\mathring{A} - 7000\,\mathring{A}$.

$\therefore \lambda_{visible} \not> \lambda_s$

so, visible light is absorbed

for diamond.

$\lambda_{visible} \not> \lambda_{diamond}$.

$\therefore$ so, visible light is transmitted.

N/ Intrinsic carrier density for Ge at 300 K is $2.4\times10^{17}\,m^{-3}$. Find its intrinsic resistivity. if electron & hole mobilities are. $0.35\,m^2V^{-1}s^{-1}$ & $0.18\,m^2V^{-1}s^{-1}$.

Soln Here,

$T = 300K$.

for intrinsic, sc, $n = p = n_i = 2.4\times10^{17}\,m^{-3}$.

$\mu_e = 0.35\,m^2V^{-1}s^{-1}$.

$\mu_h = 0.18\,m^2V^{-1}s^{-1}$.

$\rho = ?$

$$\rho = \frac{1}{n_i e(\mu_e + \mu_h)}$$

$= ___\ \Omega m$.

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N/ The energy gap in Ge is 0.75eV, compare the intrinsic conductivity of ge. at 27°c and 57°c.

Sol:

$E_g = 0.75eV = 0.75 \times 1.6 \times 10^{-19}$ J.

$T_1 = 300K$ & $T_2 = 330K$. Now, we have, $n_i = \sqrt{N_c N_v}\, e^{-E_g/2k_BT}$

$= AT^{3/2} \cdot e^{-E_g/2k_BT}$.

$\sigma = n_i e (\mu_e + \mu_h)$

$= eAT^{3/2} e^{-E_g/2k_BT} \cdot (\mu_e + \mu_h)$.

for T_1,

$\sigma_1 = eAT_1^{3/2} e^{-E_g/2k_BT_1} (\mu_e + \mu_h)$ ——

for T_2,

$\sigma_2 = eAT_2^{3/2} e^{-E_g/2k_BT_2} (\mu_e + \mu_h)$ ——

$$\therefore \frac{\sigma_1}{\sigma_2} = \frac{eAT_1^{3/2} e^{-E_g/2k_BT_1} (\mu_e + \mu_h)}{eAT_2^{3/2} e^{-E_g/2k_BT_2} (\mu_e + \mu_h)}$$

$$= \left(\frac{T_1}{T_2}\right)^{3/2} e^{\frac{-E_g}{2k_BT}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)}$$ □.

N/ A certain intrinsic sc. has band gap 0.2eV. Calculate the resistivity at 350K. if resistivity at 300K is 0.3 Ωm.

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Semi_conductor purification & IC production.

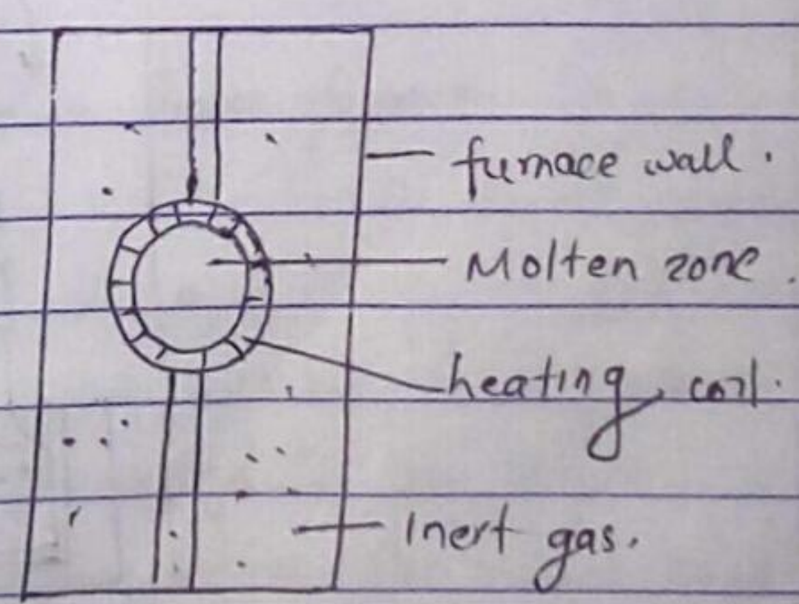
Semiconductor purification.

Silicon is mostly used semi conducting material due to following factors:

1. It is most abundent element on the earth.
2. It is easier for dopping impurities in silicon.
3. It is non-toxic and no special care is needed during its production & application.
4. It is very cheap because its raw materials are most abundent in nature.
5. There are simpler methods for crystallization & purification of silicon.
6. It is used as insulating layer (SiO_2) in MOSFET devices.
7. The energy gap for silicon is smaller 1.1eV. due to which there is the small lekage current.

Purification of silicon.

1. Zone refining:



Zone refining.

Principle: The impurities have higher solubility in molten state as compared to that of solid state.

