LECTURE #18

Note Title 11/3/2008

CHAP 8 ALL

CHAPT 9 152 - 162

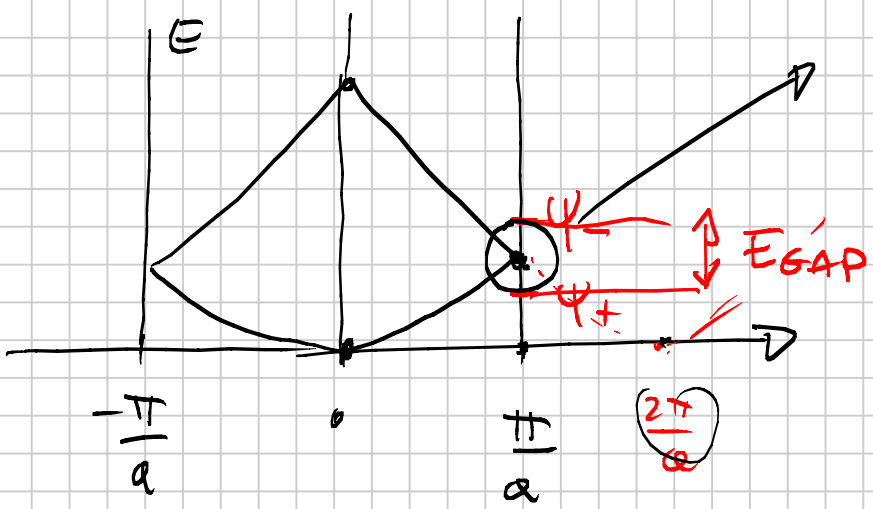
- ELECTRONS IN A WEAK PERIODIC POTENTIAL

(1) $V_{IONS} \sim 0$

(2) $E(k) \sim \frac{\hbar^2 k^2}{2m}$ (ENERGY ~ ENERGY FREE ELECTRON)

(3) $E(k) = E(k + K)$ PERIODIC IN THE RECIPROCAL LATTICE

(4) BAND FOLDING = REPRESENT ALL ELECTRONIC STATES IN THE FIRST BRILLOUIN ZONE

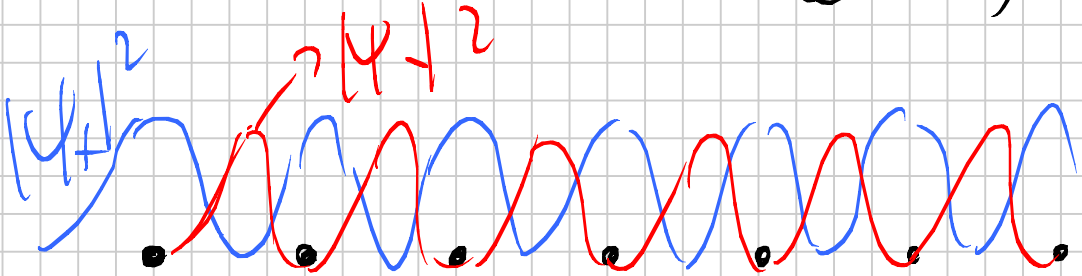


TWO DEGENERATE STATES

$$\psi_1 = e^{i\frac{\pi}{a}x}$$

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

$$\psi_+ = \psi_1 + \psi_2 \sim \cos\frac{\pi}{a}x \quad ; \quad \psi_- = \psi_1 - \psi_2 \sim \sin\frac{\pi}{a}x$$



