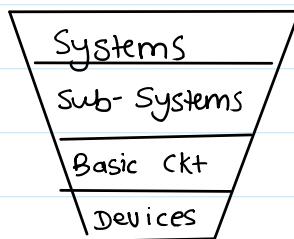


Semiconductor devices

- Conductivity \Rightarrow Insulators < Semicond. < Conductors
- Conductivity increases with increase in temperature as more electrons get energy to jump from valence band to Conduction band.
- Conductivity increases when light is incident because when light is incident more no. of free e^- are generated.
- Conductivity of semiconductors can be controlled by doping.
* PN Homojunction diode - 2 terminal
BJT = 3 terminal , MOSFET - 4 terminal

Classification :-

- Groups in periodic table - IV, III-V, II-VI, VI, I-III-VI₂ etc.
- Material type - Organic, Inorganic, Hybrid
- Structure - Crystalline, poly-Crystalline, Micro-Crystalline, Nano Crystalline, Amorphous
- Impurity - Intrinsic (pure), Extrinsic (doped / impure)
- Dimensions - 1D, 2D, 3D, 0-D

Heirarchy \Rightarrow 

Moore's law -

No. of Components on ICs showed exponential growth.
 → Plot of log. of no. of components per IC vs year showed that no. of transistors doubled in a certain period of time (sometimes 2 yrs, 18 months, yearly etc.)

→ Adding more and more Components decreased yield and increased Complexity and thus raised Cost per Component.

Koomey's law

No. of Computations per joule energy dissipated doubles every 1.57 years. (slowed down to 2.6 yrs since 2000)

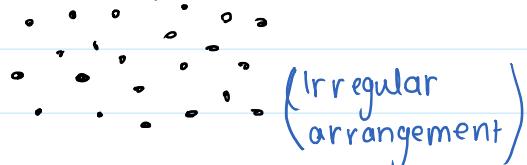
Lec-3

Semiconductor Crystal Structure

Types of Solids

- Amorphous - No pattern /geometry followed by atoms / molecules. i.e. order only within a few atomic or molecular dimensions.

Ex:- SiO_2



(Irregular arrangement)

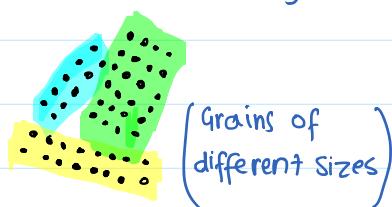
- Polycrystalline - • High degree of order over many atomic or molecular dimensions.

• Ordered regions are called GRAINS.

• Grains may vary in sizes.

• Grains are Separated by Grain boundaries.

Ex:- Poly-Si

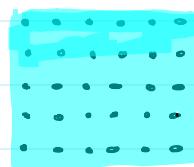


(Grains of different sizes)

- Monocrystalline / Single- Crystal - • High degree of order throughout entire volume.

• They have Superior electrical properties

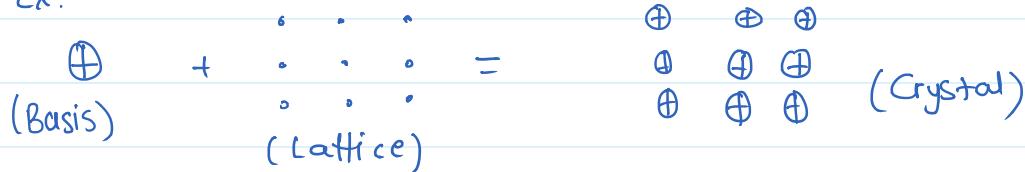
Ex:- Si



- * Lattice - Periodic arrangement of points in space.
- * Basis - Atoms / Molecules / Complex objects at each of the lattice points. (i.e. individual particle)

Basis + Lattice = Crystal

Ex:-



- * Lattice Constants - Edge length, Angle b/w edges.

Weigner - Seitz primitive cell.

Primitive cell is smallest unit cell. To find primitive cell

→ Connect all nearby lattice points

→ Draw \perp at mid point of these connected lines

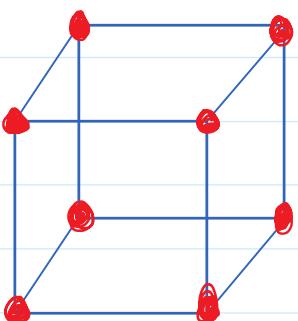
the Smallest are enclosed this way is Weigner - Seitz primitive cell.

BRAVAIS LATTICES

All possible lattices - Any lattice can be represented by one of the Bravais lattice.

- Cubic - $a=b=c$, $\alpha=\beta=\gamma=90^\circ$
- Tetragonal - $a=b \neq c$, $\alpha=\beta=\gamma=90^\circ$
- Orthorhombic - $a \neq b \neq c$, $\alpha=\beta=\gamma=90^\circ$
- Monoclinic - $a \neq c$, $\beta \neq 90^\circ$, $\alpha=\gamma=90^\circ$
- Rhombohedral - $a=b=c$, $\alpha=\beta=\gamma \neq 90^\circ$
- Hexagonal - $a=b \neq c$, $\alpha=\beta=90^\circ$, $\gamma=120^\circ$
- Triclinic - $a \neq b \neq c$, $\alpha \neq \beta \neq \gamma$

Simple Cubic Lattice



→ per atom donates $\frac{1}{8}$ to each unit cell.

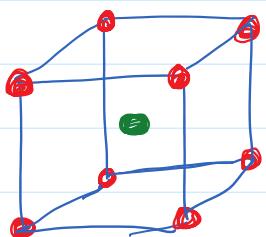
Co-ordination number = No. of nearest neighbours = 6. (at 'a')

No. of atoms / unit cell = 1.

Packing density = $(n \times \text{Vol of each Sphere}) / \text{Vol. of Cube}$

$$= \frac{4/3 \pi r^3}{a^3} \Rightarrow \left[r = \frac{a}{2} \right] \Rightarrow \frac{4/3 \pi \left(\frac{a}{2} \right)^3}{a^3} = 0.5236$$

BCC



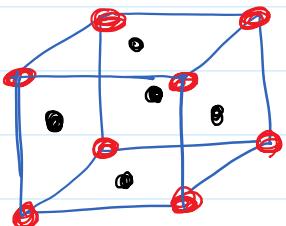
Co-ordination No. - 8 (at

No. of atoms/unit cell = $\frac{1}{8} \times 8 + 1 = 2$

Packing density = $\frac{2 \times 4/3 \pi r^3}{a^3}$

$$\left[r = \frac{\sqrt{3}}{4} a \right] = \frac{4/3 \pi \left(\frac{\sqrt{3}}{4} a \right)^3}{a^3} = 0.680$$

FCC



Co-ordination no. - 12

No. of atoms/unit cell = $\frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$

Packing density = $\frac{4 \times 4/3 \pi r^3}{a^3}$

$$r = \frac{a}{4} = 4 \times 4/3 \pi \left(\frac{a}{4} \right)^3 = 0.740$$

$$r = \frac{a}{2\sqrt{2}} = \frac{4 \times 4/3 \pi \left(\frac{a}{2\sqrt{2}}\right)^3}{a^3} = 0.740$$

Lec-4

Miller indices -

- Represents parallel planes.
- Same as reciprocal of intercepts.
- Not unique due to arbitrary choice of axes.
- representation of -ve indices is as -
Ex:- $(-100) \equiv (\bar{1}00)$

Silicon -

- Widely used for ICs

Advantages:-

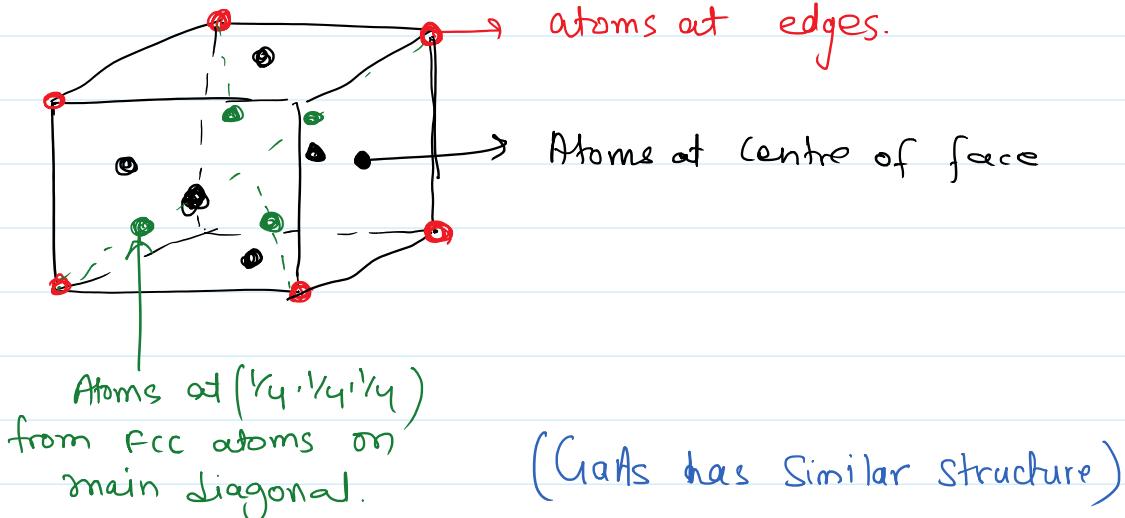
- abundantly available as sand or silica.
(Inexpensive and abundant)
- SiO_2 - highly useful for MOS
 - Easy to grow by thermal oxidation
 - Excellent electrical and mech. properties.
 - almost same thermal expansion coeff. as Si.
- High bandgap - low leakage current,
useful for ↑ temp. application.