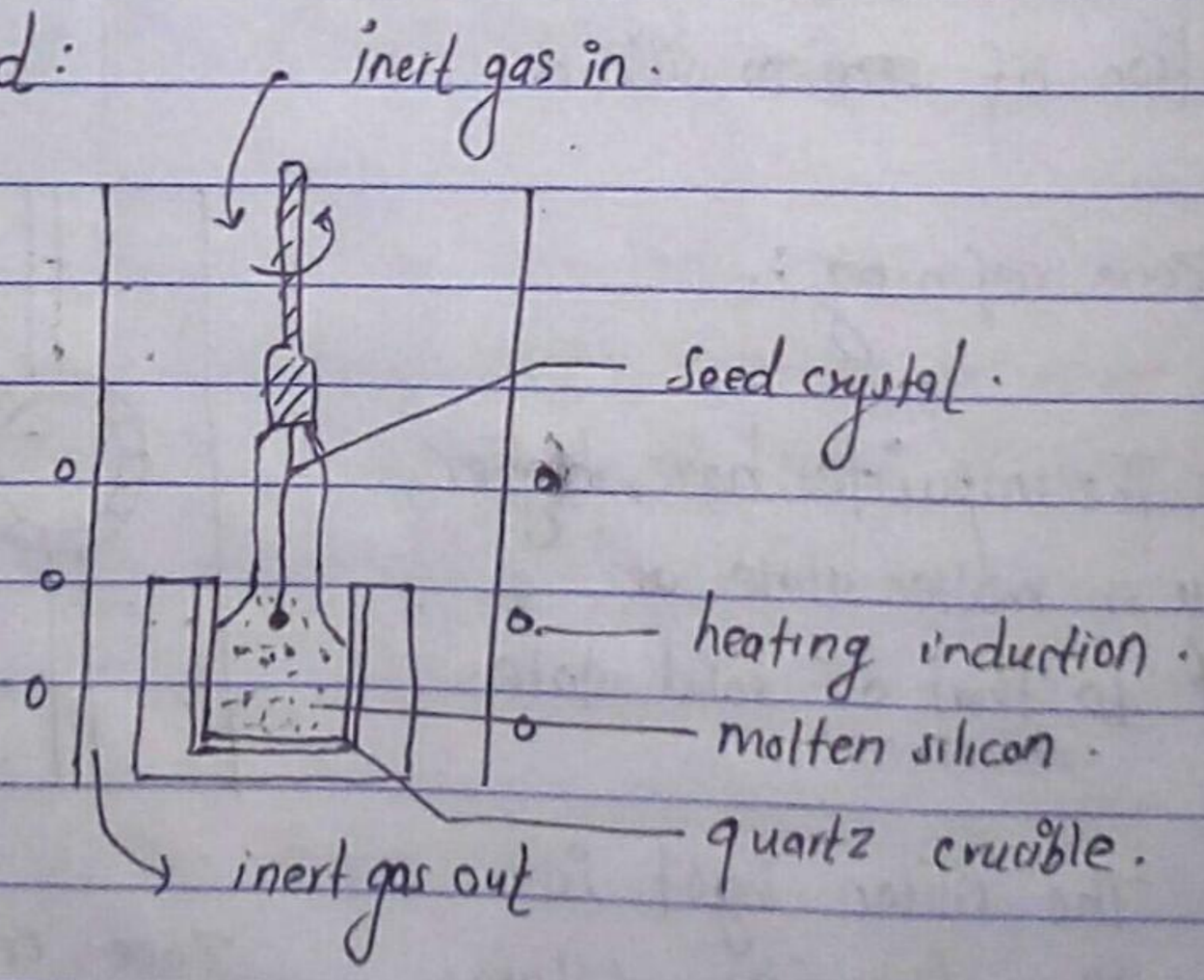
Working: The silicon ingot is polycrystalline & consists of large numbers of crystals having random orientation wrt each other.

In this process, impure silicon ingot is placed inside zone refiner under inert gas environment. The silicon ingot is surrounded

by a series of circular mobile heating coils which can move from one end to another end. At a time, the heater melts the particular zone of rod where impurity is present. As the heater moves, the previous molten state gets solidified and impurities move from one zone to another zone. Actually, impurities shift towards the molten zone of ingot. In this way, as the heater reaches to another end of ingot, all the impurities are collected there. The process is repeated continueously and finally the end at which impurities are concentrated are cut and removed.

Single Crystal growth: The process of growing large numbers of single crystals of silicon from seed crystal is called single crystal growth. Seed crystal is the small piece of single crystal material which can grow a large number of similar crystals. Some methods of single crystal growth:

a. Czochraiski method:



This method is used for manufacture of silicon wafer. The Si- wafer is a piece of SC material used in IC. It involves following steps:

