Bloch's Theorem

$$H\psi = \left(\frac{-\hbar^2}{2m}\nabla^2 + U(r)\right)\psi = \varepsilon\psi$$

$U(r) = U(r+R)$ for all R in Bravais lattice

$$T_R f(r) = f(r+R)$$

$$T_R H\psi = H(r+R)\psi(r+R) = H(r)\psi(r+R) = HT_R\psi$$

$\rightarrow [T_R, H] = 0 \quad \rightarrow \quad T_R\psi = c(R)\psi$ $\left\{\begin{array}{l}\text{simultaneous}\\ \text{eigenvalues}\end{array}\right.$

$$T_R T_{R'}\psi = T_{R'}T_R\psi = T_{R+R'}\psi$$

$$\rightarrow \quad c(R+R') = c(R)\,c(R')$$

$c(a_i) = e^{2\pi i x_i}$ {unitary

$$R = n_1 a_1 + n_2 a_2 + n_3 a_3$$

$$\rightarrow c(R) = c(a_1)^{n_1}\, c(a_2)^{n_2}\, c(a_3)^{n_3}$$

$$= e^{2\pi i(x_1 n_1 + x_2 n_2 + x_3 n_3)}$$

Define $k = x_1 b_1 + x_2 b_2 + x_3 b_3$.

$\rightarrow c(R) = e^{i\vec{k}\cdot\vec{R}}$ since $\vec{a}_i\cdot\vec{b}_j = 2\pi\delta_{ij}$

$\therefore$ Can choose eigenstates so that:

$$\boxed{T_R\psi = \psi(r+R) = e^{i\vec{k}\cdot\vec{R}}\psi(r)}$$

$$\boxed{u(r) = e^{-ik\cdot r}\psi(r) = u(r+R)}$$

Periodic boundary conditions:

$$\psi(r + N_i a_i) = \psi(r) \quad \text{for } i = 1,2,3.$$
N_i large

$$\rightarrow \psi(r + N_i a_i) = e^{iN_i \vec{k}\cdot\vec{a}_i}\, \psi(r)$$

$$\rightarrow e^{iN_i \vec{k}\cdot\vec{a}_i} = 1$$

$$\rightarrow e^{2\pi i N_i x_i} = 1$$

$$x_i = \frac{m_i}{N_i}$$

$$\vec{k} = \sum_{i=1}^{3} \left(\frac{m_i}{N_i} \vec{b}_i \right)$$

2nd proof:

$$\psi(r) = \sum_q c_q e^{iq\cdot r}$$ by periodic boundary condition

$$U(r) = \sum_K U_K e^{iK\cdot r}$$ by periodicity of lattice

$$U_K = \frac{1}{v} \int_{\text{cell}} d^3r\, e^{-iK\cdot r}\, U(r)$$

v: vol. unit cell

Take $U_0 = \frac{1}{v} \int_{\text{cell}} d^3r\, U(r) = 0$ w/out loss of generality

$U(r)$ real $\rightarrow U_K^* = U_{-K}$

If in addition we have inversion symmetry, $U(r) = U(-r)$, then $U_{-K} = U_K$.

$$\frac{p^2}{2m}\psi = \sum_q \frac{\hbar^2}{2m} q^2 C_q e^{iq\cdot r}$$

$$U\psi = \left(\sum_K U_K e^{iK\cdot r}\right)\left(\sum_q C_q e^{iq\cdot r}\right)$$

$$= \sum_{K,q} U_K C_q e^{i\underbrace{(K+q)}_{q'}\cdot r}$$

$$= \sum_{K,q'} U_K C_{q'-K} e^{iq'\cdot r}$$

dummy variables, summed over

$$\rightarrow \sum_q e^{iq\cdot r}\left\{\left(\frac{\hbar^2 q^2}{2m} - \varepsilon\right) C_q + \sum_{K'} U_{K'} C_{q-K'}\right\} = 0$$

$$\rightarrow \boxed{\left(\frac{\hbar^2 q^2}{2m} - \varepsilon\right) C_q + \sum_{K'} U_{K'} C_{q-K'} = 0}$$

Can write q as $k-K$, where k is in the first Brillouin zone.

$$\left(\frac{\hbar^2 (k-K)^2}{2m} - \varepsilon\right) C_{k-K} + \sum_{K'} U_{K'} C_{k-\underbrace{K-K'}} = 0$$

$$K' \rightarrow K' - K$$

$$K + K' \rightarrow K'$$

$$\boxed{\left(\frac{\hbar^2}{2m}(k-K)^2 - \varepsilon\right) C_{k-K} + \sum_{K'} U_{K'-K} C_{k-K'} = 0}$$

Note:

(i) Only $C_k, C_{k-K}, C_{k-K'}, \ldots$ coupled.

(ii) Thus, can take

$$\psi_k = \sum_K c_{k-K}\, e^{i(k-K)\cdot r}$$

$$= e^{ik\cdot r} \sum_K C_{k-K}\, e^{-iK\cdot r}$$

(iii) $u(r) = \sum_K C_{k-K}\, e^{-iK\cdot r}$ is periodic: $u(r) = u(r+R)$

$$\boxed{\psi(r) = e^{ik\cdot r} u(r)}$$

Remarks:

(i) k in 1st BZ. Multiple solutions for given k.
Denoted by n = band index. ψ_{nk}

(ii) $$\frac{\hbar}{i}\nabla \psi_{nk} = \frac{\hbar}{i}\nabla\left(e^{ik\cdot r} u_{nk}(r)\right)$$

$$= \hbar k\, \psi_{nk} + e^{ik\cdot r}\frac{\hbar}{i}\nabla u_{nk}(r)$$

$\hbar k$ is <u>not</u> momentum. Sometimes called crystal momentum.

