BAND STRUCTURE CALCULATION IN TIGHT BINDING MODEL

$$\psi_k = \frac{1}{\sqrt{N}} \sum_j e^{ik.r_j} \phi(r - r_j)$$

Crystal electron wave function

Atomic electron wave function

To calculate E(k) we do as follows:

$$E(k) = \langle \psi_k | H | \psi_k \rangle = \int \psi_k^* H \psi_k dv$$

$$E(k) = \frac{1}{N} \sum_j \sum_m e^{ik.(r_j - r_m)} \langle \phi(r - r_m) | H | \phi(r - r_j) \rangle$$

Just for simplicity we define that: $\{\phi_j = \phi(r - r_j), \quad \phi_m = \phi(r - r_m)$

$$E(k) = \frac{1}{N} \sum_j \sum_m e^{ik.(r_j - r_m)} \langle \phi_m | H | \phi_j \rangle$$

We calculate the above summation for an special atom located at $r_j = 0$, and then multiply it by N

$$r_j = 0, \quad \rho_m = r_m - r_j = r_m$$

$$E(k) = N \times \frac{1}{N} \sum_m e^{-ik.\rho_m} \int \phi^*(r - \rho_m) H \phi(r) dv$$

Summation is over all the atoms with respect to the atom located at the origin, i.e. $r_j = 0$

Okay, now if we consider only nearest neighbor atoms and neglect the overlap with the other atomic orbitals:

For the main atom at the origin $\rho_m = 0$ $\int \phi^*(r) H \phi(r) dv = -\alpha$

$\int \phi^*(r - \rho) H \phi(r) dv = -\gamma$ For the nearest neighbors $\rho_m = \rho$

$$E(k) = \sum_m e^{-ik.\rho_m} \int \phi^*(r - \rho_m) H \phi(r) dv$$

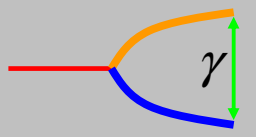
$$E(k) = -\alpha - \gamma \sum_m e^{-ik.\rho_m}$$

This term originates from the interaction of the main atom with its nearest neighbors

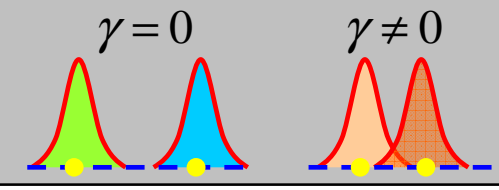
For the isolated atom, i.e. localized electrons

$$\int \phi^*(r - \rho) H \phi(r) dv = -\gamma$$

γ Is called the overlap integral. γ is a parameter that causes to be changed the energy levels to energy bands.



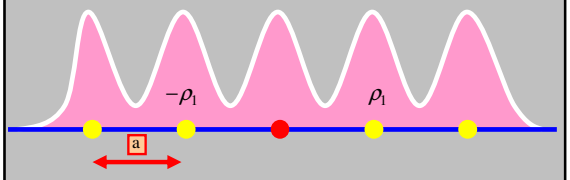
The band width depends on γ



$$E(k) = -\alpha - \gamma \sum_m e^{-ik.\rho_m}$$

Over nearest neighbors

For a 1D lattice:



$$E(k) = -\alpha - \gamma \sum_{m=-1}^{1} e^{-ik.\rho_m} = -\alpha - \gamma \left(e^{-ik.\rho_{-1}} + e^{-ik.\rho_1} \right)$$

$$= -\alpha - \gamma \left(e^{ika} + e^{-ika} \right) = -\alpha - \gamma (2\cos(ka))$$

