LECTURE # 19

Note Title 11/5/2008

ANNOUNCEMENT:

MON NOV 10 REVIEW (OUT OF TOWN)

CLASS: TA KAIJIE XU

TRY TO WORK ON PROBLEMS

BEFORE PICKING UP SOLUTION

HW # 4 DUE ON

MONDAY +90

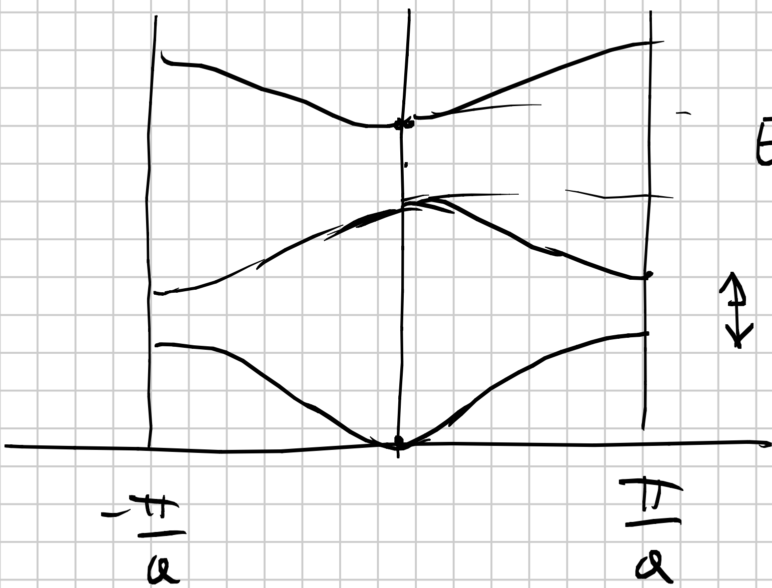
WILL BE IN THE MIDTERM

CHAP 4-5-6 8-9

CHAP 10 (TIGHT BINDING)

MT # 2 ONLY FIRST 3 PROBLEMS

- ELECTRONS WEAK PERIODIC POTENTIAL



$$E_{GAP}^{(2)} = 2\,\tilde{V}_{ION}\left(K = \frac{4\pi}{a}\right)$$

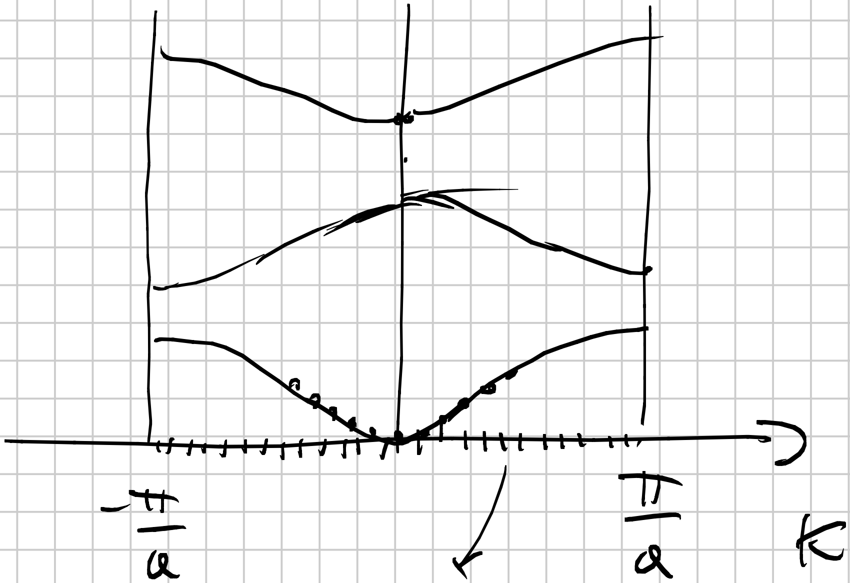
$$E_{GAP}^{(1)} = 2\,\tilde{V}_{ION}\left(K = \frac{2\pi}{a}\right)$$

