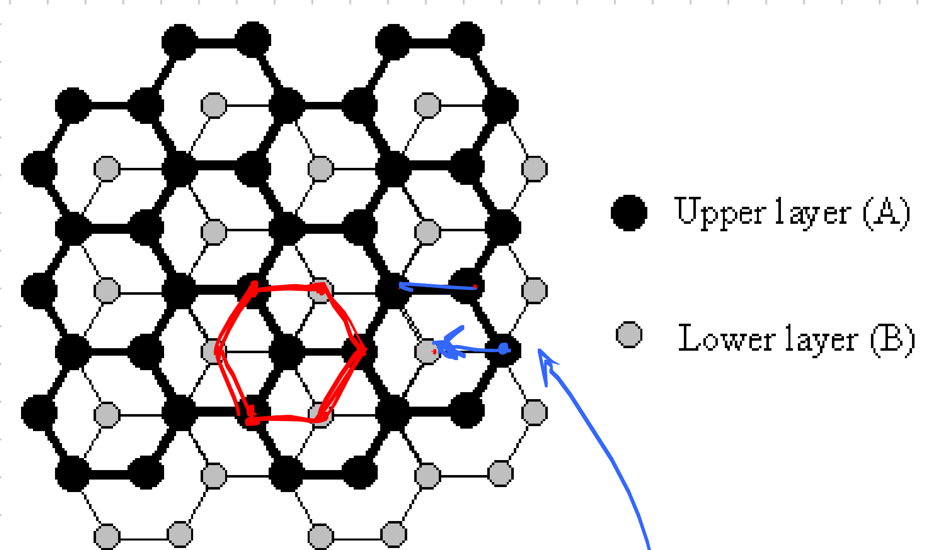
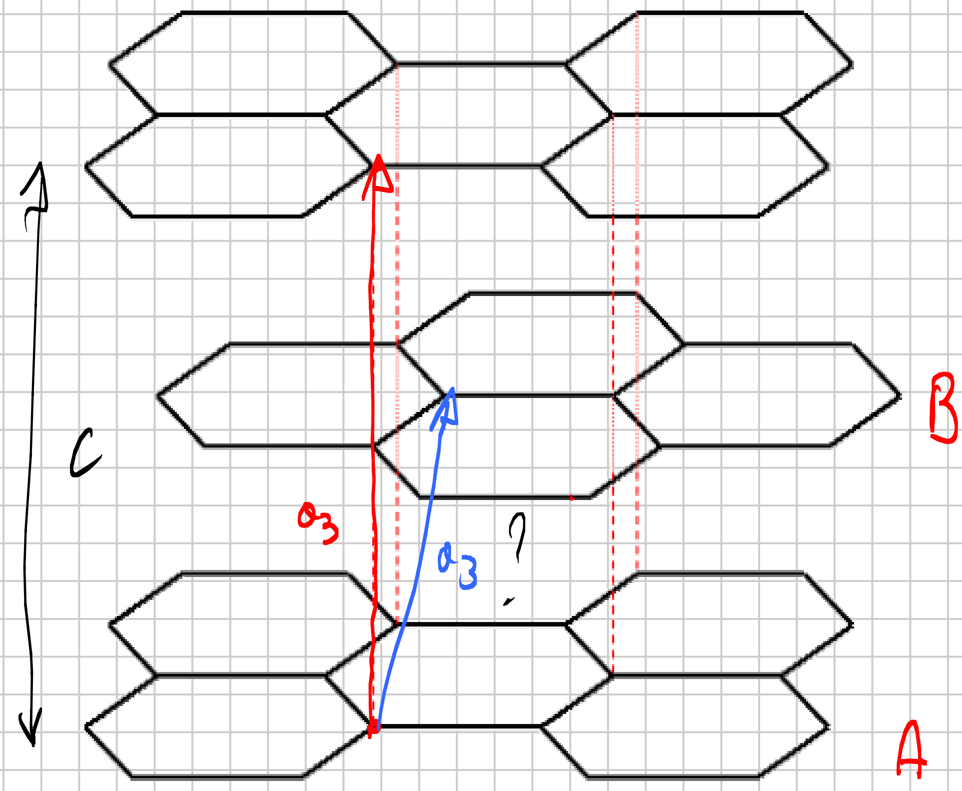
LECTURE # 15

