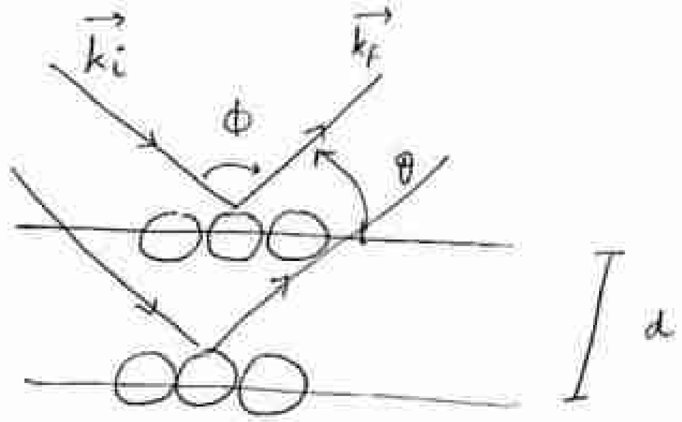
Solid State Physics & Miscellaneous Topics

There are two types of solids

(i) Amorphous

(ii) Crystalline $\longrightarrow$ internal structure can be replicated in terms of some fundamental units called crystals, therefore it has ordered arrangement of atoms.

Crystal Structure Determination



Now, $2\theta + \phi = \pi$

$$\theta = \left(\frac{\pi - \phi}{2}\right)$$

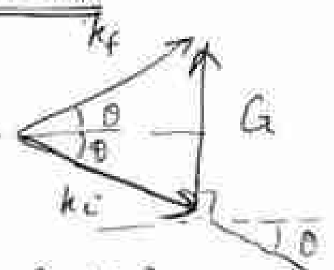
Also, $2d\sin\theta = n\lambda$ for interference constructively

Now we also also, for diffraction, $|\vec{k_f}| = |\vec{k_i}|$

Also $\underline{\vec{k_f} = \vec{k_i} + \vec{G}}$. where $G = \left(\frac{2\pi}{d}\right)$

Laue Equations

and direction is ~~parallel~~ $\perp$ to plane of diffraction



Its called Reciprocal Lattice Vector.

$$|k_f|^2 = |k_i|^2 + |G|^2 + 2\vec{k_i}\cdot\vec{G}$$

$$\Rightarrow \boxed{|G|^2 + 2\vec{k_i}\cdot\vec{G} = 0}$$

$$\Rightarrow \left(\frac{2\pi}{d}\right)^2 + 2\cdot\frac{2\pi}{\lambda}\cdot\frac{2\pi}{d}\cdot\cos(90+\theta) = 0$$

$$\Rightarrow \frac{2\pi}{d} - 2\cdot\frac{2\pi}{\lambda}\cdot\sin\theta = 0$$

$$\Rightarrow \boxed{\lambda = 2d\sin\theta}$$

Also note $\left(\frac{G}{k}\right) = \frac{2\pi}{d}\cdot\frac{\lambda}{2\pi} = \left(\frac{\lambda}{d}\right) = 2\sin\theta$ (for 1^{st} order interference)

Tools of Crystal structure determination

Optical / Conventional Microscopy is not sufficient as their resolving power is quite low. Remember that

Resolving Power $\propto \frac{1}{\lambda}$ $\qquad \lambda = 4000 - 7800\ \text{Å}$

For e^- scattering, λ is quite low $\Rightarrow$ resolving power is high

There are two types of e^- microscopy based on scattering:

1. Transmission e^- microscopy
2. Scanning e^- microscopy

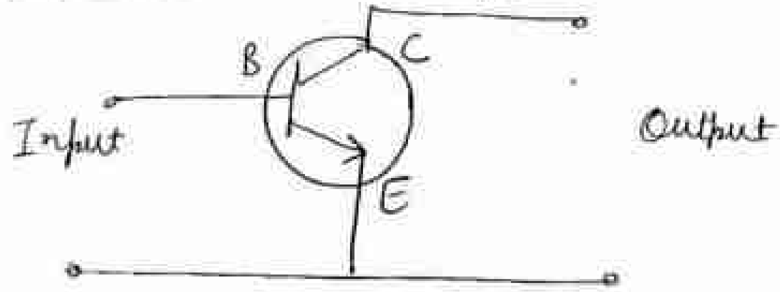
Remember that d is of the order of λ i.e. the structure to be determined should be of order of λ used. if more λ $\Rightarrow$ low resolving power, structure can't be determined.

Properties of solids

1. Magnetic Properties
   - Ferro, Para, Dia — Magnetism
   - Permeability $\mu = \mu_0\mu_r$

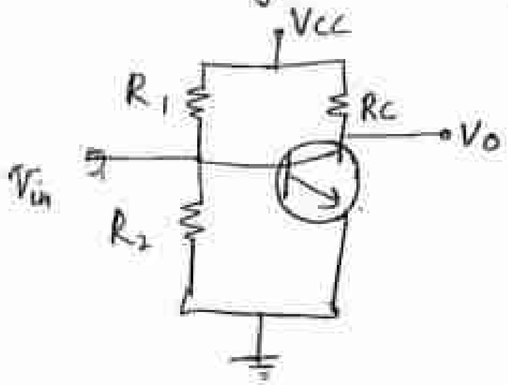
Basic BJT Amplier Configurations

(1) Common Emitter Configuration

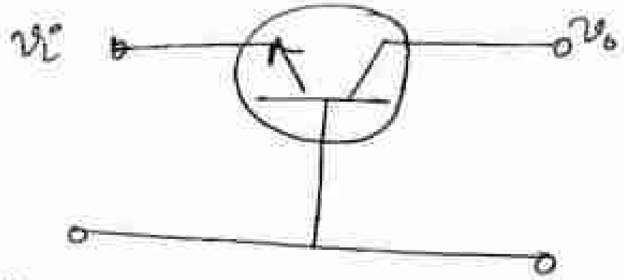


Emitter terminal is common to both input & output signals. Adv

1. Medium input impedance
2. Medium output impedance
3. high voltage gain
4. high current gain

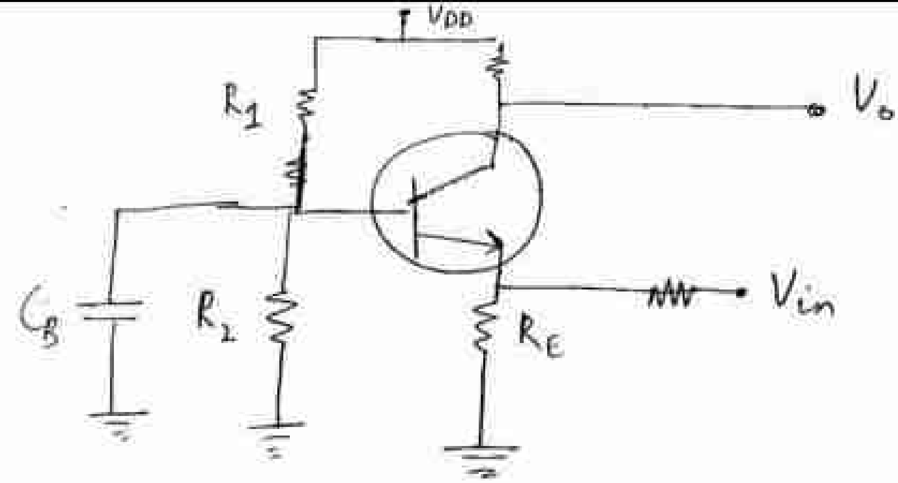


(2) Common Base Configuration

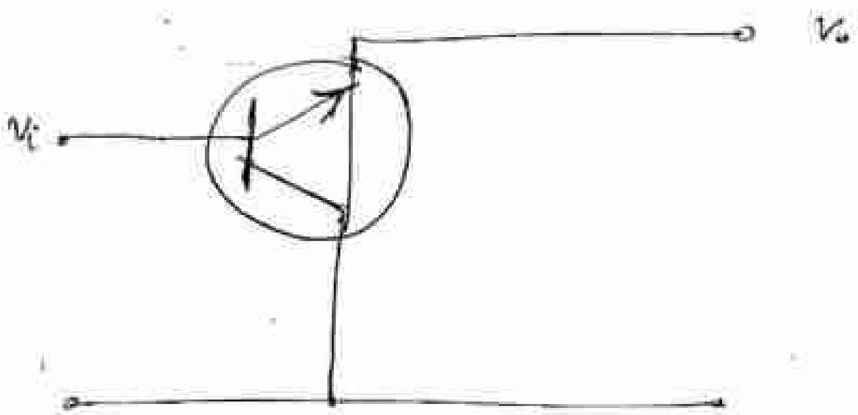


Adv

1. Used freq for RF applications
2. lower input resistance
3. high output impedance
4. Unity or less current gain
5. high voltage gain

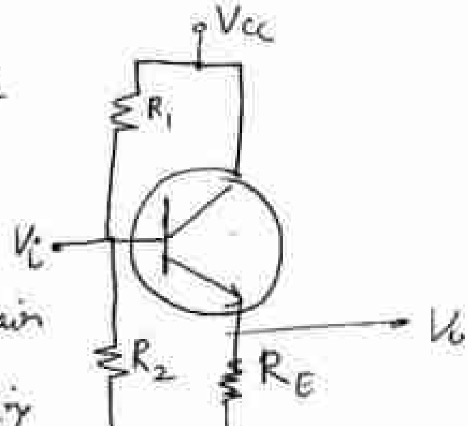


③ Common Collector Configuration



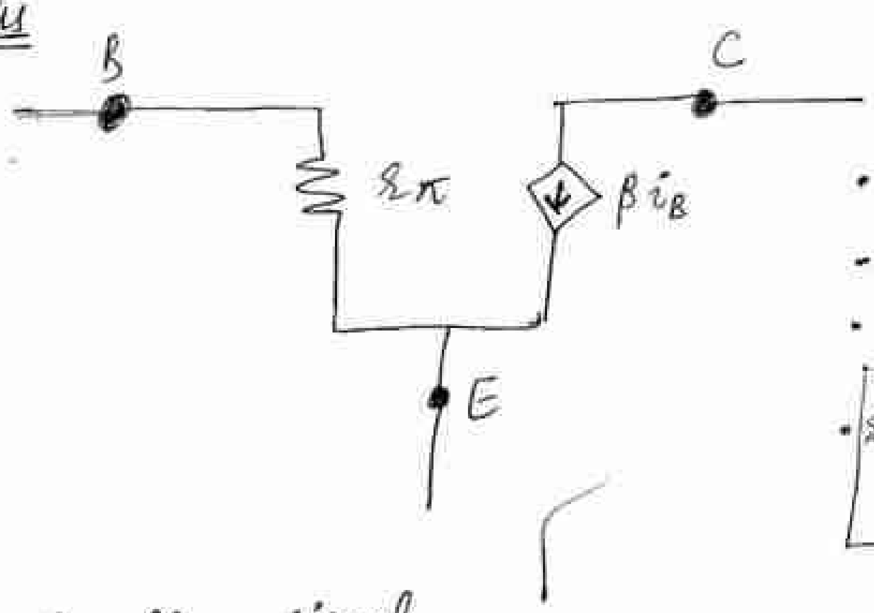
Also called emitter follower because the input signal applied at the base is "follows" quite closely at the emitter with a voltage gain close to unity. It has

1. high input impedance
2. low output impedance
3. high current gain
4. Unity or less voltage gain



Circuit is used as buffer, converting impedance or for feeding or driving long cables or low impedance loads.

Analysis



- $I_E = I_C + I_B$
- $V_{BE} = 0.7\,V$
- $\beta = \left(\frac{I_C}{I_B}\right)$ $\alpha = \left(\frac{I_C}{I_E}\right)$
- $\boxed{r_\pi = \left(\frac{0.025}{I_B}\right)}$

- Small-signal equivalent model of BJT

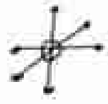
- First, find Q point via D.C. Analysis
- Then replace DC by ground, BJT by small signal model and find out gain, Rin, Rout.

③ Cubic Crystals

no. of nearest neighbours for an atom

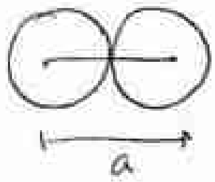
① Simple Cubic

$*$ Coordination no = 6



$*$ Packing Fraction = $\dfrac{\text{Volume of Atoms within unit cell}}{\text{Volume of Unit Cell}}$

[Polonium]



$\boxed{a = 2r}$

No. of atoms in 1 Unit cell = $\frac{1}{8} \times 8$
$= \boxed{1}$

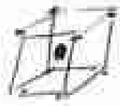
$\Rightarrow P.F. = \dfrac{\frac{4}{3}\pi r^3 \times 1}{a^3}$

$= \frac{4}{3}\pi\left(\frac{1}{8}\right) = \boxed{0.52}$

② Body Centred Cubic

[Na, K]

$*$ Coordination number = 8



$*$ Packing Fraction

$\boxed{\sqrt{3}\,a = 4r}$

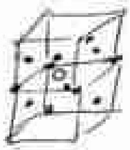
$P.F. = \dfrac{\boxed{2} \times \frac{4}{3}\pi r^3}{a^3}$

$= \frac{8}{3}\pi \, \frac{3\sqrt{3}}{64} = \boxed{0.68}$

③ Face Centred Cubic

[Cu, Ag, Au]

$*$ Coordination number = 12



12 (4 + 4 + 4)
corner, FC of top, FC of bottom

$*$ Packing Fraction

$\boxed{\sqrt{2}\,a = 4r}$

$P.F. = \dfrac{\boxed{4} \times \frac{4}{3}\pi r^3}{a^3}$

$= \frac{16}{3}\pi \, \frac{2\sqrt{2}}{64} = \boxed{0.74}$

..... ABC ABC ABC ....

7

Hexagonal Close Packing

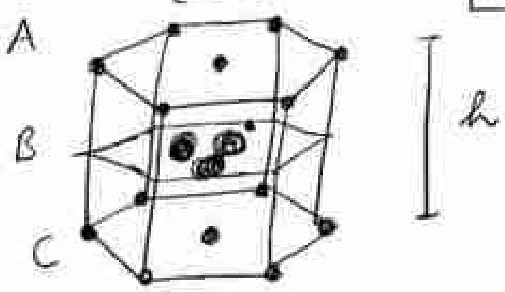
Coordination No. = 6+3+3 = 12

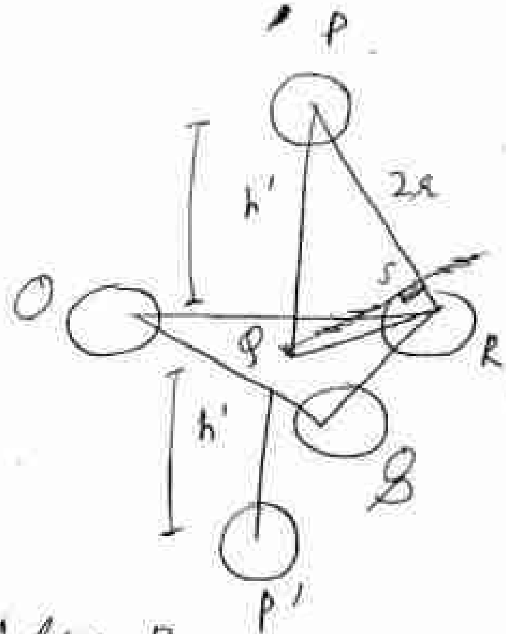
(4)

(Mg, Zn)

$\boxed{a = 2r}$

जमा ही सही है !!





(...ABABAB....)

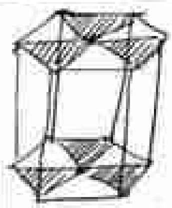
→ Centre of 1st layer A lies exactly over void of 2nd layer. B

→ Centre sphere and spheres of 2nd layer B are in touch.

