Solid State Physics: Problem Set #10

Electronic Properties of Solids: Band Structure

Due: Friday Mar. 28 by 6 pm

Reading assignment: for Monday, 9.1 (Fermi surface and Landau levels)
for Wednesday, 9.6 (electrical resistance and band mass)
for Friday, 9.7-9.8 (electrons and holes)

Problem assignment:

Chapter 7 Problems: 7.4 fcc band structure - empty lattice approximation

*A1. *CuZn alloy (brass)*. Brass is an alloy of copper and zinc in which some atoms in the fcc copper crystal are replaced by zinc. Since copper is monovalent and zinc is divalent, as the fraction of zinc to copper increases the valence electron concentration increases. This particular alloy is only stable up to a certain maximum zinc concentration. This stability limit can be identified with the point at which the free-electron Fermi sphere touches the first Brillouin zone boundary. Determine this maximum zinc to copper ratio. **[Melissa]**

A2. *Tight binding model*. In this approximation (also known as LCAO or linear combination of atomic orbitals) the electron wavefunction in an *N*-atom crystal is written as a sum of free atom wavefunctions as follows

$$\psi_k(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} C_{kj} \phi(\vec{r} - \vec{r}_j)$$

where $\phi(\vec{r})$ is the electron wavefuntion in an isolated atom and $\vec{r}_j$ is the position of atom *j*. For a periodic potential, the wavefunction must be of the Block form which requires $C_{kj} = \exp(i\vec{k} \cdot \vec{r}_j)$. The electron energy is given by the expectation value of the Hamiltonian operator as follows

$$E_k = \int \psi_k^*(\vec{r}) \hat{H} \psi_k(\vec{r}) d\vec{r} = \frac{1}{N} \sum_j \sum_m C_{jk}^* C_{mk} \int \phi^*(\vec{r} - \vec{r}_j) \hat{H} \phi(\vec{r} - \vec{r}_m) d\vec{r} .$$

In the tight binding approximation we only consider those terms where *j*=*m* and for which *j* and *m* are nearest neighbor sites.

a) Show that the above tight-binding energy can be written as

$$E_k = \varepsilon_0 - \gamma \sum_m e^{-i\vec{k} \cdot \vec{\delta}_m}$$

where the vectors $\vec{\delta}_m$ connect an atom to its nearest neighbors, $-\varepsilon_0$ is the electron energy in the isolated atom, and, in the case of spherically symmetric s-type orbitals,

$$\gamma = \int \phi^*(\vec{r} - \vec{\delta}) \hat{H} \phi(\vec{r}) d\vec{r}$$

is the "overlap" integral for nearest neighbor sites in the crystal.

b) Show that for the simple cubic lattice the tight binding energy can be written as

$$E_k = -\varepsilon_0 - 2\gamma(\cos k_x a + \cos k_y a + \cos k_z a).$$

*c) Show that for the fcc lattice the tight binding energy can be written as

$$E_k = -\varepsilon_0 - 4\gamma(\cos k_y a/2 \cos k_z a/2 + \cos k_z a/2 \cos k_x a/2 + \cos k_x a/2 \cos k_y a/2). \quad \textbf{[Peter]}$$

A3. *Tight binding energy in the 2D square lattice*.

a) Show that the tight binding energy (see A2) for the 2D square lattice can be written as

$$E_k = -\alpha - 2\beta(\cos k_x a + \cos k_y a)$$

b) Use the Maple **contourplot()** function to plot equal energy lines within the first Brillouin zone for the square lattice. The Maple syntax is as follows:

```
with(plots);
contourplot(f(x,y),x=x1..x2,y=y1..y2, contours=20);
```

(Compare your result with Fig. 7.12)

A4. *Fermi surfaces from the tight binding approximation*. The Maple function **implicitplot3d()** can be used to visualize the Fermi surfaces predicted by the tight binding model. The Maple syntax is as follows:

```
with(plots);
implicitplot3d(f(x,y,z)=a, x=x1..x2, y=y1..y2, z=z1..z2, grid=[16,16,16]);
```

Using the results of Problem A2:

a) Plot the Fermi surface for a simple cubic lattice for $E_k = -\alpha - 4.0\beta$ and $E_k = -\alpha - 1.0\beta$. Let $-\pi/a \le k_x, k_y, k_z \le \pi/a$.

b) Plot the Fermi surface for the fcc lattice for $E_k = -\alpha - 8.0\beta$, $E_k = -\alpha - 1.0\beta$, and $E_k = -\alpha + 0.4\beta$. Let $-2\pi/a \le k_x, k_y, k_z \le 2\pi/a$. (Compare the latter result with Fig. 9.1).

c) For the fcc lattice, determine the energy at which the Fermi surface first crosses the zone boundary. Plot this Fermi surface.

Note: For Maple 3D plots, by clicking on the plot and then dragging the mouse, you can rotate them to get the view from all angles. Try it!!

*To be presented in class on Friday.