IONS

$\Rightarrow$ DIFFERENT ENERGY FOR ψ_+ AND ψ_-

IN THE PRESENCE OF V_{ION}

THE EFFECT OF V_{ION} IS TO OPEN A GAP

- DRUDE CLASSICAL ELECTRONS BOX
- SOMMERFELD FERMIONIC NATURE OF ELECTRONS IN A BOX

THEY CAN ONLY EXPLAIN METALS

BLOCH ELECTRONS EXPLAIN PRESENCE OF INSULATORS

INSULATORS CAN BE EXPLAINED ONLY IF E_{GAP} EXISTS

$$\psi_1 = e^{i\frac{\pi}{a}x} \qquad \psi_2 = e^{-i\frac{\pi}{a}x}$$

$$E_1^{(0)} = E_2^{(0)} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2$$

TURN ON V_{ION}, SMALL PERTURBATION

PERTURBATION THEORY (FIRST ORDER DEGENERATE PERTURBATION THEORY)

$$\Delta E^{(1)} = \langle \psi^{(0)} | V_{ION} | \psi^{(0)} \rangle$$

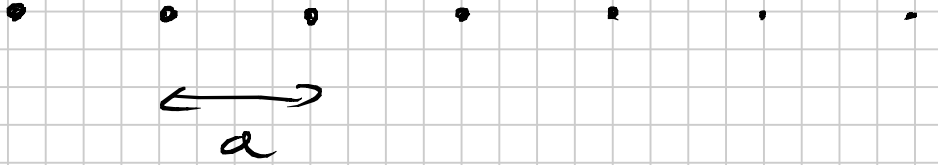
NON DEGENERATE

DEGENERATE CASE:

$$\begin{bmatrix} \langle \psi_1 | V_{ION} | \psi_1 \rangle & \langle \psi_1 | V_{ION} | \psi_2 \rangle \\ \langle \psi_2 | V_{ION} | \psi_1 \rangle & \langle \psi_2 | V_{ION} | \psi_2 \rangle \end{bmatrix} \longrightarrow \text{DIAGONALIZE} \longrightarrow \Delta E_2^{(1)}, \; \Delta E_2^{(1)}$$

$$\langle \psi_1 | V_{ION} | \psi_1 \rangle = \frac{1}{L} \int_0^L dx \; e^{-i\frac{\pi}{a}x} V_{ION}(x) e^{i\frac{\pi}{a}x} =$$

$$= \frac{1}{L} \int_0^L dx \; V_{ION}(x) = \overline{V} \quad \text{(AVERAGE POTENTIAL)}$$



$$L = a \cdot N$$

$$\langle \psi_1 | V_{ION} | \psi_2 \rangle = \frac{1}{L} \int_0^L dx \; e^{-i\frac{\pi}{a}x} V_{ION}(x) e^{-i\frac{\pi}{a}x}$$

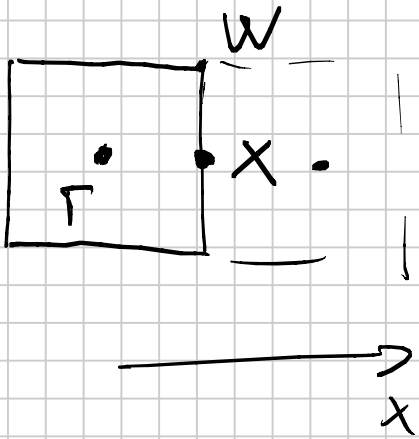
$$= \frac{1}{L} \int_0^L dx \; e^{-i\frac{2\pi}{a}x} V_{ION}(x)$$