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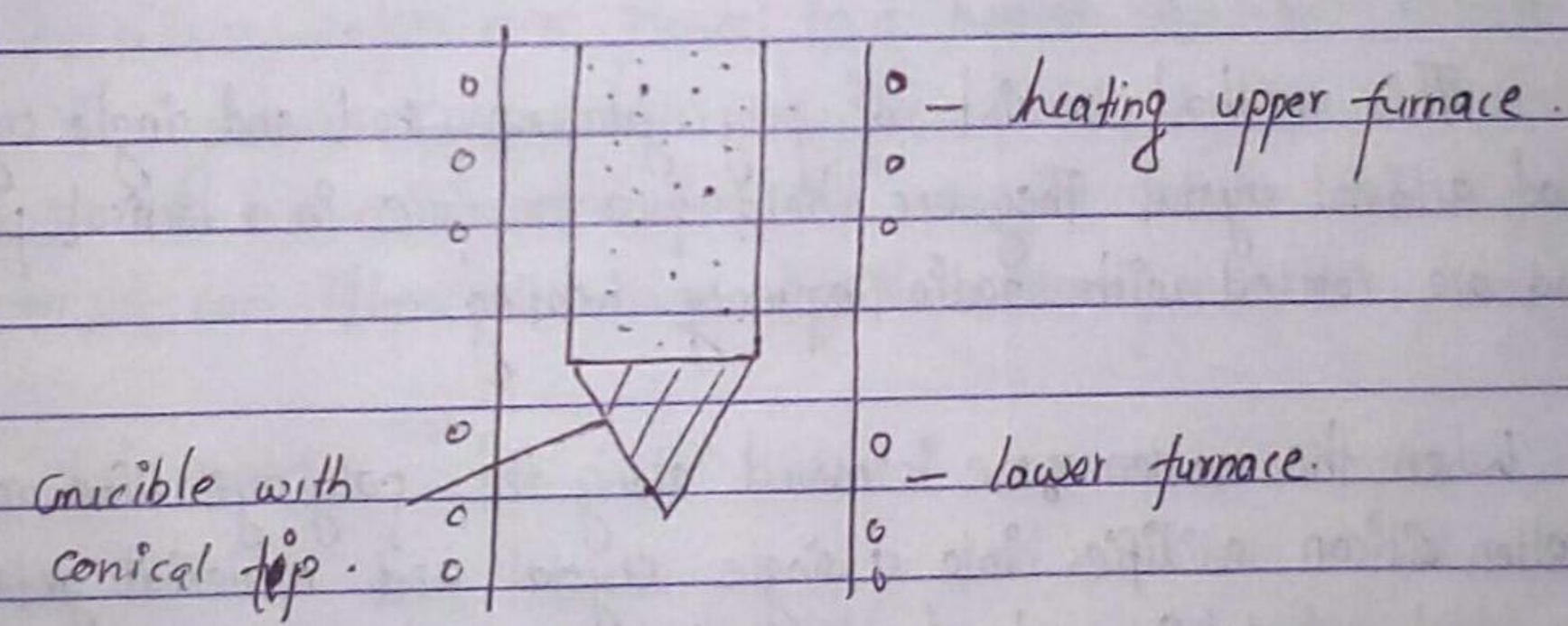
crucible to its m.p and molten si is formed.

2. Deeping the seed crystal: The seed crystal is dipped in the molten solution of silicon and it is cooled to grow large single crystals.
3. Drawing seed upward. The seed will be cooled out from molten silicon. As it is cooled upward, the molten silicon will solidify as same as seed growing. a numbers of si crystals. The size of crystal depends on cooling rate, rotation speed & temperature difference.

b. Bridgmann stockbarger method:



In this method, the material is placed in a crucible having a conical tip. The poly crystalline sample is melted in the upper furnace which is maintained at high temperature. The melted sample moves down into lower furnace having low temperature and gets slowly cooled to solidify. A small crystal is formed at the conical tip. and it behaves as the seed crystal for rest of melt. In this way, single crystal are grown by this method.

