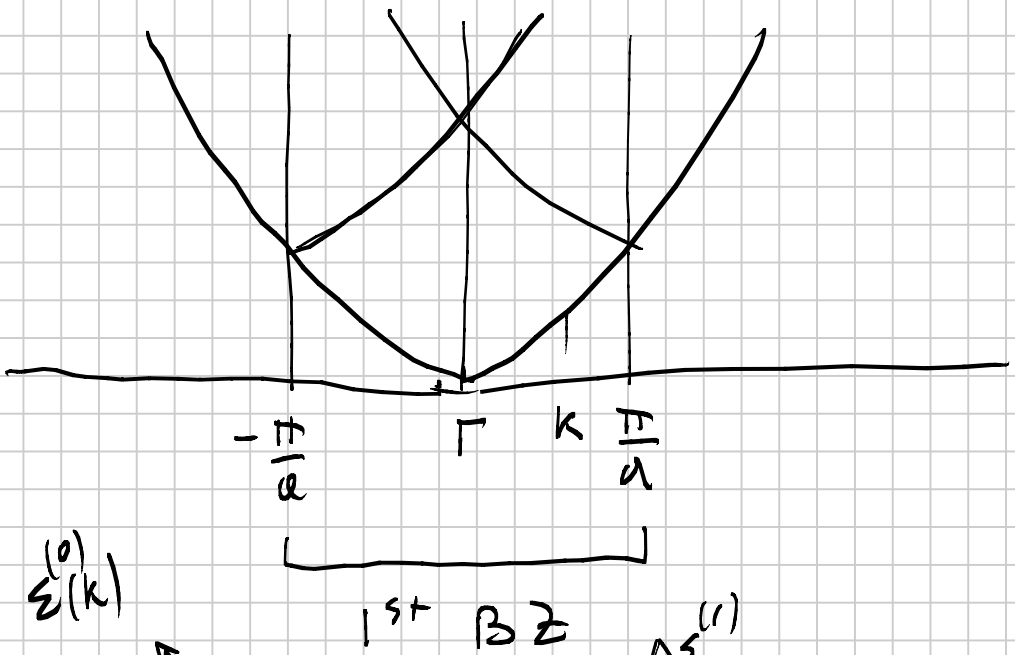
LECTURE #15

Note Title 2/15/2010

ELECTRONIC BANDS

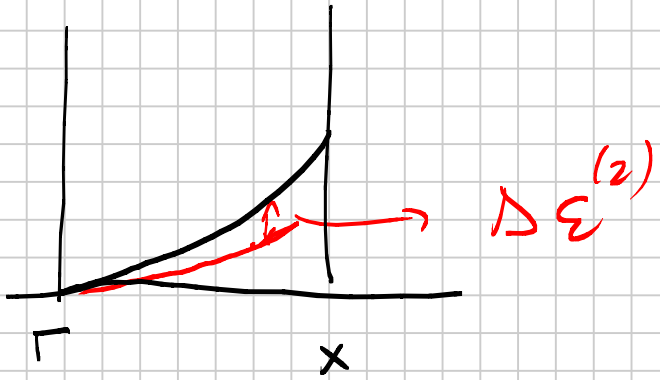
NEARLY-FREE ELECTRON APPROX



$$\varepsilon(k) = \varepsilon^{(0)}(k) = \frac{\hbar^2 k^2}{2m} + C + \Delta\varepsilon^{(1)} + \sum_{G_m} \frac{|\tilde{V}(G_m)|}{\varepsilon^{(0)}(k) - \varepsilon^{(0)}(k+G_m)} \quad \Delta\varepsilon^{(2)}(k)$$

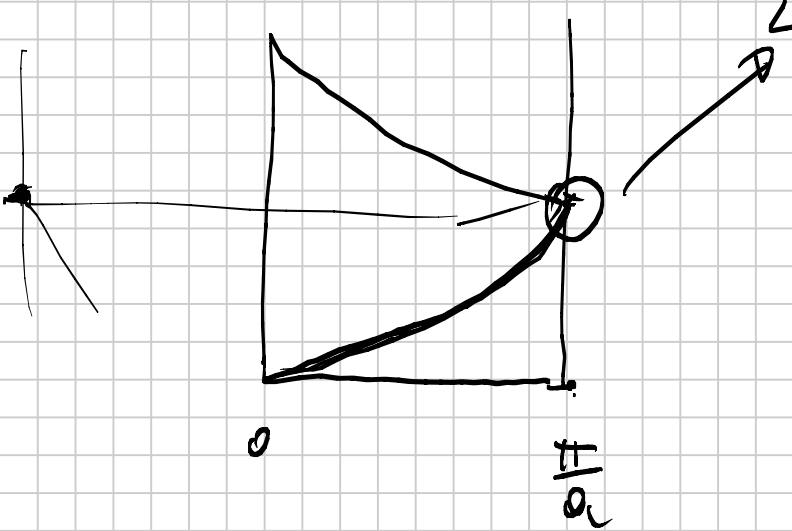
$\tilde{V}(k)$ IS FOURIER TRANSFORM $V_{ION}(\vec{r})$