$$E(k) = -\alpha - \gamma (2\cos(ka))$$

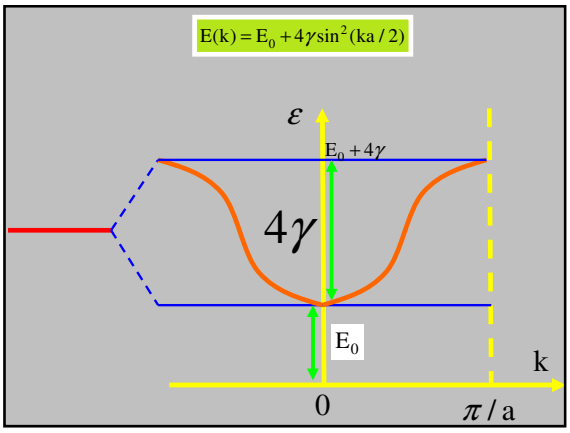
$$\cos(ka) = 1 - 2\sin^2(ka/2)$$

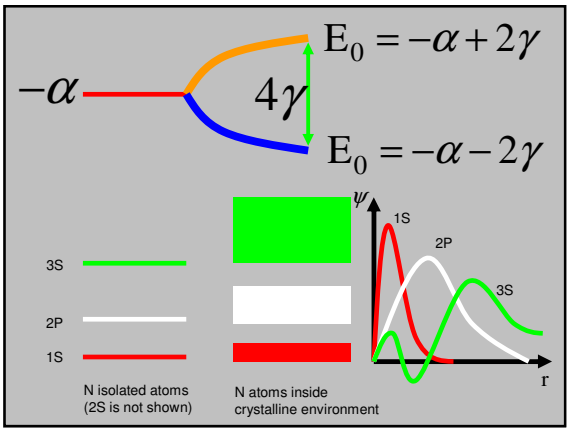
$$E(k) = -\alpha - \gamma \left(2 - 4\sin^2(ka/2) \right)$$

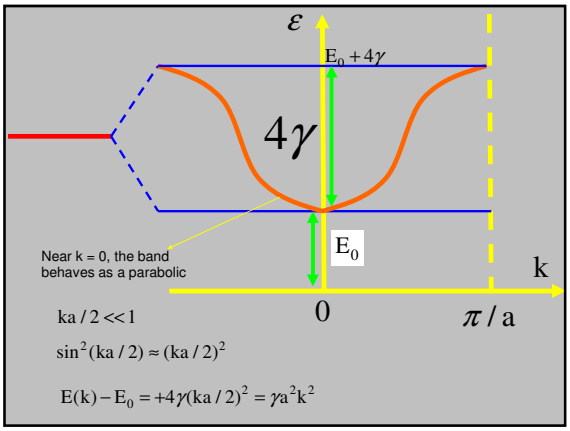
$$E(k) = -\alpha - 2\gamma + 4\gamma \sin^2(ka/2)$$

E_0

$$E(k) = E_0 + 4\gamma \sin^2(ka/2)$$







EFFECTIVE MASS

$$E(k) - E_0 = \gamma a^2 k^2$$

From the above band structure we observe that the mass of electron may be different with respect to the mass of a free electron.
For free electron we have:

$$E(k) - E_0 = \frac{\hbar^2 k^2}{2m}$$

$$m^* = \hbar^2 \left(\frac{\partial^2 E(k)}{\partial k^2} \right)^{-1}$$

$$m^* = \hbar^2 \left(\frac{\hbar^2 2}{2m} \right)^{-1} = m$$

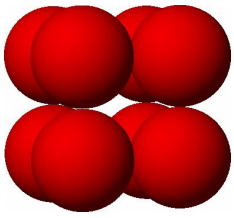
For the above TB electron:

$$E(k) - E_0 = \gamma a^2 k^2$$

$$m^* = \hbar^2 \left(\gamma a^2 2 \right)^{-1} = \frac{\hbar^2}{2\gamma a^2} \neq m$$

BAND STRUCTURE PLOTTING FOR A SIMPLE CUBIC LATTICE BASED ON TIGHT BINDING MODEL

$$\rho_m = (\pm a, 0, 0), (0, \pm a, 0), (0, 0, \pm a)$$



$$E(k) = -\alpha - \gamma \sum_{m=-3}^{3} e^{-i\mathbf{k}\cdot\boldsymbol{\rho}_m}$$

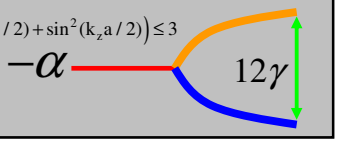
$$= -\alpha - \gamma \left(e^{ik_x a} + e^{-ik_x a} + e^{ik_y a} + e^{-ik_y a} + e^{ik_z a} + e^{-ik_z a} \right)$$

$$= -\alpha - 2\gamma \left(\cos(k_x a) + \cos(k_y a) + \cos(k_z a) \right)$$

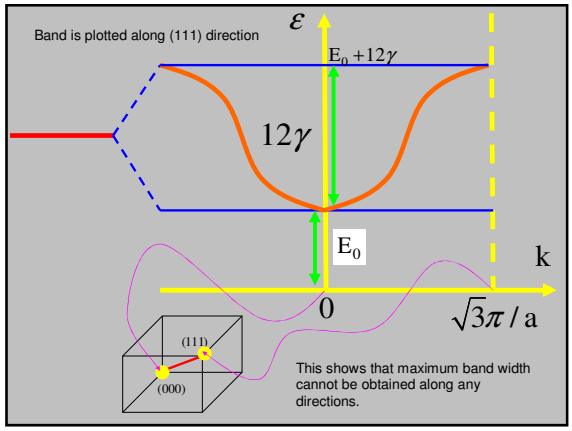
$$\cos(k_x a) = 1 - 2\sin^2(k_x a/2) \quad \cos(k_y a) = 1 - 2\sin^2(k_y a/2) \quad \cos(k_z a) = 1 - 2\sin^2(k_z a/2)$$

$$E(k) = \underbrace{-\alpha - 6\gamma}_{E_0} + 4\gamma \left(\sin^2(k_x a/2) + \sin^2(k_y a/2) + \sin^2(k_z a/2) \right)$$

$$0 \leq \left(\sin^2(k_x a/2) + \sin^2(k_y a/2) + \sin^2(k_z a/2) \right) \leq 3$$



