Nearly free electron model

Periodic potential

$$U(\vec{r}) = \sum_{\vec{G}} U_{\vec{G}}\, e^{i\vec{G}\cdot\vec{r}}$$

$$H\Psi = \epsilon\Psi$$

$$\psi(\vec{r}) \Rightarrow \qquad \psi_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} C(\vec{k}-\vec{G})\, e^{i(\vec{k}-\vec{G})\cdot\vec{r}}$$

Bloch Theorem

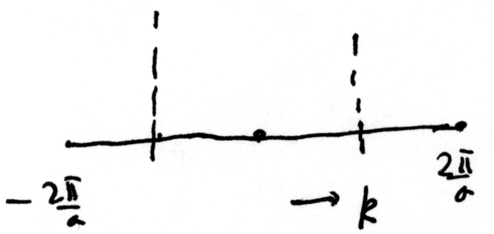
$$H = -\frac{\hbar^2}{2m}\nabla_r^2 + U(\vec{r})$$

$$\boxed{\Big(\underbrace{\frac{\hbar^2 k^2}{2m}}_{\lambda_{\vec{k}}} - \epsilon\Big) C(\vec{k}) + \sum_{\vec{G}} U_G\, C(\vec{k}-\vec{G}) = 0}$$

infinite # of Coeff. $C(\vec{k}-\vec{G})$

$$U_{\vec{G}} = \int U(\vec{r})\, e^{-i\vec{G}\cdot\vec{r}}\, dr$$

Apply to 1d $\qquad \vec{k} = k\hat{x}\ , \qquad \vec{G} = \frac{2\pi}{a}\nu\,\hat{x}$



$k \lesssim \frac{\pi}{a}$

$$\psi_k(x) = C(k)\, e^{ikx} + C(k-G)\, e^{i(k-G)x} \qquad G = \frac{2\pi}{a}$$

$$(\lambda_k - \epsilon)\, C(k) + U_G\, C(k-G) = 0$$

$$(\lambda_{k-G} - \epsilon)\, C(k-G) + U_G^*\, C(k) = 0$$

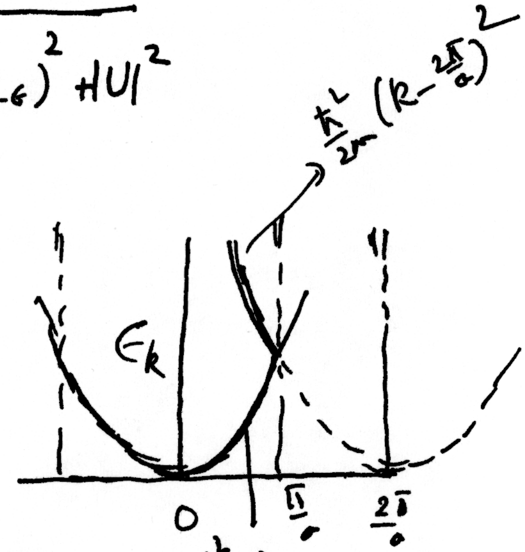
$$\det\begin{pmatrix} \lambda_k - \epsilon & U_G \\ U_G^* & \lambda_{k-G} - \epsilon \end{pmatrix} = 0 \qquad \text{~~For k~~}$$

$$\epsilon^2 - \epsilon(\lambda_k + \lambda_{k-G}) + \lambda_k\lambda_{k-G} - |U|^2 = 0$$

where $U_{G=2\pi/a} = U$

Two solutions

$$\epsilon_k^{\pm} = \frac{1}{2}\left(\lambda_k + \lambda_{k-G}\right) \pm \sqrt{\frac{1}{2}\left(\lambda_k - \lambda_{k-G}\right)^2 + |U|^2}$$



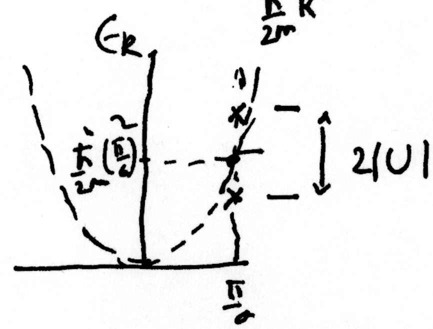
check: $|U| = 0$

$$\epsilon_k^{\pm} = \lambda_k\,,\ \lambda_{k-G}$$

$$= \frac{\hbar^2}{2m}k^2\,,\ \frac{\hbar^2}{2m}(k-G)^2$$

Check $k = \frac{\pi}{a}$ (BZ boundary)

$$\epsilon_k^{\pm} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 \pm |U|$$