COUNTING ELECTRONS

N

TOTAL

CELLS



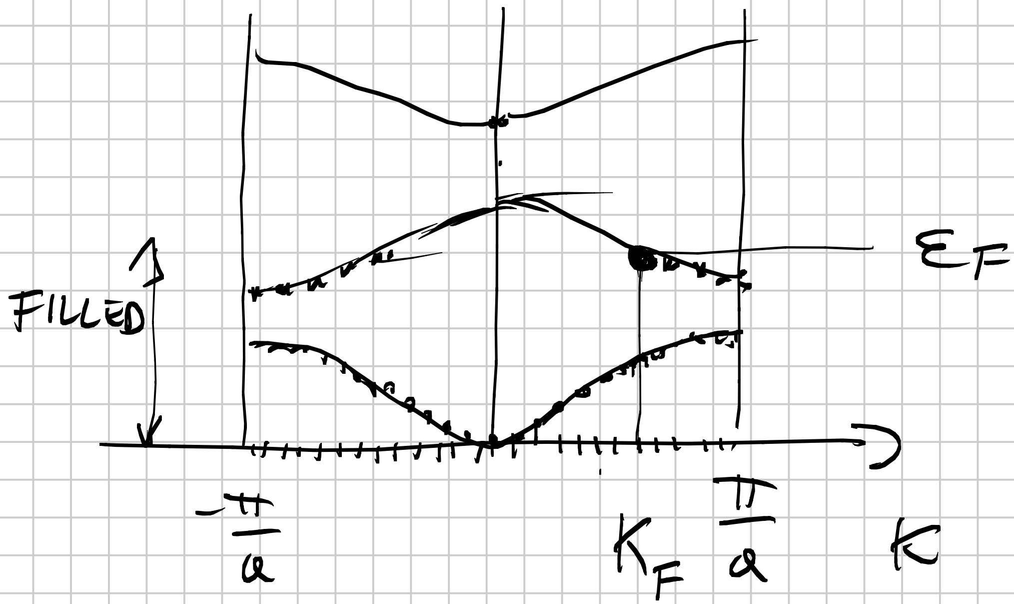
$\Delta k \sim \frac{2\pi}{Na}$

FILL UP STATES WITH

2 ELECTRONS / K POINT

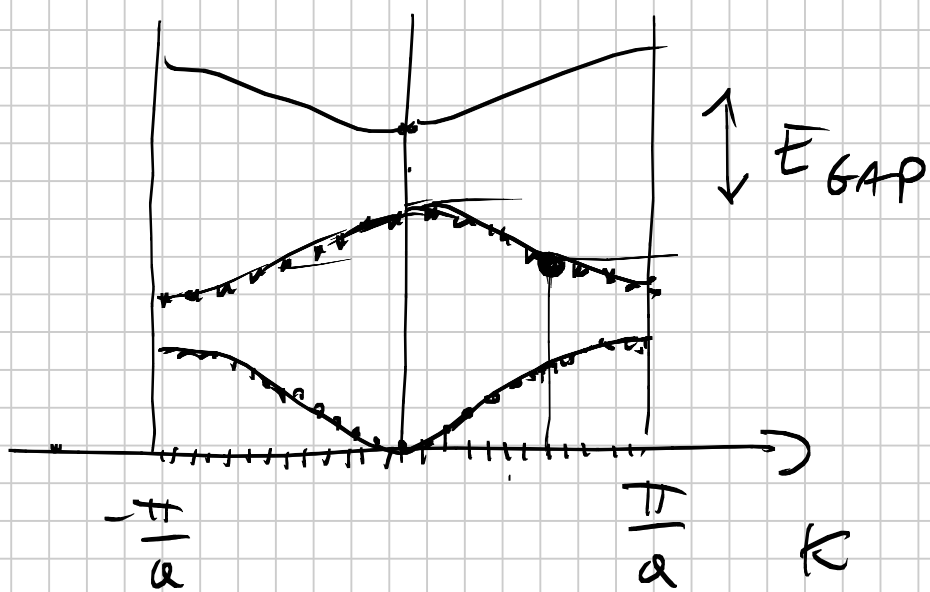
(SPIN ↑ , SPIN ↓)