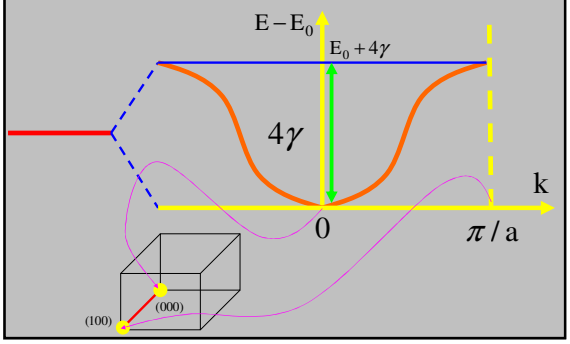
Band is plotted along (111) direction



This shows that maximum band width cannot be obtained along any directions.

How about the band width along (100) direction? $\Gamma(0,0,0) \longrightarrow X(k_x = \pi/a, k_y = 0, k_z = 0)$

$$E(k) - E_0 = 4\gamma\left(\sin^2(k_x a/2)\right) \qquad E_{max} = 4\gamma$$



Near the Γ point the band structure is spherical.

$$\left(\sin(k_x a/2) \approx k_x a/2,\ \sin(k_y a/2) \approx k_y a/2,\ \sin(k_z a/2) \approx k_z a/2\right)$$

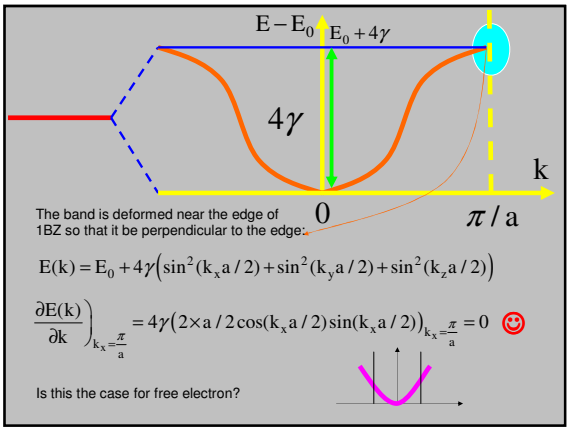
$$E(k) = E_0 + 4\gamma\left(\sin^2(k_x a/2) + \sin^2(k_y a/2) + \sin^2(k_z a/2)\right)$$

$$E(k) - E_0 \approx 4\gamma\left((k_x a/2)^2 + (k_y a/2)^2 + (k_z a/2)^2\right)$$

$$\approx \gamma a^2\left(k_x^2 + k_y^2 + k_z^2\right) = \gamma a^2 k^2$$

☺

To find the effective mass: $m^* = \hbar^2\left(\gamma a^2 2\right)^{-1} = \dfrac{\hbar^2}{2\gamma a^2} \neq m$



The band is deformed near the edge of 1BZ so that it be perpendicular to the edge:

$$E(k) = E_0 + 4\gamma\left(\sin^2(k_x a/2) + \sin^2(k_y a/2) + \sin^2(k_z a/2)\right)$$

$$\left.\frac{\partial E(k)}{\partial k}\right)_{k_x = \frac{\pi}{a}} = 4\gamma\left(2 \times a/2 \cos(k_x a/2)\sin(k_x a/2)\right)_{k_x = \frac{\pi}{a}} = 0$$ ☺

Is this the case for free electron?

