Lecture #15

Note Title 10/29/2007

Electronic states in periodic potential V_i ψ_{nk}

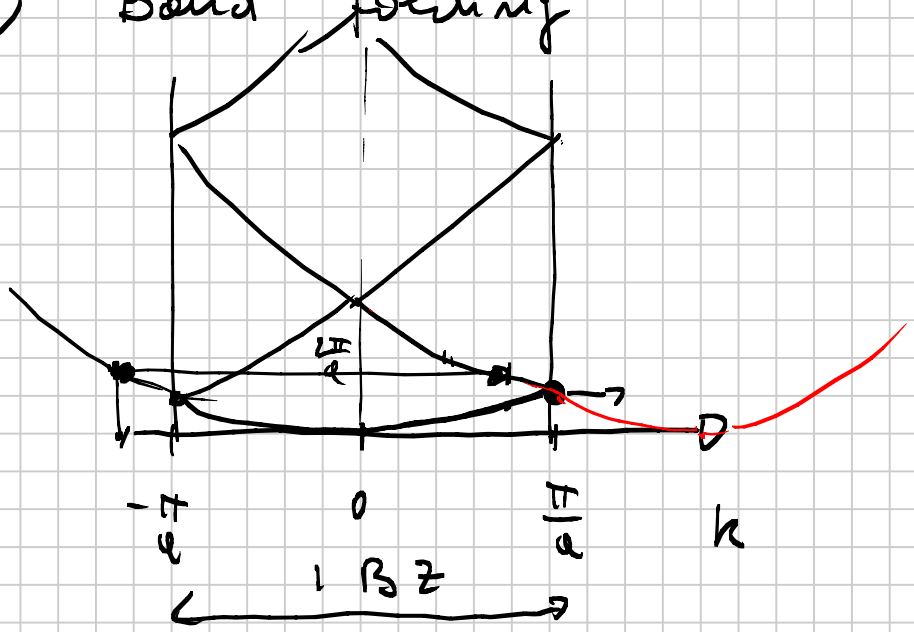
① $\vec{k}$ Crystal momentum good quantum #

② $\psi_{\vec{k}}$, $\psi_{\vec{k}+\vec{K}}$ same state

③ $E(\vec{k}) = E(\vec{k}+\vec{K})$ $\forall \vec{K}$

Energy is periodic in k space
Periodicity by Reciprocal Lattice

④ Band folding



$$E(k) = \frac{\hbar^2 k^2}{2m}$$

$$\boxed{V_i = 0}$$

V_1 small

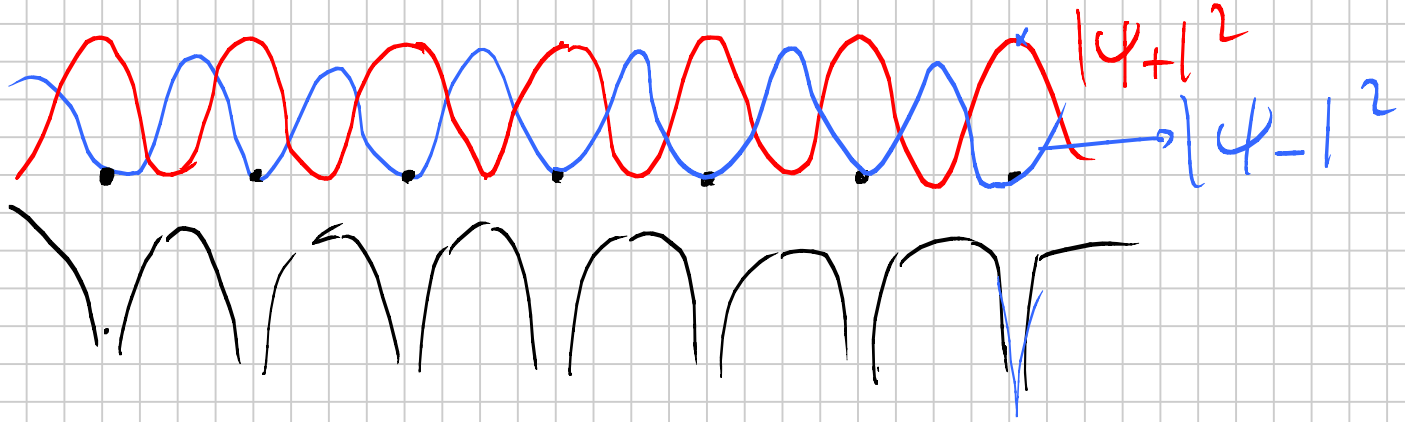
What happens at $k = \frac{\pi}{a}$ Degeneracy 2