Limitations -

- Indirect bandgap material
- Low Carrier mobility (Not suited for high Speed applications)

Properties -

- Diamond structure
- Seen as 2 penetrating FCC, shifted by $\frac{1}{4}$ along main diagonal.
- FCC lattice with extra atoms at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ distance from each FCC atoms.



$$\text{Total no. of atoms} = 8 \times \frac{1}{8} + 6 \times \frac{1}{2} + 4 = 8$$

Bond angle for Si -

$$\cos \theta = \frac{\vec{v}_1 \cdot \vec{v}_2}{|\vec{v}_1| |\vec{v}_2|}$$

$$\vec{v}_1 = (0, 0, 0)\vec{a} - \left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)\vec{g} = \left(-\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}\right)\vec{a}$$

$$\vec{v}_2 = \left(\frac{1}{2}, \frac{1}{2}, 0\right)\vec{a} - \left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right)\vec{g} = \left(\frac{1}{4}, \frac{1}{4}, -\frac{1}{4}\right)\vec{a}$$

$$\cos \theta = \frac{-\frac{1}{4} + \frac{1}{4} + \frac{1}{4}}{\left(\sqrt{3 \times \left(\frac{1}{4}\right)^2}\right)^2} = -\frac{1}{3}$$

$$\theta = 109.4^\circ$$

$$\text{for } a = 5.43 \text{ \AA}$$

$$\text{Density} = \frac{\text{no. of atoms}}{\text{Volume}} = \frac{8}{a^3} = 5 \times 10^{22} \text{ atoms/m}^3$$

for $a = 5.43 \text{ \AA}$

$$\text{Density} = \frac{\text{no. of atoms}}{\text{Volume}} = \frac{8}{a^3} = 5 \times 10^{22} \frac{\text{atoms}}{\text{cm}^3}$$

Co-ordination no. - 4

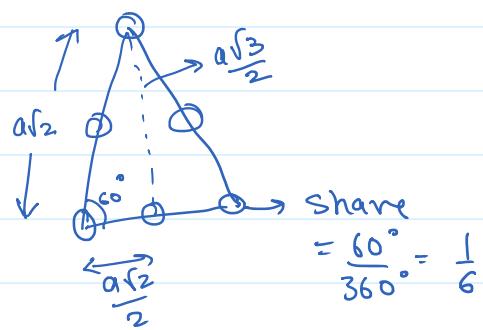
$$\text{distance of nearest neighbours} = \frac{\sqrt{3}a}{4}$$

$$R = \frac{\sqrt{3}a}{8}$$

$$\text{Packing fraction} = \frac{8 \times \frac{4}{3}\pi \left(\frac{\sqrt{3}a}{8}\right)^3}{a^3} = 0.340$$

\Rightarrow Surface atom density -

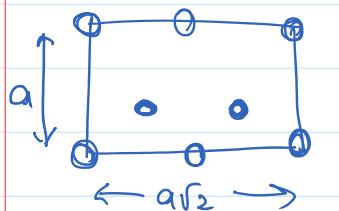
(111) plane -



$$\text{Area density} = \frac{\frac{3}{2} \times \frac{1}{6} + 3 \times \frac{1}{2}}{2 \times \frac{1}{2} \times \frac{a\sqrt{2}}{2} \times \frac{a\sqrt{3}}{2}}$$

$$= 7.83 \times 10^9 \text{ atoms/cm}^2$$

(110) plane :-



$$= \frac{4 \times \frac{1}{4} + 2 \times \frac{1}{2} + 2}{a \times a\sqrt{2}} = \frac{2\sqrt{2}}{a^2}$$

WAVE F/n - Solution to Schrodinger's wave eqⁿ,
determines all properties of particle.

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

here, $\Psi(x,t)$ = Wave f/n
 $V(x)$ = Potential f/n
 m = mass of particle

$|\Psi(x,t)|^2$ = probability density f/n
= probability of finding particle
b/w x and $x+dx$.

Now, $\Psi(x,t) = \psi(x)\phi(t)$

Only f/n of x , Only f/n of t .

$$\text{We have, } -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi = j\hbar \frac{\partial \Psi}{\partial t}$$

$$\begin{aligned}
 \Psi &= \Psi(x)\phi(t) \\
 &= -\frac{\hbar^2}{2m} \phi(t) \frac{\partial^2 \Psi(x)}{\partial t^2} + V\Psi(x)\phi(t) = j\hbar \Psi(x) \frac{\partial \phi(t)}{\partial t} \\
 &= -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x)}{\partial t^2} \times \underbrace{\frac{1}{\Psi(x)}}_{\text{f/n of } x} + V(x) = j\hbar \frac{\partial \phi(t)}{\partial t} \cdot \underbrace{\frac{1}{\phi(t)}}_{\text{f/n of } t} = \eta \text{ (say)}
 \end{aligned}$$

On solving,

$$\phi(t) = e^{-j\frac{\omega}{\hbar}t} = e^{-j\omega t}$$

E = total energy of particle
 $\omega = E/\hbar$

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

$$|\psi(x,t)|^2 = \psi(x,t) \cdot \psi^*(x,t) = \underbrace{\psi(x) \psi^*(x) \cdot \phi(t) \phi^*(t)}_{=1}$$

$$|\psi(x,t)|^2 = \psi(x) \psi^*(x)$$

Probability density $f(x)$ is independent of time i.e. particle remains in same state, such state is called stationary state.

Integrating probability density $f(x)$ over space gives 1 as particle is located somewhere in space.

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 \quad [\text{Wave fcn is NORMALIZED}]$$

⇒ Basic postulates-

- $\psi(x)$ and $\partial \psi(x)/\partial x$ must be finite, single valued and continuous for finite energies.
- Only properties of particles (Observables) are meaningful.
- $\psi(x)$ is solution to Schrodinger's eqⁿ.
- Average / expectation value of observable $O \approx$

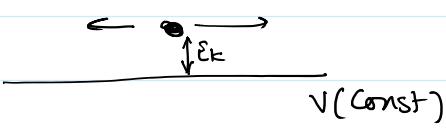
$$\langle O \rangle = \frac{\int \psi^* O \psi dx}{\int \psi^* \psi dx}$$

$$p = \frac{\hbar \mathbf{z}}{j \partial x}, \quad E_k = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}, \quad E = -\frac{\hbar^2}{j} \frac{\partial}{\partial t}$$

Free electron:-

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

$$\Psi(x, t) = \psi(x) \phi(t)$$



$$\underset{\text{Time independent}}{\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{2m_0}{\hbar^2} (E - V) \right) \psi = 0}$$

$$\downarrow$$

$$\psi = Ae^{jkn} + Be^{jkn}$$

$$k = \sqrt{\frac{2m_0(E-V)}{\hbar^2}} = \sqrt{\frac{2m_0 E_k}{\hbar^2}}$$

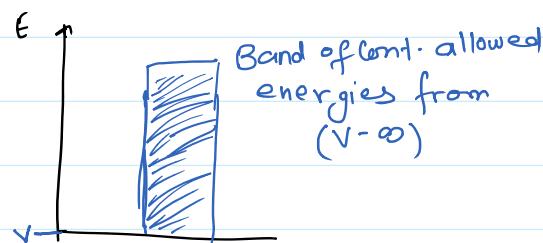
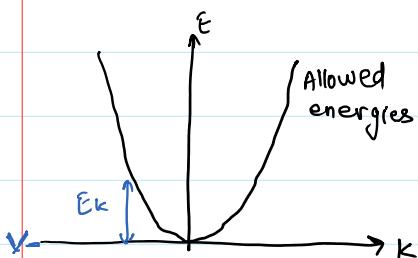
$$\frac{d\phi}{dt} + \frac{jE}{\hbar} \phi = 0 \quad \underset{\text{Time dependent}}{\left(\frac{d\phi}{dt} + \frac{jE}{\hbar} \phi = 0 \right)}$$

$$\phi = e^{\frac{jE}{\hbar} t}$$

$$\boxed{\phi = e^{-j\omega t}} \quad (E = \hbar\omega)$$

$$\Psi(x, t) = \psi(x) \phi(t) = Ae^{j(kx - \omega t)} + Be^{j(-kx - \omega t)}$$

$$E = V + \frac{\hbar^2 k^2}{2m_0} \quad \left\{ \begin{array}{l} \text{E-K relation for free } e^- \\ \text{T.E} \quad \downarrow \quad \text{P.E} \quad \downarrow \quad \text{K.E.} \end{array} \right.$$



$$\frac{\partial E}{\partial k} = \frac{\hbar^2 k}{m_0}$$

$$\frac{\partial^2 E}{\partial k^2} = \frac{\hbar^2}{m_0}$$

$$\boxed{m_0 = \frac{\hbar^2}{(\partial^2 E / \partial k^2)}}$$

Mass of particle is inversely proportional to curvature of E-k parabola.

e^- in infinite potential well:-

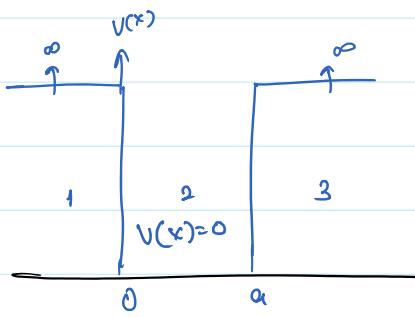
e^- in infinite potential well:-

$\psi(x) = 0$ for region 1 and 3 as

e^- with finite energy can't

Cross infinite energy

barrier. So, e^- lies in 2.