$\tilde{V}(k)$ FOURIER TRANSFORM OF $V_{ION}(x)$

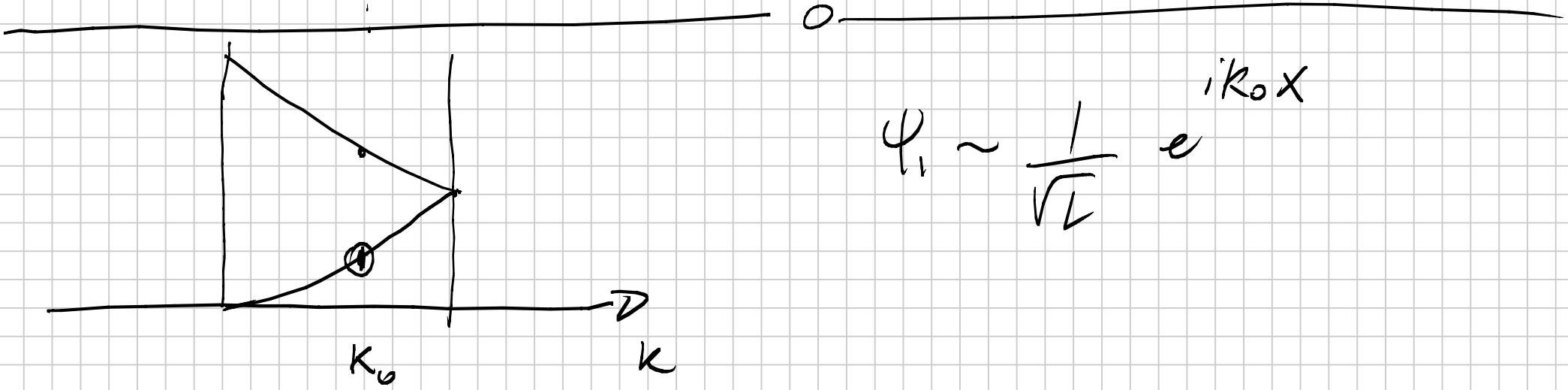
$$\langle \psi_1 | V_{ION} | \psi_2 \rangle = \tilde{V}\left(k = \frac{2\pi}{a}\right)$$

$$\begin{bmatrix} \bar{V} & \tilde{V}\left(\frac{2\pi}{a}\right) \\ \tilde{V}\left(\frac{2\pi}{a}\right) & \bar{V} \end{bmatrix} \Rightarrow \Delta\varepsilon^{(2)}_{1,2} = \bar{V} \pm \tilde{V}\left(\frac{2\pi}{a}\right)$$

$$\Rightarrow E_{GAP} = 2\tilde{V}\left(k = \frac{2\pi}{a}\right)$$



$$E_{GAP} \text{ AT } (X) = 2\tilde{V}\left(\vec{K} = \left(\frac{2\pi}{a}, 0\right)\right)$$



$$\psi_1 \sim \frac{1}{\sqrt{L}} e^{iK_0 x}$$

$$\Delta\varepsilon^{(1)} = \frac{1}{L}\int_0^L dx \; \cancel{e^{-iK_0 x}} \; V_{ION}(x) \; \cancel{e^{iK_0 x}} = \overline{V}$$

TO SECOND ORDER OF PERTURBATION

THEORY :

$$\Delta E^{(2)} = \sum_{k'} \frac{\langle k_0 | V_{ION} | k' \rangle \langle k' | V_{ION} | k_0 \rangle}{E(k_0) - E(k')}$$

$$V_{ION}(x) = V_{ION}(x + R) \qquad \forall R \text{ IN THE LATTICE}$$

$$V_{ION}(x) = \sum_{k} e^{ikx} \tilde{V}(k)$$

$$V_{ION}(x+R) = \sum_{k} e^{ikx} \underbrace{e^{ikR}}_{\text{HAS TO BE } 1} \tilde{V}(k) = V_{ION}(x)$$