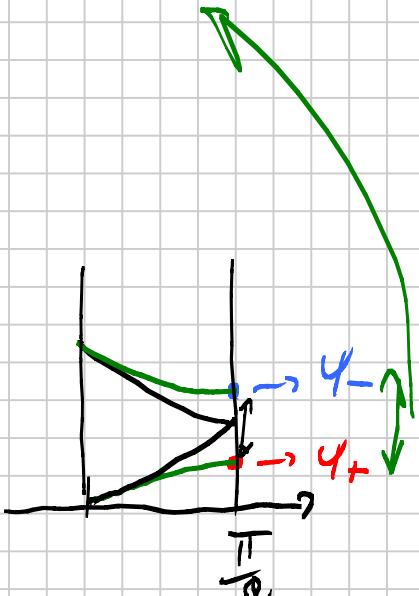
$$\psi_1 = e^{ikx} \text{ with } k = \frac{\pi}{a} \Rightarrow \psi_1 = e^{i\frac{\pi}{a}x}$$

$$\psi_2 = e^{i\left(k-\frac{2\pi}{a}\right)\cdot x} \text{ with } k = \frac{\pi}{a} \Rightarrow \psi_2 = e^{-i\frac{\pi}{a}x}$$

$$\psi_+ = \psi_1 + \psi_2 = e^{i\frac{\pi}{a}x} + e^{-i\frac{\pi}{a}x} \rightarrow \sim \cos\frac{\pi}{a}x$$

$$\psi_- = \psi_1 - \psi_2 = e^{i\frac{\pi}{a}x} - e^{-i\frac{\pi}{a}x} \rightarrow \sim \sin\frac{\pi}{a}x$$





How big is E_{gap}?

$\psi_1 = e^{i\frac{\pi}{a}x}$ $\quad\quad$ $\langle\psi_1|V_i|\psi_1\rangle$

$\psi_2 = e^{-i\frac{\pi}{a}x}$

Degenerate perturbation theory

V_i: small perturbation

Diagonalize a 2×2 matrix

$$\begin{bmatrix} \langle\psi_1|V_i|\psi_1\rangle & \langle\psi_1|V_1|\psi_2\rangle \\ \langle\psi_2|V_i|\psi_1\rangle & \langle\psi_2|V_i|\psi_2\rangle \end{bmatrix} \rightarrow \begin{matrix} \Delta E_1 \\ \Delta E_2 \end{matrix}$$

From diagonalization

$$\langle\psi_1|V_i|\psi_1\rangle = \int dx\, \cancel{e^{-i\frac{\pi}{a}x}}\, V_i(x)\, \cancel{e^{i\frac{\pi}{a}x}} = \int dx\, V_i(x) = \overline{V}$$

$$\langle\psi_1|V_i|\psi_2\rangle = \int dx\, e^{-i\frac{\pi}{a}x}\, V_i(x)\, e^{-i\frac{\pi}{a}x} = \int dx\, V(x)\, e^{-i\frac{2\pi}{a}x} =$$