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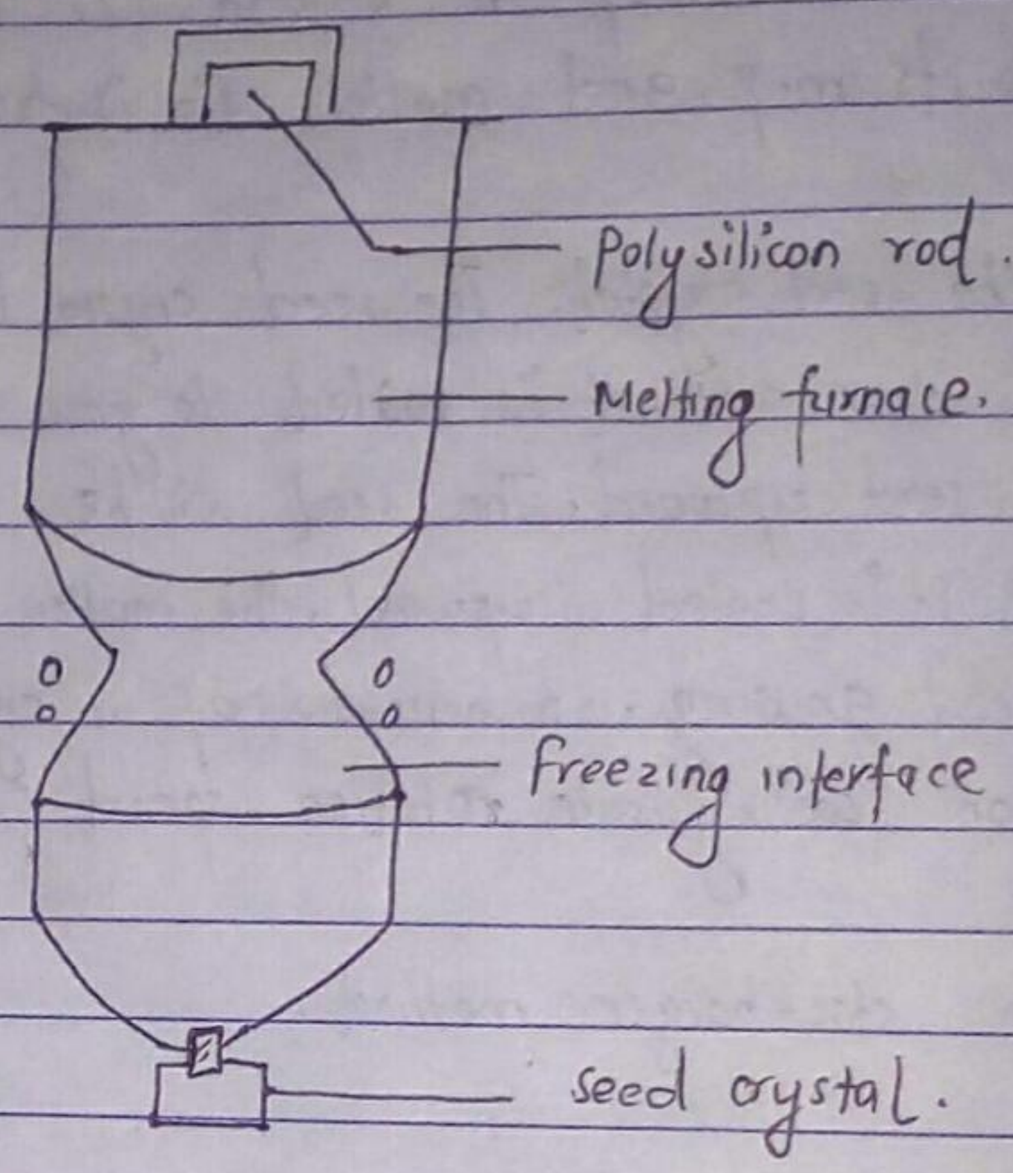
c. Floating zone method:



This method consists of polycrystalline rod and single crystal used as seed crystal. They are held face to face in a vertical position and are rotated with radio frequency heating coil.

When the molten zone is moved along the polycrystalline rod, the molten silicon solidifies into a single crystal and material gets purified. The seed crystal is used to grow the same types of the crystal. On moving the heater over the whole polysilicon rod, it converts into single crystal silicon rod.

d. Epitaxy:

The term epitaxy is a Greek word in which epi means above, and taxy means an ordered manner. Thus, the deposition of crystalline layer over the crystalline substrate is called epitaxy. Such deposited layer is called epitaxial layer.

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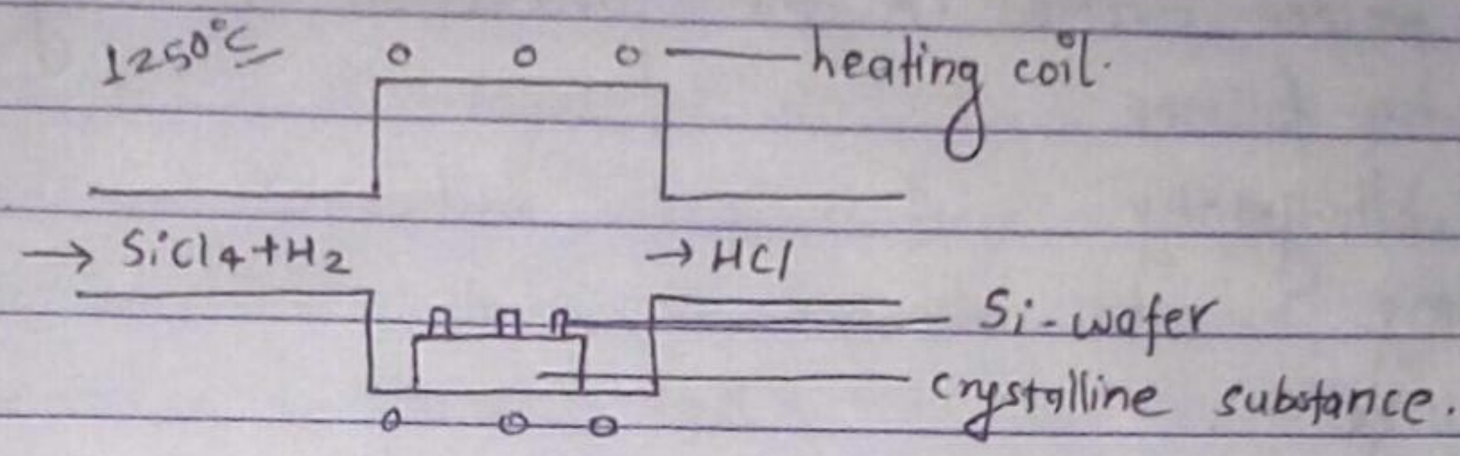
Types of epitaxy :

1. VPE (Vapour Phase Epitaxy)



In VPE, atoms of silicon from a vapour are deposited on the substrate layer. The deposited layer has the same crystal structure & orientation as that of substrate. The substrate serves as the seed crystal into which epitaxial layers grow.