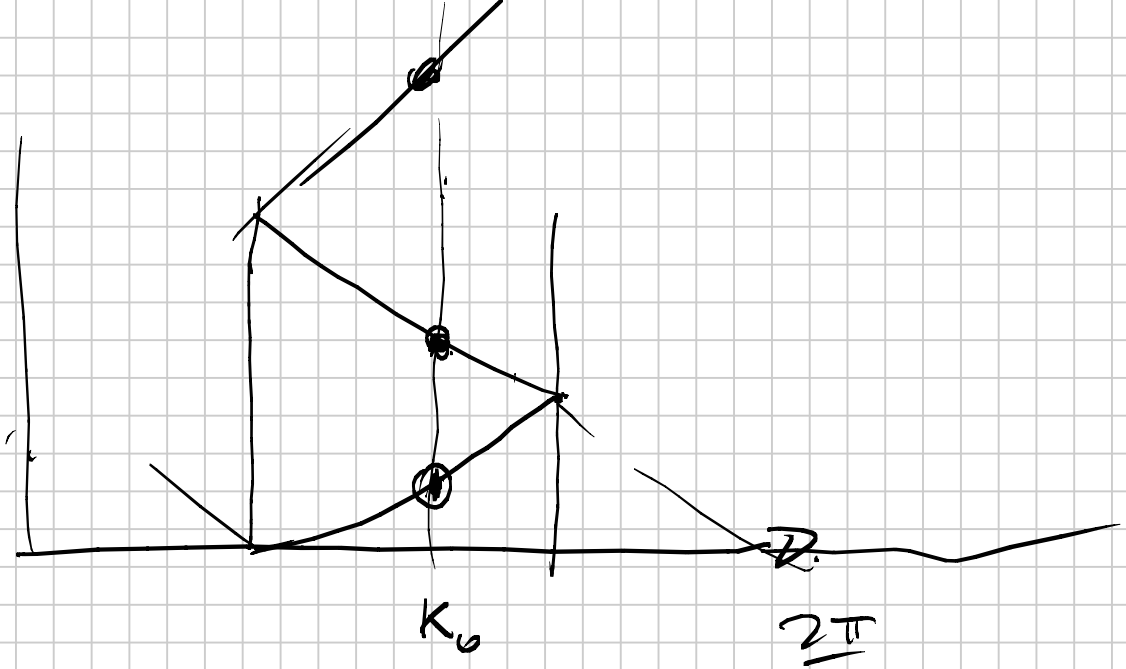
$\Rightarrow$ k HAS TO BE A RECIPROCAL

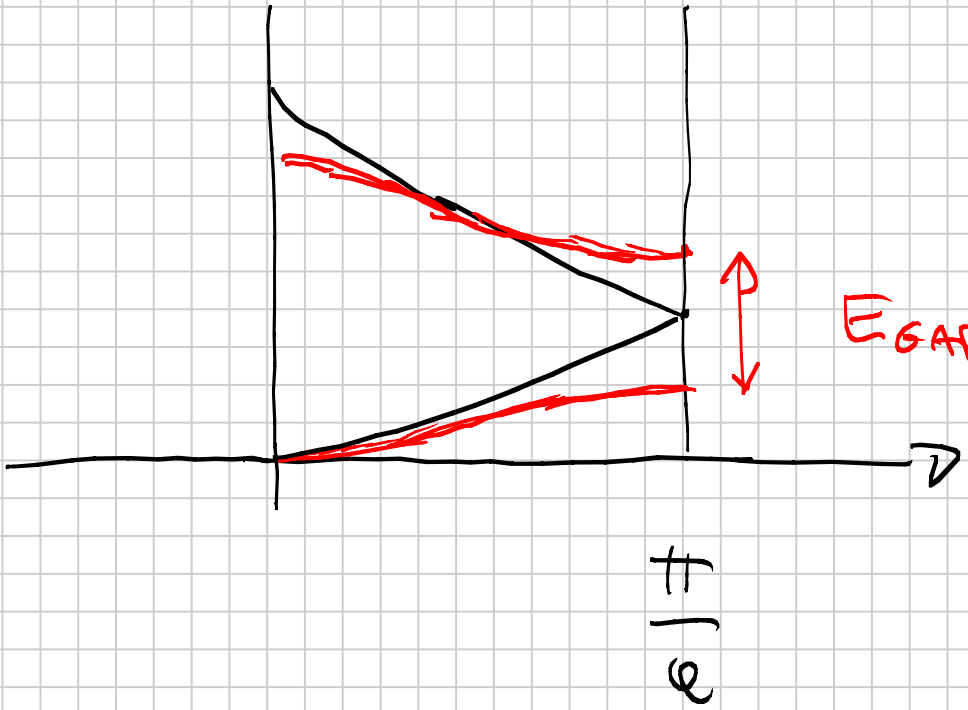
LATTICE VECTOR $\Rightarrow$ K HAS TO BE $\underline{K}$