2 CASES:



METAL

PARTIALLY FILLED BAND



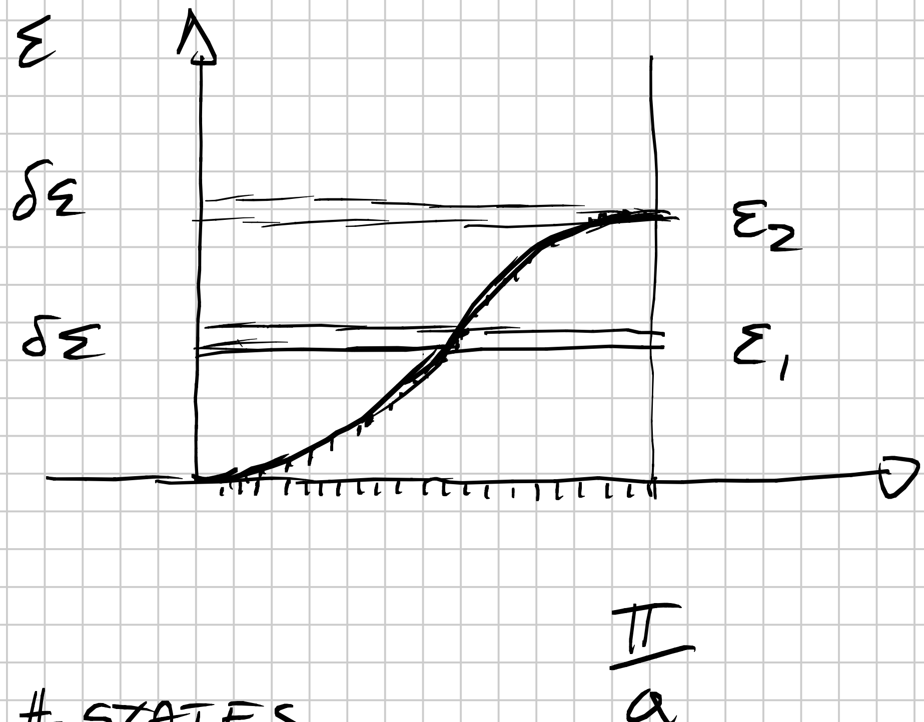
INSULATOR (OR SEMICONDUCTOR)

COMPLETELY FILLED BANDS

DENSITY OF STATES

HOW MANY ELECTRONIC STATES I HAVE

AS A FUNCTION OF ENERGY



ε_2 HAS HIGHER DENSITY OF K POINTS

$\Rightarrow$ HIGHER DENSITY OF STATES

TOTAL # STATES AT ε

$$N(\varepsilon) = \sum_{K \in BZ} \delta_{\varepsilon(K),\varepsilon}$$

WHERE

$$\delta_{\varepsilon(k),\varepsilon} \begin{cases} \to 1 & \varepsilon \leq \varepsilon(k) < \varepsilon + \delta\varepsilon \\ \to 0 & \text{OTHERWISE} \end{cases}$$

$\delta\varepsilon$ SMALL $\to$ CONTINUUM

$$\Delta k = \frac{2\pi}{L}$$

$$N(\varepsilon) = \sum_{k \in BZ} \delta_{\varepsilon(k),\varepsilon} \sim \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{\Delta k}\, \delta(\varepsilon(k) - \varepsilon)$$

$$DOS(\varepsilon) = \frac{N(\varepsilon)}{L} = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi}\, \delta(\underline{\underline{\varepsilon(k)}} - \varepsilon)$$

