Band Theory of solids.

1 D infinite chain of Atoms.

e^- $\quad \leftarrow a \rightarrow$

$\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \cdots\cdots \rightarrow x$.

Motion of free e^- under the influence of a periodic potential.

$V(x+a) = V(x)$.

$\hat{H}\psi(x) = E\,\psi(x)$. $\longrightarrow$ (1)

Hamiltonian $\longrightarrow$ Total energy op. $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right] \equiv \hat{H}$

Info 1: $\hat{H}(x+a) = \hat{H}(x)$. $\rightarrow$ Prove it.

Info 2: If we define an op. $\hat{T}_a$ such that $\longrightarrow$ "Lattice Translatory op."

$\hat{T}_a f(x) = f(x+a)$

Then as from Schrödinger eqn:

$\psi(x)$ is an eigen fn of $\hat{H}(x)$, with eigen value E.

Then $\hat{T}_a\psi(x)$ is also - - - - - - - - - - - -

Proof. Schrödinger eqn: $\hat{H}(x)\,\psi(x) = E\,\psi(x)$.

$$\hat{T}_a\left[\hat{H}\psi\right] = \hat{T}_a\left[E\psi\right].$$

$$\Rightarrow \hat{H}(x+a)\,\psi(x+a) = E\left[\hat{T}_a\psi\right].$$

$$\Rightarrow \hat{H}\left[\hat{T}_a\psi(x)\right] = E\left[\hat{T}_a\psi(x)\right].$$

$\Downarrow$

$\psi(x)$ and $\hat{T}_a\psi(x)$ or $\psi(x+a)$ both are eigen fn of Hamiltonian op. with eigen value E.

$\Downarrow$

$\hat{T}_a\psi(x) = \psi(x+a) \propto \psi(x) \;\Rightarrow\; \psi(x+a) = \lambda\,\psi(x)$ doesn't depend on x

$\lambda = ??$

Th. **Floquet's Th:** if $V(x+a) = V(x)$. Then, $\boxed{|\lambda| = 1}$.

Proof. Schrödinger eqn. $\longrightarrow$ 2nd order ~~linear~~ diff. eqn.

Two ind. soln.
Any other soln. is a linear combination of these 2 ind. soln.

u_1 u_2

$$u_1(x+a) = M_{11}\, u_1(x) + M_{12}\, u_2(x).$$
$$u_2(x+a) = M_{21}\, u_1(x) + M_{22}\, u_2(x).$$

Any general soln. of eqn (1)

$$\psi(x) = A\, u_1(x) + B\, u_2(x).$$

$$\Rightarrow \psi(x+a) = A\, u_1(x+a) + B\, u_2(x+a).$$

$$\Rightarrow \lambda \psi(x) = A\left(M_{11} u_1(x) + M_{12} u_2(x)\right) + B\left(M_{21} u_1(x) + M_{22} u_2(x)\right)$$

$$\Rightarrow \lambda A\, u_1(x) + \lambda B\, u_2(x) = \left(A M_{11} + B M_{21}\right) u_1(x) + \left(A M_{12} + B M_{22}\right) u_2(x).$$

Comparing the coeffi. of $u_1(x)$ and $u_2(x)$ in both sides.

$$\lambda A = A M_{11} + B M_{21} \Rightarrow (M_{11} - \lambda) A + M_{21} B = 0.$$
$$\lambda B = A M_{12} + B M_{22} \Rightarrow M_{12} A + (M_{22} - \lambda) B = 0.$$

For a non-trivial soln. of A and B.

$$\begin{vmatrix} M_{11} - \lambda & M_{21} \\ M_{12} & M_{22} - \lambda \end{vmatrix} = 0. \Rightarrow \text{It's a quadratic eqn. in } \lambda.$$

λ_1 λ_2

$$\psi_1(x+a) = \lambda_1 \psi_1(x).$$
$$\psi_2(x+a) = \lambda_2 \psi_2(x).$$

Define. $W(x) = \psi_1 \psi_2' - \psi_2 \psi_1'$

We can show from Schrödinger eqn. $W'(x) = 0 \Rightarrow W(x) = \text{const w.r.to } x.$

$$\Rightarrow W(x) = W(x+a).$$

$\Downarrow$

We can show.

$$\boxed{\lambda_1 \lambda_2 = 1}$$

Suppose $|\lambda| > 1 \Rightarrow$ Say. $|\lambda| = 5$,

$$\psi(x+a) = 5\,\psi(x).$$
$$\psi(x+2a) = 5\,\psi(x+a) = 5^2 \psi(x).$$
$$\vdots$$
$$\psi(x+na) = 5^n \psi(x).$$

Prob. of finding the free e^- at $P_x = |\psi\psi^*|_x$.