$\Rightarrow$ ΔORS is equilateral triangle

$\boxed{OR = 2r}$ $\Rightarrow 2\,QR\cos 30^\circ = OR$

$\Rightarrow QR = \frac{r}{\cos 30^\circ} = \left(\frac{2r}{\sqrt{3}}\right)$



in between shaded regions we have 1 atom each

$\Rightarrow QP = \sqrt{(2r)^2 - QR^2} = \sqrt{4r^2 - \frac{4r^2}{3}}$

$= \sqrt{\frac{8r^2}{3}} = \frac{2\sqrt{2}\,r}{\sqrt{3}}$

$\Rightarrow \boxed{h = 2h' = 2QP} = \boxed{\frac{4\sqrt{2}}{\sqrt{3}}\,r}$

$\Rightarrow$ Volume of Crystal $= 6 \times \frac{\sqrt{3}}{4} a^2 \times h$

$= 6 \times \frac{\sqrt{3}}{4} \times 4r^2 \times \frac{4\sqrt{2}}{\sqrt{3}} r = \underline{24\sqrt{2}\,r^3}$

Volume of atoms $= \underline{6 \times \frac{4}{3}\pi r^3}$

$\Rightarrow \boxed{P.F. = 74\%}$

①

- **Solid** < Crystals, Amorphous (glass, rubber, plastic)
  - Crystals → single crystal (diamond, mica, quartz) : Periodicity extends throughout the material
  - Crystals → poly crystalline (metals, ceramic) : Aggregate of a no. of crystallites with random orientations separated by well defined boundaries. These crystallites are called grains.

- Point Lattice / Space Lattice : ∞ no. of imaginary points in 3-dimensional space, each having identical surrounding

- Pattern Unit : Lattice contains small group of points, called pattern unit, which repeat itself in all directions, by means of a translation operator $\vec{T}$

$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$$

- $(n_1, n_2, n_3) \in \mathbb{Z}$ ⇒ Primitive translation vector
  ⇒ Primitive Unit cell

  if fraction ⇒ non-primitive

- Unit Cell : Building block for construction of complete lattice. Primitive Unit Cell is the smallest volume cell.

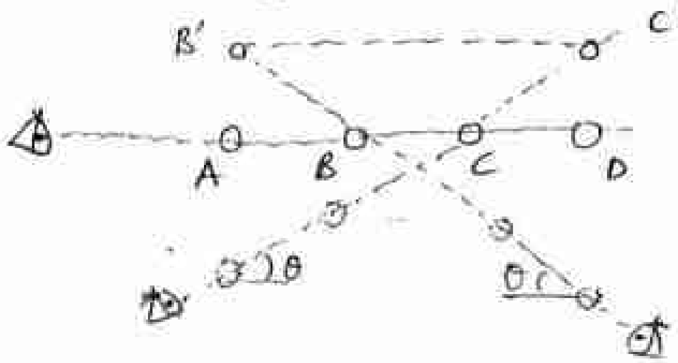
- Wigner-Seitz Cell :
  - Join nearby lattice points
  - draw ⊥ bisectors
  - volume enclosed is Wigner-Seitz Cell

- $\vec{a}, \vec{b}, \vec{c}$: Basis vectors or Crystal Axis

- Component of Crystal Lattice → Space lattice (14), Basis
  - Basis (atom or group of atom that takes the place of space lattice points) < Monoatomic (copper), Complex (Biological)

- **Symmetry Operations** : Transformation that yield the same crystal.
  - Rotation
  - Reflection (about a plane (3D) or a line (2D))
  - Translation $\vec{T}$
  - Inversion $(x\, y\, z) \rightarrow (-x, -y, -z)$

- **Multiplicity of Rotation Axis**



Let distance between lattice points = T

We must have, $B'C' = m\ BC$

$$T + 2T\cos\theta = mT$$

$$\cos\theta = \left(\frac{m-1}{2}\right)$$

$$-1 \leq \frac{m-1}{2} \leq 1$$

$$-1 < m < 3$$

$$\theta = \frac{2\pi}{1}, \frac{2\pi}{2}, \frac{2\pi}{3}, \frac{2\pi}{4}, \frac{2\pi}{6}$$

multiplicity $= \left(\frac{2\pi}{n}\right)$

$$\Rightarrow \boxed{n = 1, 2, 3, 4, 6}$$

For a given crystal, n can take values from above 5 values.

- The symmetry operations lead to different kinds of space lattice :

  5 : 2 - dimensions

  14 : 3 - dimensions

14 '3-D' lattice are defined by 6 lattice parameters :

angles : α, β, γ

dimensions : a, b, c

along with

P (Primitive Cell)

F (Face Centred Cell)

I (body Centered Cell)

② Numbers of effective lattice points belonging to a cell is given by

$$N = N_i + \left(\frac{N_f}{2}\right) + \left(\frac{N_c}{8}\right)$$

c: corner

Lattice directions and planes

→ **direction** given by $[h, k, l]$ (Bracket) where $h, k, l \in \mathbb{Z}$

negative direction is represented by $\bar{h}$.

→ angle between 2 directions

$$\cos\theta = \frac{hh' + kk' + ll'}{\sqrt{(h^2+k^2+l^2)}\sqrt{(h'^2+k'^2+l'^2)}}$$

→ **plane** Orientation is given by Miller Indices (h, k, l) (Parenthesis)

$h, k, l \in \mathbb{Z}$ and are simplified (to integer) reciprocals of intercepts to crystal axes. Intercepts are measured in (a, b, c) units

Interplanar spacing $d = \dfrac{1}{\sqrt{\left(\frac{h}{a}\right)^2 + \left(\frac{k}{b}\right)^2 + \left(\frac{l}{c}\right)^2}}$ (in general)

Interplanar spacing $d = \dfrac{a}{\sqrt{h^2+k^2+l^2}}$

for cubic lattice $(a=b=c)$

Simple Crystal Structures

- Closed Packed
  - FCC
  - HCP

  Packing Fraction = 74%

  Coordination number = 12
- Loose Packed
  - BCC: 68%, C.N. = 8
  - Simple Cubic: 52%, C.N. = 6

Composite Systems

examples include

- diamond cubic Structure: 34%, fcc + alternate tetrahedral
- NaCl structure: fcc + octahedral

Diamond Cubic (dc) structure

✓ Packing Efficiency : 34% (if both atoms are same)

✓ Coordination number : 4

✓ Nearest neighbour distance = $\frac{(\sqrt{3}\,a)}{4}$

✓ 2 Basis

1^{st} : fcc position (effectively : 4 atoms)

2^{nd} : 4 atoms at alternate tetrahedral sides (effectively : 4)

eg. - Si (Both basis : Si atoms)

- Ge (" " : Ge ")
- Diamond (" " : C ")
- ZnS (Zn : 1^{st}, S : 2^{nd})
(Zinc Blende)

✓ It can also be seen as interpenetration of 2 fcc lattices.

NaCl structure

✓ Coordination Number : 6

✓ 2 Basis

1^{st} : fcc position (4)

2^{nd} : octahedral voids (4)

✓ can be viewed as interpenetrating fcc lattices

(4) ⇒ All angle $(\alpha, \beta, \gamma) = 90$ (इनमें working आसान है, यही आएँगे)

Cubic $(a = b = c)$

Tetragonal $(a = b \neq c)$

Orthorhombic $(a \neq b \neq c)$

Q/ A plane makes intercepts of 1, 2 and 0.5 Å on the crystallo graphic axes of an Orthorhombic crystal with $a : b : c = 3 : 2 : 1$. Determine the Miller Indices of the plane

A/ Let length of basis axes vectors be 3Å, 2Å and 1Å

⇒ Intercepts in terms of basis vectors = $\left(\frac{1}{3}\right), \left(\frac{2}{2}\right) \left(\frac{0.5}{1}\right)$

$= \frac{1}{3}, 1, \frac{1}{2}$

⇒ Reciprocal of intercepts = $(3, 1, 2)$

⇒ Miller Indices of Plane are $(3, 1, 2)$

X-ray diffraction

(A) Theory (Scattering + Interference)

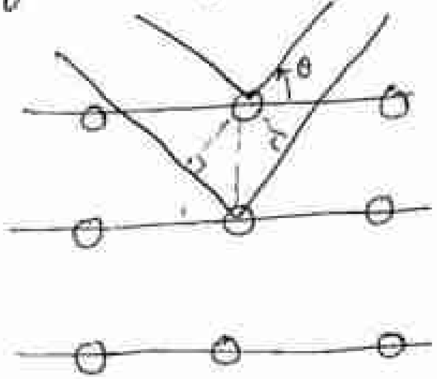
When an atomic electron is irradiated by a beam of monochromatic X-rays, it starts vibrating with frequency equal to that of incident beam. Since an accelarated charge emits radiations, the vibrating electrons present inside a crystal become source of secondary radiations having same frequency as incident X-rays. These secondary

X-rays spread out in all directions. Its called Scattering of X-rays. These secondary waves interfere Constructive only in certain directions, leading to formation of a diffraction pattern, called LAUE'S PATTERN.

(B) ANALYSIS

(1) $\boxed{\text{Bragg's Treatment}}$ (Reflection + Interference)

The direction of diffraction lines can be accounted for if X-rays are considered to be reflected from a set of parallel atomic planes, followed by constructive interference of resulting reflected rays.



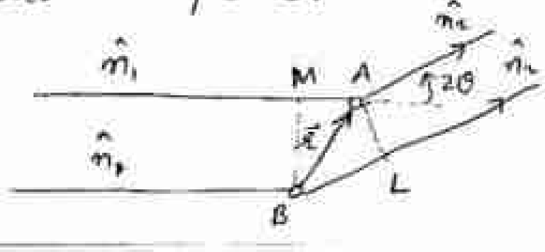
$$\boxed{2d\sin\theta = n\lambda}$$

Bragg's law

Intensity of reflected lines decreases with increase in value of n or θ. n_{max} found by $\sin\theta = 1$.

(2) $\boxed{\text{Von Laue's Treatment}}$

Von Laue considered the scattering of X rays by individual atoms in the crystal, followed by their interference. Note that here we are not considering reflection from an atomic plane. ⇒ its a more general treatment.



(5) $\Delta = BL - AM = \vec{r}\cdot\hat{n}_2 - \vec{r}\cdot\hat{n}_1 = \vec{r}\cdot(\hat{n}_2 - \hat{n}_1)$ (8)

$= \underline{\vec{r}\cdot\vec{N}}$ (where $\vec{N} = \hat{n}_2 - \hat{n}_1$)

$\Rightarrow \Delta\phi = \frac{2\pi}{\lambda}(\vec{r}\cdot\vec{N})$

In a 3-d axes, $\vec{r}$ may coincide with any of the 3 crystallographic axis, $\vec{a}$, $\vec{b}$ and $\vec{c}$. ∴ for occurrence of diffraction maxima,

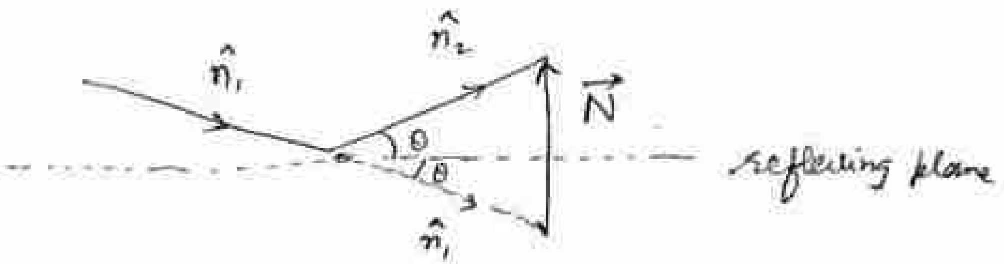
$$\frac{2\pi}{\lambda}(\vec{a}\cdot\vec{N}) = 2\pi h' = 2\pi n h$$

$$\frac{2\pi}{\lambda}(\vec{b}\cdot\vec{N}) = 2\pi k' = 2\pi n k$$

$$\frac{2\pi}{\lambda}(\vec{c}\cdot\vec{N}) = 2\pi l' = 2\pi n l$$

where h', k', l' represent 3 integers having HCF as n.

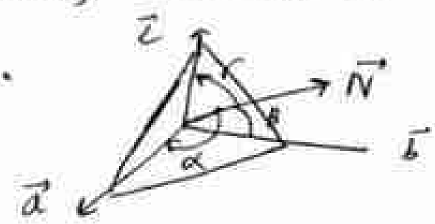
Note that $(h, k l)$ represent the miller indices of a plane which happens to be a reflecting plane (proof on next page) whose normal is $\vec{N}$.



$|\vec{N}| = 2\sin\theta$

Let α, β, γ be angles between scattering normal $\vec{N}$ and crystallographic axis $\vec{a}$, $\vec{b}$ and $\vec{c}$.

$\Rightarrow \vec{a}\cdot\vec{N} = 2a\sin\theta\cos\alpha$



Hence we can write

$$\left.\begin{aligned} \vec{a}\cdot\vec{N} &= 2a\sin\theta\cos\alpha = nh\lambda \\ \vec{b}\cdot\vec{N} &= 2b\sin\theta\cos\beta = nk\lambda \\ \vec{c}\cdot\vec{N} &= 2c\sin\theta\cos\gamma = nl\lambda \end{aligned}\right\} \text{Laue's equations}$$

1) We know <u>interplanar spacing</u>, for plane (h, k, l) is given by

$$d = \frac{a}{h}\cos\alpha = \frac{b}{k}\cos\beta = \frac{c}{l}\cos\gamma$$

Hence, we get $\boxed{2d\sin\theta = n\lambda}$

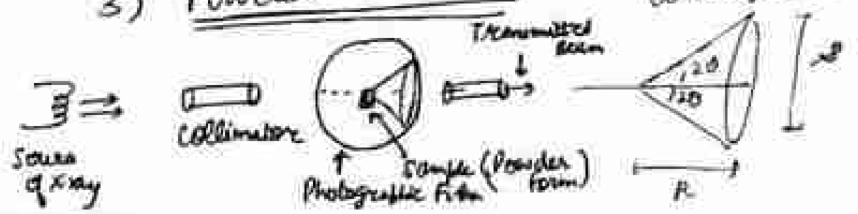
2) For fixed θ, directional cosines $\cos\alpha$, $\cos\beta$, $\cos\gamma$ of scattering normal are proportional to $\left(\frac{h}{a}\right)$, $\left(\frac{k}{b}\right)$ and $\left(\frac{l}{c}\right)$

Also, we know, directional cosines of normal to any arbitrary plane (h, k, l) are proportional to $\frac{h}{a}, \frac{k}{b}, \frac{l}{c}$

Hence, scattering normal $\vec{N}$ is same as normal to the plane (h, k, l) i.e. the arbitrary plane (h, k, l) happens to be reflecting plane.

EXPERIMENTAL METHODS

1) Laue Method
2) Rotating Crystal Method
3) <u>Powder Method</u>



$$4\theta_{(rad)} = \left(\frac{S}{R}\right) \Rightarrow 4\theta_{(degree)} = \left(\frac{57.298\,S}{R}\right)$$

(D) RECIPROCAL LATTICE

(6) Diffraction of x-rays occur from various sets of parallel planes having different orientations (slopes) and different interplanar spacings. Therefore, Ewald developed Reciprocal Lattice s.t.

1) Each Point in Reciprocal lattice corresponds to particular set of parallel planes of the direct lattice.
2) Distance of reciprocal lattice point from an arbitrarily fixed origin, is inversely proportional to the interplanar spacing of corresponding parallel planes of the direct lattice.
3) Volume of unit cell of reciprocal lattice is inversely proportional to volume of corresponding unit cell of direct lattice.

Reciprocal lattice Vector

a^* : magnitude = reciprocal of interplanar spacing d_{hkl}

direction = normal to (hkl) plane

$$a^* = \frac{1}{d_{hkl}} \hat{n}$$

Note that a vector drawn from the origin to any point in the reciprocal lattice is a Reciprocal lattice Vector.

$$a^* = 2\pi \left[\frac{\vec{b}\times\vec{c}}{\vec{a}\cdot(\vec{b}\times\vec{c})}\right] \qquad c^* = 2\pi\left[\frac{\vec{a}\times\vec{b}}{\vec{a}\cdot(\vec{b}\times\vec{c})}\right]$$

$$b^* = 2\pi\left[\frac{\vec{c}\times\vec{a}}{\vec{a}\cdot(\vec{b}\times\vec{c})}\right]$$

a, b, c :- Translation vector of direct lattice

a^*, b^*, c^* :- of reciprocal lattice

- Hence, every crystal is associated with 2 types of lattice: direct lattice and reciprocal lattice.