G_m ARE RECIPROCAL LATTICE VECTORS



NON - DEGENERATE STATES

DEGENERATE - CASE



2 DEGENERATE STATES

$$\psi_1^{(0)} = \frac{1}{\sqrt{L}} e^{i\frac{\pi}{a}x}$$

$$\psi_2^{(0)} = \frac{1}{\sqrt{L}} e^{-i\frac{\pi}{a}x}$$

V_{IONS}

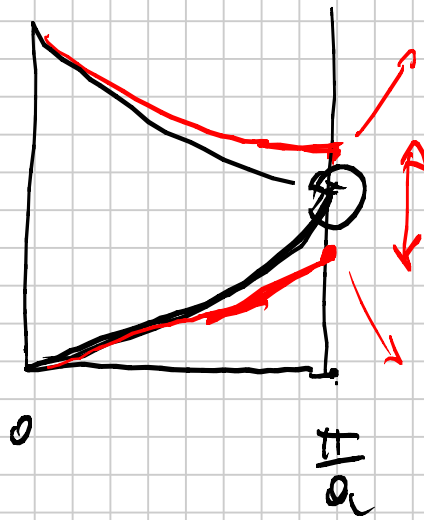
1ST ORDER PERTURBATION THEORY (DEGENERATE CASE)

$$\begin{bmatrix} \langle \psi_1|V|\psi_1\rangle & \langle \psi_2|V|\psi_1\rangle \\ \langle \psi_1|V|\psi_2\rangle & \langle \psi_2|V|\psi_2\rangle \end{bmatrix} \xrightarrow{\text{DIAGONALIZE}} \Delta E^{(1)}$$

$$\langle \psi_1|V|\psi_1\rangle = \frac{1}{L}\int dx\, V_{10N}(x) = \text{CONST} = \langle \psi_2|V|\psi_2\rangle$$

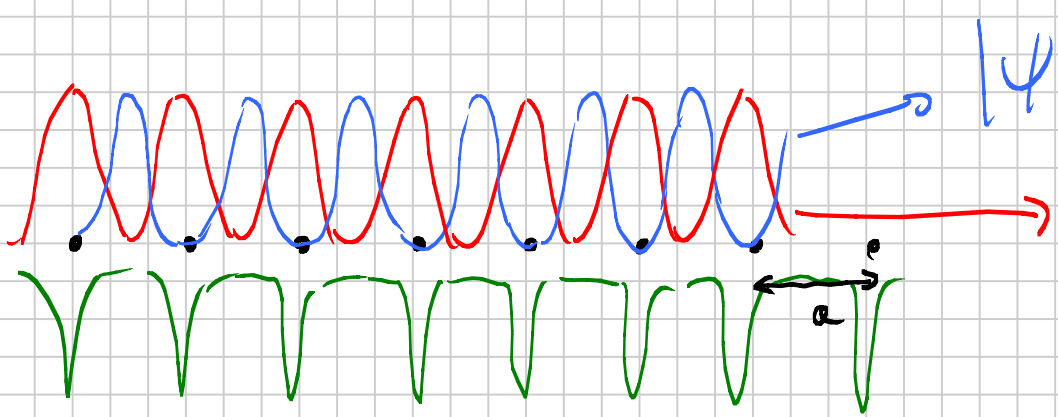
$$\langle \psi_1|V|\psi_2\rangle = \frac{1}{L}\int dx\, e^{-i\frac{2\pi}{a}x} V_{10N}(x) = \tilde{V}\left(G_1 = \frac{2\pi}{a}\right)$$

$$\begin{bmatrix} c & \tilde{V}\left(\frac{2\pi}{a}\right) \\ \tilde{V}\left(\frac{2\pi}{a}\right) & c \end{bmatrix} \rightarrow \Delta E^{(1)} = c \pm \tilde{V}\left(\frac{2\pi}{a}\right)$$