- - - - - - - - - - - $P_{x+2a} = |\psi\psi^*|_{x+2a}$

$$= (5^2)^2 |\psi\psi^*|_x.$$

If $|\lambda| > 1$. Prob. of finding the free e^- the monotonically increases as we go more inside the solid.

$P_{x+2a} > P_x$.

$P_{x+na} > P_{x+(n-1)a} > \cdots > P_x$

$\Rightarrow$ This is unphysical.

$\Downarrow$

$$|\lambda| \not> 1.$$

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If $|\lambda| < 1$ say $|\lambda| = \frac{1}{5}$.

$\Downarrow$

Pob. of finding the free e^- will monotonically decrease as we go further inside the solid.

$\Downarrow$

UNPHYSICAL

$\Downarrow$

$|\lambda| \cancel{<} 1$.

$\Downarrow$

$|\lambda| = 1$, $\lambda_1 \lambda_2 = 1$.

Best choise:

$$\lambda_{1,2} = e^{\pm i\theta}$$

$$\lambda_{1,2} = e^{\pm iKa}.$$

$\lambda_1 = e^{i\theta}$, $\lambda_2 = e^{-i\theta}$.

What is θ ?! • $[\theta] = [\text{Angle}] =$ dimensionless.

• θ ~~must~~ must be related to some kind of periodicity.

$\Downarrow$

$\theta \propto a \Rightarrow \theta = Ka$.

Const. of prop.

This is some kind of "WAVE VECTOR".

Capital K.

$[K] = \frac{1}{\text{Length}}$.

For a free particle ~~and~~ which is not under the influence of a periodic pot. $(V(x) = 0$ or const.$)$. The wave vector is denoted as 'k'

small 'k'.

$$\psi_1(x+a) = e^{iKa}\psi_1(x), \quad \psi_2(x+a) = e^{-iKa}\psi_2(x).$$

Bloch's Theorem (1 D).

for a periodic potention. $V(x+a) = V(x)$.

We can write $\psi(x+a) = e^{iKa}\psi(x)$.

and $\psi(x+na) = e^{iKna}\psi(x)$

Only when $\psi(x) = e^{iKx}\phi(x)$. where $\phi(x)$ is a periodic fn. with periodicity "a".

$$\phi(x+a) = \phi(x).$$

Demonstration that above statement is true.

Suppose, $\psi(x) = e^{iKx}\phi(x)$ with $\phi(x+a) = \phi(x)$.

$$\Rightarrow \psi(x+a) = e^{iK(x+a)}\phi(x+a).$$

$$= e^{iKa}\left[e^{iKx}\phi(x)\right].$$

$$= e^{iKa}\psi(x).$$

We call $\psi(x)$ as BLOCH WAVE FN.
and these free e^-'s as Bloch electrons.

We can show that there is a relm. between k and K.

k ↑ wave vector of a 'free' electron

K ↑ wave vector of a Bloch e^-

⇓

This relm. is call dispersion Relm.

$$k \longleftrightarrow K.$$

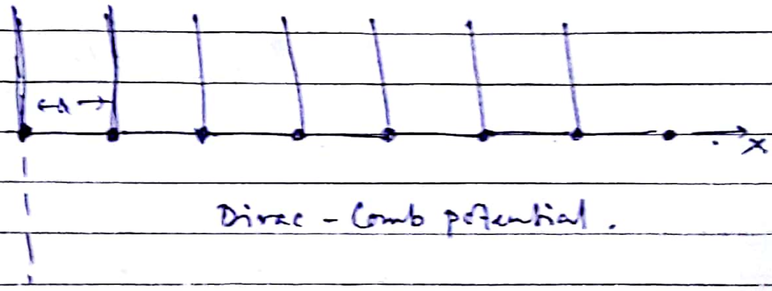
Kronig - Penney Model.

$$V(x) = \frac{\hbar^2}{m}\Omega\sum_{n=-\infty}^{+\infty} V_n(x)$$

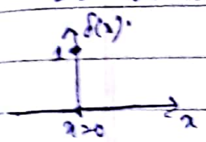
$\hbar, m, \Omega \to$ consts.

$$V_n(x) = \delta(x \pm na) = 1 \quad \text{when } x = \pm na.$$
$$= 0 \quad \text{otherwise.}$$

Dirac delta fn.



$\delta(x) = 1$ when $x=0$.
$= 0$ when $x \neq 0$.



Dirac - Comb potential.