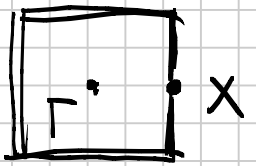
$\tilde{V}$ is the Fourier transform of $V_i(x)$

$$\langle \psi_1 | V_i | \psi_2 \rangle = \tilde{V}\left(k = \frac{2\pi}{a}\right)$$

$$\begin{bmatrix} \bar{V} & \tilde{V}\left(\frac{2\pi}{a}\right) \\ \tilde{V}\left(\frac{2\pi}{a}\right) & \bar{V} \end{bmatrix} \rightarrow \Delta\varepsilon = \bar{V} \pm \tilde{V}\left(\frac{2\pi}{a}\right)$$

$$E_{gap} = 2\,\tilde{V}\left(\frac{2\pi}{a}\right)$$

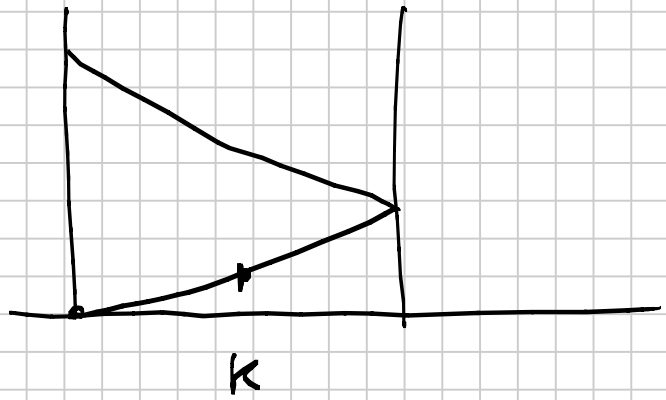
Same in 2D and 3D



$$E_{gap} \text{ at } (X) = \tilde{V}_i\left(k = \left(\frac{2\pi}{a}, 0\right)\right)$$

Strongest effects are at the Brillouin zone boundary

Brillouin zone boundary = Bragg planes



k non degenerate

$\psi_k \sim e^{ikx}$

① 1° order perturbation theory $\langle \psi_k | V_i | \psi_k \rangle = \varepsilon^{(1)}$

$$\int dx \; e^{-ikx} V_i(x) e^{ikx} = \bar{V} = \tilde{V}(0)$$

② 11° order perturbation theory

$$\varepsilon^{(2)} = \sum_{k'} \frac{\langle k | V_i | k' \rangle \langle k' | V_i | k \rangle}{\varepsilon(k) - \varepsilon(k')}$$