Also, $\vec{a}^*\cdot(\vec{b}^*\times\vec{c}^*) = \dfrac{1}{\vec{a}\cdot(\vec{b}\times\vec{c})}$

$T = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}$

$\underline{G = h\vec{a}^* + k\vec{b}^* + l\vec{c}^*}$ reciprocal lattice vector

$$e^{i(G\cdot T)} = e^{i\,2\pi[n_1h + n_2k + n_3l]} = 1$$

$\boxed{\text{Simple Cubic}}$

$\vec{a} = a\hat{i}$ $\quad \vec{a}^* = \left(\frac{2\pi}{a}\right)\hat{i}$, $\vec{b}^* = \left(\frac{2\pi}{a}\right)\hat{j}$,

$\vec{b} = a\hat{j}$

$\vec{c} = a\hat{k}$ $\quad \vec{c}^* = \left(\frac{2\pi}{a}\right)\hat{k}$

Hence reciprocal lattice is also simple cubic.

$\boxed{\text{BCC lattice}}$

$\vec{a} = \frac{a}{2}(\hat{i}+\hat{j}-\hat{k})$ $\quad \vec{a}^* = \frac{2\pi}{a}(\hat{i}+\hat{j})$

$\vec{b} = \frac{a}{2}(-\hat{i}+\hat{j}+\hat{k})$ $\quad \vec{b}^* = \frac{2\pi}{a}(\hat{j}+\hat{k})$

$\vec{c} = \frac{a}{2}(\hat{i}-\hat{j}+\hat{k})$ $\quad \vec{c}^* = \frac{2\pi}{a}(\hat{k}+\hat{i})$

negative

(एक पीछे वाले में जाइ वइ)

missing

(केवल पहले की working दिखाओ बाकी बोलो cyclically आ जाएंगे)

$\Downarrow$

Primitive translation vectors of FCC lattice

$\boxed{\text{FCC lattice}}$

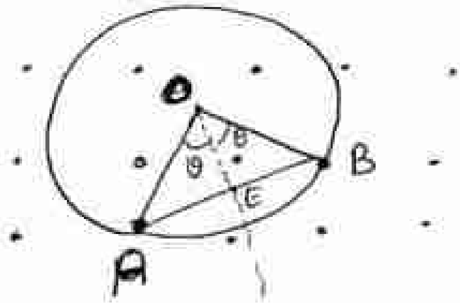
$\vec{a} = \frac{a}{2}(\hat{i}+\hat{j})$ $\quad \vec{a}^* = \frac{2\pi}{a}(\hat{i}+\hat{j}-\hat{k})$

$\vec{b} = \frac{a}{2}(\hat{j}+\hat{k})$ $\quad \vec{b}^* = \frac{2\pi}{a}(\hat{j}+\hat{k}-\hat{i})$

$\vec{c} = \frac{a}{2}(\hat{k}+\hat{i})$ $\quad \vec{c}^* = \frac{2\pi}{a}(\hat{k}+\hat{i}-\hat{j})$

Primitive Translation vector of BCC lattice

⑦ Bragg's law in Reciprocal Lattice



Ewald construction

In reciprocal lattice take any point O (not necessarily a lattice point)

draw $\vec{OA}$ of length $\left(\frac{1}{\lambda}\right)$ in direction of incident X-ray beam s.t. it terminates on a lattice point A

Draw circle from O with OA radius and define coordinate system with A at origin.

If B intersects the circle, whose coordinates are $(h', k', l') = (nh, nk, nl)$

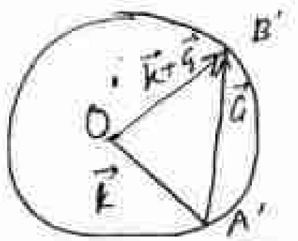
$$\Rightarrow \quad |\vec{AB}| = \left(\frac{n}{d_{hkl}}\right) \quad : \text{reciprocal lattice vector}$$

$$AB = 2\,AE = 2\,OA \sin\theta = \frac{2\sin\theta}{\lambda}$$

$$\Rightarrow \quad \frac{n}{d_{hkl}} = \frac{2\sin\theta}{\lambda}$$

$$\Rightarrow \quad \boxed{n\lambda = 2 d_{hkl} \sin\theta}$$

$\boxed{2^{nd}\text{ form}}$



Magnified Ewald Construction

$$A'O' = \left(\frac{2\pi}{\lambda}\right) \quad \text{write } \vec{A'O'} = \vec{k}$$

$A'B'$: reciprocal lattice vector $\vec{G}$

$$|O'A'| = |O'B'| \Rightarrow (\vec{k}+\vec{G})^2 = k^2 \Rightarrow \boxed{G^2 + 2\vec{k}\cdot\vec{G} = 0}$$

The 2nd form is used to Brillouin Zones.

(E) Brillouin Zones

From Ewald construction, we know all the $\vec{k}$ values for which reciprocal lattice points intersect the Ewald sphere are Bragg reflected.

A Brillouin Zone is locus of all those k-values in the reciprocal lattice which are Bragg reflected.

Simple Square Lattice (not cubic)

$$\vec{a} = a\hat{i} \qquad \vec{a}^* = \left(\frac{2\pi}{a}\right)\hat{i} \qquad \vec{G} = \frac{2\pi}{a}(h\hat{i} + k\hat{j})$$

$$\vec{b} = a\hat{j} \qquad \vec{b}^* = \left(\frac{2\pi}{a}\right)\hat{j}$$

Using 2nd form of Bragg's equation,

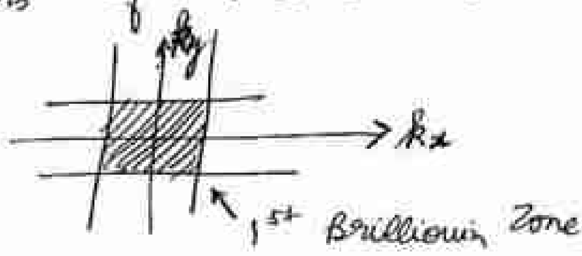
$$2\vec{k}\cdot\vec{G} + G^2 = 0$$

$$hk_x + kk_y = -\frac{\pi}{a}(h^2+k^2)$$

Consider all possible combinations of (h, k), we get

$h = \pm 1,\ k = 0 \Rightarrow k_x = \pm\left(\frac{\pi}{a}\right),\ k_y \in \mathbb{R}$

$h = 0,\ k = \pm 1 \Rightarrow k_y = \pm\left(\frac{\pi}{a}\right),\ k_x \in \mathbb{R}$



Using other values of (h, k) obtain other zones

[Boundaries of Brillouin zones represent loci of k-values that are Bragg reflected ⇒ hence, they are reflecting planes: 1st zone : 1st order reflection
2nd zone : 2nd order reflection]

2nd zone ↓ $(h,k) = (\pm 1, \pm 1)$

(8) BCC (remember we are taking reciprocal lattice here) 90

$a^* = (2\pi/a)(\hat{i}+\hat{j})$

$b^* = (2\pi/a)(\hat{j}+\hat{k})$

$c^* = (2\pi/a)(\hat{k}+\hat{i})$

$$\vec{G} = \frac{2\pi}{a}\left((h+l)\hat{i} + (h+k)\hat{j} + (k+l)\hat{k}\right)$$

Using different combinations like $(\pm1,0,0)$, $(0,\pm1,0)$, $(0,$

we get 12 vectors viz $\frac{2\pi}{a}(\pm\hat{i}\pm\hat{j})$, $\frac{2\pi}{a}(\pm\hat{j}\pm\hat{k})$, $\frac{2\pi}{a}(\pm\hat{k}\pm$

$\Rightarrow$ $\boxed{\text{Rhombic Dodecahedron}}$ (12 faced)

FCC

$\vec{a}^* = \frac{2\pi}{a}(\hat{i}+\hat{j}-\hat{k})$

$\vec{b}^* = \frac{2\pi}{a}(-\hat{i}+\hat{j}+\hat{k})$

$\vec{c}^* = \frac{2\pi}{a}(\hat{i}-\hat{j}+\hat{k})$

$$\vec{G} = \frac{2\pi}{a}\left[(h-k+l)\hat{i} + (h+k-l)\hat{j} + (-h+k+l)\hat{k}\right]$$

We get $\boxed{\text{Truncated Octahedron}}$

(F) Allowed h, k, l values for reflections

Simple Cubic : all possible values of h, k, l

$h^2+k^2+l^2$:- 1 : 2 : 3 : 4 :

BCC : even values of $h+k+l$

$h^2+k^2+l^2$:- 2 : 4 : 6 : 8
(1,1,0) (2,0,0) (2,1,1)

FCC : all odd or all even values of h, k, l

$h^2+k^2+l^2$:- 3 : 4 : 8 : 11 : ...
(1,1,1) (2,0,0) (2,2,0) (3,1,1)

Remember ① $d_{hkl} = \dfrac{a}{\sqrt{h^2+k^2+l^2}}$ for cubic crystals

a : lattice parameter

② $a^3 = \left(\dfrac{n'M}{N\rho}\right)$

n' : effective atom in a cubic crystal (FCC : 4)

M : Molecular Weight

N : Avogadro

ρ : density of crystal

$\left(\rho = \dfrac{n'\left(\frac{M}{N}\right)}{a^3}\right)$

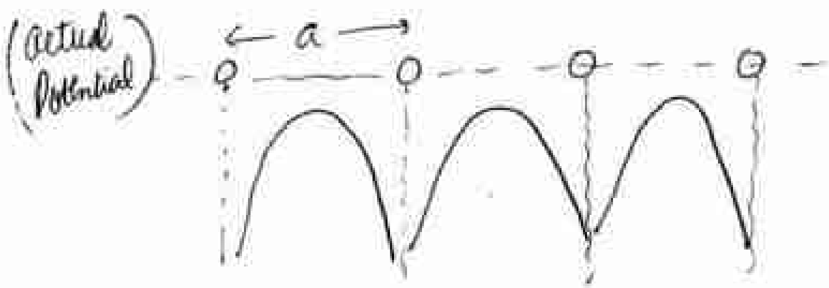
$\left(\dfrac{M}{N}\right)$: mass of 1 atom

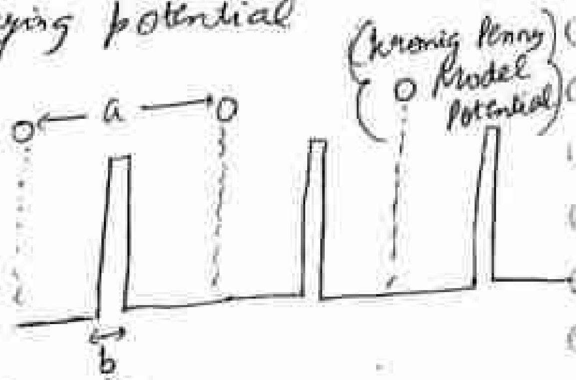
Band Theory of Solids

- If we assume free e^- i.e. no bound of Potential, then

$$\psi = e^{ikx}$$
$$E = \left(\frac{\hbar^2 k^2}{2m}\right), \quad \underline{k} \in (-\infty, \infty)$$

But in order to understand Band Structure of Solids, we have to consider a periodically varying potential





< Read Band Structure from H.C. Verma >

< Qualitative formation of Band Gaps & >

< classification of solids into conductors, insulators >

< and semiconductors. >

The movement of e- in a region of periodically varying potential, with the periodicity of the lattice, caused by ion-cores situated at the lattice points, which results in diffraction of electrons by the lattice $\left(\text{if } \lambda = h/p \approx a\right)$.

The electron undergoes Bragg's reflection.

(9) Schrödinger Solution of Kronig Penny Potential (9d)

Eigenfunction of a free electron travelling wave

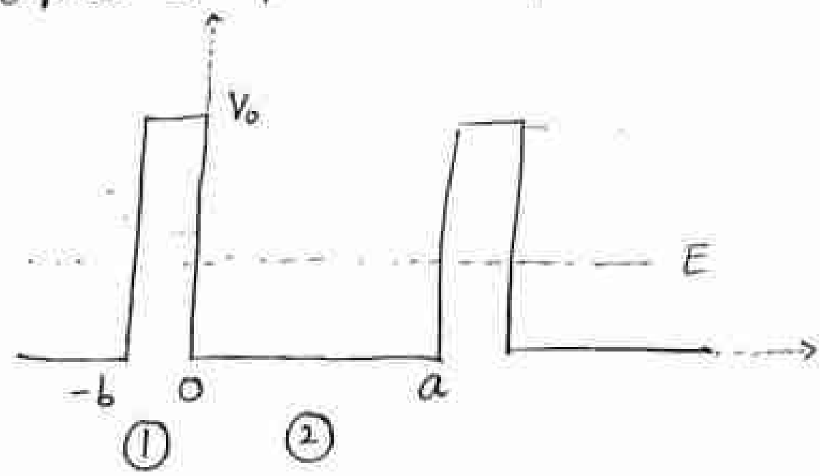
$\psi(x) = e^{\pm ikx}$ where $k = \frac{2\pi}{\lambda}$ i.e. propagation const.

For a periodic potential with periodicity a,

$\psi(x) = U_k(x)\, e^{\pm ikx}$ where $U_k(x+a) = U_k(x)$
$= U_k(x+na)$

This is called Bloch Theorem.

$U_k(x)$ depends on particular potential and value of k.



Writing eqn.

$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}(E-V_0)\psi_1 = 0 \qquad -b<x<0$$

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}E\,\psi_2 = 0 \qquad 0<x<a$$

Using $\alpha^2 = \frac{2mE}{\hbar^2}$, $\beta^2 = \frac{2m(V_0-E)}{\hbar^2}$, $\psi_1 = e^{ikx}u_1(x)$
$\psi_2 = e^{ikx}u_2(x)$

$\left[\begin{matrix}\alpha \Leftrightarrow k \\ \beta \Leftrightarrow \gamma\end{matrix}\right]$

Hence, we get

$$\left(\frac{d^2u_2}{dx^2}\right) + 2ik\left(\frac{du_2}{dx}\right) + (\alpha^2-k^2)\,u_2 = 0 \qquad 0<x<a$$

$$\left(\frac{d^2u_1}{dx^2}\right) + 2ik\left(\frac{du_1}{dx}\right) - (\beta^2+k^2)\,u_1 = 0 \qquad -b<x<0$$

For simplification, $V_0 \to \infty$
$b \to 0$

$V_0 b$: finite, called Barrier Strength

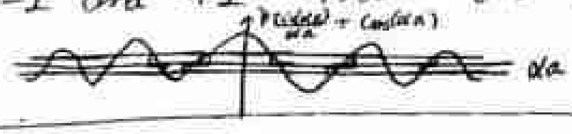
Hence, upon using continuity & differential continuity, we get (after lengthy calculation)

$$\boxed{P = \frac{mV_0 b}{\hbar^2}} \quad \left(\frac{mV_0 b}{\hbar^2 \alpha}\right) \sin(\alpha a) + \cos(\alpha a) = \cos(ka)$$

(Can also use $P = \frac{mV_0 b}{\hbar^2}$)

$$\Rightarrow \boxed{P\left(\frac{\sin(\alpha a)}{\alpha a}\right) + \cos(\alpha a) = \cos(ka)}$$

Only those values of (αa) are allowed for which L.H.S lies between -1 and $+1$. From this the following conclusions are drawn:

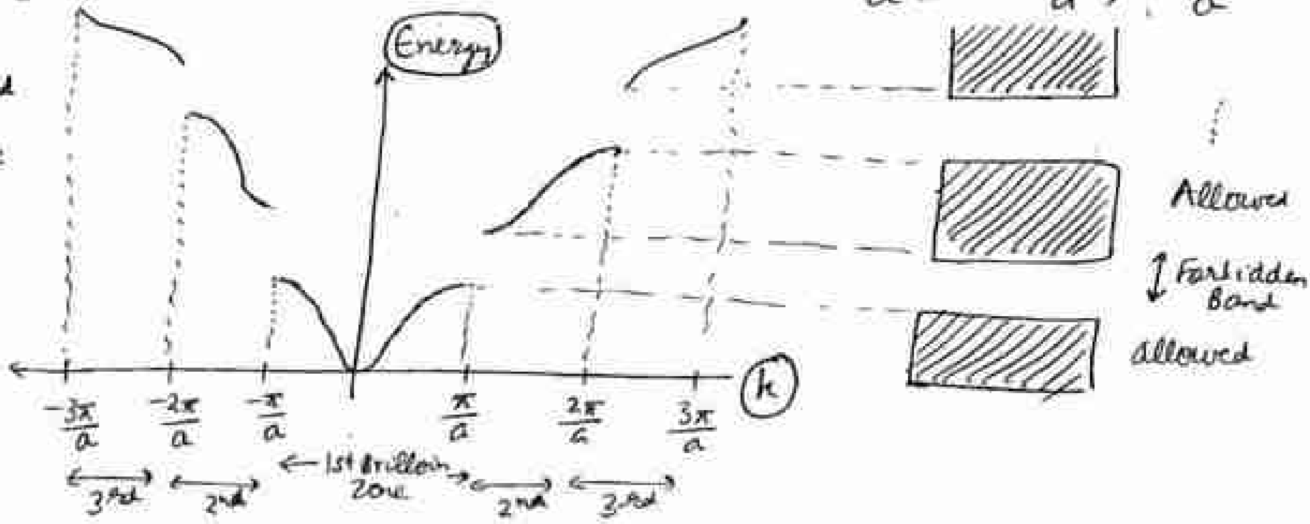


1) Energy spectrum consists of alternate regions of allowed energy bands and forbidden energy bands.
2) Width of bands increases with α (or energy).