1 DIMENSIONA

2 D $\quad DOS(\varepsilon) = \int_{BZ} \frac{d^2\vec{k}}{(2\pi)^2}\, \delta(\varepsilon(k_x, k_y) - \varepsilon)$

3D $\quad DOS(\varepsilon) = \int_{BZ} \frac{d^3\vec{k}}{(2\pi)^3} \, \delta(\varepsilon(\vec{k}) - \varepsilon)$

$$\int dx \; g(x) \; \delta(x - x_0) = g(x_0)$$

FIND x_0 SUCH THAT

$f(x_0) = 0$

$$\int g(x) \; \delta(f(x)) \, dx =$$

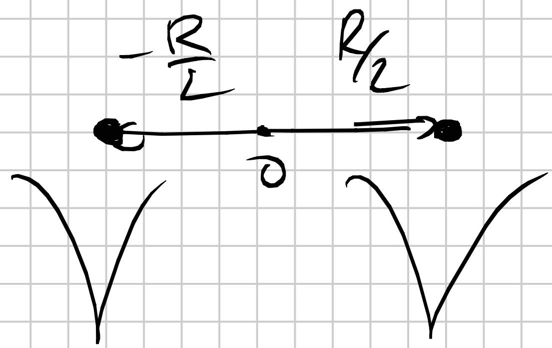
$$= \int dx \; \frac{g(x)}{|f'(x)|} \; \delta(x - x_0)$$

TIGHT BINDING MODEL (CHAPT 10 p 176-184)

START FROM ELECTRONS

LOCALIZED ON EACH ATOM

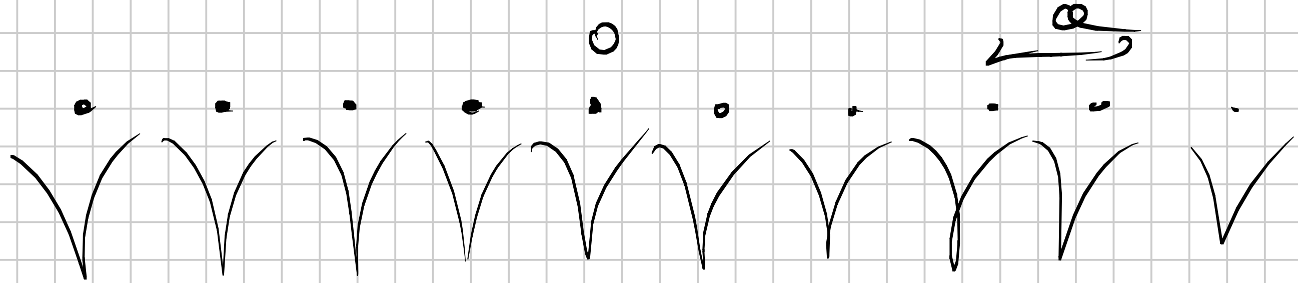
H_2^+



$$V_{IONS} = V_A\left(r - \frac{R}{2}\right) + V_A\left(r + \frac{R}{2}\right) \leftarrow$$

$$\psi_{H_2^+} = \varphi_{1S}\left(r + \frac{R}{2}\right) \pm \varphi_{1S}\left(r - \frac{R}{2}\right) \leftarrow$$

LINEAR COMBINATION OF ATOMIC ORBITALS



$\{R\}$ ALL POSITION OF ATOMS

$$V_{ion}(r) = \sum_R V_A(r-R)$$

$$\boxed{\psi_k(r) = \sum_R e^{ik\cdot R}\,\varphi_{1s}(r-R)}$$

BLOCH FUNCTION

$$\psi_k(r+R) = e^{ikR}\,\psi_k(r)$$

$$H = -\frac{\hbar^2\nabla^2}{2m} + \sum_R V_A(r-R)$$

$$\varepsilon(k) = \langle \psi_k | H | \psi_k \rangle$$ → GIVE THE TIGHT BINDING BAND

$$\sum_{RR'} \int dr\, e^{-ikR} \varphi_{1s}(r-R) \left(T + \sum_{R''} V_{AT}(r-R'')\right) \varphi_{1s}(r-R') e^{ikR'}$$