ENERGY CONTOUR IN K-SPACE

In order to plot energy contour, we would first plot the Fermi surface, and then find intersections of an specific plane with the Fermi surface:

$$E(k) = -\alpha - 6\gamma + 4\gamma\left(\sin^2(k_x a/2) + \sin^2(k_y a/2) + \sin^2(k_z a/2)\right)$$

$$= \text{cons tan t}$$

$$\sin^2(k_x a/2) + \sin^2(k_y a/2) + \sin^2(k_z a/2) = \text{cons tan t}$$

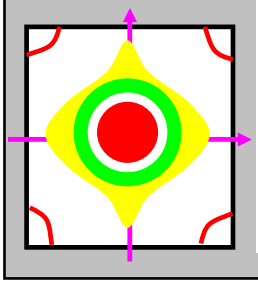
PRACTICE

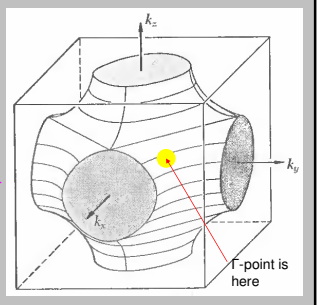
Plot the above Fermi surface in 3 wave vector space dimensional space.

The result of the last practice will be similar to the following Fermi surface:

Near the Γ-point the shape of the Fermi surface is spherical. But far from it the deviation is observed.

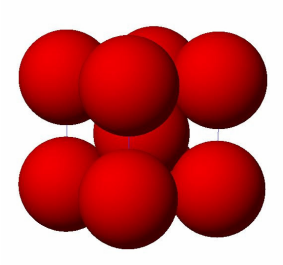
A typical energy contour can be as follows:





BAND STRUCTURE PLOTTING FOR A BODY CENTERED CUBIC LATTICE BASED ON TIGHT BINDING MODEL

$$\rho_m = (\pm a/2, \pm a/2, \pm a/2)$$



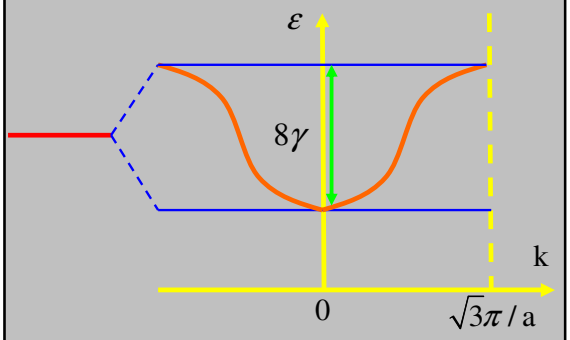
$$E(k) = -\alpha - \gamma \sum_{m=-3}^{3} e^{-i\mathbf{k}.\boldsymbol{\rho}_m}$$

$$= -\alpha - \gamma \left\{ e^{-i(k_x a/2 + k_y a/2 + k_z a/2)} + e^{i(k_x a/2 + k_y a/2 + k_z a/2)} + e^{-i(k_x a/2 - k_y a/2 + k_z a/2)} + e^{i(k_x a/2 - k_y a/2 + k_z a/2)} + e^{-i(k_x a/2 k_y a/2 - k_z a/2)} + e^{i(k_x a/2 - k_y a/2 - k_z a/2)} \right\}$$

$$E(k) = -\alpha - \gamma \{ 2\cos(k_x a/2 + k_y a/2 + k_z a/2) + 2\cos(k_x a/2 - k_y a/2 + k_z a/2) + 2\cos(k_x a/2 + k_y a/2 - k_z a/2) \}$$

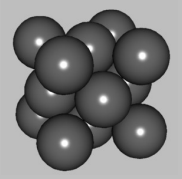
$$E(k) = -\alpha - 8\gamma \cos(k_x a/2)\cos(k_y a/2)\cos(k_z a/2)$$

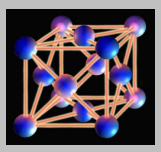
Band is plotted along (111) direction



PRACTICE

Find the band structure of a fcc lattice based on the tight binding model:





$$E(k) = -\alpha - 4\gamma \left(\cos(k_x a/2)\cos(k_y a/2) + \cos(k_x a/2)\cos(k_z a/2) + \cos(k_y a/2)\cos(k_z a/2) \right)$$

PRACTICE

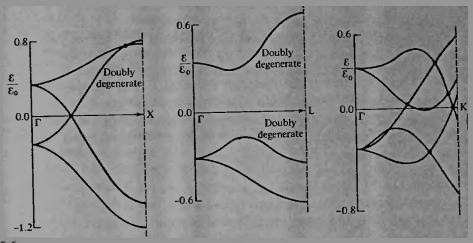


Figure 10.6
A tight-binding calculation of the 3*d* bands of nickel. (G. C. Fletcher, *Proc. Phys. Soc.* A65, 192 (1952).) Energies are given in units of $\mathcal{E}_0 = 1.349$ eV, so the bands are about 2.7 volts wide. The lines along which $\mathcal{E}$ is plotted are shown in Figure 10.5. Note the characteristic degeneracies along ΓX and ΓL, and the absence of degeneracy along ΓK. The great width of the bands indicates the inadequacy of so elementary a treatment.