LECTURE 13

Note Title 2/10/2010

$$\left(-\frac{\hbar\nabla^2}{2m_e} + V(\vec{r})\right)\psi_e(\vec{r}) = E\,\psi_e(\vec{r}) \qquad (\mathrm{I})$$

$$\underline{V(\vec{r}) = V(\vec{r}+\vec{R}_i)} \qquad \forall\, R_i \text{ IN A BRAVAIS LATTICE} \qquad (\mathrm{II})$$

<u>BLOCH THEOREM</u> : SOLUTION OF PROBLEM (I) WITH V SATISFYING (II) HAS ALWAYS THE FORM

$$\boxed{\begin{aligned} \psi_{m\vec{k}}(\vec{r}) &= e^{i\vec{k}\cdot\vec{r}}\,\underline{u_{mk}}(\vec{r}) \\ u_{m\vec{k}}(\vec{r}+\vec{R}_i) &= u_{m\vec{k}}(\vec{r}) \quad \longrightarrow \text{ IS PERIODIC} \end{aligned}}$$

$\psi_{m\vec{k}}(\vec{r})$ IS NOT PERIODIC

$$\boxed{\psi_{m\vec{k}}(\vec{r}+\vec{R}_i) = e^{i\vec{k}\cdot\vec{R}_i}\,\psi_{m\vec{k}}(\vec{r})} \qquad \forall\ R_i$$

$\vec{k}$ QUANTUM # $\Longleftrightarrow$ HOW STATES TRANSFORMS UNDER TRANSLATIONS R_i IN THE LATTICE

FREE PARTICLE

$\forall r'$ IN SPACE

$$\psi_p(r+r') = e^{ip\cdot r'}\,\psi_p(r)$$

CONTINUOUS TRANSLATIONAL SYMMETRY

p LINEAR MOMENTUM

p GROUP REPRESENTATION

LATTICE

$$\psi_k(\vec{r}+\vec{R}_i) = \underbrace{e^{i\vec{k}\cdot\vec{R}_i}}\,\psi_k(\vec{r})$$

DISCRETE TRANSLATIONAL SYMMETRY (BRAVAIS)

$\underline{k \text{ CRYSTAL MOMENTUM}}$ $\neq$ LINEAR MOMENTUM OF ELECTRON.

POSSIBLE VALUES OF $\vec{k}$!

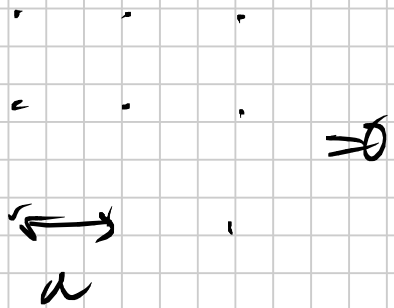
SEE WHAT HAPPEN $\vec{k} \rightarrow \vec{k} + \vec{G}$

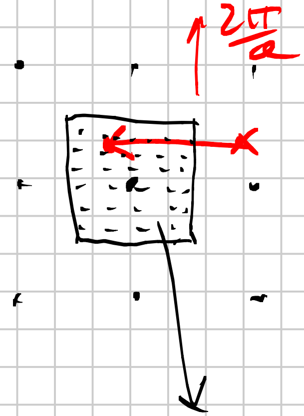
$\vec{G}$ IS A VECTOR OF THE RECIPROCAL LATTICE

$$\psi_{\vec{k}+\vec{G}}(\vec{u} + \vec{R}_i) = e^{i(\vec{k}+\vec{G})\cdot\vec{R}_i}\,\psi_{\vec{k}+\vec{G}}(\vec{u}) \qquad e^{iG\cdot R_i} = 1$$