The silicon wafers are placed in a heated chamber called reactor. The gaseous compound of silicon $SiCl_4$ together with the reactant gas H_2 are introduced into the reactor. At the suitable temp of reactor, it can liberate silicon by the decomposition of compound

$$SiCl_4 + 2H_2 \xrightarrow[\Delta]{1250^\circ C} Si + 4HCl.$$

The silicon atom released in this process are deposited on the substrate forming epitaxial layer.

2. LPE (Liquid Phase Epitaxy)

In LPE, the substrate is dissolved into the molten state of material to be deposited.

3. SPE (solid phase Epitaxy)

In SPE, a film of amorphous material is deposited on the crystalline substrate.

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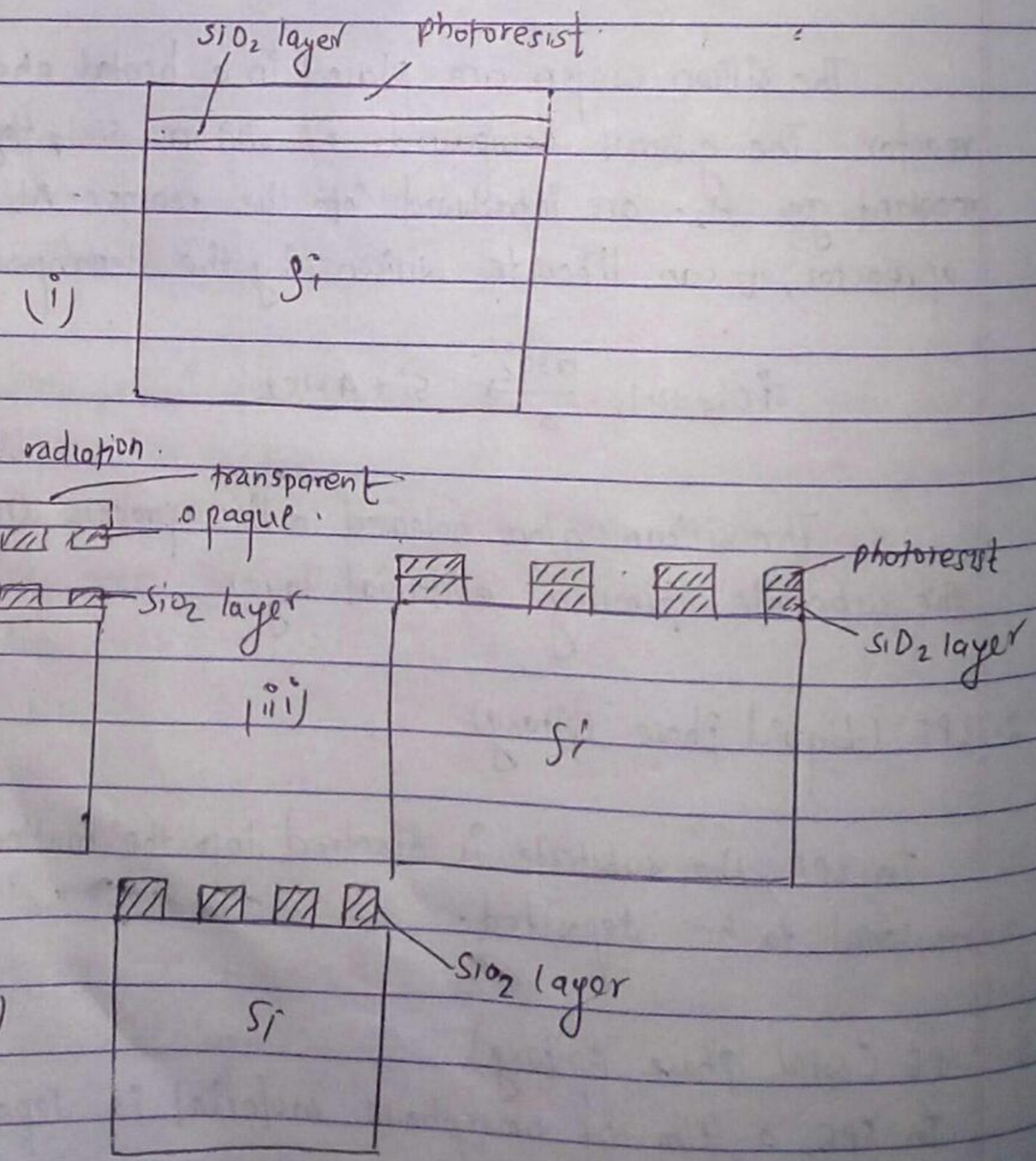
Process of IC production:

The process involved in the production of integrated circuit are as follows:

1. photo lithography
2. Dopping
3. Metallization.