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

$$V(x) = 0$$

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

$$\psi(x) = A \cos(kx) + B \sin(kx)$$

$$k = \sqrt{2mE/\hbar^2}$$

$$\psi(0) = A = 0 \rightarrow \psi(x) = B \sin(kx)$$

$$\psi(a) = B \sin(ka) = 0 \quad (B \neq 0)$$

$$\text{so } \sin(ka) = 0 \rightarrow ka = n\pi \quad k = n\pi/a$$

$$k = \sqrt{2mE/\hbar^2} = n\pi/a \Rightarrow$$

$$\boxed{E = \frac{n^2 \pi^2 \hbar^2}{2ma^2}} \quad \left\{ E = \text{quantized} \right\}$$

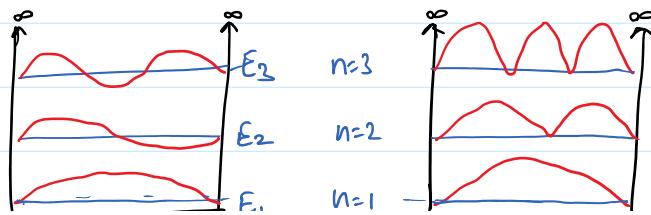
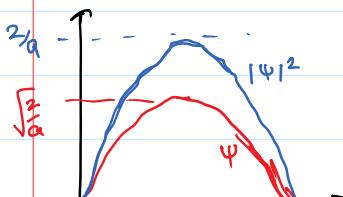
We have $\int_0^a |\psi(x)|^2 dx = 1$

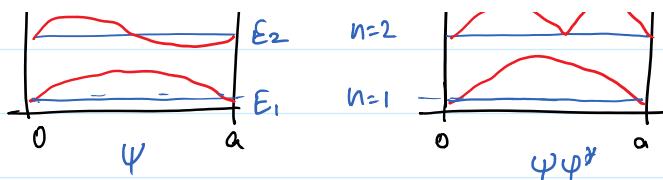
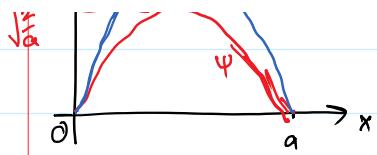
$$\int_0^a B^2 \sin^2 \left(\frac{n\pi}{a} x \right) dx = 1$$

$$B \frac{a}{2} = 1$$

$$B = \sqrt{\frac{2}{a}}$$

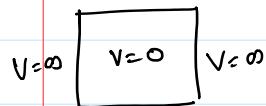
$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi}{a} x$$





= Observations -

- Confinement leads to discrete energy levels.
- $\Delta E \propto 1/a^2$
- ↑ Confinement ($\downarrow a$) \rightarrow ↑ energy, ↑ separation b/w energy levels.
- Zero Confinement \rightarrow limiting case of free e⁻.
- As energy ↑, probability of finding e⁻ at any x becomes more uniform.



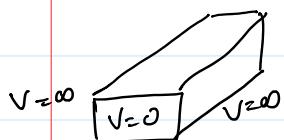
$$\left[\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right] + \frac{2m}{\hbar^2} [E - V(x,y)] \psi = 0 \rightarrow \psi = \frac{z}{d} \sin\left(\frac{n_x \pi}{d} x\right) \sin\left(\frac{n_y \pi}{d} y\right)$$

$$E = \frac{\hbar^2 \pi^2 (n_x^2 + n_y^2)}{2m d^2} \quad (2 \text{ quantum nos})$$



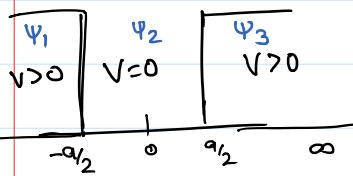
$$\psi = \left(\frac{2}{d}\right)^{3/2} \sin\left(\frac{n_x \pi}{d} x\right) \sin\left(\frac{n_y \pi}{d} y\right) \sin\left(\frac{n_z \pi}{d} z\right)$$

$$E = \frac{\hbar^2 \pi^2}{2m} \frac{(n_x^2 + n_y^2 + n_z^2)}{d^2}$$



$$E = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{d_x^2} + \frac{n_y^2}{d_y^2} + \frac{n_z^2}{d_z^2} \right)$$

e⁻ in finite potential well :-



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

$$\Psi_1 = C e^{\alpha x} \quad \Psi_2 = C e^{-\alpha x}$$

$$\Psi_2 = A \cos kx$$

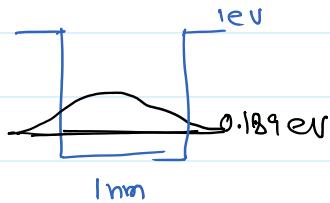
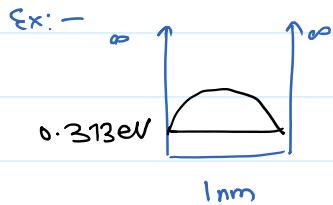
$$\sqrt{\beta^2 - k^2} = k \tan\left(\frac{ka}{2}\right)$$

$$\beta = \sqrt{2mV/\hbar^2}$$

$$k = \sqrt{2mE/\hbar^2}$$

Imp. Observations -

- * Wave fn Spills out of potential well.
- * Probability of finding particle outside well $\neq 0$
- * $E_n(\text{cowell}) > E_n(\text{finite well})$



Lec-6

ENERGY BAND FORMATION :-

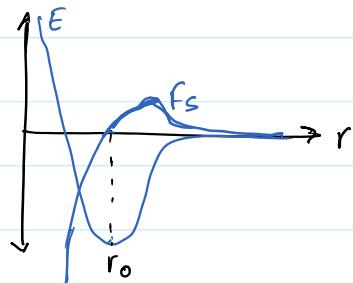
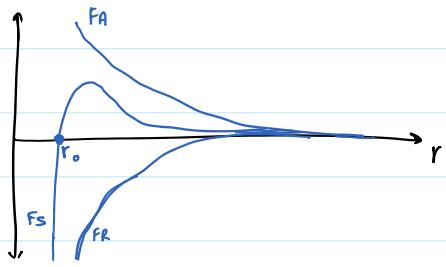
When two atoms are far attractive forces are dominant.

When brought close, repulsive force increases. and e^- clouds starts overlapping.

$$\text{Total force} = \vec{F}_{(\text{Rep})} + \vec{F}_{(\text{Att})}$$

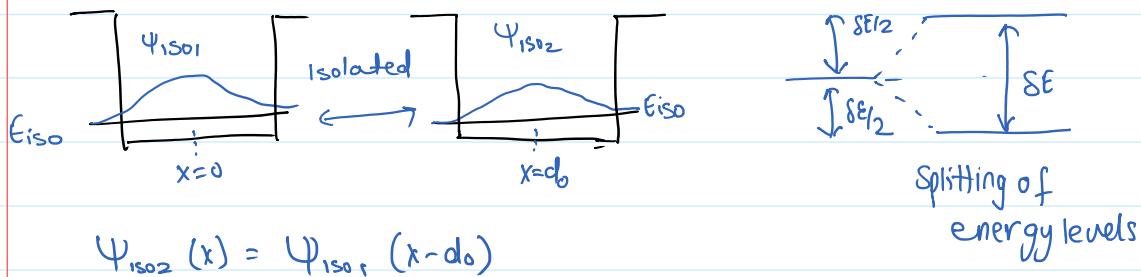
When,

$F_{\text{Net}} = 0$ ($e g m$) \rightarrow Bonding occurs &
this dist is bond length.



E_g^m and bonding occurs at min energy.

Coupled quantum well :-



On bringing potential wells closer, wave fn begin to overlap at some distance.

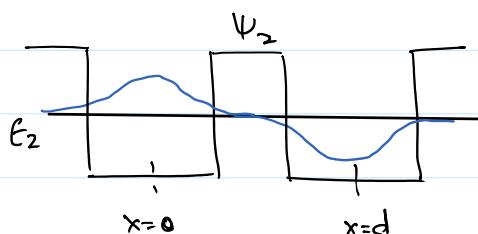
Both wells become ONE SYSTEM.

Energy levels split into two and wave fns will also be two.

These energy levels and wave fn belongs to the System (both wells).



- One System
- Two Soln to TISE
- Symm & Assym wave fns



$$\Psi_1 = \frac{1}{\sqrt{2}} (\Psi_{iso1} + \Psi_{iso2})$$

$$\Psi_2 = \frac{1}{\sqrt{2}} (\Psi_{iso1} - \Psi_{iso2})$$

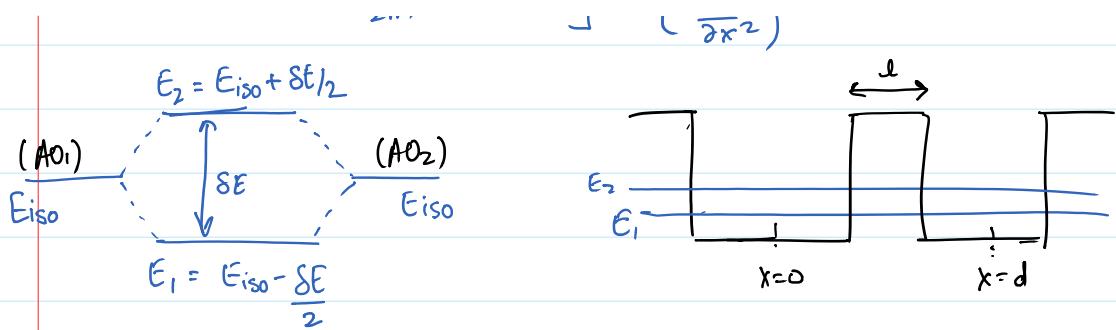
$$E_1 = \int_{-\infty}^{\infty} \Psi_1^* \hat{H} \Psi_1 dx$$