$\cos ka = \pm 1$ (for discontinuity) $\Rightarrow ka = \pm n\pi$

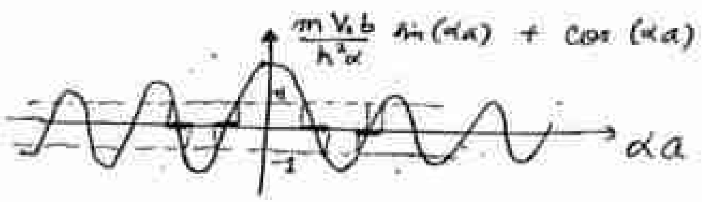
$\Rightarrow$ Bands are discontinuous at $k = \pm\frac{\pi}{a}, \pm\frac{2\pi}{a}, \pm\frac{3\pi}{a} \ldots$

Extended Zone scheme of E–k curve



Note that these values of k define the boundaries of the Brillouin zones. The Bragg reflections at these boundaries result in discontinuities in E-k curve.

L.H.S. curve

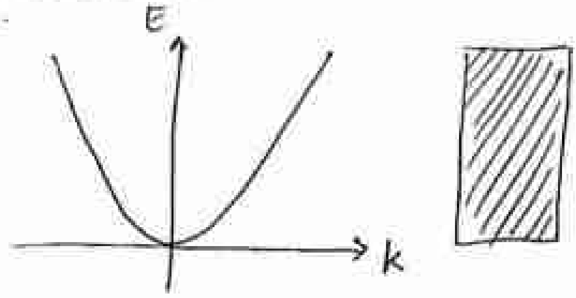


— allowed Bands

(E=0 नहीं allowed है, in extended zone scheme)

The previous E-k curve is for intermediate Bound

For loosely bound, $V_0 b \to 0$



loosely bound case

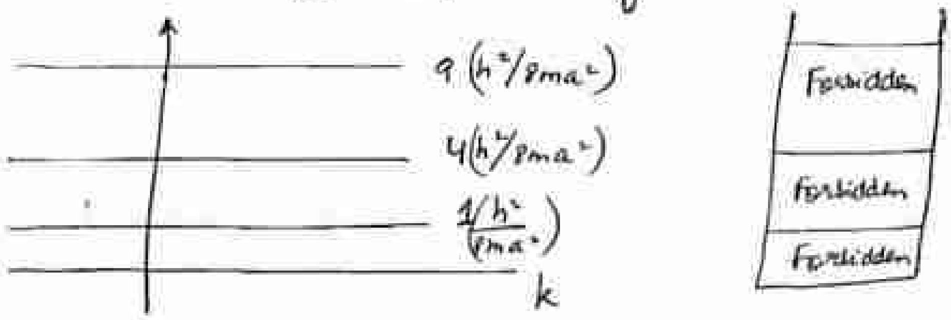
For tight bound, $V_0 b \to \infty$

$$\Rightarrow \sin \alpha a = 0$$

$$\alpha a = n\pi$$

$$\Rightarrow E = \left(\frac{n^2 h^2}{8ma^2}\right) \quad (n = 1, 2, 3, \ldots)$$

i.e. independent of k



Similar to 1-D ∞ box

Explanation by Brillouin Zones

We know for diffraction $2\vec{k}\cdot\vec{G} + G^2 = 0$

For one-dimension case,

Primitive lattice vector (base) $\vec{a}_1 = a\hat{x}$

$\Rightarrow$ Reciprocal lattice vector (base) $\vec{a}_1^* = \left(\frac{2\pi}{a}\right)\hat{x}$

$\Rightarrow$ Reciprocal lattice vector $\vec{G} = n_x \vec{a}_1^* = \frac{2\pi n_x}{a}\hat{x}$

Let us write $\vec{k} = k_x\hat{x} + k_y\hat{y} + k_z\hat{z}$

$$\Rightarrow 2\vec{k}\cdot\vec{G} + G^2 = 0 \Rightarrow 2 \cdot \frac{2\pi n_x k_x}{a} + \left(\frac{2\pi n_x}{a}\right)^2 = 0 \Rightarrow k_x = \left(\frac{n_x \pi}{a}\right.$$

No. of Wavefunctions in a Band

For a crystal of length L & no. of primitive cells $= N$,

$$\psi(x+L) = \psi(x)$$

$$\Rightarrow e^{ik(x+L)} u_k(x+L) = e^{ikx} u_k(x)$$

$$\Rightarrow e^{ikL} = 1$$

$$\Rightarrow \boxed{k = \left(\frac{2n\pi}{L}\right)} \qquad n = \pm 1, \pm 2, \pm 3, \ldots$$

$$\Rightarrow k = \pm\left(\frac{2\pi}{L}\right), \pm\left(\frac{4\pi}{L}\right), \pm\left(\frac{6\pi}{L}\right), \ldots$$

$$\Rightarrow dk = \left(\frac{2\pi}{L}\right) dn \Rightarrow dn = \left(\frac{L}{2\pi}\right) dk$$

$$\Rightarrow \text{Total no. of states} = \int dn$$

$$= \int_{-\pi/a}^{\pi/a} \frac{L}{2\pi} \, dk$$

$$= \frac{L}{2\pi} \cdot \frac{2\pi}{a}$$

$$\left(\text{assuming } b \to 0, \; N = \frac{L}{a+b} = \left(\frac{L}{a}\right)\right) \quad = \left(\frac{L}{a}\right)$$

$$= N$$

But each state can occupy 2 electrons

$\Rightarrow$ each band has a maximum $2N$ electron state

i.e. can accomodate $2N$ electrons.

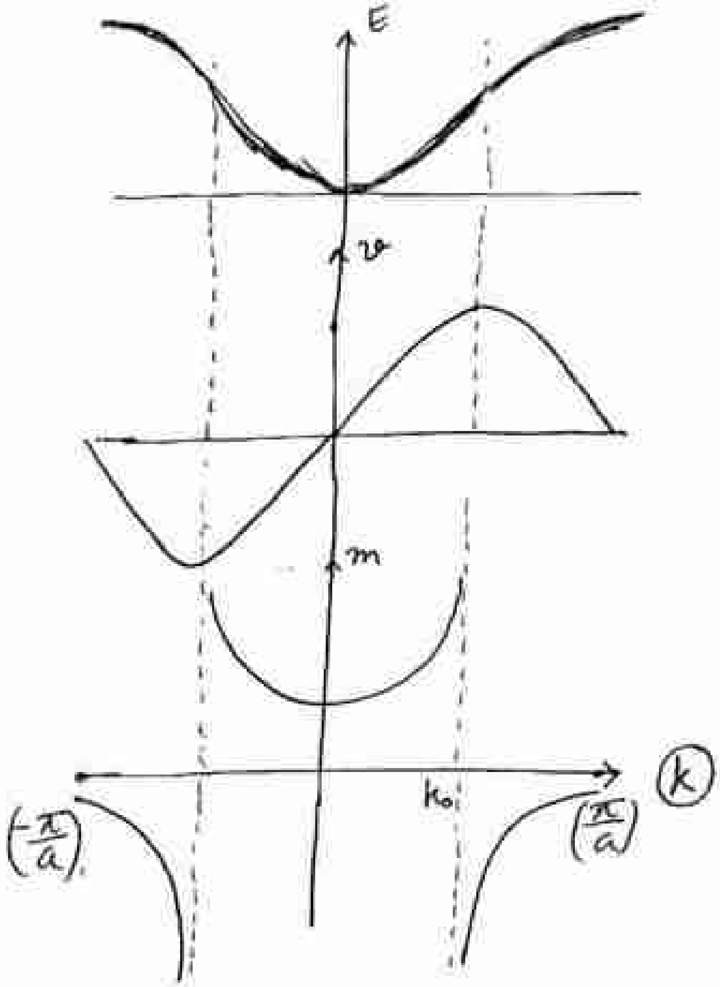
Effective Mass

a particle moving with velocity v is equivalant to a wave packet moving with a group velocity v_g

$$v = v_g = \left(\frac{d\omega}{dk}\right)$$

Also $E = \hbar\omega \Rightarrow \boxed{v = \frac{1}{\hbar}\left(\frac{dE}{dk}\right)}$

Considering the first brillouin zone



k_0 : inflexion point of E(k) curve

The mass of an electron in a crystal, in general, appears different from free e- mass, and is referred to as m^* from a semi-classical model. We find expression for m^* from a

$$\text{Accelaration } a = \left(\frac{dv}{dt}\right) = \frac{1}{\hbar}\left(\frac{d^2E}{dk^2}\right)\cdot\left(\frac{dk}{dt}\right)$$

Let us consider electron to be placed in an electric field E_0 s.t. work done by electric field on the electron, at a particular k, will increase the energy by dE

$$dE = eE_0 dx = eE_0 v\, dt = \frac{eE_0}{\hbar}\left(\frac{dE}{dk}\right)\cdot dt$$

$$\Rightarrow \left(\frac{dE}{dt}\right) = \frac{eE_0}{\hbar}\left(\frac{dE}{dk}\right)$$

$$\Rightarrow \left(\frac{dE}{dk}\right)\left(\frac{dk}{dt}\right) = \frac{eE_0}{\hbar}\left(\frac{dE}{dk}\right) \Rightarrow \left(\frac{dk}{dt}\right) = \frac{eE_0}{\hbar}$$

$$\Rightarrow m^* = \frac{F}{a} = \frac{eE_0}{\frac{1}{\hbar}\left(\frac{d^2E}{dk^2}\right)\left(\frac{dk}{dt}\right)} = \frac{eE_0}{\frac{1}{\hbar}\left(\frac{d^2E}{dk^2}\right)\frac{eE_0}{\hbar}} = \frac{\hbar^2}{\left(\frac{d^2E}{dk^2}\right)}$$

Concept of negative mass

Effective mass, taking negative values can be understood by Bragg's reflection when k is close to $\pm\left(\frac{\pi}{a}\right)$. Due to Bragg's reflection, a force applied in one direction will lead to gain of momentum in the opposite direction, resulting in negative effective mass.

For alkali metals, partially filled band implies conduction taking place mainly through electrons. However in crystals for which energy band is nearly full, except for a few electron vacancies at top of band, these negative charge & negative mass vacancies may be considered as positive charge & positive mass particles called HOLES, which act as ⊕ve charged carriers to produce conduction.

[Negative charge, negative mass वाली states की vacancy = hole equivalent to position in fermi model]

Effective no. of free electrons

Let $f_k = \frac{m}{m^*} = \frac{m}{\hbar^2}\left(\frac{d^2E}{dk^2}\right)$

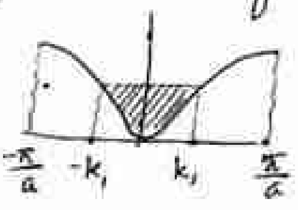
Measure of extent to which electron behaves as a free electron

$f_k = 1 \Rightarrow e^-$ behaves totally as free electron

If $f_k < 1 \Rightarrow e^-$ behaves as a heavy particle : less mobility & therefore less conduction.

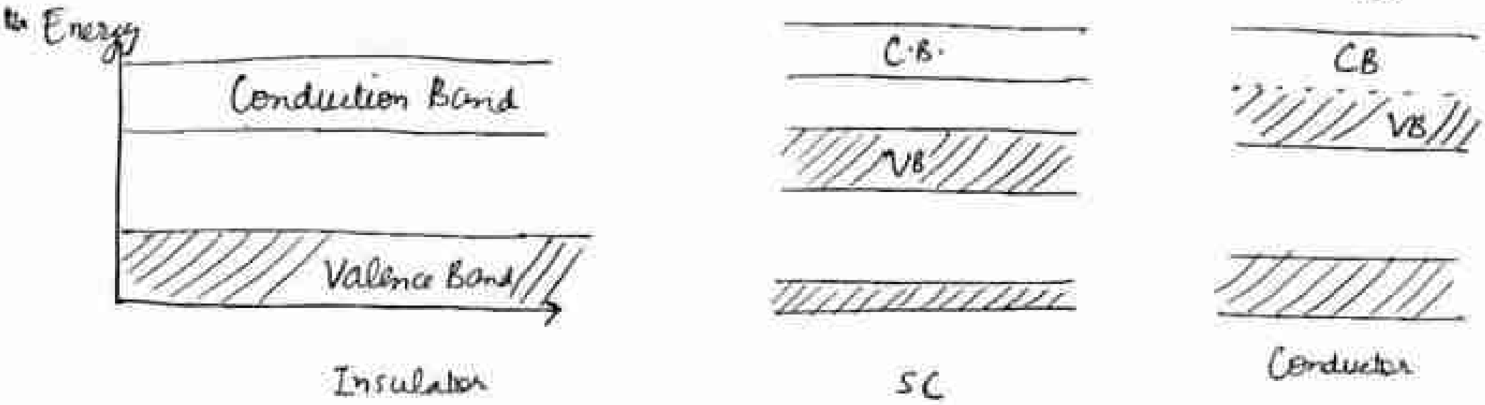
Let energy band be filled upto $k = k_1$.

We know $dn = \frac{L}{\pi} dk$



$$N_{eff} = \int_{-k_1}^{k_1} f_k \, dn = \frac{2mL}{\pi\hbar^2}\int_0^{k_1}\left(\frac{d^2E}{dk^2}\right) dk$$

$$\boxed{N_{eff} = \frac{2mL}{\pi\hbar^2}\left(\frac{dE}{dk}\right)_{k=k_1}}$$



$\boxed{@\ T = 0K}$

→ For completely filled band, $\left(\frac{dE}{dk}\right) = 0 \Rightarrow N_{eff} = 0 \Rightarrow$ insulator

→ For maximum N_{eff}, band should be filled upto inflexion point
⇒ Partly filled Band has metallic Character

Magnetism in Solids

Diamagnetism

- Magnetism, in general, in solids is due to
  - spin of electrons
  - orbital motion of electrons
  - spin of nuclei
- (1) Weak effect; in (2) solids which do not contain permanent magnetic moment; due to (3) orbital motion of electrons; directed (4) opposite to applied magnetic field.
- Induced current due to change of electron motion, according to Lenz's law
- Diamagnetism exists in all materials but is usually suppressed due to presence of stronger effects like paramagnetism, ferromagnetism e
- Manifested by small & negative value of χ.