What's ϵ_k for $k \lesssim \pi/a$

Define $\tilde{k} = \frac{\pi}{a} - k$, $\tilde{k}$ is small.

$$\lambda = \frac{\hbar^2}{2m}(\pi/a)^2$$

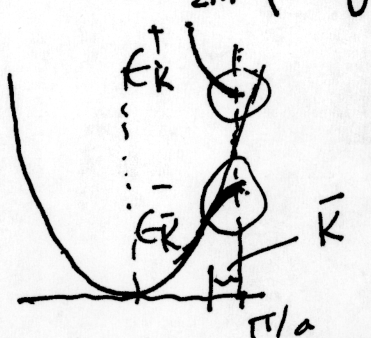
$$\epsilon_{\tilde{k}}^{\pm} = \lambda + \frac{\hbar^2}{2m}\tilde{k}^2 \pm U\left[1 + \frac{4\lambda}{U^2}\underbrace{\left(\frac{\hbar^2}{2m}\tilde{k}^2\right)}_{\text{small}}\right]^{\frac{1}{2}} \qquad |U| = U$$

$$\epsilon_{\tilde{k}}^{+} = \lambda + U + \frac{\hbar^2}{2m}\left(1 + \frac{\lambda}{U}\right)\hat{k}^2$$

$$\epsilon_{\tilde{k}}^{-} = \lambda - U + \frac{\hbar^2}{2m}\left(1 - \frac{\lambda}{U}\right)\hat{k}^2$$

$\lambda = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 > U$

weak potential



Parabolic

$\epsilon_{\hat{k}}^{+} \rightarrow$ positive mass

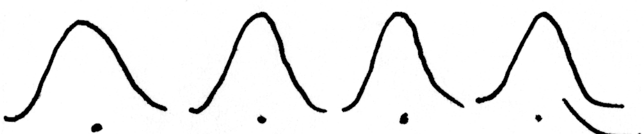
$\epsilon_{\hat{k}}^{-} \rightarrow$ negative mass

Tight binding model to get Band Structure $\epsilon_{\vec{k}}$

Chapter 9 Eqn. 4

$$H\psi = \epsilon\psi \quad , \quad H = \frac{p^2}{2m} + U(\vec{r})$$

Linear combination of atomic orbitals



$\phi(\vec{r}-\vec{r}_j)$

$\vec{r}_j \Rightarrow$ Direct lattice vectors.

$$\psi_{\vec{k}}(\vec{r}) = \sum_j C_{\vec{k},j}\,\phi(\vec{r}-\vec{r}_j)$$

$\downarrow$

Should be a Bloch function

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}}\sum_j e^{i\vec{k}\cdot\vec{r}_j}\,\phi(\vec{r}-\vec{r}_j)$$

$\checkmark$

check $\psi_{\vec{k}}(\vec{r}+\vec{T}) = \frac{1}{\sqrt{N}}\sum_j e^{i\vec{k}\cdot\vec{r}_j}\,\phi(\vec{r}+\vec{T}-\vec{r}_j)$

Define $\vec{r}_j - \vec{T} = \vec{r}_m$

$$= \frac{1}{\sqrt{N}}\sum_{\cancel{j}\,m} e^{i\vec{k}\cdot(\vec{T}+\vec{r}_m)}\,\phi(\vec{r}-\vec{r}_m)$$

$$= e^{i\vec{k}\cdot T}\frac{1}{\sqrt{N}}\sum_m e^{i\vec{k}\cdot\vec{r}_m}\,\phi(\vec{r}-\vec{r}_m)$$

$$= e^{i\vec{k}\cdot\vec{T}}\,\psi_{\vec{k}}(\vec{r})$$

$\checkmark$ Yes a true Bloch function.

$$\epsilon_{\vec{k}} = \frac{\langle \psi_{\vec{k}} | H | \psi_{\vec{k}} \rangle}{\langle \psi_{\vec{k}} | \psi_{\vec{k}} \rangle}$$

Slightly different from the book.

$$\langle \psi_{\vec{k}} | \psi_{\vec{k}} \rangle = \int dv \, \frac{1}{N} \sum_j \sum_m e^{-i\vec{k}\cdot\vec{r}_j} e^{i\vec{k}\cdot\vec{r}_m} \langle \varphi(\vec{r}-\vec{r}_j) | \phi(\vec{r}-\vec{r}_m) \rangle$$

$$= \frac{1}{N} \sum_j \int dv \langle \varphi(\vec{r}-\vec{r}_j) | \varphi(\vec{r}-\vec{r}_j) \rangle + \frac{1}{N} \sum_{j \neq m} e^{-i\vec{k}\cdot(\vec{r}_j - \vec{r}_m)} \langle \varphi(\vec{r}-\vec{r}_j) | \varphi(\vec{r}-\vec{r}_m) \rangle$$

only nn overlap S

$$\boxed{\langle \psi_{\vec{k}} | \psi_{k} \rangle = 1 + S \sum_{j\,(nn)\text{ of a chosen origin}} e^{-i\vec{k}\cdot\vec{r}_j}}$$

