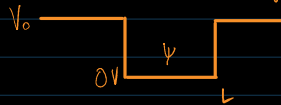


## Drawbacks of Classical $e^-$

- Compton, photo electric, black-body | Electrical conductivity (Wiedmann-Franz  $\left(\frac{k}{dT}\right)$  at low temp.
- ferromagnetism, Quantum free  $e^-$  theory,  $4.5R \neq 3R$

## Sommerfeld Model

- $e^-$  move freely in constant potential within boundaries of metal
- discrete energy values, pauli exclusion princpl, ( $e^-$  & lattice,  $e^-$  &  $e^-$ ) neglect.



$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE\psi}{\hbar^2} = 0 \quad \rightarrow \quad E = \frac{n^2 \hbar^2 \pi^2}{2mL^2}$$

## Density of States

- in solid energy level of  $e^-$  spread over (energy band) range. Each band has no. of state.
- $g(E)$  = no. of quantum/energy state / Energy / Volume.

$$g(E) = \frac{\frac{\text{no. of energy state b/w } (E, E+dE)}{dN(E)}}{\frac{dE}{V}} \rightarrow g(E) dE = dN(E)$$

$$\text{When using fermi} \rightarrow n = \frac{N}{V} = \int \frac{dN(E)}{V} dE = \int \underbrace{f(E)}_{\text{fermi-dirac}} g(E) dE$$

no. of particle per unit volume.

$$E \text{ for 3D} = E = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2) \quad (\text{Give sphere example})$$

$$\begin{aligned} dN(E) dE &= \frac{1}{8} \left[ \frac{4}{3} \pi (n+dn)^3 \right] - \left( \frac{4}{3} \pi n^3 \right) \\ &= \frac{\pi}{6} (3 n^2 dn) = \frac{\pi}{2} (n(n+dn)) \end{aligned}$$

$$E = \frac{n^2 \hbar^2 \pi^2}{2ma^2} = \frac{n^2 \hbar^2}{8ma^2} \quad \begin{cases} \rightarrow n dn = \left( \frac{8ma^2}{\hbar^2} \right) \times \frac{1}{2} dE \\ \rightarrow n = \left( \frac{8ma^2 E}{\hbar^2} \right)^{1/2} \end{cases}$$

$$dN(E) dE = \frac{\pi}{2} \left( \frac{8m}{\hbar^2} \right)^{3/2} a^3 E^{1/2} dE \Rightarrow \frac{dN(E) dE}{a^3} = \frac{\pi}{2} \left( \frac{8m}{\hbar^2} \right)^{3/2} E^{1/2} dE = g(E)$$

$$n = \int f(E) g(E) dE \quad \text{for } T=0 \quad f(E) = 1 \rightarrow n = \frac{\pi}{3} \left( \frac{8m}{\hbar^2} \right)^{3/2} E_F^{3/2} \rightarrow \boxed{E_F = \left( \frac{3}{\pi} \right)^{2/3} \left( \frac{\hbar^2}{8m} \right) n^{2/3}}$$

## Block Theorem

- In a periodic potential, the wavefunctions of electrons can be represented as product of plane wave & periodic function with same periodicity as crystal lattice.
- assumed: 'a' dis b/w lattice points.
- Zero at site center
- max b/w 2 core

$$\psi(x) = e^{i\vec{k}\vec{r}} \underbrace{u_k(r)}_{\text{modulating function}} \rightarrow \left\{ \psi(x) = e^{i\vec{k}\cdot\vec{x}} u(x) \right\} \quad \text{1-D}$$

Verify it by putting  $x = x + Na$ .

∴ Na

modulating function

$\rightarrow$  max b/w 2 core  
 Verify it by putting  $x = x + Na$ .  
 we get  $\psi(x + Na) = e^{ikNa} \psi(x)$

modulating function

## Kronig Penny Model

$\rightarrow$  Assumed: 'a'  $\rightarrow$  gap distance, 'b' square potential width.