Langevin's Classical theory

Let electron revolve around nucleus in a circular orbit (of radius ρ) with frequency ω_0.

$$\Rightarrow m\omega_0^2 \rho = \frac{Ze^2}{4\pi\varepsilon_0 \rho^2}$$

$$\Rightarrow \omega_0 = \sqrt{\frac{Ze^2}{4\pi\varepsilon_0 m\rho^3}}$$

Now an external magnetic field $\vec{B}$ is applied.

$$\vec{F}' = e(\vec{v}\times\vec{B}) = e\rho\omega B$$

$\Rightarrow$ Net force $= \vec{F}_{nucleus} + \vec{F}' = m\omega^2\rho$

$$\Rightarrow m\omega^2\rho = \frac{Ze^2}{4\pi\varepsilon_0\rho^2} - e\rho\omega B$$

$$= m\omega_0^2\rho - e\rho\omega B$$

$$\Rightarrow \omega^2 + \left(\frac{eB}{m}\right)\omega - \omega_0^2 = 0$$

$$\Rightarrow \boxed{\omega \approx \omega_0 - \frac{eB}{2m}} \qquad \left(\text{Considering } \omega_0 >> \frac{eB}{2m}\right)$$

Larmor Theorem

$$\Rightarrow \Delta\nu = \frac{1}{2\pi}\frac{eB}{2m}$$

Due to change in frequency, current is altered in the current loop

Additional Current in 1 loop $= e *$ additional frequency

$$= -\left(\frac{e^2B}{4\pi m}\right)$$

$$\Rightarrow \text{Magnetic Moment} = -\left(\frac{e^2B\rho^2}{4m}\right)$$

- For Z electrons, total induced magnetic moment

$$\mu_T = -\frac{Ze^2 B}{4m} \langle \rho^2 \rangle$$ (Z का multiple और $\langle \rho^2 \rangle$ का average)

now note that if field along z-axis, then

$$\langle \rho^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle$$

= mean of squares of $\perp$ distances from axis of the field

Also $\langle r^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle$

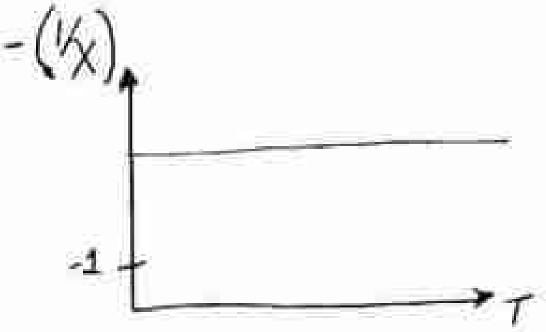
= mean square distance of electron from nucleus.

For spherical distⁿ of charge, $\langle x^2 \rangle = \langle y^2 \rangle = \langle z^2 \rangle$

$$\Rightarrow \quad \mu_T = -\frac{Ze^2 B}{4m} \cdot \frac{2}{3} \langle r^2 \rangle = -\frac{Ze^2 B}{6m} \langle r^2 \rangle$$

For a solid containing N atoms per unit volume.

$$\chi_{dia} = \frac{M}{H} = \frac{N \mu_T \mu_0}{B} = \underline{-\frac{N Z e^2 \mu_0}{6m} \langle r^2 \rangle}$$



χ_{dia} is independent of temperature

Paramagnetism (O_2, metals, Unpaired electron atoms)

- In those atoms that have permanent magnetic dipole moment. In absence of magnetic field, moments are randomly oriented, but when $\vec{B}_{ext}$ is applied, dipoles are oriented $\parallel$ to field.

It leads to magnetization in the direction of field.

- χ is small, positive & temperature dependent.
- Observed paramagnetism in :
  - metals
  - atoms / molecules having odd number of electrons
  - O_2 molecule
  - rare earth & actinide elements

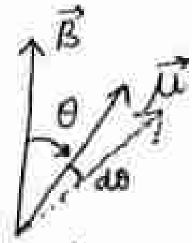
Langevin's Classical Theory

Consider a paramagnetic gas containing N atoms per unit volume, each having permanent magnetic moment μ.

In absence of magnetic field, they are randomly oriented
$\Rightarrow$ net moment $= 0$

When $\vec{B}_{ext}$ is applied, dipoles orient themselves in the direction of the field to minimize their energy $(E = -\vec{\mu}\cdot\vec{B})$
But due to thermal energy, not exactly $\parallel$, but rather at an angle θ with the direction of field.

$$\Rightarrow E = -\vec{\mu}\cdot\vec{B} = -\mu B\cos\theta$$



Now from Maxwell Boltzmann distribution,

no. of dipoles having orientation $\theta \quad \propto \quad e^{\left(\frac{\mu B\cos\theta}{kT}\right)}$

No. of dipoles within solid angle $d\omega$ lying between 2 hollow cones of semi angle θ and $\theta + d\theta$, are

$$dn \propto e^{\left(\frac{\mu B\cos\theta}{kT}\right)} d\omega$$

$$= k \; e^{\left(\frac{\mu B\cos\theta}{kT}\right)} \; 2\pi\sin\theta \; d\theta$$

where k is a constant.

Each one contributes moment $\mu \cos\theta$ to $\vec{M}$.

$$\Rightarrow M = \int \mu \cos\theta \, dn = \frac{N\int \mu \cos\theta \, dn}{\int dn}$$

$$= \mu N \frac{\int_0^{\pi} \sin\theta \, e^{\left(\frac{\mu B \cos\theta}{kT}\right)} \cos\theta \, d\theta}{\int_0^{\pi} \sin\theta \, e^{\left(\frac{\mu B \cos\theta}{kT}\right)} \, d\theta}$$

let $\left(\frac{\mu B}{kT}\right) = \lambda$

N: No. of dipoles per unit volume.

$$\Rightarrow \boxed{M = \mu N f(\lambda)}$$

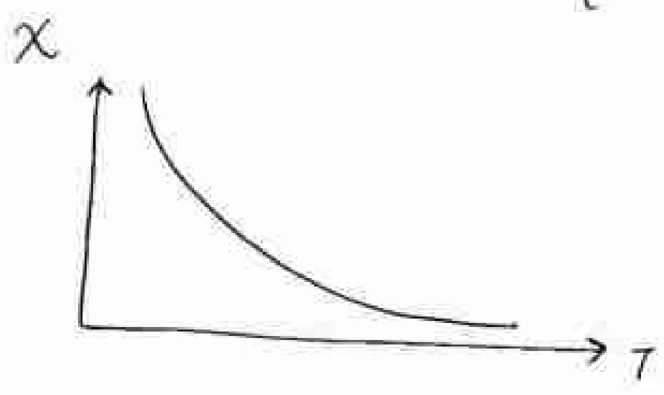
$f(x)$: Langevin function

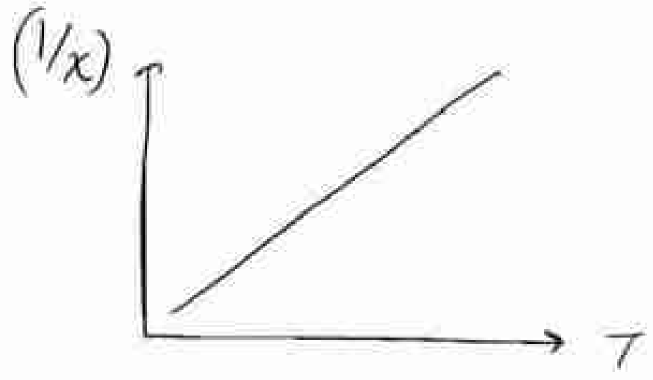
$\boxed{\text{For small } \lambda}$, $f(\lambda) \approx \left(\frac{\lambda}{3}\right) = \left(\frac{\mu B}{3kT}\right)$

$$\Rightarrow M = \left(\frac{\mu^2 N B}{3kT}\right)$$

$$\chi_{para} = \frac{\mu_0 M}{B} = \left(\frac{\mu_0 \mu^2 N}{3kT}\right) = \left(\frac{C}{T}\right)$$

C: Curie's const $= \left(\frac{\mu_0 N \mu^2}{3k}\right)$





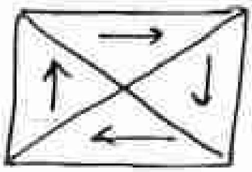
For large λ $\left(\begin{array}{l}\text{large } \lambda \Rightarrow \text{small } T \Rightarrow \text{all dipoles get aligned} \\ \Rightarrow M = \mu N\end{array}\right)$

$$f(\lambda) \approx 1$$

$$\boxed{M = \mu N} \Rightarrow \text{saturation magnetization}$$

Ferromagnetism (Fe, Ni, Co)

- Also associated with permanent dipole moment, but here magnetic moments of adjacent atoms are aligned in a particular direction even in the absence of applied magnetic field.



This magnetization that exists even in the absence of applied magnetic field is called SPONTANEOUS MAGNETIZATION. It exists below a critical temperature T_c, called CURIE TEMPERATURE.

- Above Curie Temperature, thermal effects offset the spin alignment and ferromagnetic substance becomes paramagnetic
- χ is large and positive, varies with temperature as well as applied field (hysteresis loop)

Weiss Theory of Ferromagnetism

2 hypothesis

① Ferromagnetic material contains a no. of small regions which are spontaneously magnetized. called domains

Magnitude of spontaneous magnetization of specimen as a whole is given by vector sum of magnetic moment of individual domains.

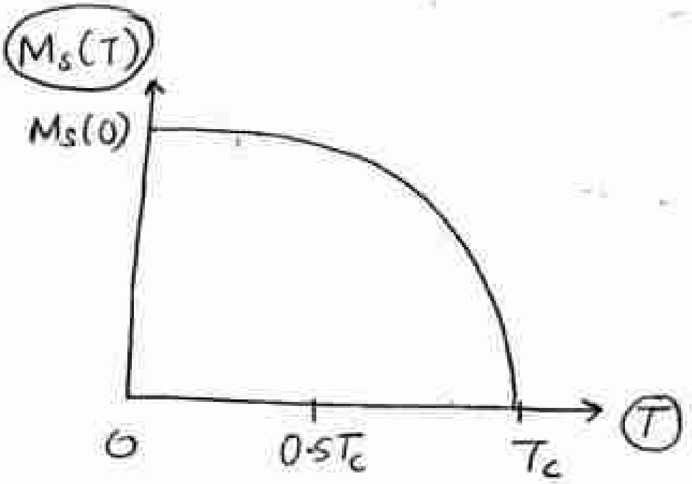
(2) Spontaneous magnetization of each domain is due to presence of an exchange field B_E, which tends to produce a parallel alignment of atomic dipoles.
Field B_E is assumed to be proportional to the magnetization M of each domain.

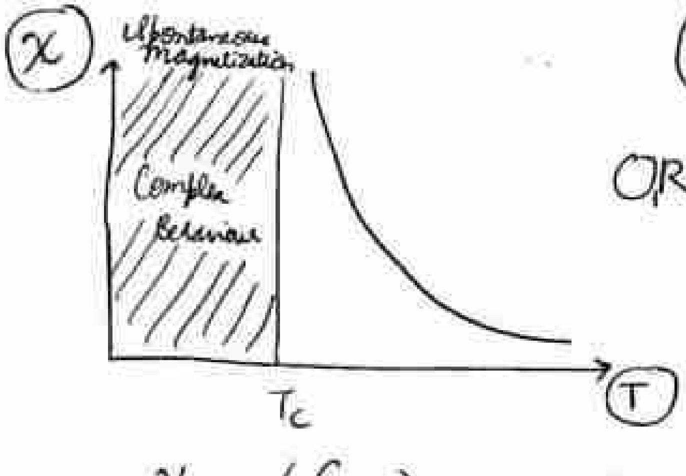
$$B_E = \lambda M$$: Weiss Field / Exchange Field / Molecular Field

λ: Weiss Field Constant (independent of temperature)

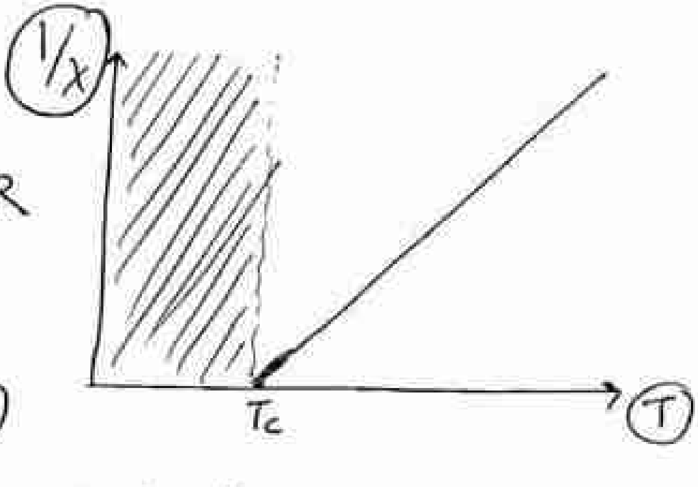
B_E is quite strong as compared to applied field ($\approx 1000\,T$) ($\approx 1\,T$)

From quantum theory, we can derive 2 curves





OR



$$\chi = \left(\frac{C}{T - T_c}\right)$$: Curie-Weiss law

Origin of Weiss Field was explained by Heisenberg who proposed the field to be a Consequence of quantum mechanical exchange interaction between atoms. Interaction arises due to Pauli's exclusion principle (any change in relative orientation of 2 spins would disturb spatial dist^n of charge, thus producing interaction between two atoms)

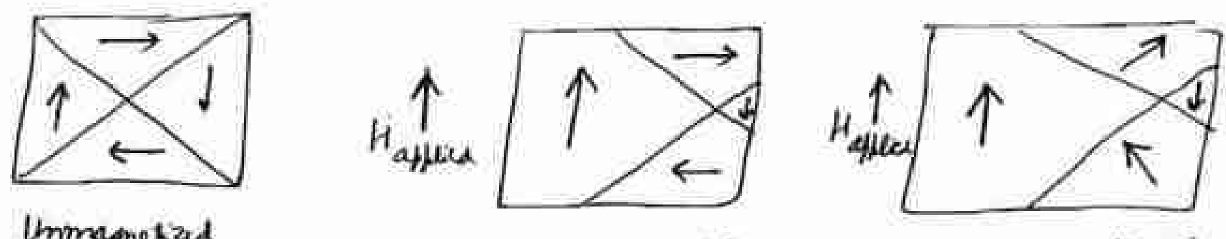
Hence, the exchange interactions between neighbouring dipoles in a ferromagnetic substance generates an internal exchange field B_E, which aligns them in a particular direction.

Domain Structure

According to Neel, domain structure is such that there is minimization of total energy (magnetic field energy + anisotropic energy + domain wall energy) [MAD]

magnetization produced in ferromagnetic material is due to

1) Growth is size of || domains at expense of anti parallel domains w.r.t. applied $\vec{B}$
2) Rotation of direction of magnetization, along field direction



Unmagnetized specimen

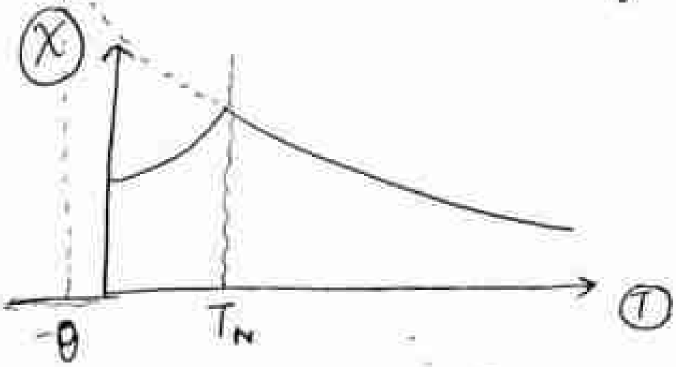
magnetization by domain growth

magnetization by domain rotation

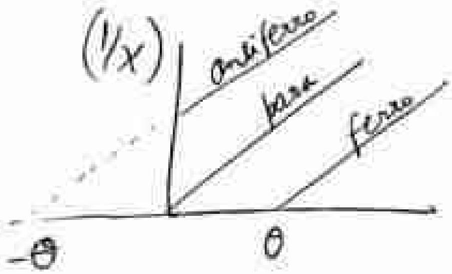
- Apart from them we have

Antiferromagnetism (MnO)

- Adjacent Moments are equal & opposite to each other
$\Rightarrow$ complete cancellation of moments.



$$\chi = \left(\frac{C}{T+\theta}\right) \quad \text{for } T > T_N$$



Ferrimagnetism ($Fe_3O_4 = FeO \cdot Fe_2O_3$)
(ferrites)

- Identical to antiferromagnetism except magnetization is not completely cancelled.
- Resembles ferromagnetism as
  - both possess spontaneous magnetization
  - both exhibit hysteresis

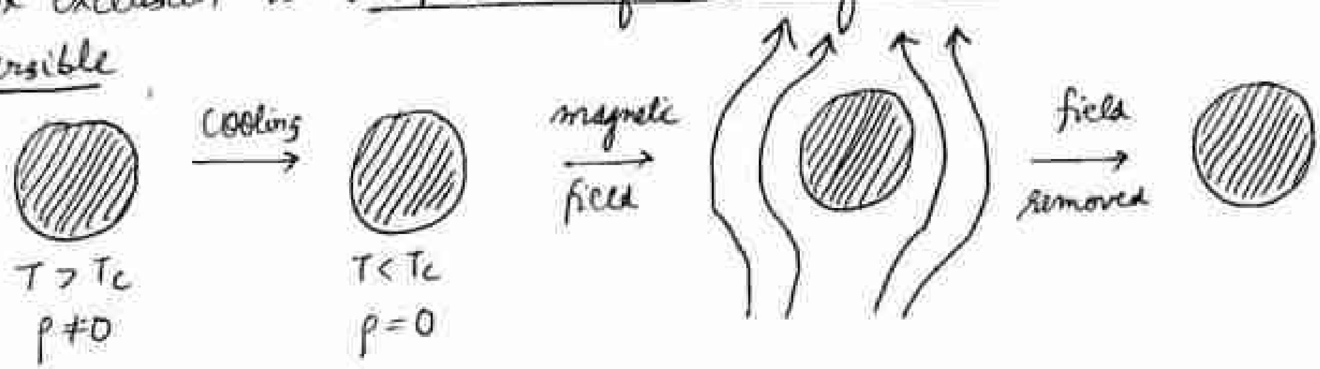
Superconductivity

- An electromagnet made up of a superconductor can function for years together even after removal of supply voltage. However due to requirement of very low temp., it was not feasible to manufacture such devices.