$$E_2 = \int_{-\infty}^{\infty} \Psi_2^* \hat{H} \Psi_2 dx$$

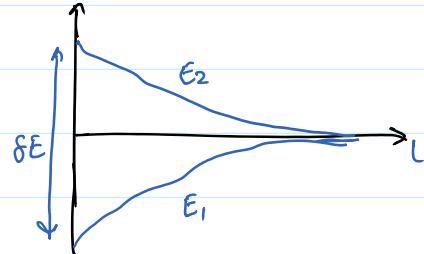
$$\left[E_{op} = \hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V \right] \quad \begin{matrix} \text{Curvature } \uparrow \rightarrow \text{KET} \rightarrow \text{ET} \\ \left(\frac{\partial^2}{\partial x^2} \right) \end{matrix}$$

$$E_2 = E_{iso} + \Delta E/2$$

$$\xleftrightarrow{d}$$



- $l \downarrow \rightarrow \uparrow \text{ Energy diff}$
- Bonding Orbitals \rightarrow Overlapping wave fn
- Atomic orbitals Combine to form molecular orbitals



$$\Psi = C_0 \Psi_{\text{iso}1} + C_1 \Psi_{\text{iso}2}$$

$$E_0 = \int \Psi_1^* \hat{H} \Psi_1 dx = \int \Psi_2^* \hat{H} \Psi_2 dx$$

$$I_{12} = \int \Psi_1^* \hat{H} \Psi_2 dx = \int \Psi_2^* \hat{H} \Psi_1 dx$$

$$E = \frac{\int \Psi^* \hat{H} \Psi dx}{\int \Psi^* \Psi dx} \approx \frac{E_0 c^2 + 2C_0 I_{12} + E_0 c^2}{c^2 + C_1^2}$$

$$\frac{\partial E}{\partial C_0} = 0 \Rightarrow E_G = E_0 C_0 + I_{12} C_1$$

$$\frac{\partial E}{\partial C_1} = 0 \Rightarrow E_G = I_{12} C_0 + E_0 C_1$$

$$\begin{pmatrix} E_0 & I_{12} \\ I_{12} & E_0 \end{pmatrix} \begin{pmatrix} C_0 \\ C_1 \end{pmatrix} = E \begin{pmatrix} C_0 \\ C_1 \end{pmatrix} \Rightarrow$$

$$E = E_0 - I_{12}$$

$$C_0 = \frac{1}{\sqrt{2}}, \quad C_1 = \frac{1}{\sqrt{2}}$$

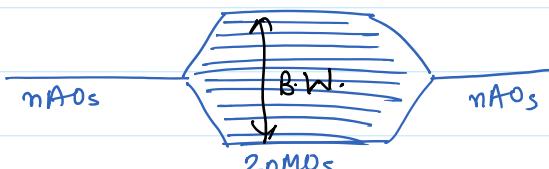
$$\Psi \approx \frac{1}{\sqrt{2}} (\Psi_1 + \Psi_2)$$

$$E = E_0 + I_{12}$$

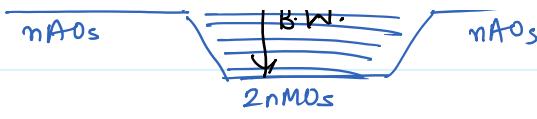
$$C_0 = \frac{1}{\sqrt{2}}, \quad C_1 = -\frac{1}{\sqrt{2}}$$

$$\Psi = \frac{1}{\sqrt{2}} (\Psi_1 - \Psi_2)$$

→ If we consider a solid, it contains a lot of atoms so, the levels of energy of each set of atoms are closely spaced, giving cont. energy band.



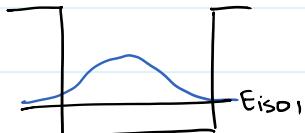
BWL depends on
Strength of Overlap



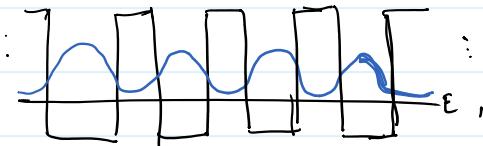
Strength of overlap
(coupling b/w wells)

Narrow B.W. \Rightarrow Weak Coupling.

Strong Overlap \Rightarrow Large B.W.

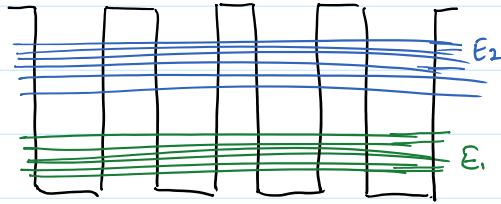
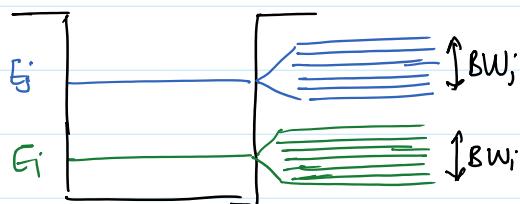


Localised state

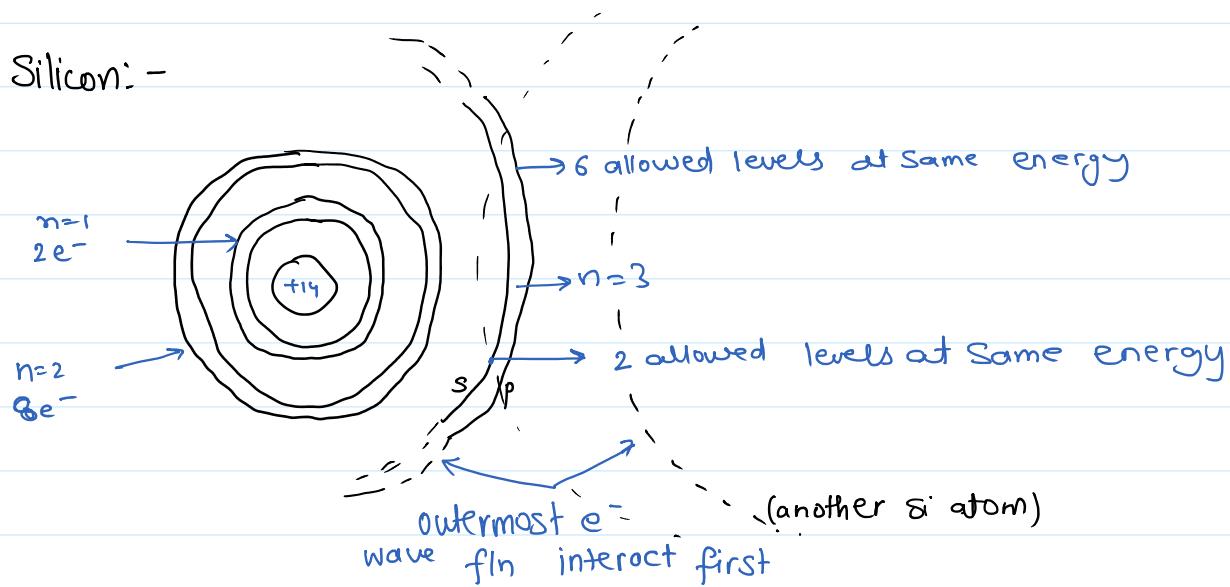


Delocalised state

In any state, the particle isn't confined to any particular potential well.



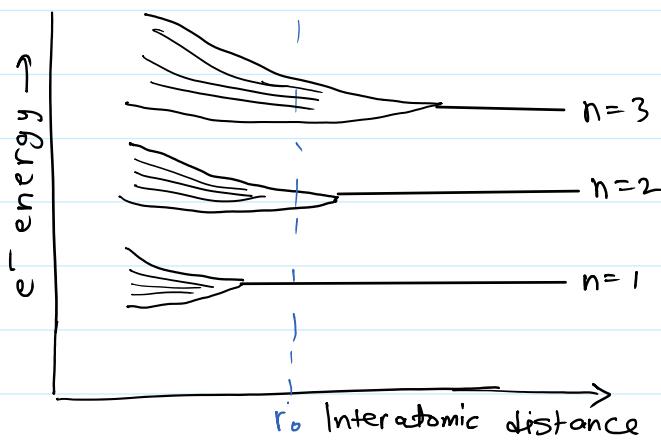
Silicon:-



Si e^- configuration = $1s^2 2s^2 2p^6 3s^2 3p^2$
(4 3p states are empty)

• N atoms \Rightarrow

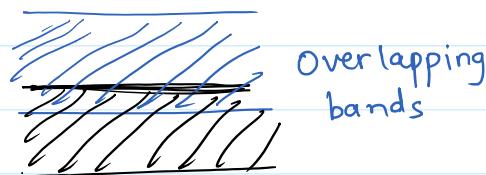
$2N$ 3s states, $6N$ 3p states
(4N 3p states empty)



- At 0 K e^- occupy lowest energy states available.
($4N$ are lowest available energy states in Si in the VB)
- $4N e^-$ occupy $4N$ states \rightarrow V.B will be full.
- CB will be empty \rightarrow No Conduction in CB of Si
- For an e^- to move there must be an empty State but no empty state in V.B \Rightarrow No. Conduction in V.B.

Thus, Semiconductors are insulators at 0 K.

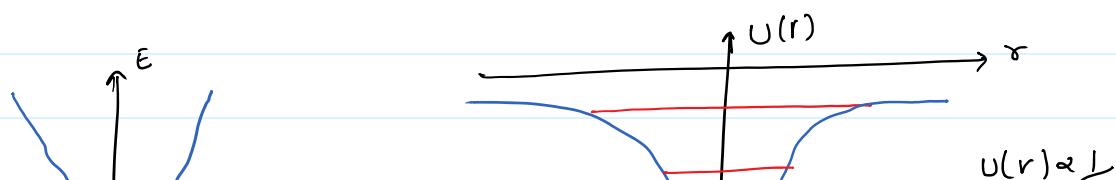
Metals:- Partially filled CB / CB and VB Overlap
hence, conductivity.