TIGHT BINDING IN FIRST NEIGHBOR APPROX

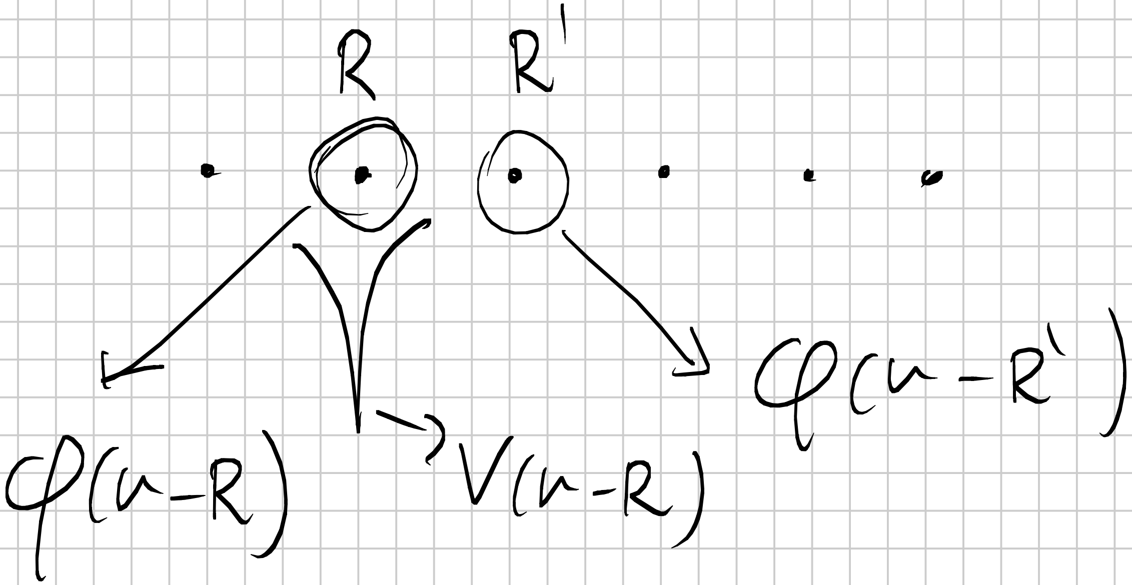
KEEP ONLY

① $R = R' = R''$

$$\int dr\, \varphi_{1s}(r-R) \left(T - V(r-R)\right) \varphi_{1s}(r-R)$$

$$= \varepsilon_{1s}$$

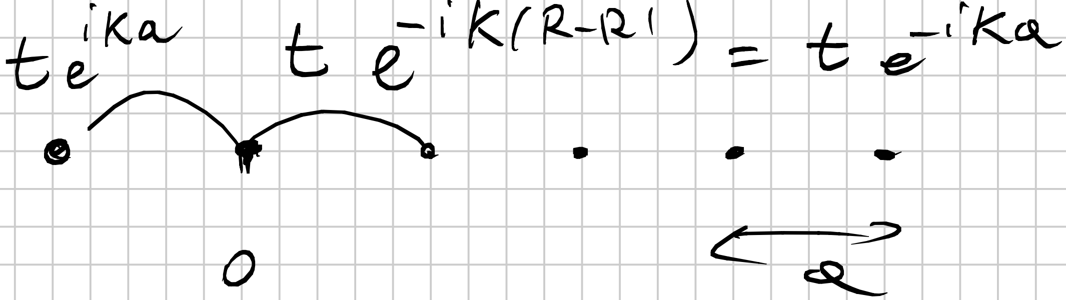
② $$\overbrace{\int dr\ \varphi(r-R)\ V_A(r-R)\ \varphi(r-R')}^{**}\ e^{-iK\cdot(R-R')}$$



