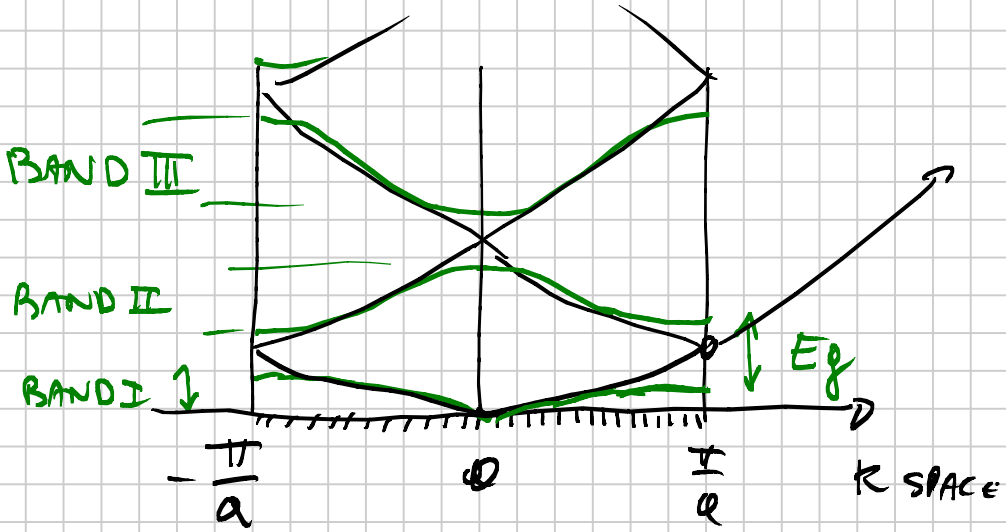
LECTURE # 16

Note Title 10/31/2007

Nearly free electrons



$\psi_K^\circ \quad \psi_{K-K}^\circ$ Doubly degenerate states

$E_g = 2\tilde{V}_{ion}(K)$

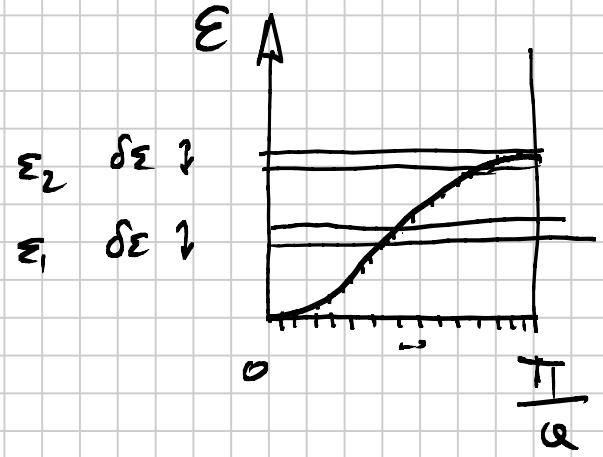
#K POINTS IN 1° BZ = N Unit cells

$\forall$ K POINT $\rightarrow$ 2 electons $k\uparrow$

FILL COMPLETELY BAND $\rightarrow$ INSULATOR

OTHERWISE $\rightarrow$ METAL

Important to know # states as a function of the energy → Density of states



ε_2 has a higher density of k points (of states)

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

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

$\delta\varepsilon$ SMALL → CONTINUUM LIMIT

$L = Na =$ total length chain

$$N(\varepsilon) = \sum_{k \in BZ} \delta_{\varepsilon(k),\varepsilon} \longrightarrow \frac{L}{(2\pi)} \int_{-\pi/a}^{\pi/a} dk \; \delta(\varepsilon(k) - \varepsilon)$$

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

$\varepsilon(k)$ (1D)

$$DOS(\varepsilon) = \frac{N(\varepsilon)}{S} = \int_{BZ} \frac{d^2k}{(2\pi)^2}\, \delta(\varepsilon(k) - \varepsilon) \qquad 2D$$