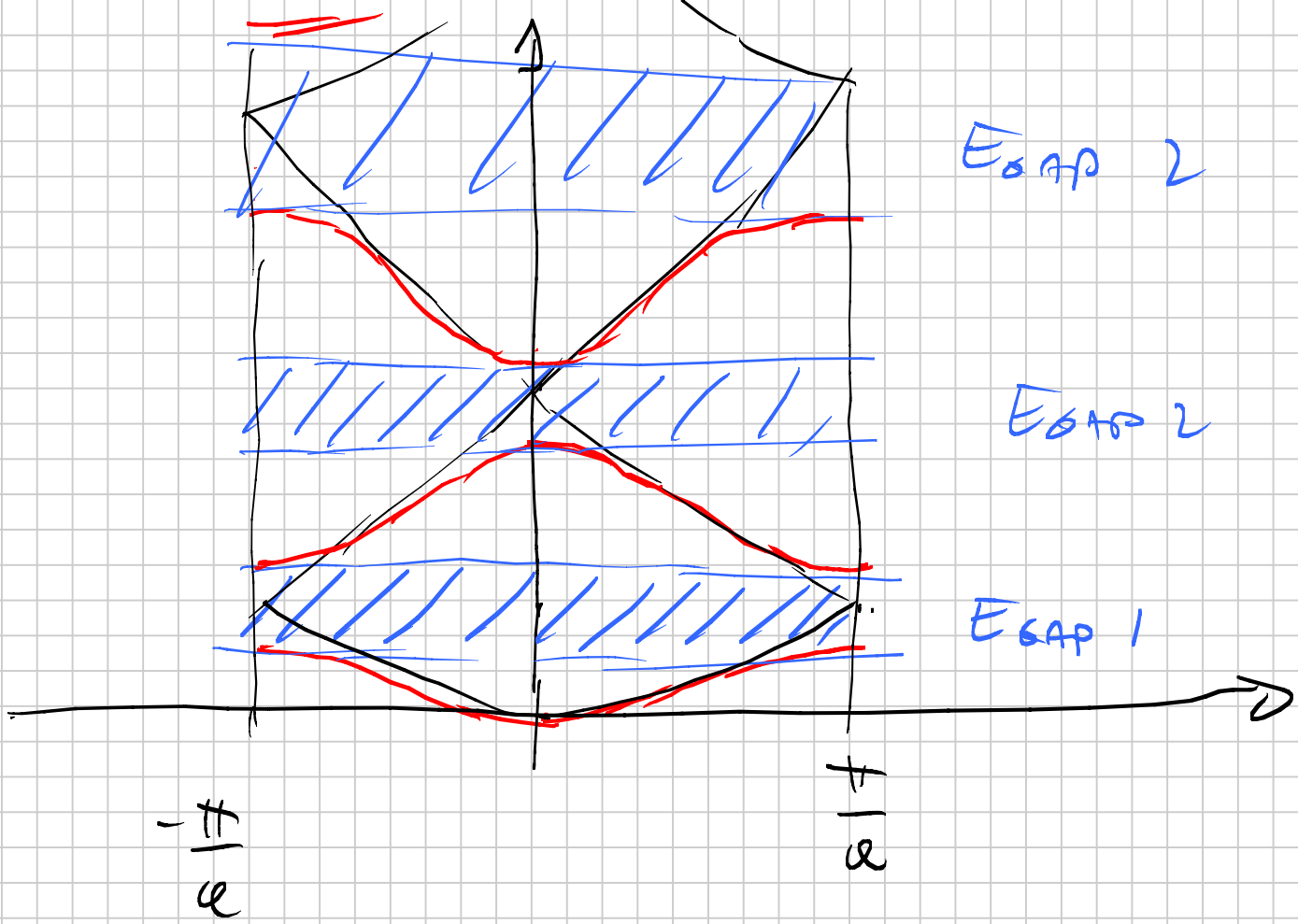
FOURIER COMPONENTS OF $V_{ION}(x)$ ARE $\neq 0$ ONLY ON $\underline{K} \in$ RECIPROCAL LATTICE