Note Title 2/16/2009





I CAN SUPERPOSE A → B

BY THE SHIFT ←

HOWEVER, IF I APPLY ←

AGAIN I DO NOT OBTAIN

A (I OBTAIN THE RED LATTICE) ⇒ $\vec{a}_3 = c\,\hat{z}$

INDEPENDENT ELECTRONS

ION POTENTIAL $V(\vec{r})$ $V(\vec{r}+\vec{R}_i) = V(\vec{r}) \quad \forall \vec{R}_i$

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

SYMMETRY UNDER TRANSLATIONS R_i $\Longleftrightarrow$ QUANTUM # CRYSTAL MOMENTUM k

BLOCH THEOREM

$$\boxed{\psi_k(\vec{r}+\vec{R}_i) = e^{ik\cdot R_i}\,\psi_k(\vec{r})}$$

$$\psi_k(\vec{r}) = e^{ik\cdot r}\,u_k(\vec{r}) \qquad u_k(\vec{r}) = u_k(\vec{r}+\vec{R}_i)$$

u_k PERIODIC

WHAT ARE POSSIBLE VALUES FOR K

$\vec{K} \longrightarrow \vec{K} + \vec{G}$ $\quad$ $\vec{G}$ IS A VECTOR OF THE RECIPROCAL LATTICE

$$\psi_{\underbrace{\vec{K}+\vec{G}}}(\vec{r}+\vec{R}_i) = e^{i(\vec{K}+\vec{G})\cdot\vec{R}_i}\,\psi_{\vec{K}+\vec{G}}(\vec{r}) = \quad (e^{iG\cdot R_i} = 1)$$

$$e^{ik\cdot R_i}\,\psi_{\vec{K}+\vec{G}}(\vec{r})$$

ψ_k

ψ_{k+G}

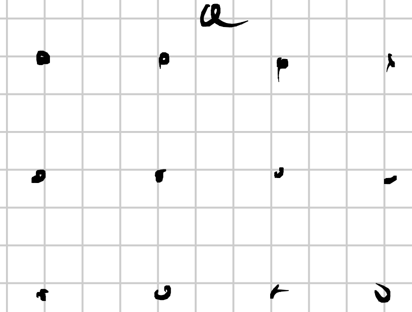
$\downarrow$

SAME PHASE AS FOR QUANNM # K

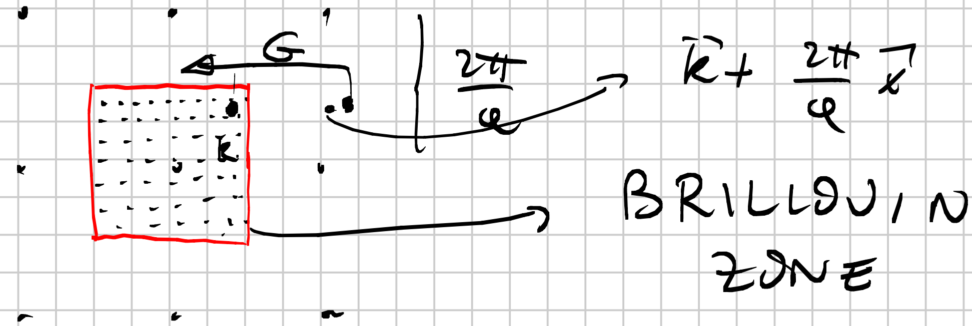
$\Downarrow$

K AND K + G REPRESENT THE **SAME** STATE

REAL



K SPACE



$$\psi(\vec{r}) = e^{ik\cdot r} u_k(r) \longrightarrow \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right)\psi(\vec{r}) = E\,\psi(\vec{r})$$

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

FIX $k \longrightarrow u_n(k)\,,\; E_n(k)$

ELECTRONIC BANDS

GROUP VELOCITY FOR ψ_{mk}

$$\vec{v}_g = -\frac{1}{\hbar} \frac{\partial E_m(\vec{k})}{\partial \vec{k}}$$

$$\boxed{\varepsilon(k) = \frac{\hbar^2 k^2}{2m}}$$ FREE

EFFECTIVE MASS

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

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

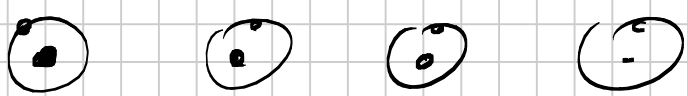
HOW DO WE FIND $\varepsilon_n(k)$ $u_{nk}(\vec{r})$?

