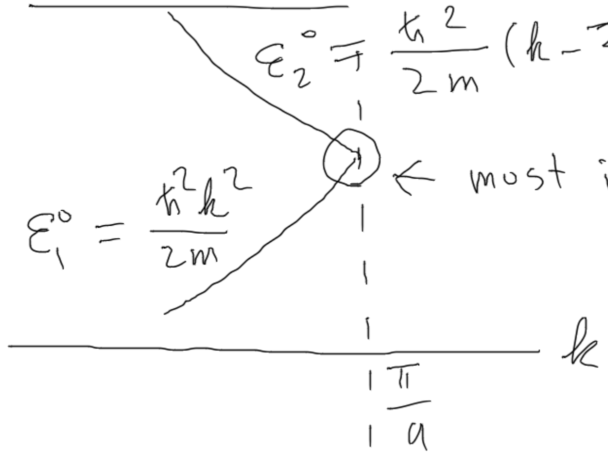
BARE BONE NEARLY FREE ELECTRON BAND



← most important when crystal pot. is small (nearly free e^-)

More generally $\quad \varepsilon_1^\circ = \frac{\hbar^2}{2m}\vec{k}^2$

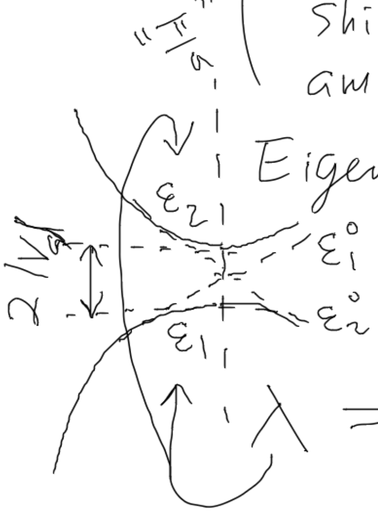
$$\varepsilon_2^\circ = \frac{\hbar^2}{2m}\left(\vec{k} - \vec{G}\right)^2$$

Zone boundary $\quad |\vec{k}| = |\vec{k} - \vec{G}|$

Unperturbed states $\quad |\vec{k}\rangle$ and $|\vec{k} - \vec{G}\rangle$

Relevant pot $\quad V_{\vec{G}} \sim \int d\vec{x}\, V(\vec{x})\, e^{-i\vec{G}\cdot\vec{x}}$

(Also $V_0 \sim \int d\vec{x}\, V(\vec{x}) \longrightarrow$ But this simply shifts energies $\varepsilon_1^\circ, \varepsilon_2^\circ$ by the same amount --- just a constant)



Eigenvalue prob. $\quad \begin{vmatrix} \varepsilon_1^\circ - \lambda & V_{\vec{G}}^{*} \\ V_{\vec{G}} & \varepsilon_2^\circ - \lambda \end{vmatrix} = 0$

$$\lambda = \frac{\varepsilon_1^\circ + \varepsilon_2^\circ}{2} \pm \frac{1}{2}\sqrt{\left(\varepsilon_1^\circ - \varepsilon_2^\circ\right)^2 + 4|V_{\vec{G}}|^2}$$

$\Rightarrow$ group velocity, FS distortion, standing wave, effective mass in semi-conductor ...

BARE BONE TIGHT BINDING

Hydrogen 1S in 1D

$H = T + V$ $\quad$ V: periodic pot.

$|\psi\rangle = \sum_n e^{ikna} |n\rangle$

$\langle n|H|n\rangle \equiv \varepsilon$ $\quad$ (throw in atomic energy -2β and so on)

$\langle m|H|n\rangle = -t$ if $m-n = \pm 1$

(keep nearest neighbor only)

t is called a "hopping" matrix element

$\langle m|n\rangle = \delta_{mn}$ $\quad$ (somewhat of a over-simplification but an often-used approx)

$H|\psi\rangle = \varepsilon_k |\psi\rangle$

$\Downarrow$

$\langle m|H|\psi\rangle \Rightarrow e^{ikna}\varepsilon_k$

$$\varepsilon_k = \varepsilon - 2t \cos ka$$

If $t \to 0$, ε_k becomes flat

$m^* \to \infty$

$t \to \infty$, ε_k becomos very wide

$m^* \to 0$

ease of hopping or hopping probability or tunneling probability