1. photo lithography: The process of transferring the geometrical patterns from a mask to the silicon wafer is called photo lithography.

Steps:



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Step 1: Oxidation. (Coating of silicon with oxide and then with photoresist)

Initially, silicon wafer is heated at about 1000°C - 1200°C in a furnace to form a thin layer of SiO_2. The thickness of such layer depends on temperature, oxidation time and atmosphere.

The si-wafer is then coated with radiation sensitive layer called photoresist. as shown in fig (i).

Step2: Exposer of radiation & develop the pattern.

UV-radiation is allowed to fall on photoresist through mask. Mask is the glass plate having the alternate opaque and transparent regions The radiation from the transparent region of mask are exposed to photoresist and hence they can remove photoresist The mask pattern is transferred on the top of the wafer as shown in fig (ii)

Step 3: Oxide removal

The substance is kept in dilute HF solution so that the SiO_2 layer crossponding to transparent region of mark are remove as shown in fig (iii)

Step4: Photoresist remover.

All the photoresist is removed by using photoresist remover solution The regions crossponding to transparency of mask have no oxide. but the regions crossponding to opaque regions of mask have oxide. the pattern of SiO_2 on si-wafer. as shown in fig (iv)

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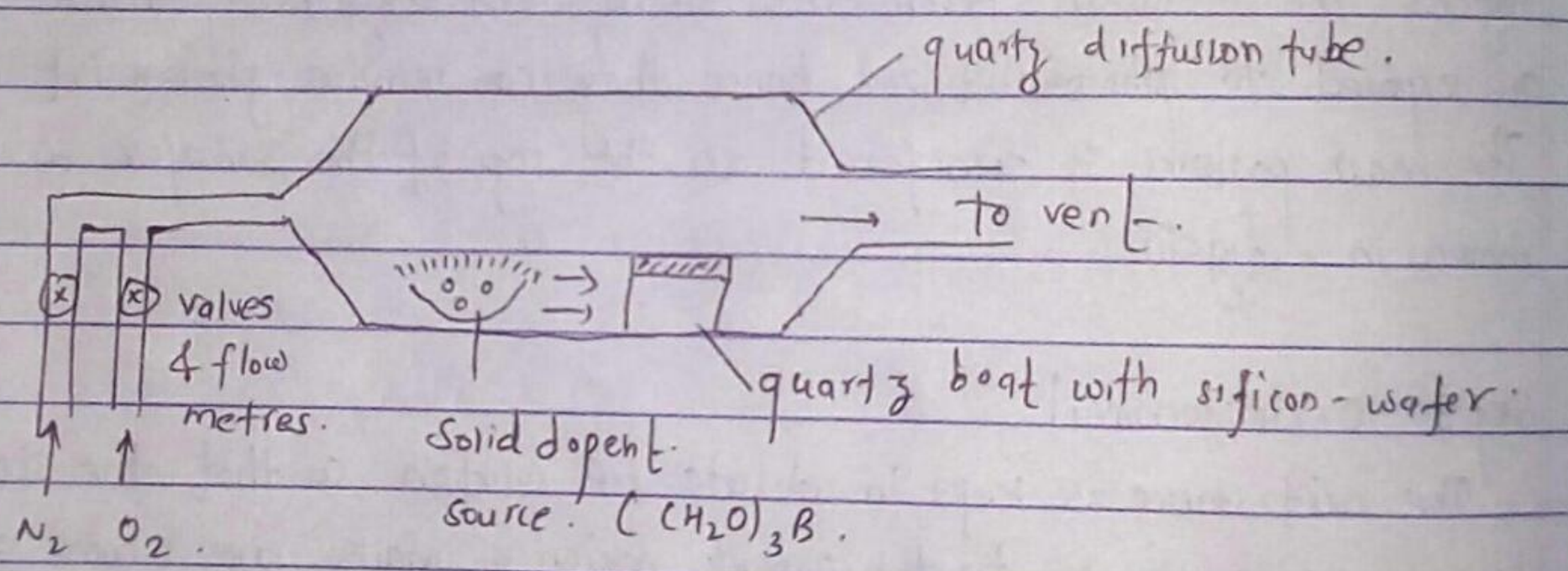
Dopping: It is the process of keeping the dopents in the region of si-wafer having no oxide. It has two methods:

a. Diffusion (solid, liquid & gas sources)

b. Ion implantation

a. Diffusion: When the silicon is heated upto 1000°c, some of its atoms may leave the lattice sites leaving the empty spaces in lattice. The impurity atoms can move (diffuse) into such vacant sites at higher temperature.

i. Solid source diffusion:



In this method, dopent source is in solid form. The carrier gases O_2 & N_2 sweeps up the vapour from the dopent source. Finally, dopent source are deposited in the surface of wafer. The common source of boron is TMB (Borate).

$$\underset{TMB}{(CH_2O)_3B} + O_2 \longrightarrow B_2O_3$$

$$2B_2O_3 + 2Si \longrightarrow 4B + 2SiO_2$$

Common solid source of phosphorus pentaoxide (P_2O_5).