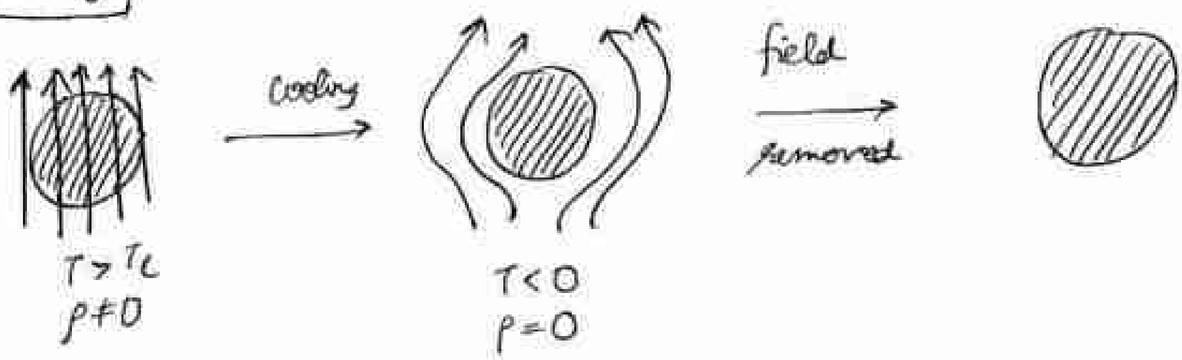
- Initial aim was to have a superconductor with transition temperature equal to or higher than 77k, the liquid N_2 temperature. With discovery of <u>Ceramic superconductors</u> ($T_c \approx 90k$) eg $YBa_2Cu_3O_7$ and <u>Thallium cuprates</u> ($T_c \approx 125k$), now the aim is to find superconductors at room temperature.

Meissner Effect (explained by London equations)

- Flux exclusion is <u>independent of order of events</u>. as well as <u>reversible</u>



ρ : resistivity



- difference between perfect conductor ($\rho = 0$) & Superconductor ($\rho = 0$)

For conductor, $\rho = 0 \Rightarrow$ Ohm's law $E = \overset{\text{resistivity}}{\rho} J = 0$

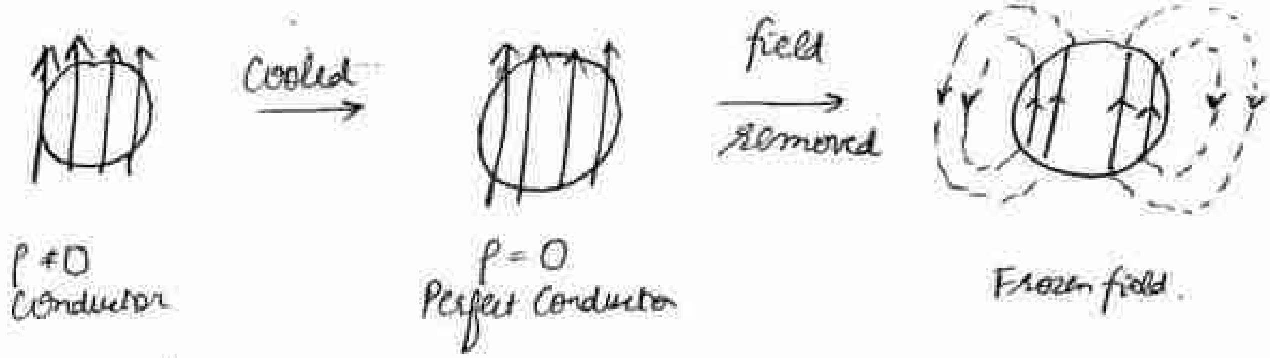
i.e. no electric field inside perfect conductor

From Maxwell eqs,

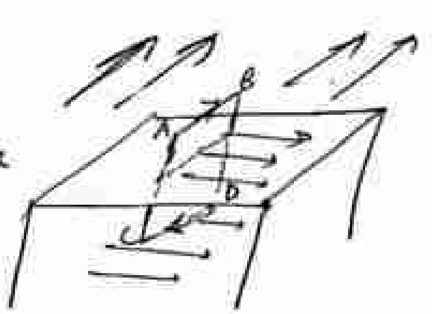
$$\vec{\nabla} \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$\Rightarrow B =$ const (and not zero)

i.e. when conductor is cooled in the magnetic field until its resistance becomes 0 (becomes perfect conductor), the magnetic field in the material gets frozen in & cannot change irrespective of applied field.



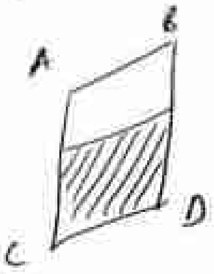
Penetration Depth



Consider a superconductor with a plane surface, with magnetic field He acting parallel to surface. From Ampere's law,

$$H_e(AB) = I_{enc}$$

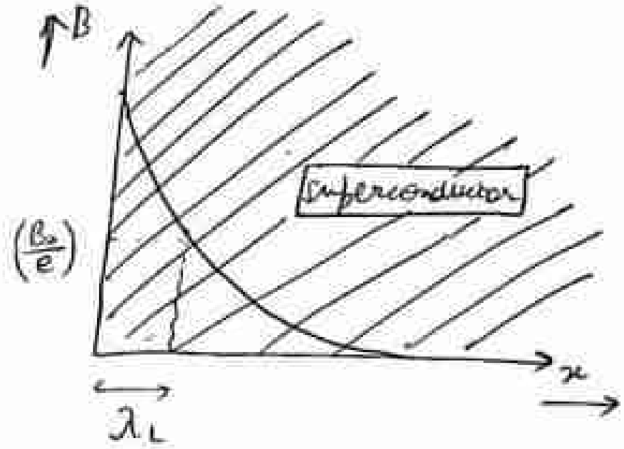
(Note that $H_{inside} = 0$ due to meissner)



I_{enc} or surface current per unit length $= H_e$. This surface current produces a magnetization $\vec{M}$ which exactly cancels $\vec{H_e}$ inside superconductor. Due to 0 resistivity, this current will remain almost constant indefinitely. Such currents are known as $\boxed{\text{supercurrents}}$.

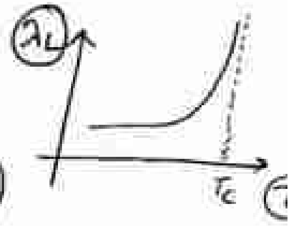
keeping AB constant, I_{enc} remains same.

now if width AC of the loop is reduced, current remai unchanged ⇒ current density or $\vec{J}$ increases (remember that there is no perfect surface current). For zero loop are current density approaches ∞, which is not possible physical ⇒ supercurrent cannot become absolute zero as one move from surface to interior. This is possible only if applied magnetic field penetrates the superconductor up to a small thickness near the surface.



λ_L: Characteristic length or london Penetration depth

$\approx 10^3$ Å

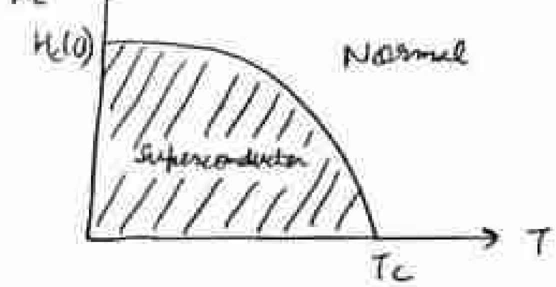


Experimentally, $H_c(x) = H_c(0)\, e^{-\left(\frac{x}{\lambda_L}\right)}$

(derived from london equations)

Critical field

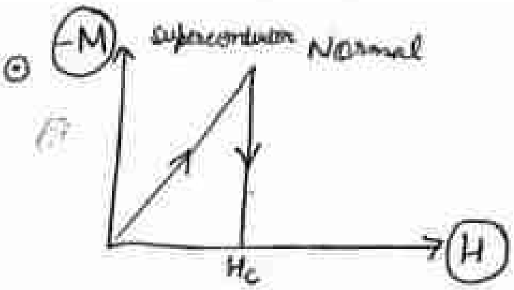
Superconducting stage is stable only in some definite ranges of Temperature & Magnetic Field.



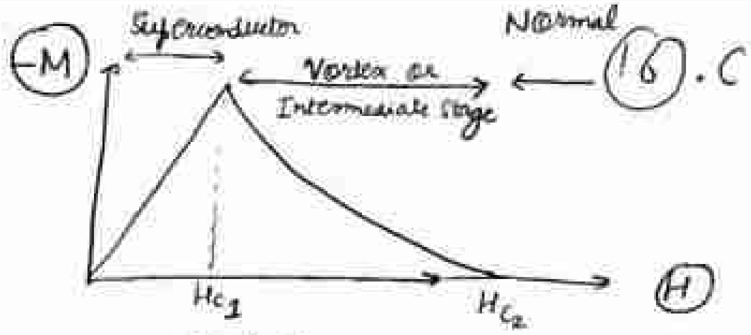
$$H_c(T) = H_c(0)\left[1 - \left(\frac{T}{T_c}\right)^2\right]$$

Type 1 and Type 2

Classification depending on behaviour in external magnetic field i.e. how strictly they follow Meissner effect

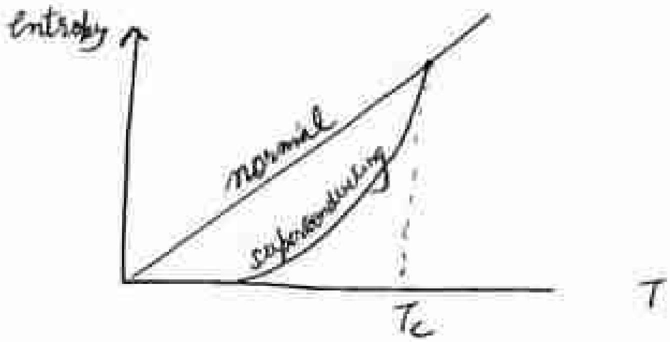


- Type 1
- (Pb)
- Soft superconductors
- due to very low H_c, very limited applications



- Type 2
- Pb-Bi Alloy
- Hard superconductor
- Practical applications
- After H_{c_1}, flux begins to penetrate the specimen & for $H = H_{c_2}$, flux penetrates completely

Entropy



- S-T curve depends on the process like PV curve. y = m~~x~~ given adjacent is assumed for a process.
  - → marked decrease in entropy in superconducting stage.
  - → Electronic structure is mainly affected during superconducting transition.

→ Some or all the thermally excited electrons in the normal state are **ordered** in the superconducting stage. Such an order may extend up to a distance of the order of 10^{-6}m in Type 1 superconductors. This range is called $\boxed{\text{Coherence length}}$ (ξ_0)

[This helps to give another definition of type 1 & type 2 superconductors:
I : $\left(\frac{\lambda_L}{\xi_0}\right) < \frac{1}{\sqrt{2}}$ II : $\left(\frac{\lambda_L}{\xi_0}\right) > \frac{1}{\sqrt{2}}$]

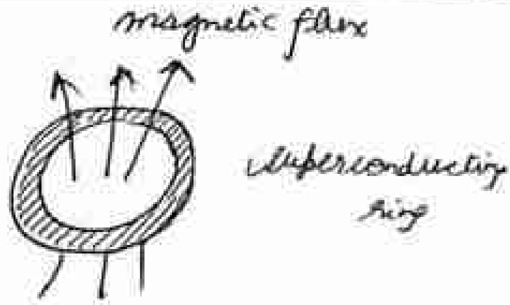
Isotope Effect

(मोटे आदमी को superconducting बनाना बहुत मुश्किल होता है)

$$T_c \propto \frac{1}{\sqrt{M}}$$

M : isotopic mass
T_c : transition temp.

Flux Quantization



$$\phi = n\left(\frac{h}{2e}\right)$$

$$= n \text{ fluxoid}$$

where $1 \text{ fluxoid} = \frac{h}{2e} = 2.07 \times 10^{-15}$ Weber

3 Josephson Effects

a) d.c. Josephson Effect

due to tunnelling of superconducting electrons through a very thin insulator (1-5 nm) sandwitched between two superconductors, d.c. current flows across the junction even when no voltage applied.

b) a.c. Josephson Effect

When d.c. voltage V applied across junction, a.c. current of r.f. flows.

$$f = \left(\frac{2e}{h}\right) V$$

For $1\,\mu V$, $f = 483.6$ MHz

Units

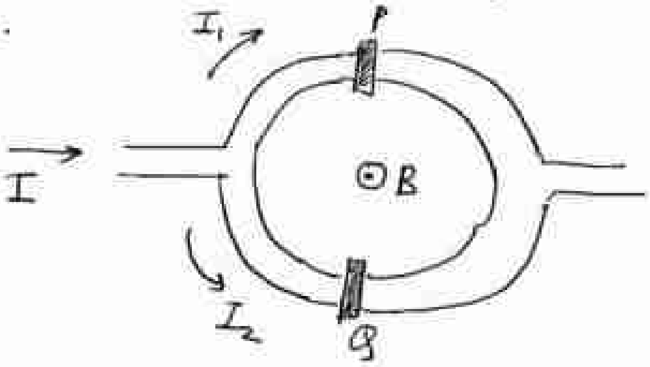
$V = \left(\frac{d\phi}{dt}\right)$

$f = \frac{V}{\phi} = \frac{V}{\left(\frac{h}{2e}\right)}$

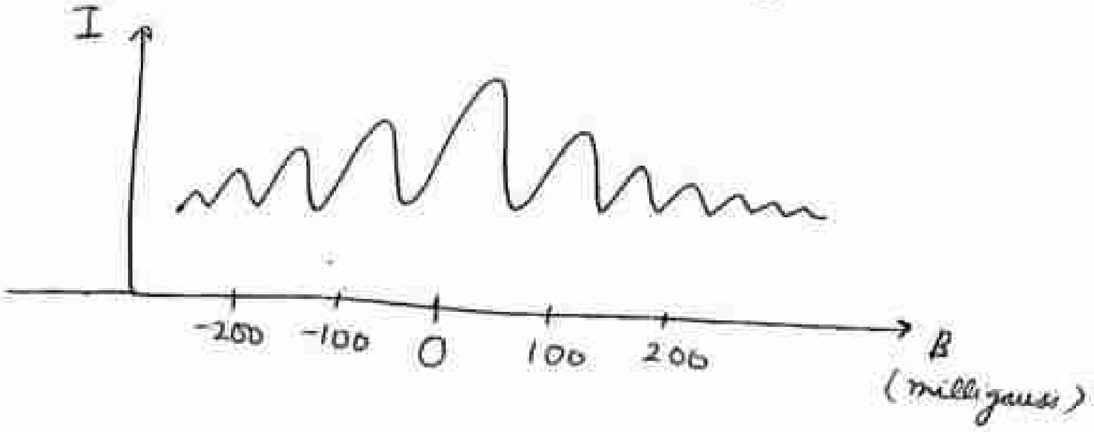
c) Quantum Interference

If a constant magnetic field is applied through a superconducting circuit containing 2 junctions, the maximum supercurrent shows interference effects depending on intensity of magnetic field.

device used to show quantum interference is called SQUID.