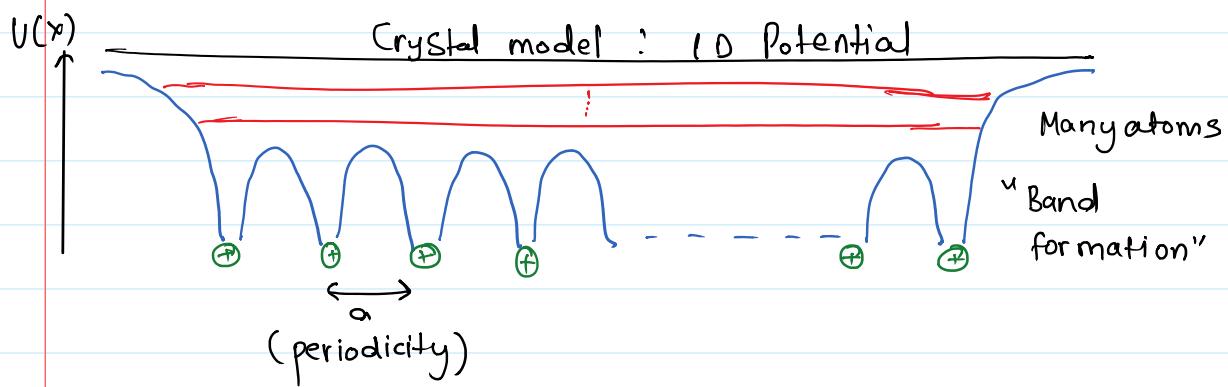
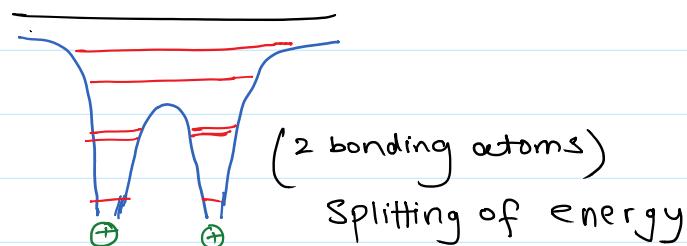
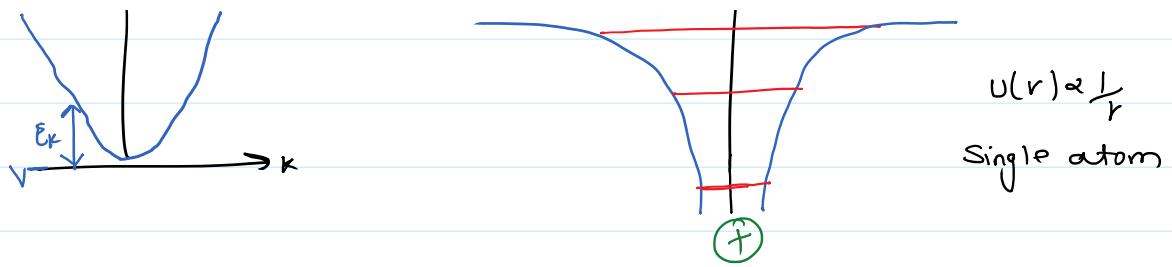


↑ _____ Possible bands for metals _____ ↑

Lec-7

BAND THEORY FROM QM :-





→ Surface effects can be neglected (Considering e^- deep within the solid)

→ Real crystals have defects (missing atoms, impurities, etc.),

Vibrating atoms at operating temp. So,

Assumptions \Rightarrow No defects
fixed atoms

Bloch Theorem -

If $U(x)$ = periodic s.t. $U(x+a) = U(x)$ then,

$$\Psi(x+a) = e^{ik_a a} \Psi(x) \quad \text{or}$$

$$\Psi(x) = e^{ik_a x} u(x)$$

$$\Psi(x,t) = \Psi(x) \phi(t)$$

$$\phi(t) = e^{-(jE/\hbar)t}$$

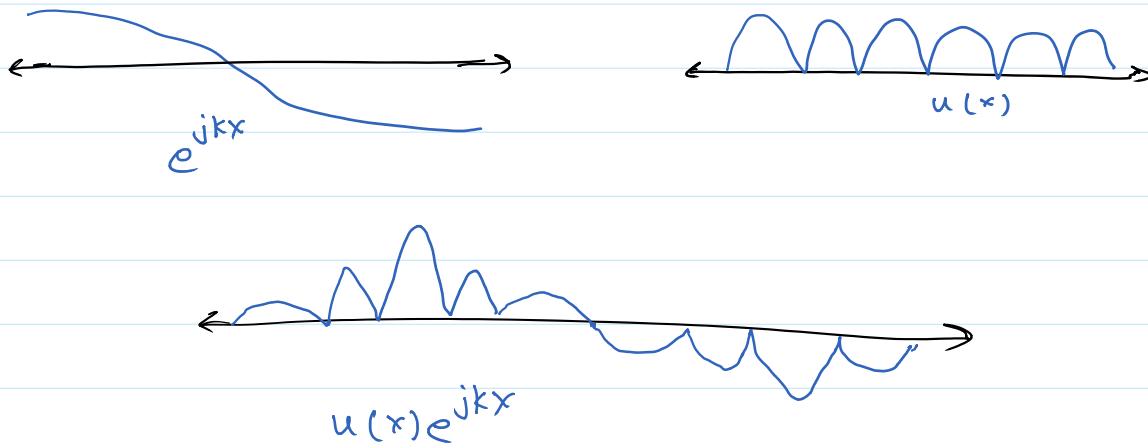
$$\Psi(x,t) = e^{jkx} u(x) e^{-(jE/\hbar)t}$$

$$\Psi(x,t) = u(x) e^{j(kx - E/\hbar)t}$$

Represents motion of e^- in single crystal

The e^- can move throughout the lattice but under the influence of a periodic potential.

→ Wave fn of e^- in periodic potential is equivalent to that of free e^- modulated by $u(x)$.



Allowed 'K' values in ideal 1D crystal-

→ 2 distinct K for each allowed E.

→ $K \pm \frac{2\pi}{a}$ gives same wave fn soln.

Range of K values = $-\pi/a$ to π/a (1st Brillouin zone)

→ K should be real if Crystal is infinite

→ Finite Crystal \rightarrow Boundary Cond' lack. So, periodic boundary Cond' is assumed i.e. starting and ending pt of Crystal are Same.

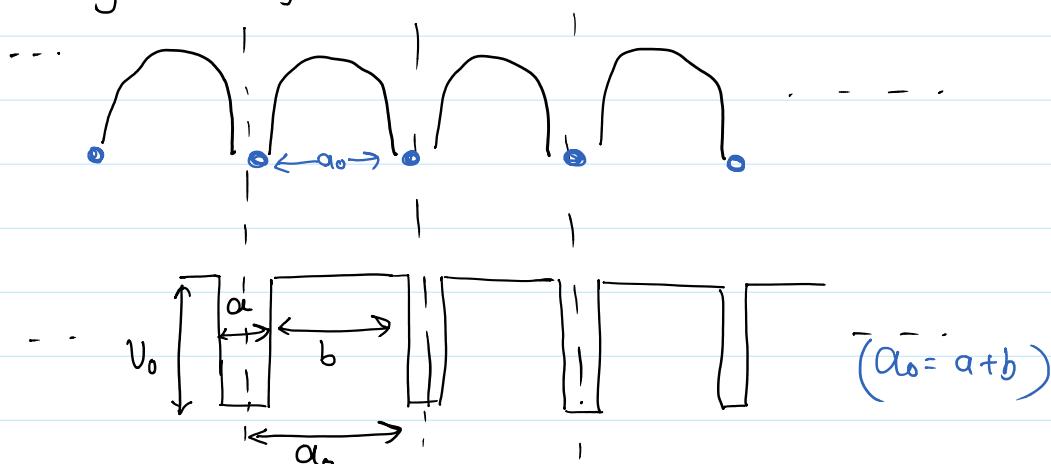
Closed ring of N atoms with interatomic Spacing = a

$$\Psi(x+Na) = \Psi(x)$$

$$\Psi(x) = \Psi(x+Na) = e^{jka} \Psi(x) \Rightarrow e^{jka} = 1$$

$$k = \frac{2\pi n}{Na} \quad \left(\begin{array}{l} \text{Total distinct } k = N \\ \text{for large } N \Rightarrow \text{close values of } k \text{ (quasi continuum)} \end{array} \right)$$

Kronig - Penney model



$$\text{from finite potential well : } \sqrt{\beta^2 - k^2} = k \tan\left(\frac{k a_0}{2}\right)$$