$V_i(x) = V_i(x+R)$ V_i is PERIODIC

$$V_i(x) = \sum_k e^{ikx}\,\tilde{V}_i(k)$$

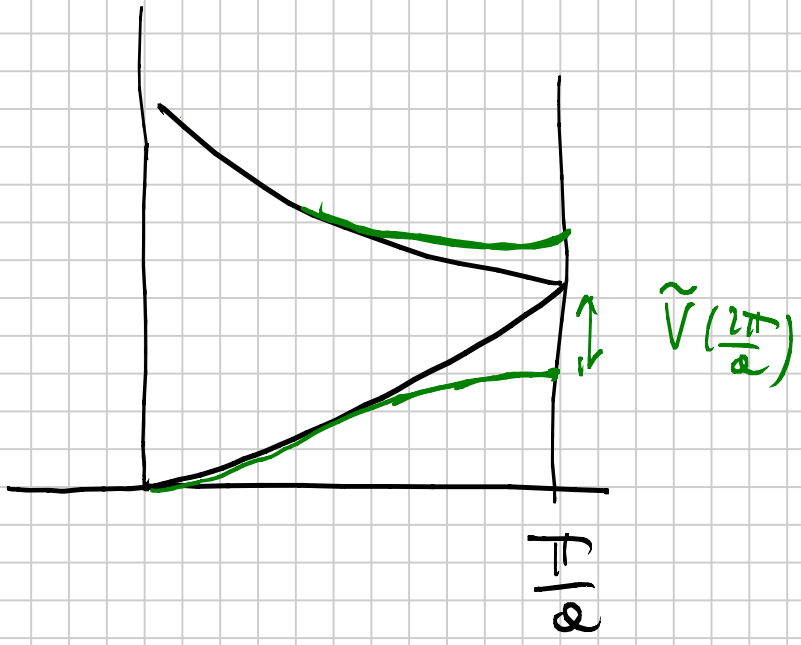
K HAS TO BE A RECIPROCAL LATTICE VECTOR

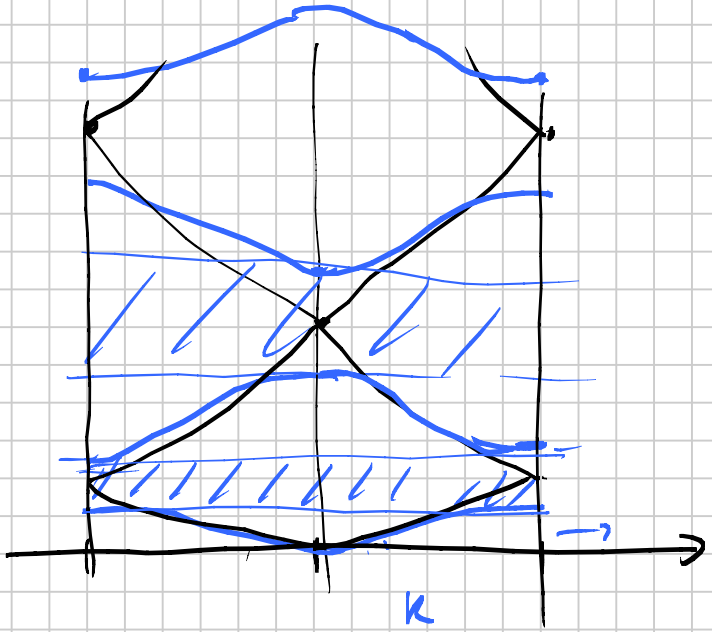
$$\Rightarrow V_i(x) = \sum_K e^{iK\cdot x}\,\tilde{V}(K_i)$$

$$V_i(x+R) \rightarrow e^{ikR}\,V(x)$$

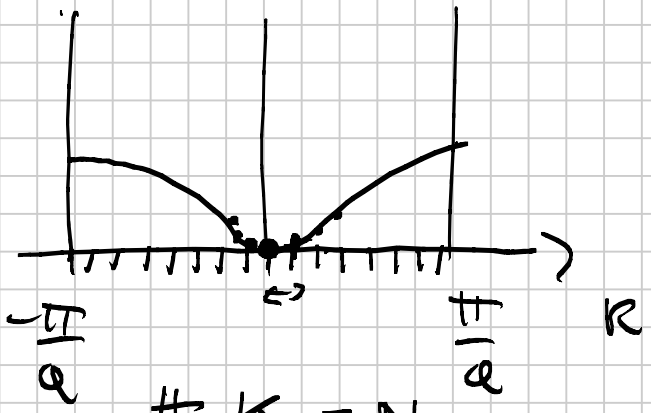
$$\varepsilon_k^{(2)} = \sum_K \frac{|\tilde{V}(K)|^2}{\varepsilon_k - \varepsilon_{k+K}}$$