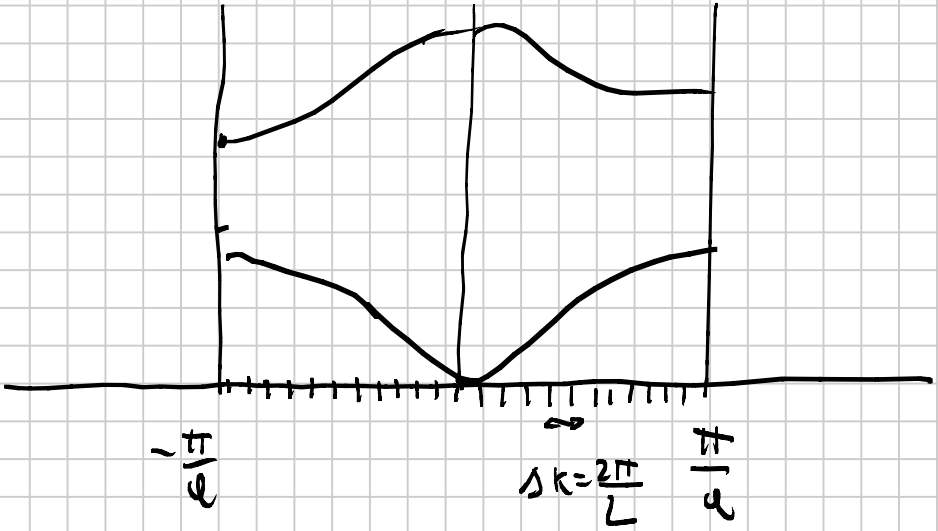


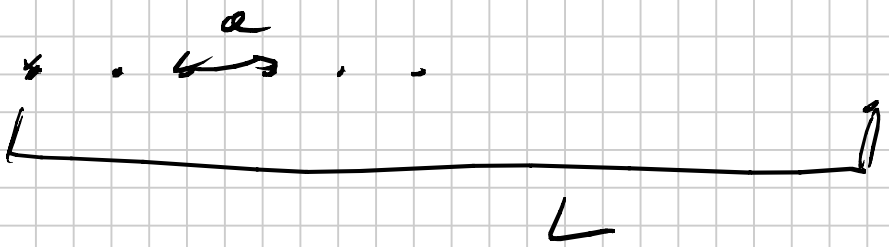
$$\psi_- \sim e^{i\frac{\pi}{a}x} - e^{-i\frac{\pi}{a}x} \sim \sin\frac{\pi}{a}x$$

$$\psi_+ \sim \ldots + \ldots \sim \cos\frac{\pi}{a}x$$



$\mathcal{E}_+ \neq \mathcal{E}_-$

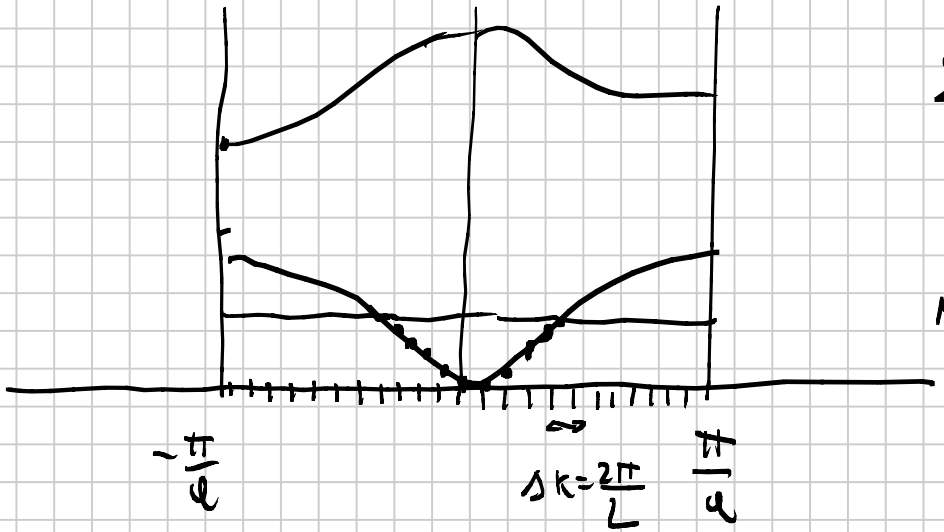




$$\#\ K\ \text{STATES} = \frac{\frac{2\pi}{a}}{\Delta K} = \frac{\frac{2\pi}{a}}{\frac{2\pi}{L}} = \frac{L}{a} = \#\ \text{IONS}$$