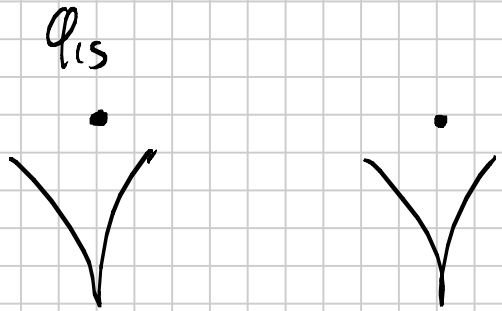
$$3D \quad DOS(\varepsilon) = \int_{BZ} \frac{d^3k}{(2\pi)^3}\, \delta(\varepsilon(k) - \varepsilon)$$

$$\int dx \quad \delta(f(x)) \rightarrow \int dx \quad \frac{1}{|f'(x)|}\, \delta(x - x_0) \qquad f(x_0) = 0$$

TIGHT BINDING MODEL

Start from electrons completely localized at atomic sites + add hopping

H_2^+

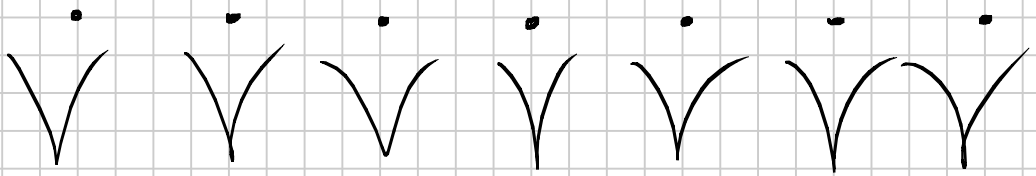


$$V_{ions}(r) = V_c\left(r - \frac{R}{2}\right) + V_c\left(r + \frac{R}{2}\right)$$

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

Linear
Combination
Atomic
Orbitals

LCAO



$$V_{ions}(\vec{r}) = \sum_{R} V_{at}(\vec{r} - \vec{R})$$

$$\psi_k(\vec{r}) = \sum_R e^{ik\cdot R} \varphi_{1s}(\vec{r} - R) \rightarrow \text{Satisfies Bloch Theorem}$$

$$\psi_k(\vec{r} + \vec{R}') = \sum_R e^{ik\cdot R} \varphi_{1s}(\vec{r} - \underbrace{\vec{R} + \vec{R}'}_{R''}) \rightarrow$$

$$e^{ik\vec{R}'} \boxed{\sum_{R''} e^{ik\vec{R}''} \varphi_{1s}(n - \vec{R}'')}$$

$$\psi_k(n)$$

$$\boxed{\psi_k(n+R) = e^{ik\cdot R} \psi_k(n)}$$

$$T$$

$$H = \frac{-\hbar^2 \vec{\nabla}^2}{2m} + \sum_R V_{at}(n - R)$$

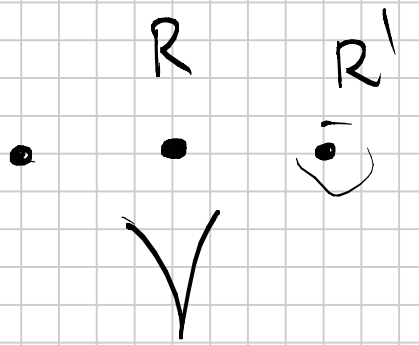
$$E(k) = \langle \psi_k | H | \psi_k \rangle =$$

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

$$R = R' = R''$$

$$\int dr \; \varphi_{1s}(r-R) \left(T + V(r-R) \right) \varphi_{1s}(r-R) = \varepsilon_{1s}$$