$\rightarrow$  0 at core, max b/w  $\oplus$  core.

for gap

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2} \psi = 0$$

$$\alpha^2 = \frac{2mE}{\hbar^2}$$

for peak

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m(E - V_0)}{\hbar^2} \psi = 0$$

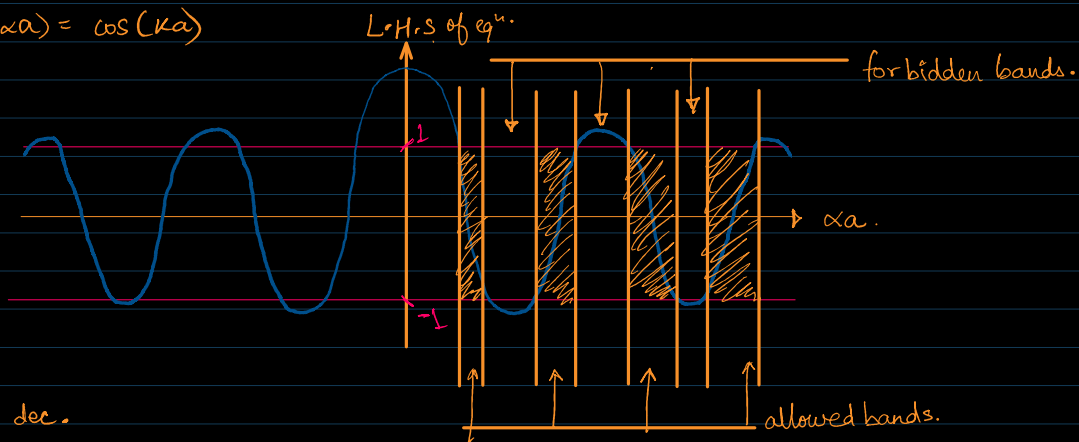
$$\beta^2 = \frac{2m}{\hbar^2} (V_0 - E)$$

$$P \frac{\sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka)$$

- due to RHS  $\cos$  b/w  $(-1, 1)$  hence bounded.

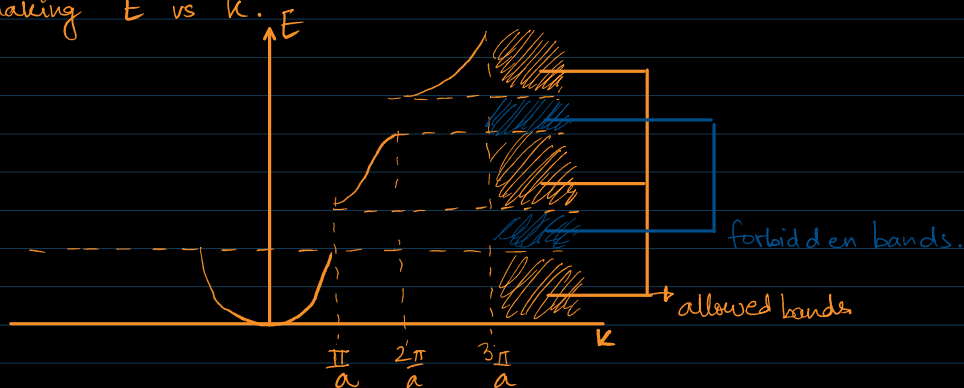
- periodicity  $= \left(n \frac{\pi}{a}\right)$

- $\alpha a$  inc, forbidden dec.



from  $\downarrow$  When making  $E$  vs  $k$ .

$$\left( \frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2} \psi = 0 \right)$$



- $P \rightarrow$  measure of potential barrier strength.  
 $P \uparrow \rightarrow$  electron bound more strongly to wells.

$$P = \infty \rightarrow \frac{\sin \alpha a}{\alpha a} + \frac{\cos \alpha a}{P} = \frac{\cos ka}{P}$$

$$\sin \alpha a = 0 \rightarrow \alpha = \frac{n\pi}{a} \rightarrow \alpha^2 = \frac{n^2 \pi^2}{a^2}$$

$$\frac{2mE}{\hbar^2} = \frac{n^2 \pi^2}{a^2} \rightarrow E = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

Pot. Well energy

$$P = 0 \rightarrow \cos \alpha a = \cos ka \rightarrow \alpha = k = \frac{2\pi}{a}$$

$$\frac{2mE}{\hbar^2} = k^2 \rightarrow E = \frac{\hbar^2 k^2}{2m} \approx \frac{1}{2} m v^2$$

free  $e^-$  energy

- $k$ -values define boundaries of Brillouin zone.
- $e^-$  moving have energies from allowed, band sep by forb zone.
- Discontinuity at  $\left(k = \frac{n\pi}{a}\right) \rightarrow$  Brillouin zone  $_1 = \left(-\frac{\pi}{a}, \frac{\pi}{a}\right)$ , Brillouin zone  $_2 = \left(\frac{\pi}{a}, \frac{2\pi}{a}\right)$  &  $\left(\frac{\pi}{a}, \frac{2\pi}{a}\right)$
- Each portion a band.