अरे अच्छा I const रहते ही हैं... Resistance of superconductor can vary... ⇒ I can vary. Now with change in flux, resistance varies ⇒ I varies, showing maxima at certain B.



- Since current is sensitive to small changes in magnetic field, SQUID can be used as a very sensitive galvanometer.

- Superconductor is characterized by a single wave function. Flow of supercurrent takes place between any 2 points where the wave function has different phases. Change in phase can also be brought about by applied electric & magnetic fields. States having different phases can be superimposed in SQUIDS.

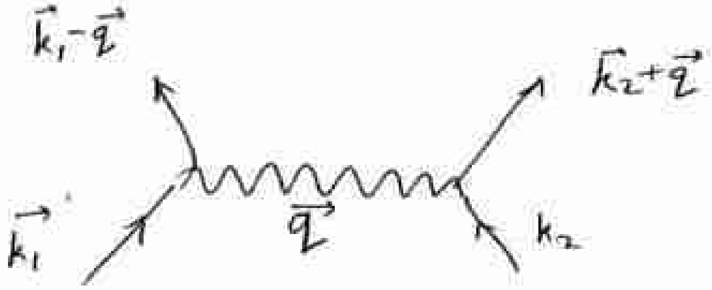
BCS Theory

- Electron-Phonon-Electron interaction is the basis of formation of a Cooper pair which results in superconduction.

- When an electron moves through a crystal, it produces lattice distortion & sets heavier ions into slow forced oscillations. Since the electron moves very fast, it leaves the region much before oscillations could die off. Meanwhile, if another electron happens to pass through this distorted region, it experiences an attractive force. This attraction lowers the energy of the electron, forming Cooper Pair.

(Note that repulsive force between electrons is small since Coulomb force is instantaneous while attraction mediated by lattice distortion is highly retarded in time)

- Smaller the mass of the ion, larger is the energy of the phonons emitted & hence larger should be transition temperature. Same conclusion is drawn from isotope effect. The isotope effect suggested that superconductivity is related to ions too $\Rightarrow$ foundation for BCS theory.



$\vec{k}_1, \vec{k}_2$: 2 electrons
$\vec{q}$: lattice distortion or phonon production

(electron - phonon - electron interaction)

Low Temperature Phenomenon

Binding Energy of Cooper Pair, called energy gap $E_g \simeq 10^{-3}$ eV
Hence temperature $\approx \frac{10^{-3}\,\text{eV}}{k} \approx 10\,\text{K}$. Above that Cooper pair will be broken.

Superconductivity due to Cooper Pair

Electron in a cooper pair have opposite spin $\Rightarrow$ Total spin = 0 $\Rightarrow$ Bosons i.e. any number of them can exist in same quantum state at the same time. A single wave function represents this system, whose total energy is less than that of system of same no. of e^- with fermi-energy distribution.

Therefore, a current in a superconductor involves all the cooper pairs acting as a single unit. To alter such a current, huge amount of energy is required (as lattice scattering is not enough, as in normal conductors) ⇒ current persists indefinitely.

Critical field

- As magnetic field applied is increased, energy of cooper pair increases (b'coz they exclude the field from interior of superconductor for Meissner effect). Beyond critical value, cooper pair is dissociated.

Meissner Effect

- Following Lenz's law, cooper pairs move without any resistance & adjust their motion to produce a magnetic field opposite to applied field.

(2) Electrical Properties ← Conductivity σ, Permittivity $\epsilon_r \epsilon_0$, Susceptibility χ_E, Resistivity ρ

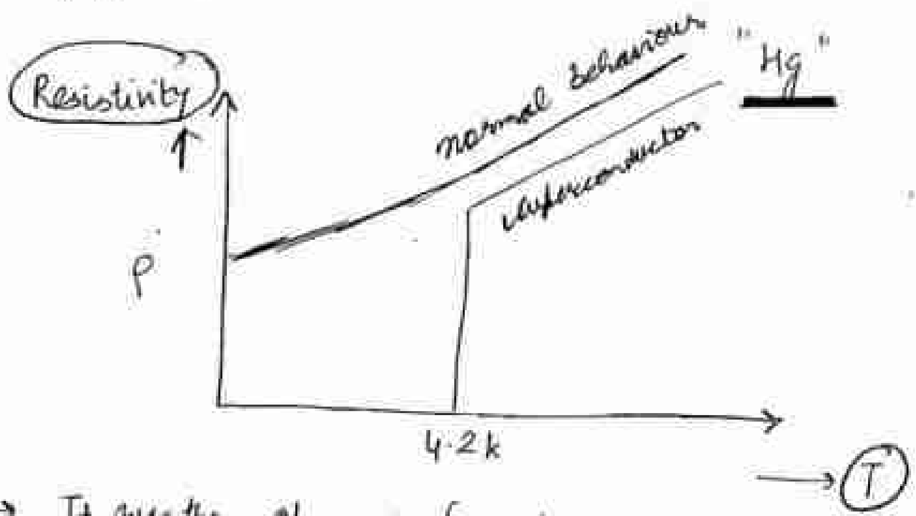
(3) Thermal Properties C_p, C_v
(Eistein, Debye's, Dulong)

(4) Optical Properties refractive index (n)

(5) Superconductivity ← Meissner Effect, Josephson Effect, High Temperature Superconductivity

Superconductivity

(Kamerlingh Onnes)
1911 K. Onnes



→ It was then observed for other materials also
→ Till 1957, there was no theory to explain it.
Joseph Bardin gave quantum theory to explain this.
Its called BCS theory or Bardeen, Cooper & Shriffer Theory
It offers quantum mechanical explanation for supercondivity

→ There are multiple properties but we are interested only in few properties.

✓ In superconductor, current has been seen to flow for years. Some application of superconductors include:

1. Storage element in memory of computer
2. Design of Maglevs
3. Design of very sensitive Magnetometers $\approx 10^{-11}$ Tesla measurement.

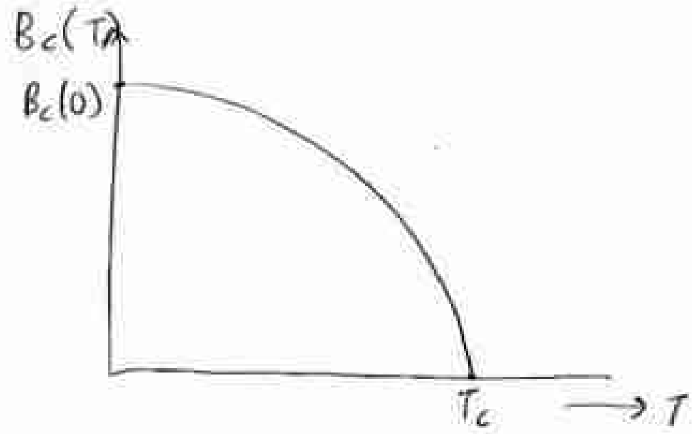
① Critical Magnetic Field

✓ By applying magnetic field, superconductivity can be destroyed.

$B_c(T)$ = Critical Magnetic field at Temp "T" to destroy superconductivity

$B_c(0)$ = critical magnetic field at Temp 0k to destroy superconductivity

$$\boxed{B_c(T) = B_c(0)\left[1 - \left(\frac{T}{T_c}\right)^2\right]}$$



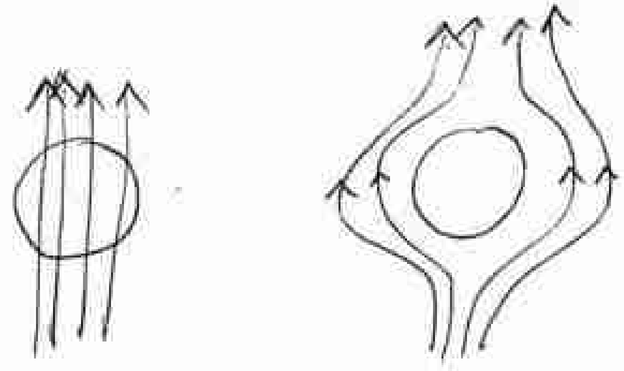
Parabolic Curve

→ इसमें B ज्यादा है, इसलिए superconductor के grains की alignment ही change कर देगा !!

② Meissner Effect

✓ Whenever specimens of superconducting materials in cooled down to lower temperatures, Magnetic Field inside the superconducting material is removed

i.e. for $T < T_c$, $B_{inside} = 0$



Meissner effect

important diagram

Magnetic field lines are "oozed out" of superconducting material below $T = T_c$

We know,

$$\vec{B} = \mu_0 (\vec{H} + \vec{M})$$

Now $\vec{B} = 0$ below T_c

$$\Rightarrow \boxed{\frac{M}{H} = -1}$$

or

$$\boxed{\chi = -1}$$

$\frac{M}{H}$ is called Magnetic susceptibility χ (a dimensionless quantity)

usually $\chi \approx 10^{-6}, 10^{-7}$ but here χ is a large negative quantity.

[Materials are classified on basic of susceptibility as Paramagnetic, Diamagnetic, Ferromagnetic.]

if $\chi = -10^{-7}$ to -10^{-6} : dipoles are aligned opposite to applied field.
They are Diamagnetic Material

$\chi = 10^{-6}$ to 10^{-7} : dipoles are aligned parallel to applied field
They are Paramagnetic Material

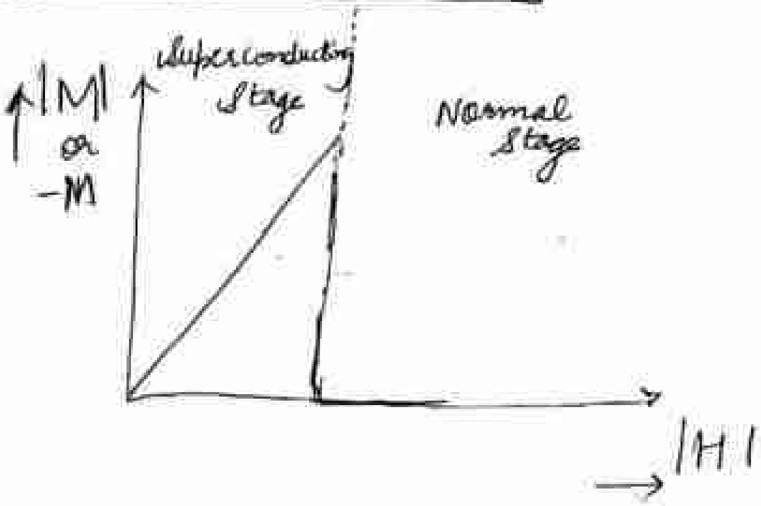
χ : large (+)ve : Ferromagnetic

$\chi = -1 \Rightarrow$ Perfect Diamagnetic

This property of superconductivity is exhibited as Meissner effect.

On the basis of Meissner Effects, we have 2 superconductor types:

1) $\boxed{\text{Type I Super Conductor}}$



$\left(\frac{M}{H}\right) = -1$

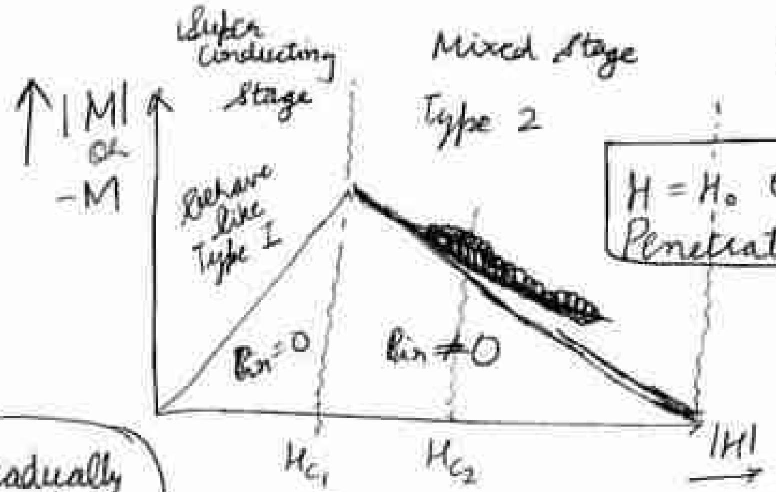
eg. Lead (Pb)

$B_{inside} = 0$

Suddenly drops

1) $\boxed{\text{Type II superconductor}}$

Some amount of Magnetic Field will remain.



$H = H_0 \, e^{-(x/\lambda)}$

Penetration depth

x: distance from surface

eg. Pb - In Alloy (Lead - Indium)

Gradually drops

$H_{c_2} = H_{c_1} e^{-1}$ at $x = \lambda$

λ: Penetration depth

There are two parameters demarcating Type II superconductors

(1) Penetration Depth : λ

(2) Coherence length : ξ_0

$k = \left(\frac{\lambda}{\xi_0}\right)$ determines whether material is Type I or Type II

* अच्छे superconductor के लिए $\lambda \simeq 0 \Rightarrow k$ very small

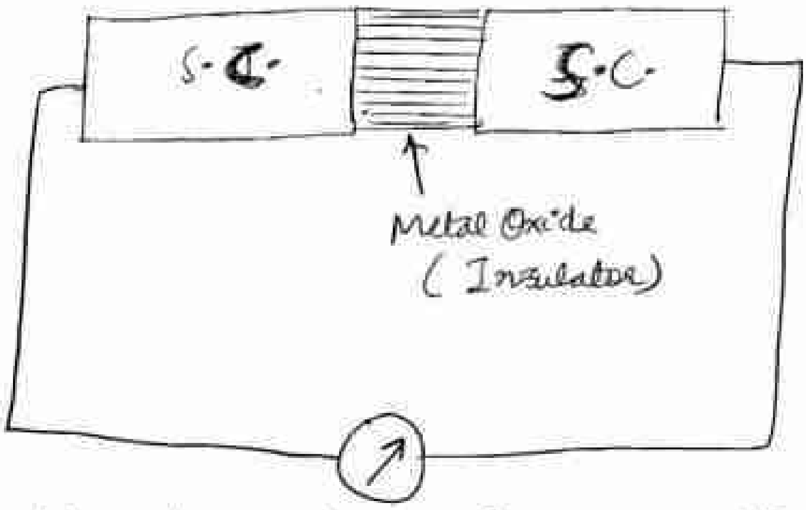
$k < \frac{1}{\sqrt{2}}$ Type I Material

$k > \frac{1}{\sqrt{2}}$ Type II Material

B.C.S. Theory will successfully explain whole Meissner Effect.

(3) Josephson Effect or Josephson Junction

Junction is made out of two superconductors (identical) with a very thin insulating layer in between, typically a Metal Oxide (sandwiched)



We observe Direct Current without application of any Potential. This is $\boxed{\text{D.C. Josephson Effect}}$

Note that no $\vec{E}$ or $\vec{B}$ is applied, yet D.C. is created.

We also have $\boxed{\text{A.C. Josephson Effect}}$ if a source of Electric Field, a battery is applied.

AC Josephson Effect

$$\hbar\omega = 2eV$$ { $2e$ charge due to Cooper pair }

$$\Rightarrow \boxed{\omega = \frac{2eV}{\hbar}}$$ A.C. Josephson Effect

for $V=0$, $\omega=0$ $\Rightarrow$ D.C. Josephson Effect

$$\Rightarrow \boxed{\nu = \frac{2eV}{h}}$$

3 applications of Josephson effect

① Measurement of very low Potential differences (10^{-6} volts)

- For $1\mu V$, we have

$$\nu = \frac{2 \times 1.6 \times 10^{-19} \times 1 \times 10^{-6}}{6.6 \times 10^{-34}} \text{ Hz}$$

$$= \frac{3.2}{6.62} \times 10^{9} \text{ Hz}$$

$$\boxed{\nu = 483.3 \text{ MHz}}$$

I cannot discriminate b/w $1\mu V$ and $2\mu V$ but I can differentiate $\nu = 483.3$ MHz and 2ν. Hence very sensitive device can be created.