$\#$ OF UNIT CELLS

CASE (1) $\qquad \#e = \#\ \text{IONS}$



2e ON EACH K POINT

METAL ELECTRONS FILL BAND PARTIALLY

CASE (2) 2e / ION → COMPLETELY FILLED BAND

→ INSULATOR

$$\mathcal{E}^{(0)}(k_x, k_y, k_z) = \frac{\hbar^2(k_x^2 + k_y^2 + k_z^2)}{2m}$$

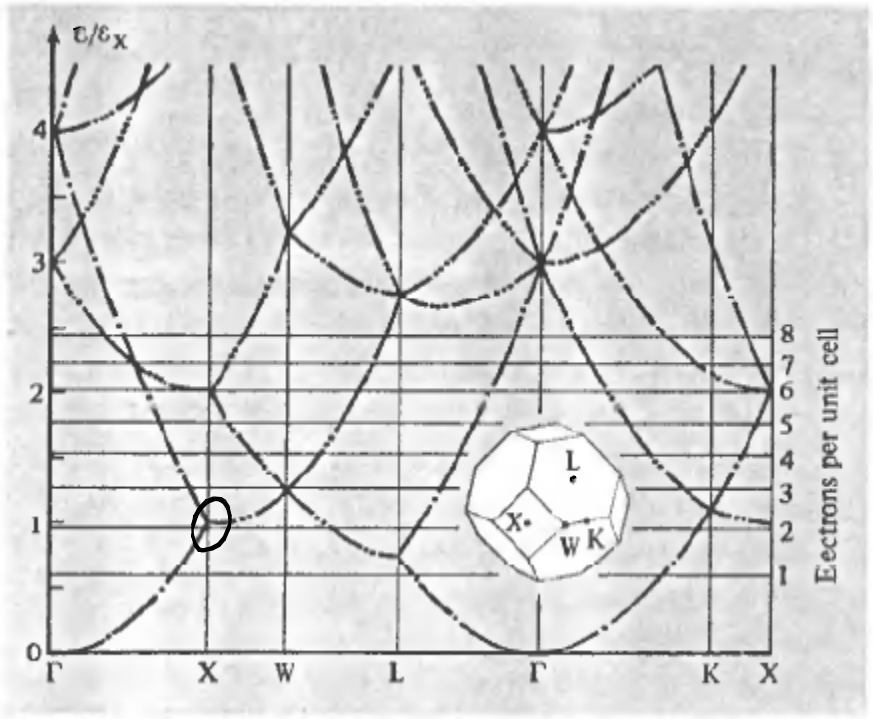


Figure 9.5
Free electron energy levels for an fcc Bravais lattice. The energies are plotted along lines in the first Brillouin zone joining the points $\Gamma(\mathbf{k} = 0)$, K, L, W, and X. ε_x is the energy at point X ($[\hbar^2/2m][2\pi/a]^2$). The horizontal lines give Fermi energies for the indicated numbers of electrons per primitive cell. The number of dots on a curve specifies the number of degenerate free electron levels represented by the curve. (From F. Herman, in *An Atomistic Approach to the Nature and Properties of Materials*, J. A. Pask, ed., Wiley, New York, 1967.)

