BAND STRUCTURE CALCULATION IN TIGHT BINDING MODEL

\[ \psi_{\alpha} = \frac{1}{\sqrt{N}} \sum_{j} e^{i \mathbf{k} \cdot \mathbf{r}_j} \phi(\mathbf{r} - \mathbf{r}_j) \]

\[ \text{Crystal electron wave function} \]

\[ \text{Atomic electron wave function} \]

To calculate \( E(k) \) we do as follows:

\[ E(k) = \langle \psi_{\alpha} | H | \psi_{\alpha} \rangle = \int \psi_{\alpha}^{*} H \psi_{\alpha} \, dv \]

\[ E(k) = \frac{1}{N} \sum_{m} \sum_{j} e^{i \mathbf{k} \cdot (\mathbf{r}_m - \mathbf{r}_j)} \langle \phi(\mathbf{r} - \mathbf{r}_j) | H | \phi(\mathbf{r} - \mathbf{r}_j) \rangle \]

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

\[ \int \rho^*(\mathbf{r} - \mathbf{p}) H \rho(\mathbf{r}) \, dv = -\gamma \]

\( \gamma \) is called the overlap integral. \( \gamma \) is a parameter that causes to be changed the energy levels to energy bands.

\[ \gamma = 0 \quad \gamma \neq 0 \]

The band width depends on \( \gamma \)

For the isolated atom, i.e. localized electrons:

\[ E(k) = -\alpha - \gamma \sum_{n=1}^{\infty} e^{-\beta \rho_{n1}} \]

For a 1D lattice:

\[ E(k) = -\alpha - \gamma \left(2 \cos(ka)\right) \]

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

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

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

\[ E(k) = E_0 + 4\gamma \sin^2(ka/2) \]
BAND STRUCTURE PLOTTING FOR A SIMPLE CUBIC LATTICE BASED ON TIGHT BINDING MODEL

\[ \rho_m = (\pm a, 0, 0), (0, \pm a, 0), (0, 0, \pm a) \]

Near \( k = 0 \), the band behaves as a parabolic

\[ \frac{\hbar^2 k^2}{2m} \approx \frac{1}{2} \left( \frac{\hbar^2}{2m} \right)^2 \]

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

\[ m' = \frac{\hbar^2}{2\gamma a^2} \neq m \]

\[ E(k) = -\alpha - 6\gamma \left( \sin^2 \left( \frac{ka}{2} \right) + \sin^2 \left( \frac{ka}{2} \right) + \sin^2 \left( \frac{ka}{2} \right) \right) \]

\[ \sum_{n=0}^1 e^{-ikx} \]

\[ E(k) = -\alpha - 2\gamma \left( \cos(k_{1a}) + \cos(k_{2a}) + \cos(k_{3a}) \right) \]

\[ 0 \leq \left( \sin^2 \left( \frac{ka}{2} \right) + \sin^2 \left( \frac{ka}{2} \right) + \sin^2 \left( \frac{ka}{2} \right) \right) \leq 3 \]
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:

\[ E(k) = E_0 + 4\gamma \left( \sin^2\left(\frac{k_x}{a}/2\right) + \sin^2\left(\frac{k_y}{a}/2\right) + \sin^2\left(\frac{k_z}{a}/2\right) \right) \]

To find the effective mass:

\[ m^* = \frac{\hbar^2}{2\gamma a^2} = \frac{\hbar^2}{2m} \]

Near the \( \Gamma \) point the bandstructure is spherical.

\[
\begin{align*}
(\sin(k_x/a)/2) &= k_x/a/2, & (\sin(k_y/a)/2) &= k_y/a/2, & (\sin(k_z/a)/2) &= k_z/a/2
\end{align*}
\]

\[ E(k) = E_0 + 4\gamma \left( \sin^2\left(\frac{k_x}{a}/2\right) + \sin^2\left(\frac{k_y}{a}/2\right) + \sin^2\left(\frac{k_z}{a}/2\right) \right) \]

\[ E(k) - E_0 = 4\gamma \left( \sin^2\left(\frac{k_x}{a}/2\right) + \sin^2\left(\frac{k_y}{a}/2\right) + \sin^2\left(\frac{k_z}{a}/2\right) \right) \]

\[ = \gamma a^2 \left( k_x^2 + k_y^2 + k_z^2 \right) = \gamma a^2 k^2 \]

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

\[ E(k_x) - E_0 = 4\gamma \left( \sin^2\left(\frac{k_x}{a}/2\right) \right) \]

\[ E_{\text{max}} = 4\gamma \]

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

Near the \( \Gamma \) 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:

**Practice**

Plot the above Fermi surface in 3 wave vector space dimensional space.
BAND STRUCTURE PLOTTING FOR A BODY CENTERED CUBIC LATTICE BASED ON TIGHT BINDING MODEL

\[ \rho_m = (\pm a/2, \pm a/2, \pm a/2) \]

\[
E(k) = -\alpha - \gamma \sum_{m=1}^{3} e^{-ik_m}
= -\alpha - \gamma \left[ e^{-ik_x a/2} + e^{ik_x a/2} + e^{-ik_y a/2} + e^{ik_y a/2} + e^{-ik_z a/2} + e^{ik_z a/2} \right]
\]

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

PRACTICE

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

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

Figure 10.6

A tight-binding calculation of the 4 bands of an fcc lattice. It illustrates the intrinsic degeneracy of the lowest band at \( k = 0 \) and the absence of degeneracy along \( k \). The figure shows the bands along which \( E \) is plotted, as shown in Figure 10.3. Note the characteristic degeneracy along \( X \) and \( X \), and the absence of degeneracy along \( K \). The great width of the bands indicates the inadequacy of an elementary treatment.