(iii) k restricted to primative cell (usually 1st BZ).
Extended zone scheme:

$$\psi_{n,k+K}(r) = \psi_{nk}(r)$$

$$\varepsilon_{n,k+K} = \varepsilon_{nk} \leftarrow \text{Band structure}$$

(iv) Velocity:

$$\mathcal{E}_n(k+q) = \mathcal{E}_n(k) + \underbrace{\vec{\nabla}_k \mathcal{E}_n}_{\text{wish to evaluate}} \cdot \vec{q} + \text{higher order terms}$$

$$\frac{\hbar^2}{2m}(k-K)^2 C_{k-K} + \sum_{K'} U_{K'-K} C_{k-K'} = \mathcal{E}_k C_{k-K}$$

$$\frac{\hbar^2}{2m}(k+q-K)^2 C_{k+q-K} + \sum_{K'} U_{K'-K} C_{k+q-K'} = \mathcal{E}_{k+q} C_{k+q-K}$$

$$\Delta H = \text{perturbation} = \frac{\hbar^2}{2m}(k+q-K) - \frac{\hbar^2}{2m}(k-K)^2$$

$$= \frac{\hbar^2}{m} q \cdot (k-K)$$

$$\psi_k = e^{ik\cdot r} \sum_K C_{k-K} e^{-iK\cdot r}$$

$$\rightarrow \frac{\vec{\nabla}}{i}\psi_k = \sum_K (\vec{k}-\vec{K}) C_{k-K} e^{-iK\cdot r}$$

$$\rightarrow \Delta H = \frac{\hbar^2}{m}\vec{q}\cdot\frac{\vec{\nabla}}{i}$$

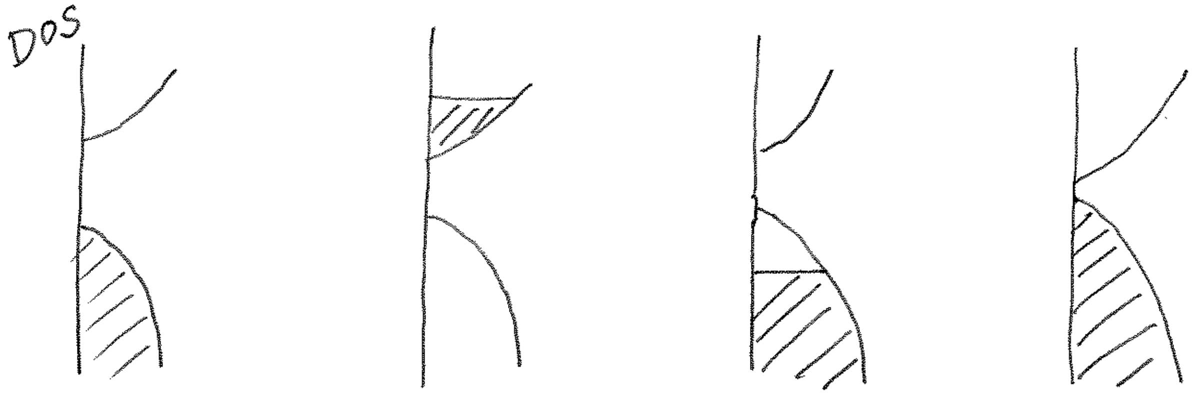
$$\rightarrow \Delta E = \mathcal{E}_n(k+q) - \mathcal{E}_n(k)$$

$$= \langle \psi_{nk} | \frac{\hbar^2}{m}\vec{q}\cdot\frac{\vec{\nabla}}{i} | \psi_{nk}\rangle$$

$$= \vec{q}\cdot\frac{\hbar^2}{m}\int d^3r\, \psi_{nk}^* \frac{\vec{\nabla}}{i}\psi_{nk}$$

$$\rightarrow \boxed{\frac{1}{\hbar}\vec{\nabla}_k \mathcal{E}_n(k) = \frac{\hbar}{m}\int d^3r\, \psi_{nk}^* \frac{\vec{\nabla}}{i}\psi_{nk} = \vec{v}_{nk}}$$ mean velocity

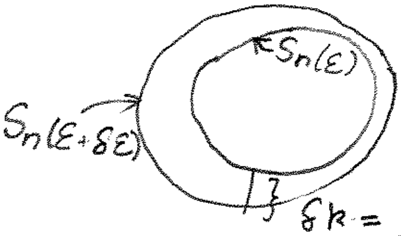
Fermi surface: $E = \varepsilon_F$ = boundary between occupied and empty @ $T=0$



insulator   metal   metal   Semiconductor

Definition:
$$\boxed{g_n(\varepsilon) = 2\int_{\text{cell}} \frac{d^3k}{(2\pi)^3}\,\delta(\varepsilon - \varepsilon_k)}$$

$$g(\varepsilon) = \sum_n g_n(\varepsilon)$$



$$\delta k = \frac{\delta\varepsilon}{|\nabla_k \varepsilon_n|}$$

$$g_n(\varepsilon)\,\delta\varepsilon = \int_{S_n(\varepsilon)} \frac{dS}{4\pi^3}\,\delta k$$

$$\rightarrow \boxed{g_n(\varepsilon) = \int_{S_n(\varepsilon)} \frac{dS}{4\pi^3}\,\frac{1}{|\nabla \varepsilon_n(k)|}}$$

Because $\varepsilon_n(k)$ is period, there are points where $\vec{\nabla}\varepsilon = 0$. Integrable in 3D.