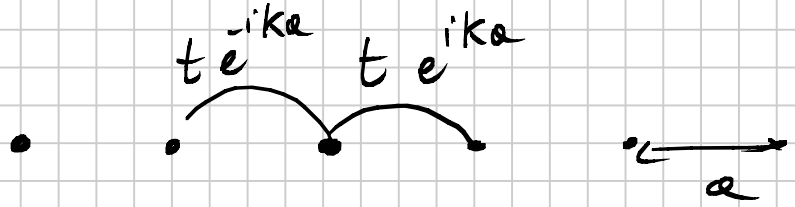
On site energy



$$\rightarrow \underbrace{\int dr \varphi(r-R) \, V(r-R) \, \varphi(r-R') \, e^{ik(R-R')}}$$

HOPPING TERM "t"

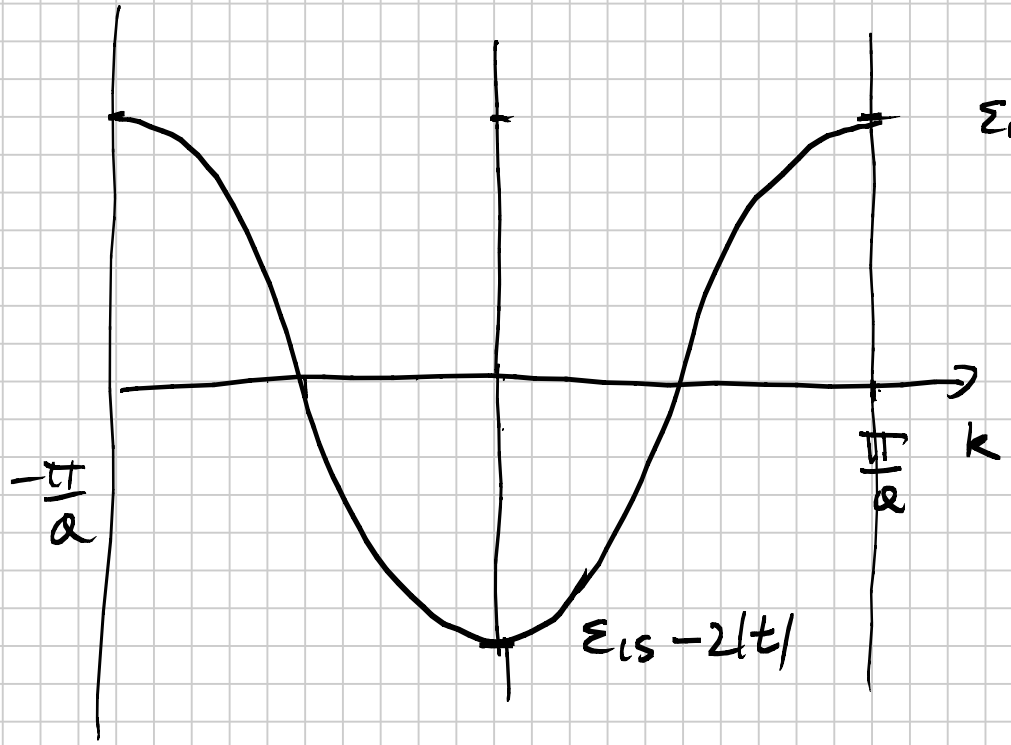
USUALLY $t < 0$



$e^{ik(R-R')}$

$$\mathcal{E}(k) = \mathcal{E}_{1s} + te^{ika} + te^{-ika} \Rightarrow \mathcal{E}_{1s} + 2t\cos ka$$

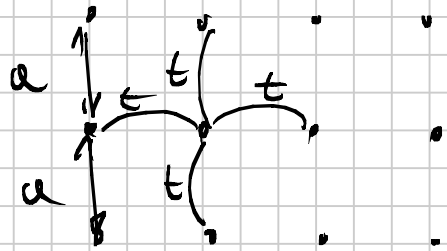
$$\mathcal{E}_{1s} - 2|t|\cos ka$$



q_{1s}

FOR $ka << 1$

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



$$\mathcal{E}(k_x, k_y) = \mathcal{E}_{1s} - 2|t|\cos k_x a - 2|t|\cos k_y a$$

CALCULATE DOS(E)

FOR FREE ELECTRONS IN 3D

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

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

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

$$f(x_0) = 0$$