$$= e^{ik\cdot\vec{R}_i}\,\psi_{\vec{k}+\vec{G}}(\vec{u})$$

$\vec{k}$ AND $\vec{k}+\vec{G}$ REPRESENT THE SAME QUANTUM NUMBER





$\updownarrow \frac{2\pi}{a}$

$$\boxed{\vec{p} = \vec{K}_i} + \vec{G}_i$$

K POSSIBLE

$$\psi(\vec{r}) = e^{ik\cdot r} u_k(r)$$

$$\downarrow$$

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V(r)\right)\psi = E\psi$$

$$\downarrow$$

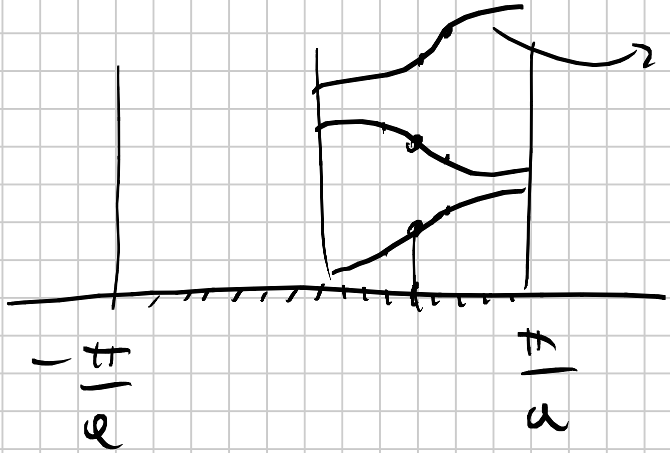
$$\left[\frac{\hbar^2}{2m}\left(-i\nabla + k\right)^2 + V(r)\right] u_k(r) = E(k)\, u_k(r)$$

$$p = -i\vec{\nabla}$$

$$-i\nabla e^{ik\cdot r} u_n(r) = k\psi \underbrace{- i e^{ik\cdot r} \nabla u_n(r)}$$

$$-i\nabla \psi_p(\vec{r}) = p\psi$$

FIX K $\rightarrow$ $u_{nk}(\vec{r})$ $\nearrow$ FUNCTION $\quad E_n(k)$ $\nearrow$ EVALUES



$E(k)$ ENERGY BANDS

GROUP VELOCITY $\qquad \vec{v}_g = -\frac{1}{\hbar}\frac{\partial E_n(k)}{\partial \vec{k}}$

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m} \to \frac{1}{m} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon(k)}{dk^2}$$

$$\left(\frac{1}{m}\right)_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon(\vec{k})}{\partial k_i \partial k_j} \qquad i \in \{x, y, z\}$$

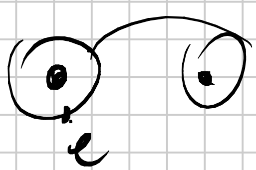
HOW DO WE FIND $\varepsilon_n(k)$ $\psi_{nk}(\vec{r})$?

① NEARLY-FREE ELECTRONS (CHAPT 9)

SOMMERFELD MODEL + V_{ION} WEAK

$\Rightarrow$ PERTURBATION THEORY

② TIGHT BINDING METHOD



START FROM COMPLETELY LOCALIZED ELECTRONS + HOPPING

PERTURBATION THEORY

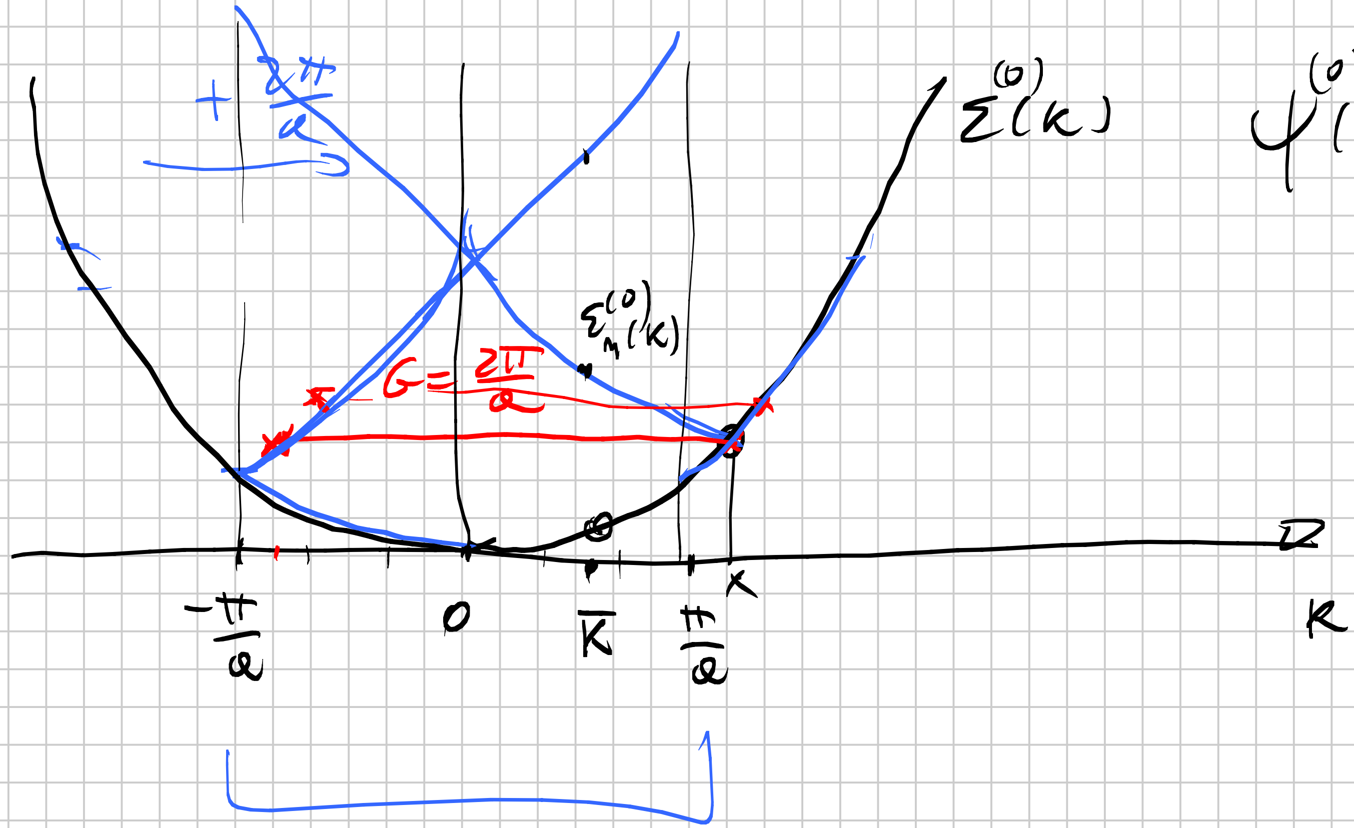
$$\psi_k^{(0)} = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} \qquad \varepsilon^0(k) = \frac{\hbar^2 k^2}{2m}$$