WITH R & R' FIRST NEIGHBORS

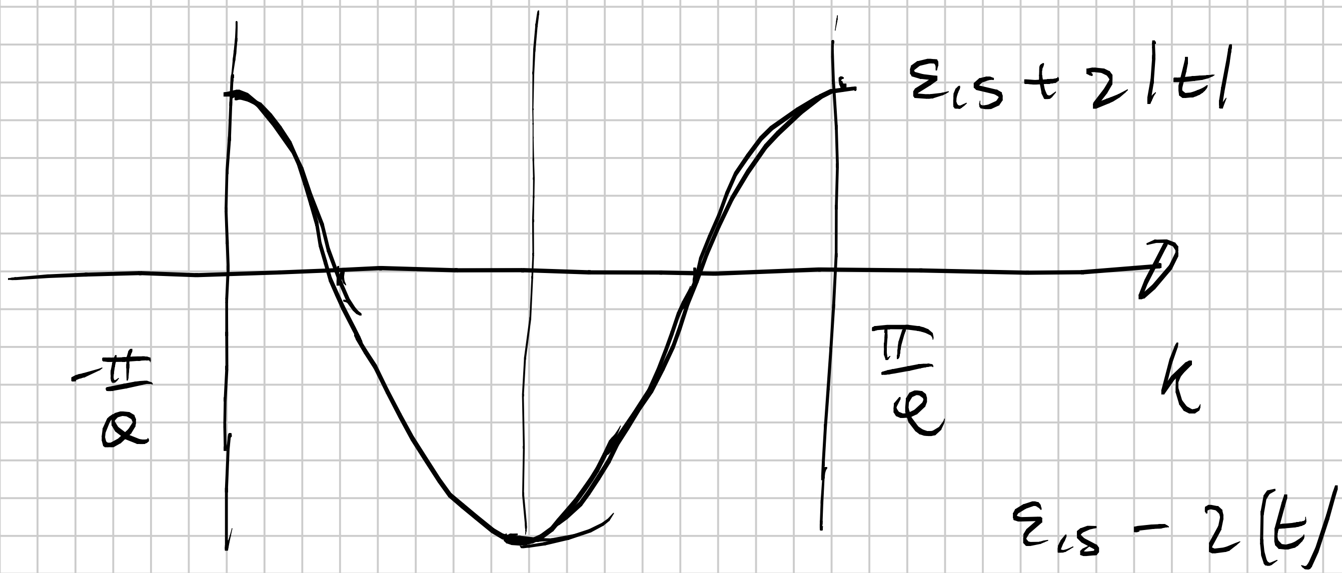
** HOPPING INTEGRAL "t"

USUALLY $t < 0$



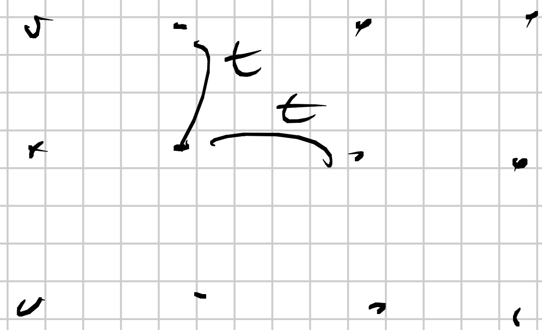
$$\varepsilon(k) = \varepsilon_{1s} + t e^{ika} + t e^{-ika} =$$

$$= \varepsilon_{1s} + 2t\cos ka = \varepsilon_{1s} - 2|t|\cos ka$$



GW 6

$$\cos ka \sim 1 - \frac{(ka)^2}{2}$$



$$DOS(\varepsilon) = \int \frac{d^3k}{(2\pi)^3}\, \delta(\varepsilon(\vec{k}) - \varepsilon)$$

$$\varepsilon(\vec{k}) = \frac{\hbar^2(k_x^2 + k_y^2 + k_z^2)}{2m}$$

DOS(ε) FOR FREE ELECTRON

FIND x_0 SUCH THAT

$$\int g(x)\, \delta(f(x))\, dx =$$

$$f(x_0) = 0$$

$$= \int dx \, \frac{g(x)}{|f'(x)|} \, \delta(x - x_0)$$

$$f(x_0) = 0$$

$$\int dx \, \delta(f(x)) = \int dx \, \frac{\delta(x - x_0)}{|f'(x)|}$$

$$df = \left| \frac{df}{dx} \right| dx$$