② Most sensitive measurement of $\left(\frac{h}{e}\right)$ can be done

$$\left(\frac{h}{e}\right) = \left(\frac{2V}{\nu}\right)$$ (Now can apply, say, 1V)

(3) To device very sensitive Magnetic galvanometers. or Magnetometers ($B = 10^{-11}$ Tesla) or (10^{-7} gauss)

This is Explained on basis of fourth Property: Quantization of Magnetic Flux.

(4) Quantization of Magnetic Flux

Note that "c" केवल CGS units में आएगा. Remove "c" in S.I. un

If we make a closed loop of superconducting material, magnetic flux will be quantized.

$$\boxed{\vec{B}\cdot\vec{A} = \Phi = S\left(\frac{h}{2e}\right)} \qquad S \in \mathbb{N} \ (1, 2, 3, \ldots)$$

due to Cooper Pair, there will always be 2e

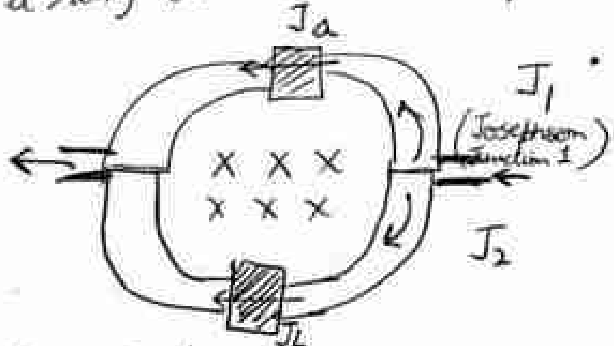
$$\frac{2e\,\Phi}{h} = 2\pi S = 2\pi, 4\pi, 6\pi \ldots$$

~~Thi[illegible]~~

Application

SQUIDS : Superconducting QUantum Interference DeviceS ; [in order to make very sensitive magnetometers]

Here we 2 josephson junctions in parallel in order to form a ring i.e. closed loop. Hence quantized flux.



- Now Apply external perpendicular field

$$\Phi = \left(\frac{h}{2e}\right) n$$

- Now A.C. is produced

Proof of Quantization (leave it)

$$J_1 = J_0 \sin\left[\delta(0) - \underbrace{\frac{e\Phi}{\hbar}}_{\text{dimensionally correct}}\right]$$

↑ current

(Quantization) बस ऐसे ही लिखना है !!

$$J_2 = J_0 \sin\left[\delta(0) + \frac{e\Phi}{\hbar}\right]$$

In absence of magnetic field $\delta = \delta(0)$ i.e. the two phases are equal

But when magnetic field is applied

$J_a = J_0 \sin(\delta_a)$

$J_b = J_0 \sin(\delta_b)$

$$\left.\begin{aligned} \delta_a &= \delta_0 + \left(\frac{e\phi}{\hbar}\right) \\ \delta_b &= \delta_0 - \left(\frac{e\phi}{\hbar}\right) \end{aligned}\right]$$

This is written because we know phase difference $\theta_2 - \theta_1$ around a closed circuit which encompasses a magnetic flux ϕ is

$$\theta_2 - \theta_1 = \left(\frac{2e}{\hbar}\right)\phi$$

$J = J_1 + J_2$ (interference)

$$\Rightarrow J = \overbrace{J_0\, 2\sin\,\delta(0)}^{\text{const.}}\ \overbrace{\cos\left(\frac{e\Phi}{\hbar}\right)}^{\text{function of }\phi}$$

For maximum current,

$$\left|\cos\left(\frac{e\phi}{\hbar}\right)\right| = 1$$

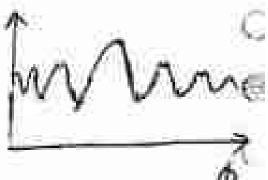
$$\Rightarrow \frac{e\phi}{\hbar} = n\pi$$

$$\Rightarrow \boxed{\frac{2e\phi}{h} = n} \quad \Rightarrow \boxed{\Phi = n\left(\frac{h}{2e}\right)}$$

Hence we have derived that flux in closed loop of superconductor is quantized, and current becomes maximum

1st maxima of current @ $\Phi = \left(\frac{h}{2e}\right)$

2nd maxima of current @ $\phi = \left(\frac{2h}{2e}\right)$



Hence observation of current maxima will give us the numerical values.

$$\phi = \frac{h}{2e} \approx 10^{-7} \text{ Weber} = 10 \text{ Maxwell}$$

$(1 \text{ Maxwell} = 10^{-8} \text{ Wb})$

Crosssection Area of Squid $\approx 1 \text{ cm}^2$

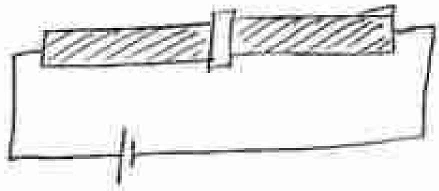
$\Rightarrow B \approx 10^{-11}$ Tesla $\approx 10^{-7}$ gauss

1 gauss of $B = 10^{-4}$ Te

Use of squid:

1) very sensitive magnetometer
2) oil prospecting
3) to detect amount of iron in body.

Proof of AC Josephson Effect



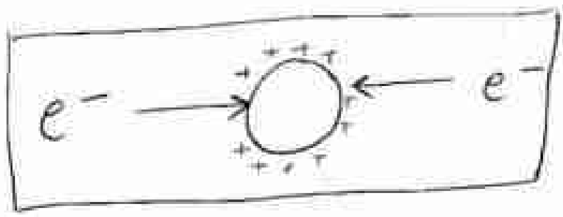
V

$\boxed{\text{BCS Theory}}$

Resistivity is due to coulumb repulsion of free electrons

If somehow I am able to change coulumb repulsion into attractive interaction, then ρ is reduced.

Direction repulsion is replaced by indirect interaction via lattice (phonon) i.e. e^-- lattice interaction whereby $2e^-$ form a closed pair



Interaction via lattice

e^- collides or interacts with lattice. Energy of lattice is reduced. Other e^- is attracted

Now the individual e^- (fermions) becomes a pair of e^- (boson) with $\vec{p}_1 = -\vec{p}_2$ and $\vec{s}_1 = -\vec{s}_2$

This is called Cooper Pair of electrons.

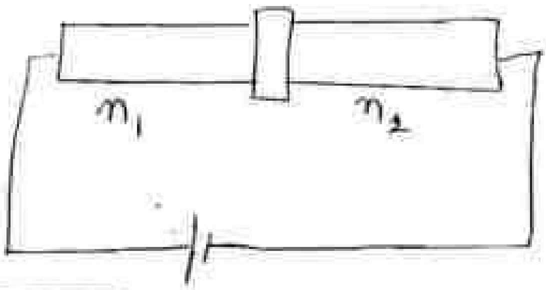
Now superconductivity is flow of cooper pairs of e^-

Each Cooper pair is a boson.

All the properties are explained via this model.

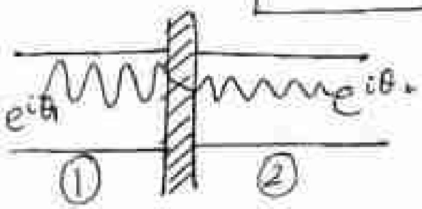
Here $q = 2e$: quantum of cooper pair

BCS theory's explanation of Josephson effect



n : Cooper Pair per unit volume

if identical superconductor $n_1 = n_2$



$$\psi_1 = \sqrt{n_1}\, e^{i\theta_1}$$

$$\psi_2 = \sqrt{n_2}\, e^{i\theta_2}$$

$$\boxed{\begin{array}{l} |\psi|^2 \propto n_1 \\ \Rightarrow |\psi| \propto \sqrt{n_1} \end{array}}$$

Quantum Solution $\quad H\psi = E\psi$

Non stationary state phenomenon

$\Rightarrow$ time dependent

$$\Rightarrow H\psi = i\hbar \frac{\partial \psi}{\partial t}$$

For region 1,

$$i\hbar \frac{\partial \psi_1}{\partial t} = \hbar T \psi_2 - eV_0 \psi_1 \quad \text{--- ①}$$

For region 2,

$$i\hbar \frac{\partial \psi_2}{\partial t} = \hbar T \psi_1 + eV_0 \psi_2 \quad \text{--- ②}$$

(T is the interaction having dimension $\frac{\partial}{\partial T}$ "multiplication operator")

(you can also same sign of V_0 as battery i.e. $+eV_0\psi_1$ in 1st eqn)

For D.C. Josephson Effect, corresponding equations are:

$$i \frac{\partial \psi_1}{\partial t} = T\psi_2$$

$$i \frac{\partial \psi_2}{\partial t} = T\psi_1$$

In ① and ②, replacing Ψ from definitions (7) (22)

$$i\frac{1}{2\sqrt{n_1}}\frac{dn_1}{dt}e^{i\theta_1} - \sqrt{n_1}\,e^{i\theta_1}\left(\frac{d\theta_1}{dt}\right) = T\sqrt{n_2}\,e^{i(\theta_2)} - \frac{eV_0}{\hbar}\sqrt{n}\,e^{i\theta}$$

$$\Rightarrow \frac{1}{2\sqrt{n_1}}\frac{dn_1}{dt}\,i - \sqrt{n_1}\frac{d\theta_1}{dt} = -\frac{eV_0}{\hbar}\sqrt{n_1} + T\sqrt{n_2}\,e^{i(\theta_2-\theta_1)}$$

Put $\underline{\theta_2-\theta_1 = \delta}$

$$\Rightarrow e^{i(\theta_2-\theta_1)} = \cos\delta + i\sin\delta$$

Separating real & imaginary components,

$$\frac{1}{2\sqrt{n_1}}\frac{dn_1}{dt} = T\sqrt{n_2}\sin\delta \quad \text{— ③}$$

$$\sqrt{n_1}\frac{d\theta_1}{dt} = \frac{eV_0\sqrt{n_1}}{\hbar} - T\sqrt{n_2}\cos\delta \quad \text{— ④}$$

$$\frac{d\theta_1}{dt} = \frac{eV_0}{\hbar} - T\sqrt{\frac{n_2}{n_1}}\cos\delta \quad \text{— ⑤}$$

Similarly ② yields (V will be $-V$, δ will be $-\delta$)

$$\frac{1}{2\sqrt{n_2}}\frac{dn_2}{dt} = -T\sqrt{n_1}\sin\delta \quad \text{— ⑥}$$

$$\frac{d\theta_2}{dt} = -\frac{eV_0}{\hbar} - T\sqrt{\frac{n_2}{n_1}}\cos\delta \quad \text{— ⑦}$$

replace V_0 by $-V_0$ and δ by $-\delta$

Now $\left(\frac{dn_1}{dt}\right) = -\left(\frac{dn_2}{dt}\right)$ because current is same

Also can be seen from comparing 3 and 6

subtracting 7 from 5

$$\frac{d}{dt}(\theta_2 - \theta_1) = -\frac{2eV_0}{\hbar}$$

$$\boxed{\frac{d\delta}{dt} = -\left(\frac{2eV_0}{\hbar}\right)}$$

remember $\frac{d\phi}{dt}$ = frequency $\qquad\phi$: Phase of function

$$\Rightarrow \boxed{\omega = \mp\frac{2eV_0}{\hbar}}$$

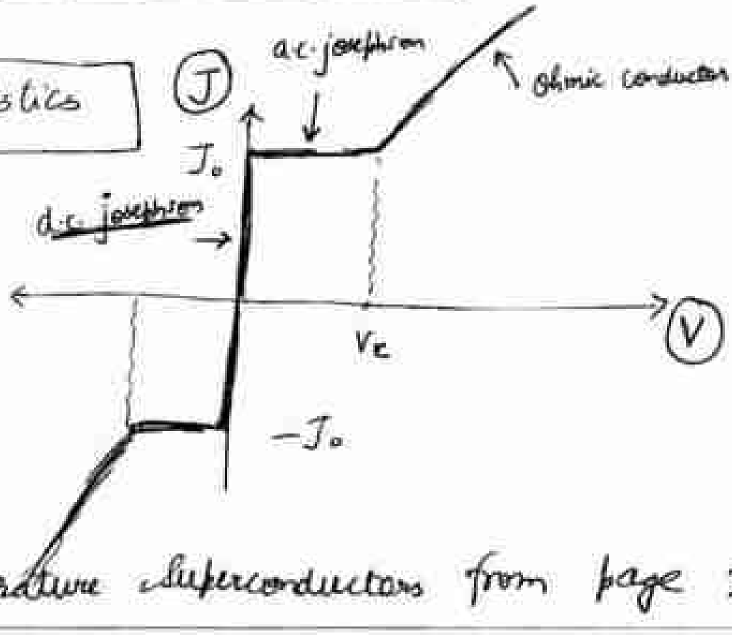
$$\int_{\delta(0)}^{\delta(t)} d\delta = -\frac{2eV_0}{\hbar}\int_{t=0}^{t} \delta t = -\frac{2eV_0}{\hbar}t$$

$$\Rightarrow \delta(t) = \delta(0) - \frac{2eV_0 t}{\hbar}$$

$$\boxed{J = J_0 \sin\left(\delta(0) - \frac{2eV_0 t}{\hbar}\right)}$$

$\boxed{\text{Josephson Characteristics}}$

$$V_c = \frac{(\text{Energy Gap})}{e}$$



< Read High Temperature Superconductors from page 299, 300

London Equations

London Equations explain the phenomenon of magnetic flux penetration inside a superconductor.

1st eqn

let n, v be density & velocity of superconducting electrons.

Now, inside the superconductor

$$m\left(\frac{d\vec{v}}{dt}\right) = -e\vec{E}$$

$$\Rightarrow \left(\frac{d\vec{v}}{dt}\right) = -\left(\frac{e\vec{E}}{m}\right) \quad \text{— (1)}$$

Also $\vec{J} = -ne\vec{v}$

$$\Rightarrow \frac{d\vec{J}}{dt} = -ne\left(\frac{d\vec{v}}{dt}\right) \quad \text{— (2)}$$

$$\Rightarrow \boxed{\frac{d\vec{J}}{dt} = +\left(\frac{ne^2}{m}\right)\vec{E}}$$ London's 1st equation

2nd eqn

Taking curl of 1st equation of London,

$$\vec{\nabla}\times\left(\frac{d\vec{J}}{dt}\right) = +\left(\frac{ne^2}{m}\right)(\vec{\nabla}\times\vec{E})$$

From maxwell equation, $\vec{\nabla}\times\vec{E} = -\left(\frac{\partial\vec{B}}{\partial t}\right)$

Hence $$\vec{\nabla}\times\left(\frac{\partial\vec{J}}{\partial t}\right) = -\frac{ne^2}{m}\left(\frac{\partial B}{\partial t}\right)$$

$$\Rightarrow \boxed{\vec{\nabla}\times\vec{J} = -\frac{ne^2\vec{B}}{m}}$$ London's 2nd equation

Explanation of flux penetration

From Maxwell Equations,

$$\vec{\nabla}\times\vec{B} = \mu_0\vec{J}$$

Taking curl,

$$\vec{\nabla}\times(\vec{\nabla}\times\vec{B}) = \mu_0(\vec{\nabla}\times\vec{J})$$

(from London equation)

$$\Rightarrow \vec{\nabla}(\vec{\nabla}\cdot\vec{B}) - \nabla^2\vec{B} = \mu_0\left[-\frac{ne^2}{m}\vec{B}\right]$$

$$\Rightarrow \nabla^2\vec{B} = \left(\frac{\mu_0 ne^2}{m}\right)\vec{B}$$

let $\sqrt{\frac{m}{\mu_0 ne^2}} = \lambda$: London's penetration depth

$$\Rightarrow \nabla^2\vec{B} = \frac{1}{\lambda^2}\vec{B}$$

$$\Rightarrow \boxed{B = B_0\, e^{-\frac{x}{\lambda}}}$$

where B_0 is the field at surface & x is the depth inside the superconductor.