BAND FOLDING

1D MODEL

$$\psi^{(0)}(k) = \frac{1}{\sqrt{L}} e^{ikx}$$

L SIZE 1D CRYSTAL



FIX $\bar{k}$ $\psi^{(0)}(\bar{k})$ NON DEGENERATE $\varepsilon(\bar{k})$

$$\Delta \varepsilon^{(1)}_{\bar{k}} = \langle \psi^{(0)}(\bar{k}) | V | \psi^{(0)}(\bar{k}) \rangle = \frac{1}{L} \int dx \, \cancel{e^{-ikx}} V(x) \cancel{e^{ikx}}$$

$$\Delta \varepsilon^{(2)}_{\bar{k}} = \sum_{k'} \frac{\langle \psi^{(0)}_{\bar{k}} | V | \psi^{(0)}_{k'} \rangle \langle \psi^{(0)}_{k'} | V | \psi^{(0)}_{\bar{k}} \rangle}{\varepsilon^{(0)}_{\bar{k}} - \varepsilon^{(0)}_{k'}}$$

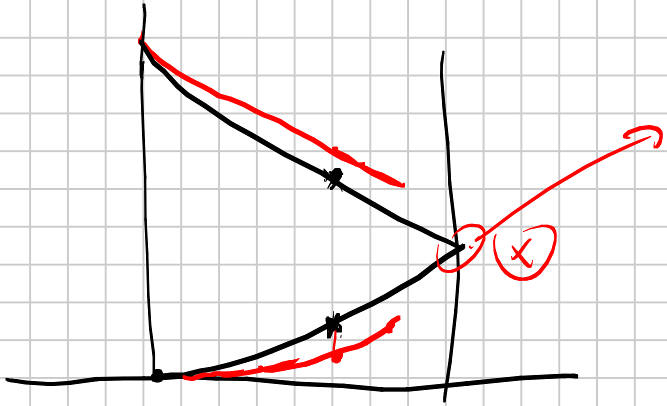
$$\langle \psi^{(0)}_{\bar{k}} | V | \psi^{(0)}_{k'} \rangle = \frac{1}{L} \int e^{i(\bar{k}-k')x} V(x)\, dx \to \tilde{V}(\bar{k}-k')$$

FOURIER TRANFORM OF V

V IS PERIODIC $\tilde{V} \neq 0$ ONLY IF

$\vec{k} - \vec{k}'$ IS $\vec{G}_m$ A REC LATTICE VECTOR

$$\Delta \varepsilon^2 = \sum_{\vec{G}_m \neq 0} \frac{|\tilde{V}(G_m)|^2}{\varepsilon^{(0)}_{\bar{k}} - \varepsilon^{0}_{\bar{k}+\vec{G}_m}}$$



DEGENERATE PERTURBATION THEORY