FCC REAL SPACE

↓

BCC REC SPACE

FOLDING ONLY

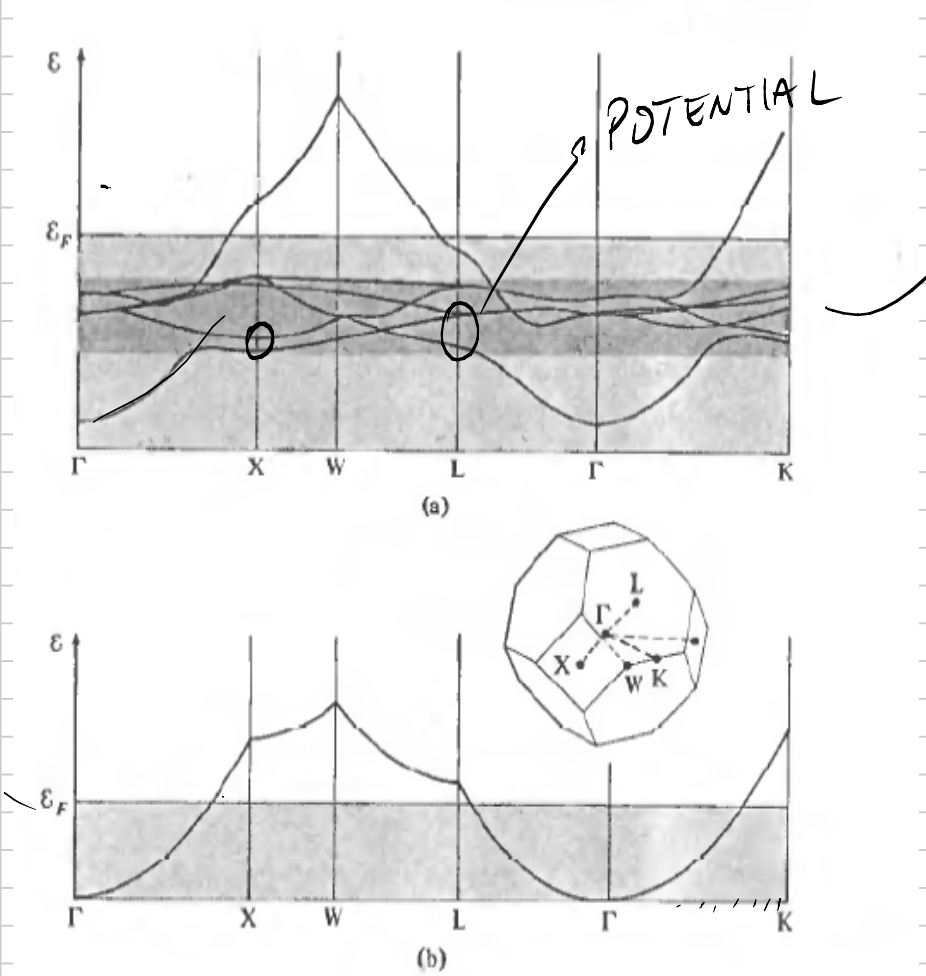
Cu → FCC

$[Ar](3d)^{10}(4s)^1$

$\ell = \pm 2$

$\ell = \pm 1$

$\ell = 0$



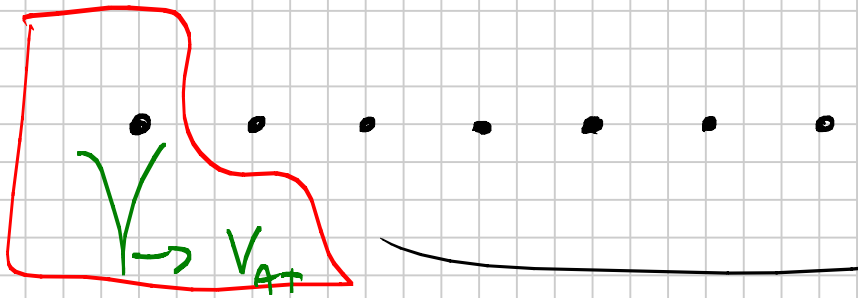
POTENTIAL

d ORBITALS ARE INCLUDED

S-d HYBRIDIZATION

→ d-LIKE BAND

TIGHT - BINDING (CHAPT 10)



→ SOLVE S.E FOR 1 e IN V_{ATOMIC}

ε_m $\varphi_m(r)$

$$V(\vec{r}) = \sum_{\vec{R}} V_{AT}(\vec{r} - \vec{R})$$

$\{\vec{R}\} \in$ BRAVAIS LATTICE

BLOCH FUNCTIONS

$$\psi_{km} = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \varphi_m(\vec{r} - \vec{R})$$

m INDEX FOR THE ATOMIC ORBITAL

ψ_{km} SATISFY BLOCH'S THEOREM:

$$\psi_{km}(\vec{r} + \vec{R}) = e^{i\vec{k}\cdot\vec{R}} \psi_{km}(\vec{r})$$

$$\Psi_k(\vec{r}) = \sum_m b_m(k) \psi_{km}(\vec{r})$$

m 6 DIFFERENT ATOMIC ORBITALS

$\hookrightarrow$ FIND $b_m(k)$ THAT DIAGONALIZE H

LCAO
LINEAR COMBINATION OF ATOMIC ORBITALS

$$H\Psi_k = E(k)\,\Psi_k$$

Ψ_{mk} BASIS WITH 6 ORBITALS

$$\left|\Psi_{1s\,k},\ \Psi_{d_1}\ \Psi_{d_2}\ \Psi_{d_3}\ \Psi_{d_4}\ \Psi_{d_5}\right.$$

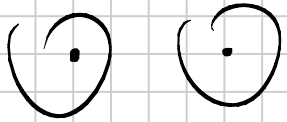
DIAGONALIZE MATRIX

6×6 MATRIX

$$\text{DET}\ \left\| \langle \Psi_{mk}|H|\Psi_{m'k}\rangle - E(k)\langle \Psi_{mk}|\Psi_{m'k}\rangle \right\| = 0$$

DIAGONALIZE $\longrightarrow$ b_m

CASE OF 1 ORBITAL / SITE $\quad m = 1s$



$\varphi_{1s}(\vec{r})$

$$\Psi_{k,1s} = \sum_R e^{ik\cdot R}\,\varphi_{1s}(\vec{r}-\vec{R})$$