Book uses $S = 0$

$$\langle \psi_{\vec{k}} | H | \psi_{\vec{k}} \rangle = \frac{1}{N} \sum_j \sum_m \int dv \, e^{-i\vec{k}\cdot\vec{r}_j} e^{i\vec{k}\cdot\vec{r}_m} \langle \varphi(\vec{r}-\vec{r}_j) | H | \phi(\vec{r}-\vec{r}_m) \rangle$$

nn

$$= \frac{1}{N} \sum_j \langle \varphi(\vec{r}-\vec{r}_j) H \phi(\vec{r}-\vec{r}_j) \rangle + \frac{1}{N} \sum_{\substack{j \neq m \\ (nn)}} e^{i\vec{k}\cdot(\vec{r}_m - \vec{r}_j)} \langle \quad \rangle$$

$$= -\alpha - \gamma \sum_{m(nn)} e^{-i\vec{k}\cdot\vec{r}_m}$$

$$\alpha = -\langle \varphi(\vec{r}) | H | \varphi(\vec{r}) \rangle$$

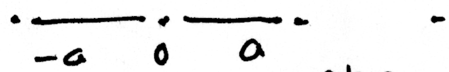
$$\gamma = -\langle \varphi(\vec{r}) | H | \varphi(\vec{r}-\vec{r}_m) \rangle$$

nn

$$\therefore \boxed{\epsilon_{\vec{k}} = \frac{-\alpha - \gamma \sum_{m(nn)} e^{-i\vec{k}\cdot\vec{r}_m}}{1 + S \sum_{m(nn)} e^{-i\vec{k}\cdot\vec{r}_m}}}$$

$s = 0$

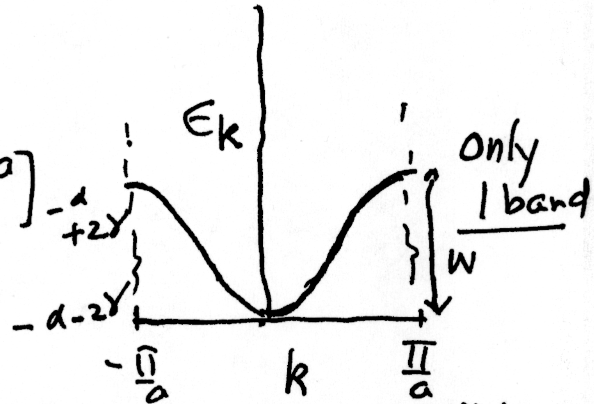
1d:



$$\epsilon_k = -\alpha - \gamma \sum_{m(nn)} e^{-ikr_m}$$

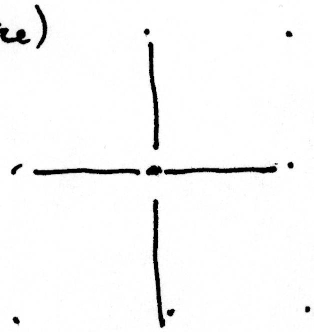
$$= -\alpha - \gamma\left[e^{-ika} + e^{+ika}\right]$$

$$\boxed{\epsilon_k = -\alpha - 2\gamma \cos ka}$$



W = Band width $= 4\gamma$

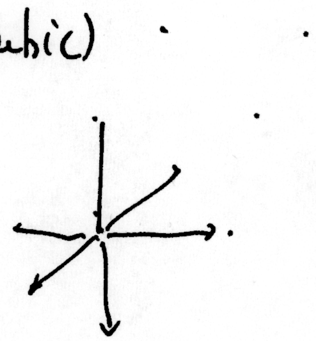
2d (square)



$$\epsilon_{k_x,k_y} = -\alpha - \gamma\left[e^{-ik_xa} + e^{+ik_xa} + e^{-ik_ya} + e^{+ik_ya}\right]$$

$$\epsilon_{\vec{k}} \equiv = -\alpha - 2\gamma\left[\cos k_xa + \cos k_ya\right]$$

3d (cubic)



$$\epsilon_{\vec{k}} \equiv \epsilon_{k_x,k_y,k_z} = -\alpha - 2\gamma\left[\cos k_xa + \cos k_ya + \cos k_za\right]$$

$$\boxed{\begin{aligned} W &= 2\gamma \times \#\text{ of nearest neighbors} \\ &= 2\gamma z \end{aligned}}$$