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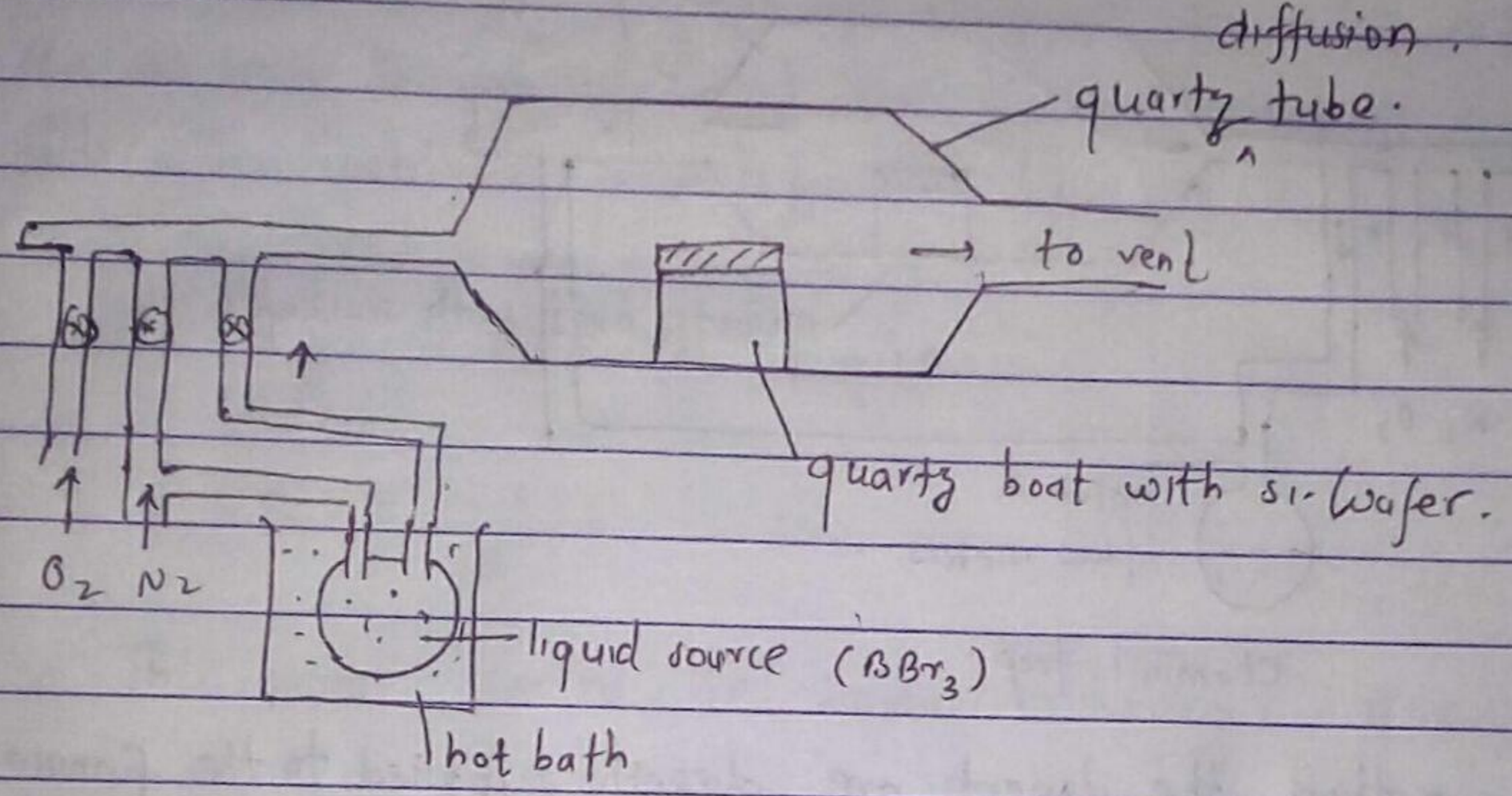
ii. liquid source diffusion:



In this method, the dopent is in liquid form. The carrier gases are passed to the liquid source where it picks up the vapour of liquid source. The carrier carries vapour into the furnace tube where it reacts with surface of si-wafer.

The common liquid source of Boron is BBr_3 (Boron tribromide)

$$BBr_3 + O_2 \longrightarrow B_2O_3 + Br_2^-$$

The common liquid source of phosphorus is $POCl_3$ (P oxychloride).

$$POCl_3 + O_2 \longrightarrow P_2O_5 + Cl_2$$

$$P_2O_5 + Si \longrightarrow P + SiO_2$$

(c) gas source diffusion:

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In this method, the plasma of impurity atom are produced inside ion source the analyser magnet of magentic field B, bends the ion beam to 90° and the beam is made fine by slits. The centripetal force is provided by mf. ie.