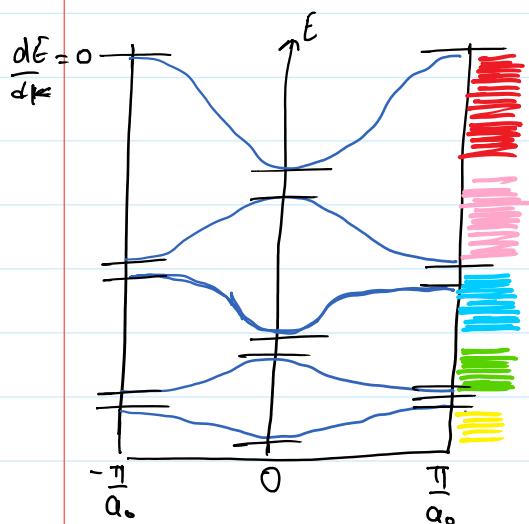
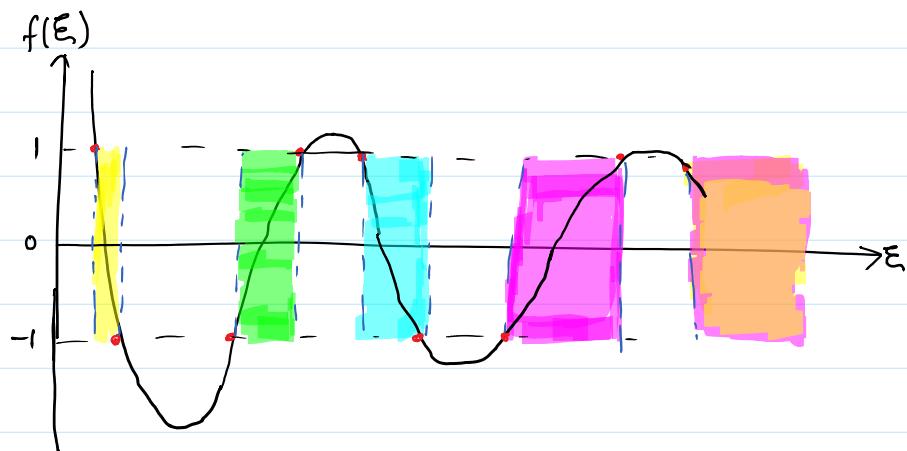
$$\xi = E/V_0 \quad a_0 = \sqrt{\frac{2mV_0}{\hbar^2}}$$

$$\frac{1-2\xi}{2\sqrt{\xi(1-\xi)}} \sin(a_0 a \sqrt{\xi}) \sinh(a_0 b \sqrt{1-\xi}) + \cos(a_0 a \sqrt{\xi}) \cosh(a_0 b \sqrt{1-\xi}) = \cos(k a_0) \quad 0 < \xi < V_0$$

$$\frac{1-2\xi}{2\sqrt{\xi(\xi-1)}} \sin(a_0 a \sqrt{\xi}) \sin(a_0 b \sqrt{\xi-1}) + \cos(a_0 a \sqrt{\xi}) \cos(a_0 b \sqrt{\xi-1}) = \cos(k a_0) \quad \xi > V_0$$

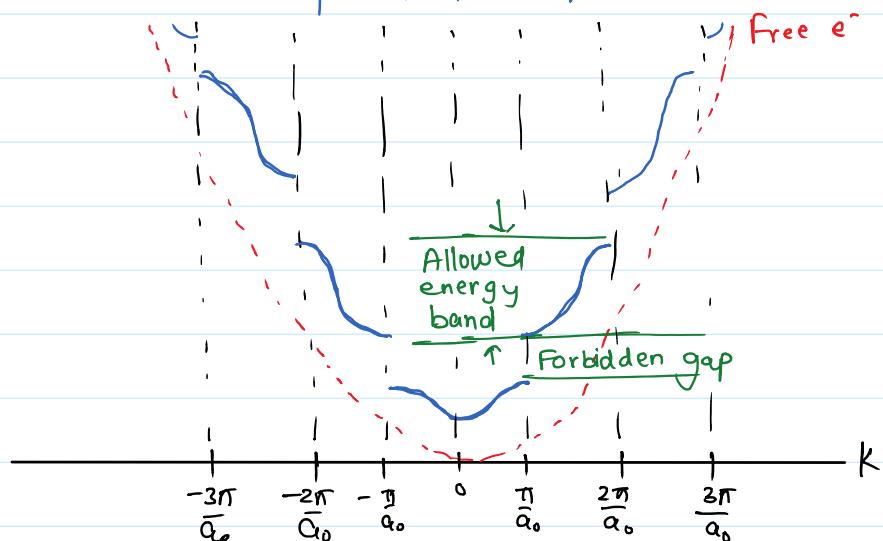
$$f(E)$$

$$E > U_0$$



- Changing by $\frac{2n\pi}{a_0}$ doesn't change allowed energy level.
- E-k Soln outside $\left[-\frac{\pi}{a_0}, \frac{\pi}{a_0}\right]$ duplicates that inside it
- $\frac{dE}{dk} = 0$ at k-zone boundaries
i.e. $k=0, k=\pm\pi/a_0$

⇒ Extended Zone representation :



- Segments due to periodic potential.
- Modification is highest at lower energies, eq's merging

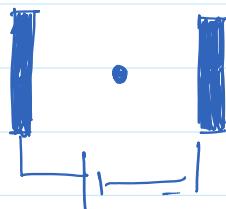
at higher energies.

→ Greater e^- energy $\Rightarrow \downarrow$ importance of periodic potential.

Effective mass -

In Crystal, e^- isn't free, periodic potential acts.
 e^- acceleration is relative to lattice.

When there's external force on e^- , it can be treated as free e^- with different mass i.e. effective mass.



$$F_{ext} = -qE = m_0 a$$

$$a_2 \frac{F_{ext}}{m_0}$$

$$F_{ext} + F_{int} = m_0 a$$

$$a = \frac{F_{ext} + F_{int}}{m_0} = \frac{F_{ext}}{m^*}$$

(m^* = effective mass)

$$\Psi(x, t) = A e^{j(kx - \omega t)} + B e^{j(-kx - \omega t)}$$

$$E = \hbar\omega$$

$$E = V + \frac{\hbar^2 E^2}{2m_0}$$

$$\frac{\partial E}{\partial k} = \frac{\hbar^2 k}{2m_0}$$

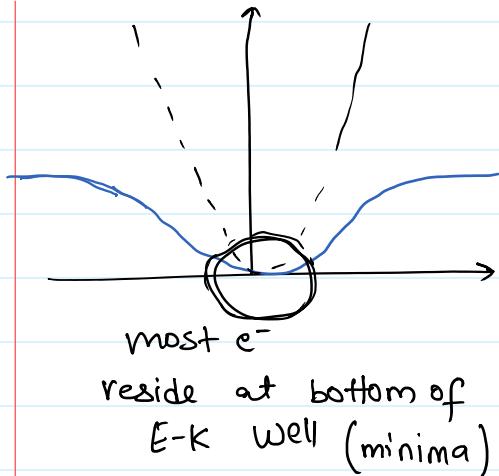
$$m_0 = \frac{\hbar^2}{(\partial^2 E / \partial k^2)}$$

$$p = \hbar k$$

$$v = \frac{\hbar k}{m_0} = \frac{1}{\hbar} \frac{\partial E}{\partial k}$$

$$F_{ext} = \frac{dp}{dt} = \frac{\hbar dk}{dt}$$

$$F_{ext} = m_0 \frac{dv}{dt} = m_0 \frac{\partial^2 E}{\partial k^2} \frac{dk}{dt}$$



$$E \approx c k^2$$

$$c = \frac{\hbar^2}{2m_0}$$

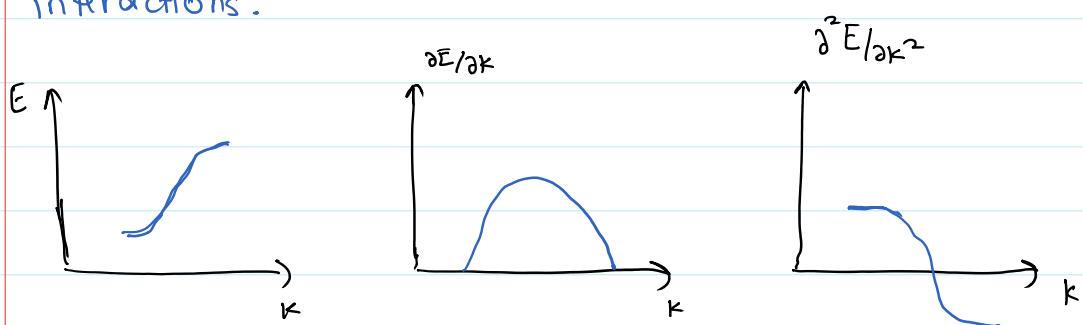
$$\frac{d^2 E}{dk^2} = 2c$$

$$m^* = \frac{\hbar^2}{(\frac{d^2 E}{dk^2})} = \frac{\hbar^2}{2c}$$

$$C = \frac{\hbar^2}{2m^*}, \quad E \approx \frac{\hbar^2}{2m^*} k^2$$

Advantages of effective mass:-

- All internal forces and quantum mech. properties are taken in account through m^* .
- e^- at bottom of E-k \rightarrow Classical particle so, motion interpretation by Newton's laws.
- Vibration of atoms can be taken as e^- phonon interactions.



- $m^* = +ve$ near the bottom of bands
 $= -ve$ near top of bands
- $-ve m^* \equiv e^-$ accelerates in opposite to expected direction.
- Holes $\Rightarrow F_{ext} = m_h^* a$

$$J = -q \sum_{j \neq k}^N v_j = -q \sum_1^N v_j - (-q v_k) = q v_k$$

$j \neq k$

$\sum_{j \neq k} v_j = 0$ bcoz of symmetric bands

[for every e^- at $+k$, there's an e^- at $-k$ So, net Current = 0 for fully filled bands.]

Current Carried by $(N-1)e^-$ in VB = Current by missing e^- with +ve charge.

\Rightarrow effect of all e^- s can be modelled as a +ve charge particle - Hole.

$\rightarrow E-x$ doesn't give info about wave vector (wave length, dirⁿ of motion)

$\rightarrow E-k$ doesn't give info about position.

Real Space $E-k$ and $E-x$ Compliment each other.