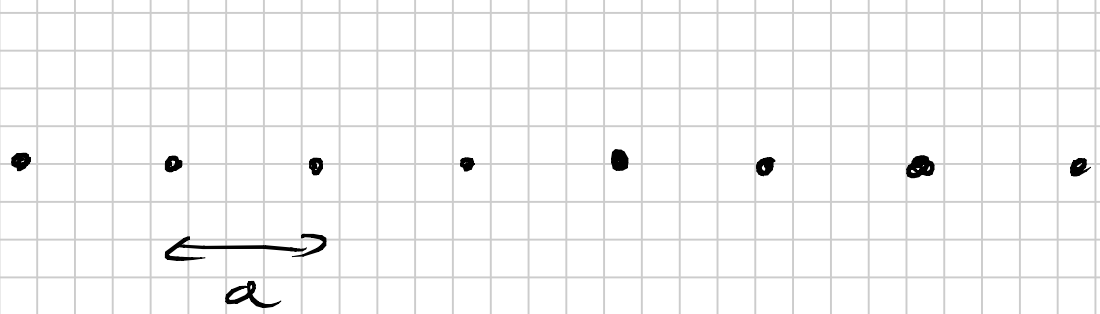
$$k' = k_0 + \underline{K}$$

$$\Delta E^{(2)}_{k_0} = \sum_{\underline{K}} \frac{|\tilde{V}(\underline{K})|^2}{E_{k_0} - E_{k_0+\underline{K}}}$$


k_0
$\frac{2\pi}{a}$


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





$$L = a \cdot N$$

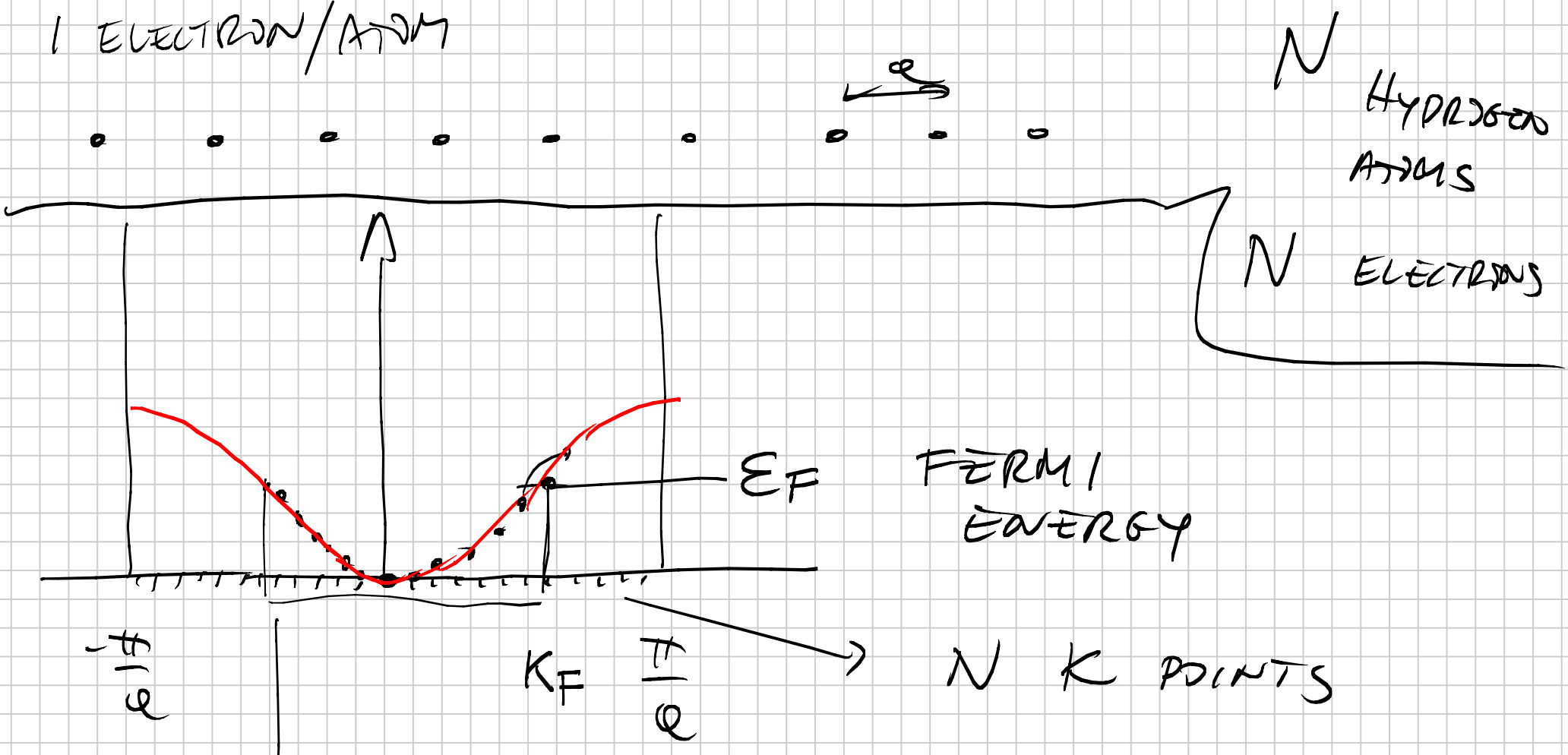
BOUNDARY CONDITIONS:

$$K = -\frac{\pi}{a} + \frac{2\pi}{Na} m \qquad ma \in [0, N-1]$$

FIRST 2 ELECTRONS $\rightarrow$ $K = 0$ (TWO SPINS)

CRYSTAL OF HYDROGEN ATOMS

1 ELECTRON/ATOM



METAL E_F

K_F = LAST K STATE OCCUPIED

$$m = \pm \frac{N}{4}$$

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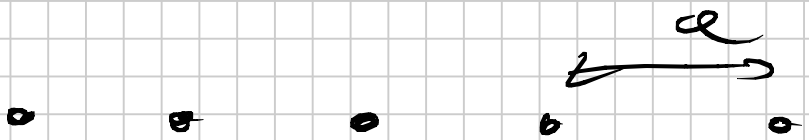
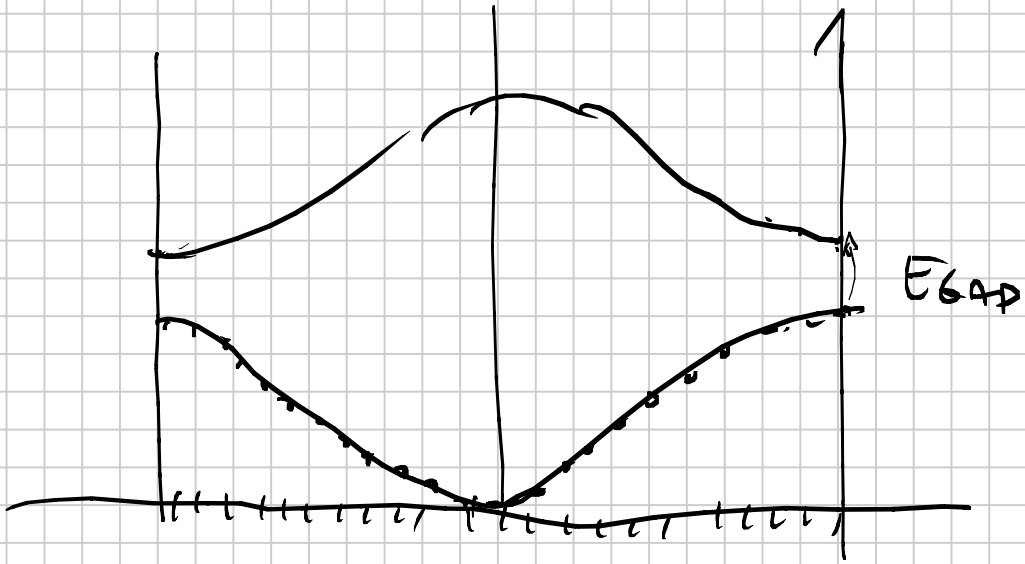
(2) CRYSTAL OF He



N # SITES

2N ELECTRONS



He CRYSTAL

FILLS UP

EXACTLY ONE BAND

N # K POINTS

$\Rightarrow$ INSULATOR

REAL INSULATOR

$E_{GAP} >> K_B T$

SEMICONDUCTORS

$E_{GAP} \sim K_B T$