TWO SIMPLE APPROACHES

1. NEARLY FREE ELECTRONS

   SOMMERFELD + V_{ION} WEAK $\Rightarrow$ PERTURBATION THEORY ON V

2. TIGHT - BINDING METHOD

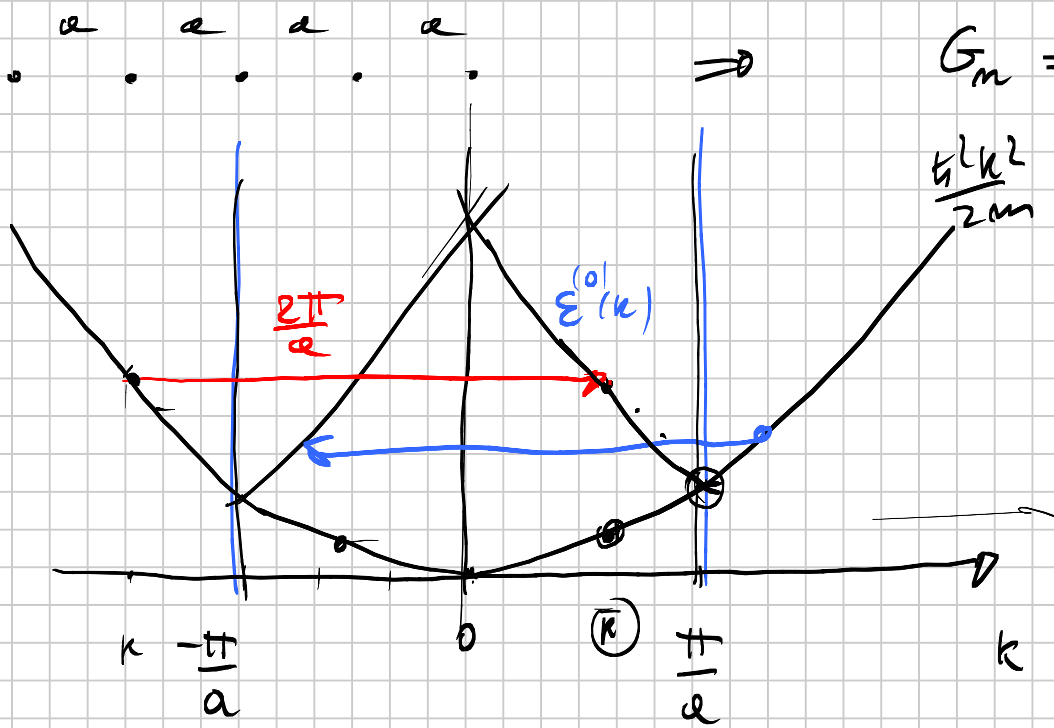


COMPLETELY LOCALIZED BASIS + HOPPING TERM

① PERTURBATION THEORY OF V

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

BAND FOLDING



$$\Rightarrow G_m = \frac{2\pi}{a} m$$

$$\frac{\hbar^2 \bar{k}^2}{2m} \qquad \frac{e^{i\bar{k}x}}{\sqrt{L}}$$

k

APPLY PERTURBATION THEORY !

LOOK ONLY POSITIVE $\bar{k}$

STATES ARE NON-DEGENERATE

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

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

$\langle \psi^{(0)}_{\bar{k}} | V | \psi^{(0)}_{k'} \rangle \rightarrow$ FOURIER TRANSFORM OF $V(x)$

$$\frac{1}{L} \int e^{i(k'-\bar{k})x} \, V(x) \, dx = \tilde{V}(k'-\bar{k})$$

$V(x)$ IS PERIODIC $\Rightarrow$ $k' - \bar{k} = G_m$

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