= Extension to 3-D

* Bloch wave :-

$$1D: \psi(x) = U_k(x) e^{ikx}$$

$$3D: \psi(\vec{r}) = U_k(\vec{r}) e^{i\vec{k}\vec{r}}$$

* $E-k$ relation in any band is periodic in k -Space with periods $\frac{2\pi}{a}, \frac{2\pi}{b}, \frac{2\pi}{c}$

a, b, c = periodicity of x, y, z respectively

* Group velocity of e^- in 3D:-

$$\vec{v} = \frac{1}{\hbar} \left(\hat{i} \frac{\partial E}{\partial k_x} + \hat{j} \frac{\partial E}{\partial k_y} + \hat{k} \frac{\partial E}{\partial k_z} \right)$$

* Near extremum, Curvature of $E-\vec{k}$ plot depend on dirⁿ of \vec{k} and thus dirⁿ of travelling of e^- . In such cases, m^* is direction dependent =

Tensor

$$m_x^* = \frac{\hbar^2}{\left(\frac{\partial^2 E}{\partial k_x^2}\right)}, \quad m_y^* = \frac{\hbar^2}{\left(\frac{\partial^2 E}{\partial k_y^2}\right)}, \quad m_z^* = \frac{\hbar^2}{\left(\frac{\partial^2 E}{\partial k_z^2}\right)}$$

* for SemiConductors with Cubic unit cell structure,

$k=0$, dirⁿ independent and

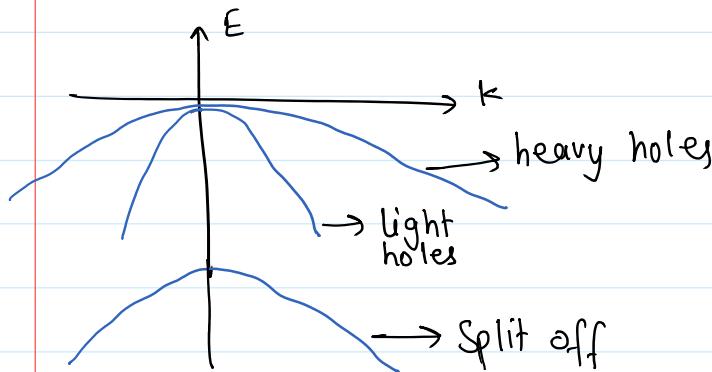
$$m^* = m_x^* = m_y^* = m_z^* \text{ (Scalars)}$$

* In K Space, slope of $E-k=0$ at edges of Brilloin zone.

Where two bands coincide the edge, sum of slopes = 0
for Cubic Crystal.

\Rightarrow V.B. of Si \rightarrow

- 3 overlapping bands, all with absolute maxima at $k=0$ and different curvature.
- 2 bands have same energy at $k=0 \rightarrow$ heavy holes and light holes.
- 3rd band is shifted by energy Δ = Split-off.
- Few holes at top of split off band (Ignorable)

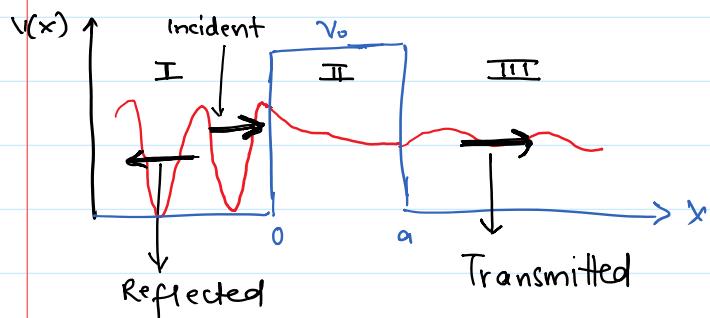


Tunneling through potential barrier -

Lec-8

If E is not much smaller than V_0 , then there's probability of e^- to transmit through the barrier into region $x>a$.

probability of e^- to transmit through the barrier into region $x>a$.



$$V(x) = \begin{cases} V_0 & 0 \leq x \leq a \\ 0 & x < 0, x > a \end{cases}$$

e^- Energy = E

$$\Psi_I = A e^{ik_1 x} + B e^{-ik_1 x} \quad x < 0$$

$$\Psi_{II} = C e^{ik_1 x} + D e^{-ik_1 x} \quad x > a$$

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

(No reflection Component, $D=0$)

$$\Psi_{III} = F e^{k_2 x} + G e^{-k_2 x} \quad 0 < x < a$$

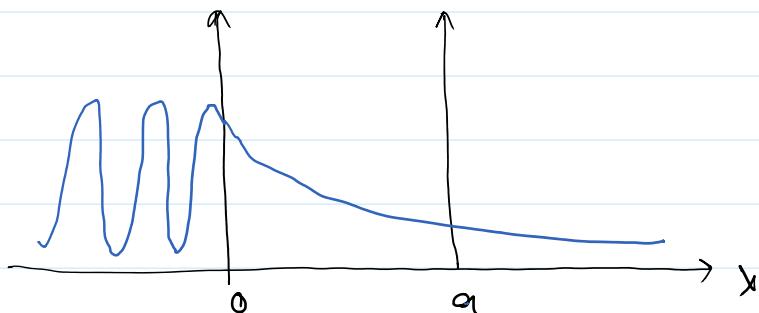
$$k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$$\Psi_I(0) = \Psi_{II}(0)$$

$$\frac{d\Psi_I}{dx} = \frac{d\Psi_{II}}{dx} \quad (\text{at } x=0)$$

$$\Psi_{II}(a) = \Psi_{III}(a)$$

$$\frac{d\Psi_{II}}{dx} = \frac{d\Psi_{III}}{dx} \quad (\text{at } x=a)$$



Probability density f/n $\Psi\Psi^*$

$x > a$:- Pure travelling wave \rightarrow Const. probability f/n.

$x < 0$:- Reflected wave + Incident wave

amplitude of reflected wave is small so,
the wave is neither purely standing nor travelling.

$$\text{Reflection Coefficient } (R) :- \frac{|\Psi_{\text{reflected}}|^2}{|\Psi_{\text{incident}}|^2} = \frac{|B|^2}{|A|^2}$$

$$\text{Transmission Coefficient } (T) :- \frac{|\Psi_{\text{transmitted}}|^2}{|\Psi_{\text{incident}}|^2} = \frac{|C|^2}{|A|^2}$$

$$T = \left[1 + \frac{1}{4} \left(\frac{V^2}{E(V-E)} \right) \left[\frac{e^{k_2 a} + e^{-k_2 a}}{2} \right]^2 \right]^{-1}$$

$$T \approx 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0} \right) e^{-2k_2 a}$$

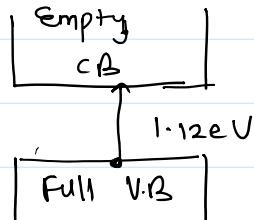
* \downarrow barrier thickness $\rightarrow \uparrow(T)$

* e^- in i-Si at room temp (300K)

Band gap Si = 1.12 eV

Thermal energy = $KT = 0.026 \text{ eV}$

(It's the avg. energy,
Some e^- have high energy than average)



$\frac{1.12}{0.026} = 43$ times \uparrow energy req.

43 e^- must collide to give an e^- the required energy

Probability of 1 Collision = p

that of 43 Collisions = p^{43} ($\sim 10^{-12}$ very low)

$$n_i = p_i = N \cdot p^{\frac{E_c}{kT}}$$

$n_i = \text{intrinsic conc}' \text{ of } e^-$
 $p_i = \text{.. .. sqf } h^+$

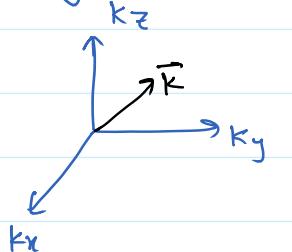
$$n_i = p_i = N \cdot p \quad \left. \begin{array}{l} n_i = \text{intrinsic conc' of } e^- \\ p_i = \text{" " " of } h^+ \end{array} \right\}$$

$$\ln(n_i) \propto \frac{1}{T}$$

Lec-9

CHARGE CARRIER DENSITY -

Imagine Space with wave vectors 'k'



$$\begin{aligned} k^2 &= k_x^2 + k_y^2 + k_z^2 \\ \vec{k} &= \vec{a} k_x + \vec{b} k_y + \vec{c} k_z \end{aligned}$$

⇒ To obtain I-V characteristics of Semiconductors, we need to know:-

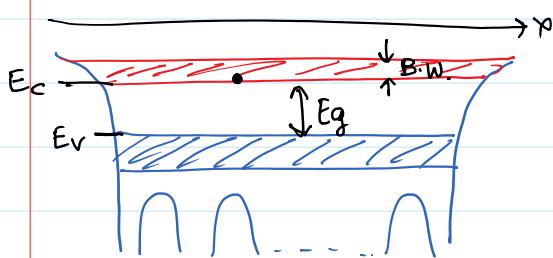
No. of charge carriers for conduction

Distribution of states available

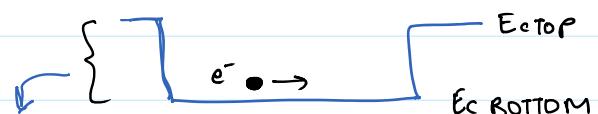
Probability of occupation →

(Density of allowed states
as a fn of energy)

(Fermi dirac stats)



e^- at bottom of C.B. can be imagined as e^- in potential well



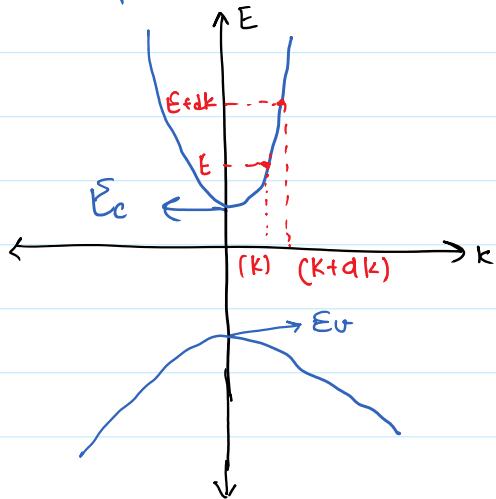
Barrier height = B.W.

for 3-D Crystal → assume e^- in 3-D potential well.

$$g(E)dE = \frac{(\text{No. of states with } E \text{ b/w } E \text{ and } E+dE)}{\dots}$$

Vol. of Crystal

Integrating DOS fcn $g(E)$ b/w $E_1 - E_2$ gives allowed states/Vol. available to e^- in this energy range.