Centripetal force = magnetic force.

ie. $\frac{mv^2}{r} = qvB\sin\theta = qvB$

$$\Rightarrow r = \frac{mv}{qB} \quad \ldots (i)$$

This means $r \propto m$. ie. impurities having diff. mass diff radius.

Such ions are accelerated by the accelerator tubes having accelerating voltage of 20–250 kV and are scanned by vertical & horizontal scanners to provide proper deflection. & finally, the ions are implanted on the si-wafer target.

Here, the accelerating voltage provides necessary K.E ie.

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

$$v = \sqrt{\frac{2qV}{m}} \quad \ldots (ii)$$

using (ii) in (i)

$$r = \frac{mv}{qB} = \sqrt{\frac{2mV}{qB^2}} \quad \ldots (iii)$$

The ion implantation method allows the implantation without distrubing previously implanted layers. so, it is superior than diffusion.

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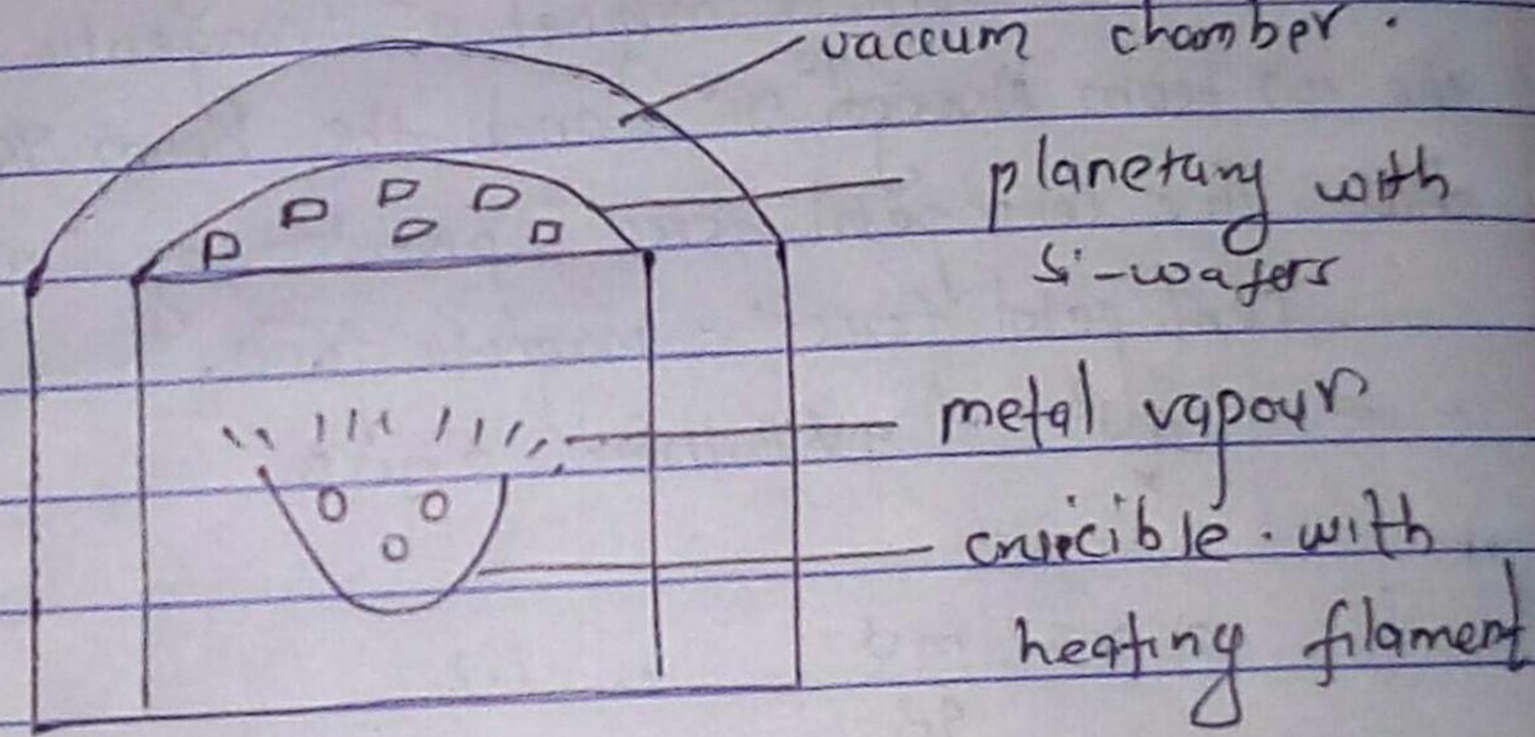
c. Metallization:



Metallization is performed by metallic thin film evapouration. The metal like ~~alloo~~ al. is place in crucible and Si-wafer are place in a doulce called planetary above the crucible. The heater heats the crucible and metal vapours are produced. such vapours heats the wafer and condenses to form thin metallic layers that connects the different sections of IC chips.

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