

Drawbacks of Classical e^-

- Compton, photo electric, black-body
- ferromagnetism, Quantum free e^- theory, $4.5R \neq 3R$
- | Electrical conductivity (Wiedmann-Franz) $(\frac{K}{\delta T})$ at low kT .

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.
- $g(E) = \text{no. of quantum energy state / energy / Volume}$

$$g(E) = \frac{dN(E)}{dE} \underset{V}{\int} \rightarrow g(E) dE = dN(E)$$

↑ no. of energy state b/w $(E, E+dE)$

$$\text{When using fermi} \rightarrow n = \frac{N_{\text{total}}}{V} = \int \frac{dN(E)}{V} dE = \int_{\text{fermi-dirac}} f(E) g(E) dE$$

no. of particle per unit volume.

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

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

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

$$\rightarrow n = \left(\frac{8ma^2}{\hbar^2} E \right)^{1/2}$$

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

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

Bloch 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 point.

- zero at site center
- max b/w 2 core

$$\Psi(r) = e^{i\vec{k}\vec{r}} u_k(r) \rightarrow \left\{ \Psi(r) = e^{i\vec{k}r} u(r) \right\} \text{ 1-D}$$

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

$\therefore u(r) \rightarrow$ modulating function

l max b/w 2 core

Verify it by putting $x = n\pi/a$.

$$\text{we get } \Psi(x+n\pi/a) = e^{ikn\pi/a} \Psi(x)$$

modulating function

Kronig-Penney Model

Assumed : 'a' → gap distance, 'b' square potential width.

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

for gap

$$\frac{\delta^2 \Psi}{\delta x^2} + \frac{2mE}{\hbar^2} \Psi = 0$$

for peak

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

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

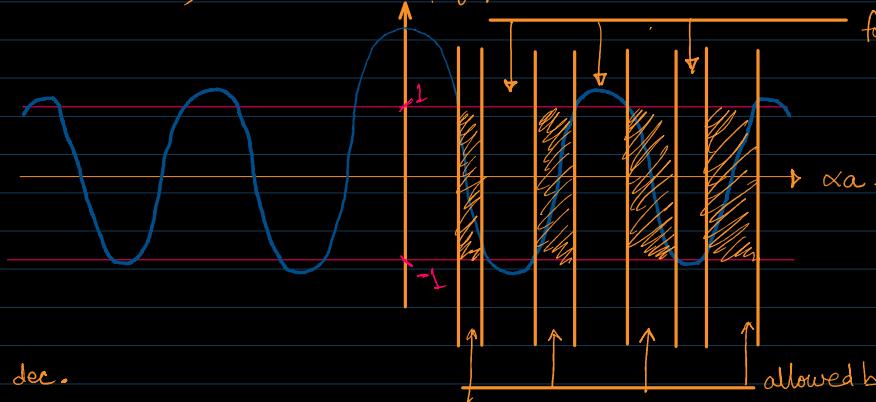
$$\beta^2 = \frac{2m}{\hbar^2} (V_0 - E)$$

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

L.H.S of eqn.

forbidden bands.

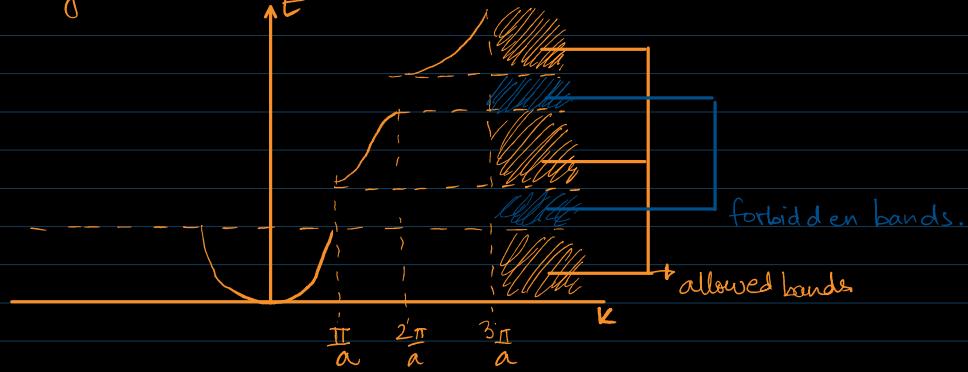
- due to RHS
cos b/w (-1, 1)
hence bounded.



- periodicity = $(n\pi/a)$
- αa inc, forbidden dec.

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

When making E vs k .



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

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

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

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

pot. Well energy

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

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

free e^- energy

- k -values define boundaries of Brillouin zone.

- e^- moving have energies from allowed band sep by forb zone.

- Discontinuity at $(k = n\pi/a)$ → Brillouin zone₁ = $(-\frac{\pi}{a}, \frac{\pi}{a})$, Brillouin zone₂ = $(-\frac{2\pi}{a}, \frac{\pi}{a})$ & $(\frac{\pi}{a}, \frac{2\pi}{a})$
- Each portion a band.