Assume parabolic E-k relation.

No. of free e^- (h^+ 's) << available states.

They occupy only bottom of CB and top of VB.

So, our assumptions is not bad at bottom & top of CB and VB respectively.

→ To find allowed states b/w E and $E+dE$

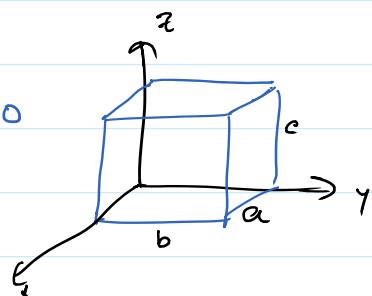
$$E = E_c + \frac{\hbar^2 k^2}{2m_c^*}$$

$$E = E_v - \frac{\hbar^2 k^2}{2m^*}$$

Consider particle of mass m , energy E Confined in
Crystal size d 3D box.

$$\left[\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right] + \frac{2m}{\hbar^2} \left[E - V(x, y, z) \right] \Psi = 0$$

$E - V(x, y, z)$
= 0
(assume for convenience)



$$\left[\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right] + \frac{2m}{\hbar^2} E \Psi = 0 \quad , \quad E = \frac{\hbar^2 k^2}{2m}$$

We will solve for this and finally, put $E - E_C$ or $E_V - E$ at place of E .

$$\textcircled{1} \left[\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right] + k^2 \Psi = 0 \quad x \in (0, a), y \in (0, b), z \in (0, c)$$

Now, Separate Variables :— $\Psi = \Psi_x \Psi_y \Psi_z$

Substitute Ψ in $\textcircled{1}$ and divide by Ψ

$$= \left[\underbrace{\frac{1}{\Psi_x} \frac{\partial^2 \Psi_x}{\partial x^2} + \frac{1}{\Psi_y} \frac{\partial^2 \Psi_y}{\partial y^2} + \frac{1}{\Psi_z} \frac{\partial^2 \Psi_z}{\partial z^2}}_{\text{fn of individual coordinates}} \right] + k^2 = 0$$

↓
constant

each of them = const so, that

sum = const.

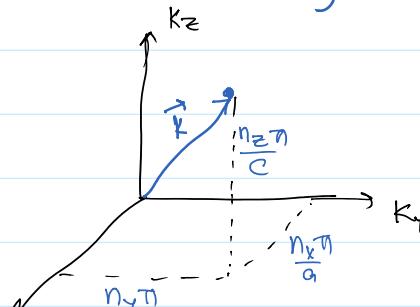
$$\frac{1}{\Psi_x} \frac{\partial^2 \Psi_x}{\partial x^2} + k_x^2 = 0 \Rightarrow \Psi_x = D \sin k_x x \quad \text{so,}$$

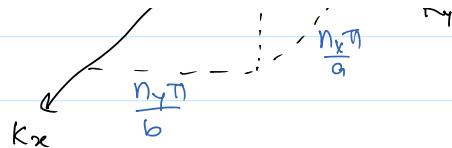
$$k_x = \frac{n_x \pi}{a} \quad \text{Similarly, } k_y = \frac{n_y \pi}{b}, \quad k_z = \frac{n_z \pi}{c}$$

$$\Psi = A \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{b} y\right) \sin\left(\frac{n_z \pi}{c} z\right)$$

Every K point, is associated with a K-Space vector where $\vec{a}, \vec{b}, \vec{c}$ are unit vectors along K-Space Co-ordinate axis.

$$\vec{R} = \vec{a} k_x + \vec{b} k_y + \vec{c} k_z$$

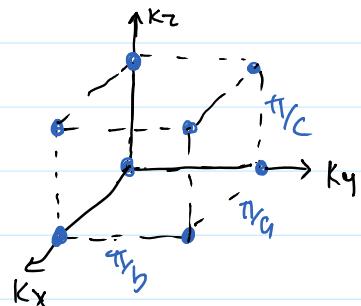




k -Space unit cell \rightarrow

Smallest possible $k_x = \frac{\pi}{a}$, $k_y = \frac{\pi}{b}$, $k_z = \frac{\pi}{c}$

So, k -Space unit cell Vol = $\frac{\pi}{a} \times \frac{\pi}{b} \times \frac{\pi}{c}$



No. of k / unit cell = 1

So 1 soln in Vol $\frac{\pi^3}{abc}$,

Soln / Vol = $\frac{abc}{\pi^3}$

No. of allowed states \neq No. of soln.

for instance, the 8 combinations by

$n_x = \pm 1$, $n_y = \pm 1$, $n_z = \pm 1$

are all same allowed state.

8 soln \Rightarrow 1 allowed state

So, allowed states per unit Vol = $\frac{1}{8} \times \frac{abc}{\pi^3}$

due to spin, 2 states are possible so,

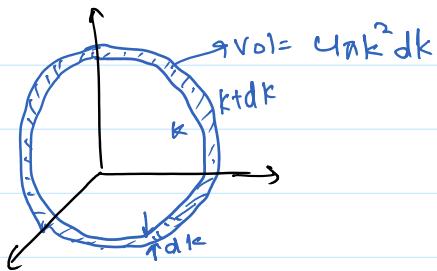
Allowed states per unit Vol of k -Space = $\frac{1}{4} \times \frac{abc}{\pi^3}$

No. of energy states b/w k and $k+dk$ per unit k -Space

Vol = $(\text{Vol b/w } k \text{ and } k+dk) \times \frac{1}{4} \times \frac{abc}{\pi^3}$

$$\text{Vol} = 4\pi k^2 dk$$

$$= \dots , 2$$



$$\begin{aligned}
 &= 4\pi k^2 dk \times \frac{1}{4} \times \frac{abc}{\pi^3} \\
 &= \frac{k^2 abc}{\pi^2} dk
 \end{aligned}$$

For energy states with E b/w E and $E+dE \Rightarrow$

$$k = \frac{\sqrt{2mE}}{\hbar} \rightarrow dk = \frac{1}{\hbar} \sqrt{\frac{m}{2E}} dE$$

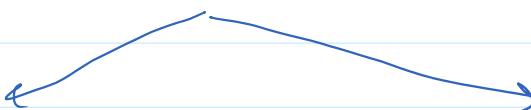
$$\frac{2mE}{\hbar^2} \frac{abc}{\pi^2} \frac{1}{\hbar} \sqrt{\frac{m}{2E}} dE$$

$$= (abc) \frac{m}{\pi^2 \hbar^3} \sqrt{2mE} dE$$

↓ divide by Vol. of Crystal = abc

$$g(E)dE = \frac{m}{\pi^2 \hbar^3} \sqrt{2mE} dE$$

$$g(E) = \frac{m}{\hbar^3 \pi^2} \sqrt{2mE} \quad \left(\text{We got this with assumption} \right)$$



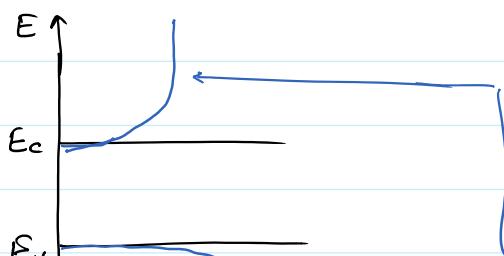
Translation for CB

Translation for VB

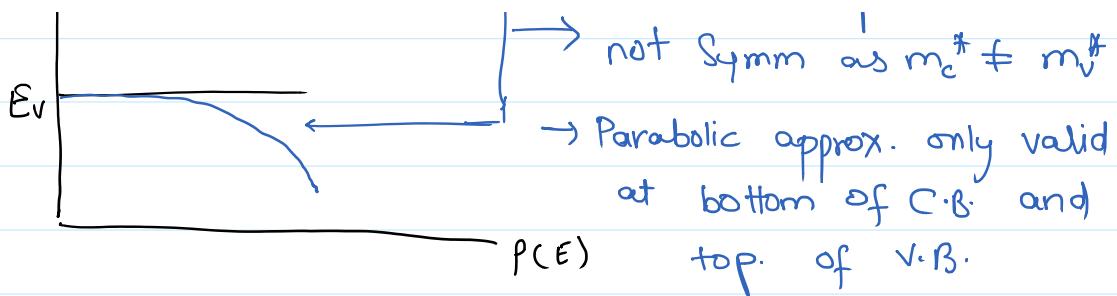
(will use $P(E)$ (density of states))

$$P(E) \Big|_{CB} = \frac{\sqrt{2}}{\pi^2} \left(\frac{m_c^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_c}$$

$$P(E) \Big|_{VB} = \frac{\sqrt{2}}{\pi^2} \left(\frac{m_v^*}{\hbar^2} \right)^{3/2} \sqrt{E_v - E}$$



Both these parabolae are not symm as $m_c^* \neq m_v^*$



No. of quantum states b/w E and $E+dE$ (N)

$$N = \int_E^{E+dE} p(E) dE$$