$\Downarrow$

Using this potential in Schrödinger eqn we get the dispersion reln. as follows:

$$\cos Ka = \cos ka + \frac{\Omega}{k}\sin ka.$$

$$|\cos Ka| \leq 1 \Rightarrow \left|1\cdot\cos ka + \frac{\Omega}{k}\sin ka\right| \leq 1.$$

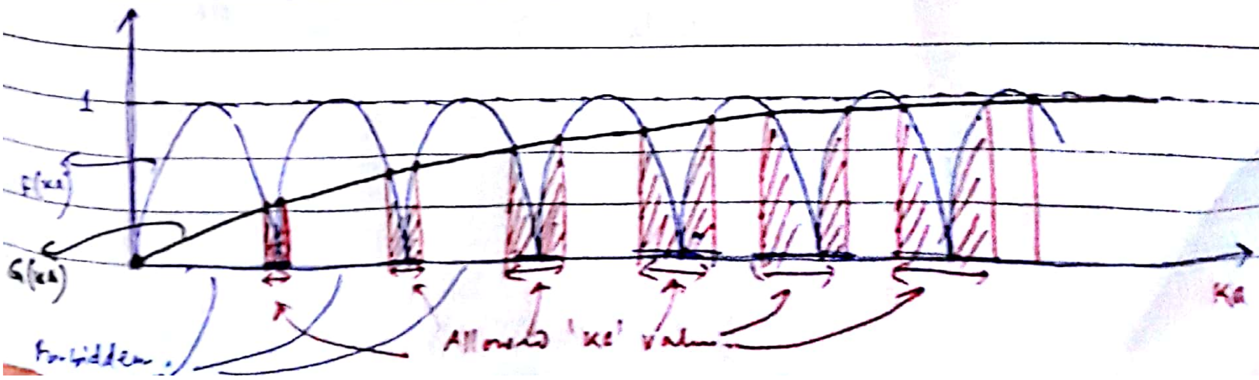
$\Downarrow$ Restriction on the value of 'k'.

say, $1 = \xi\cos\gamma$, $\frac{\Omega}{k} = \xi\sin\gamma$ $\quad \xi = \sqrt{1+\left(\frac{\Omega a}{ka}\right)^2}$, $\gamma = \tan^{-1}\left(\frac{\Omega a}{ka}\right)$

$$|\xi\cos(ka-\gamma)| \leq 1.$$

$$\Rightarrow \left|\cos\left(ka - \tan^{-1}\left(\frac{\Omega a}{ka}\right)\right)\right| \leq \frac{1}{\left|\sqrt{1+\left(\frac{\Omega a}{ka}\right)^2}\right|}$$

$$\Rightarrow F(ka) \leq G(ka).$$



Effective Mass.

$f(x-x_0) = f(x_0) + \dots$

$E = E(k)$.

Using taylor series expn.

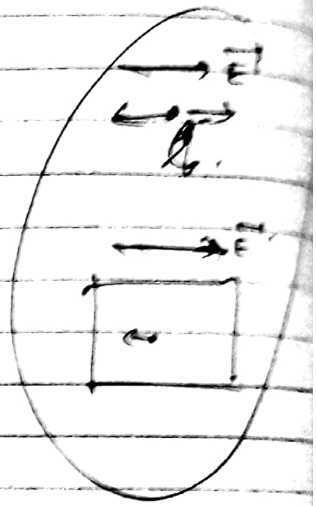
$$E(k) = E_0 + \left.\frac{\partial E}{\partial k}\right| k + \left.\frac{\partial^2 E}{\partial k^2}\right| \frac{k^2}{2} + \dots$$

$E(-k) = E(k)$ → energy of the e^- does not depend on the dirn of motion.

even fn. of 'k'

Const. adjust it to 0.

cannot be there.



$$E(K) = \frac{d^2E}{dk^2} \cdot \frac{k^2}{2} \longrightarrow (1)$$

For a free e^- we know

$$E(k) = \frac{\hbar^2 k^2}{2m} \longrightarrow (2)$$

Comparing (1) and (2) we get.

$$\frac{1}{2}\frac{d^2E}{dk^2} = \frac{\hbar^2}{2m}.$$

$$\Rightarrow \boxed{m^* = \frac{\hbar^2}{d^2E/dk^2}}$$

→ -ve ⇒ Hole.

→ +ve ⇒ electron.

Effective Mass.

Velocity of a free e^- inside a solid.

$$v_g = \frac{d\omega}{dk} = \frac{1}{\hbar}\frac{d(\hbar\omega)}{dk} = \frac{1}{\hbar}\frac{dE}{dk}$$

$$\boxed{v_g(k) = \frac{1}{\hbar}\frac{dE}{dk}.}$$

As $E(-k) = E(k)$.

$$\Rightarrow v_g(-k) = -v_g(k).$$

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Linear mom. of an e^- travelling along $\vec{k}$ dirn.

$$\vec{p} = m v_g(k)$$
$$= (-m)\{-v_g(k)\}.$$
$$= (-m)\, v_g(-k).$$

$\Rightarrow$ Motion of a particle with mass $(-m)$ travelling along $(-k)$ dirn

HOLE.

Current density. $\vec{j} = n e v_g(k)$.
$$= n(-e)\{-v_g(k)\}.$$
$$= n(-e)\, v_g(-k).$$

HOLE.