$$|k| \sim |k+K|$$





N ions



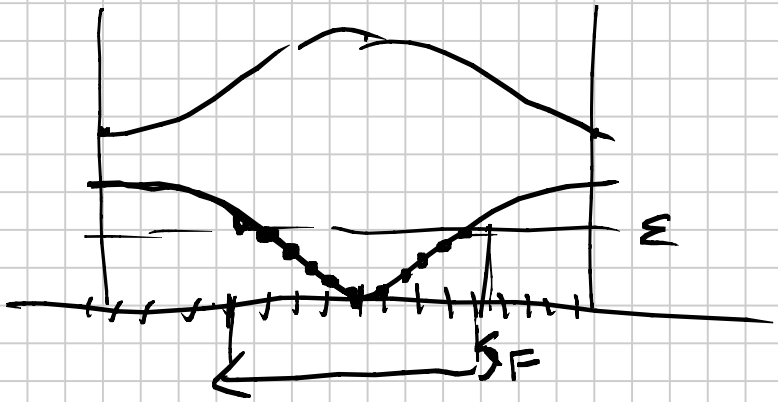
$\# K = N$

FIRST 2 electrons → $\vec{K}=0$

ADD 2 MORE $K = \frac{2\pi}{Na}$

Lattice of Hydrogen

H • • • • • • • • N sites



N K points

N electons

$\frac{N}{2}$ $\vec{K}$ points with $2\bar{e}$ each

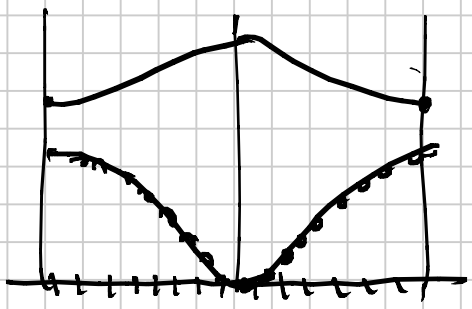
METAL BAND NOT FILLED

ε_F OF LAST FILLED STATE

FERMI ENERGY

K_F IS LAST K STATE OCCUPIED

He He He He He He



N R state

N sites

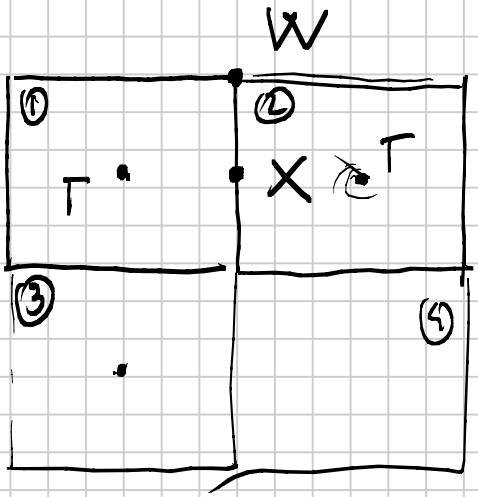
2N electrons

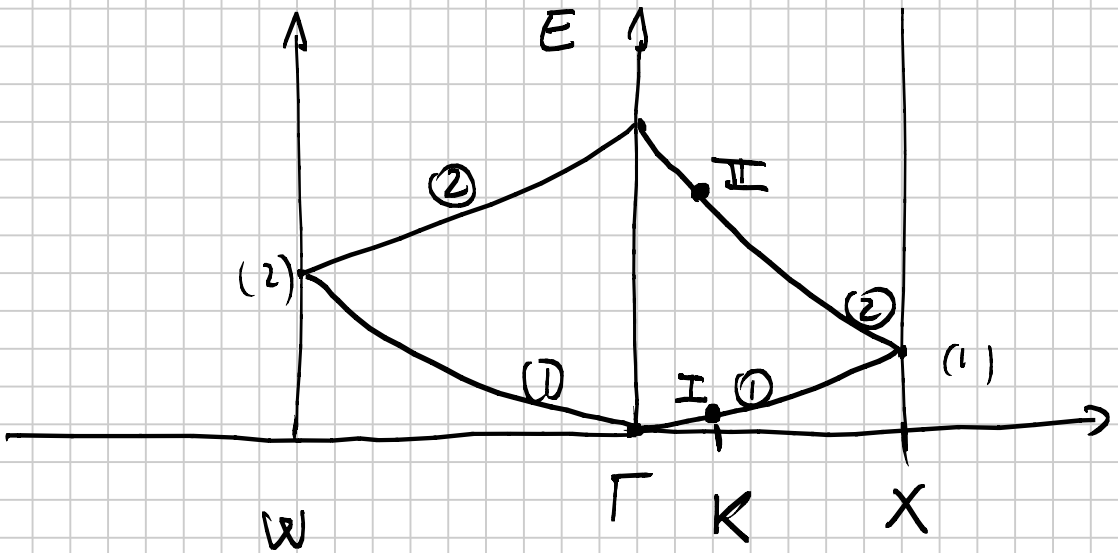
→ Insulator

Band completely filled

- Insulator $E_g > K_B T$
- Semiconductor $E_g \sim K_B T$

Nearly free electrons in 2D





$$k = (.5\,\text{Å}^{-1}, 0)$$

ψ STATE I

ψ STATE II

$$\psi = e^{ik\cdot x}\, u(x,y)$$