§10 – Fermi Surface

10.1 Fermi Surface

Let us return to the electronic properties of solids. We have considered some important concepts in solid state physics:

1. The reciprocal lattice;
2. The free electron model;
3. Opening of band gaps.

We want to look at the details of how these can be combined to produce special properties of metals.

10.2 Reduced Zone Scheme

The free electron model ignores the crystal lattice, so there are no zones. However, as soon as we introduce band gaps, we have to keep track of them in three-dimensions.

The tight-binding approximation inherently incorporates the crystal lattice. The resulting band structure is strictly periodic. All electrons in tight-binding crystals obey Bloch's theorem:

$$\psi(\vec{r}) = \exp\left(i\vec{k}\cdot\vec{r}\right)u_k(\vec{r}) \tag{10.1}$$

Where: u_k is a periodic function.

The first Brillouin zone is the unique volume of reciprocal space surrounding the origin. Any wavevector can be mapped onto the first Brillouin zone by addition of a reciprocal lattice vector:

$$\forall \vec{k}\,;\ \ \vec{k}\,' = \vec{k} + \vec{G} \tag{10.2}$$

So, we can write the Bloch wave as:

$$\psi_k(\vec{r}) = \exp\left(i\vec{k}\,'\cdot\vec{r}\right)\underbrace{\left(\exp\left(-i\vec{G}\cdot\vec{r}\right)u_k(\vec{r})\right)}_{=u_{k'}(\vec{r})} \tag{10.3}$$

This new function $u_{k'}$ is also periodic, since the exponential term is periodic by construction.

Once we map k onto k', we have an equivalent Bloch wave within the first Brillouin zone.

All possible states can be mapped into the first Brillouin zone in this manner. Multiple states for each Bloch vector are independent.: they have the same plane wave term, but different u_k functions and different energies.

10.3 Periodic Zone Scheme

The periodic zone scheme involves shifting all Bloch vectors by all possible values of the reciprocal lattice vector. This is equivalent to a repetition of the reduced zone scheme over all *k*-space.

The energies are the same in all of these copies, so the band structure is periodic. The wavefunctions u_k are similar but not identical because they have an extra $e^{-\vec{G}\cdot\vec{r}}$ term.

The periodic zone scheme is particularly useful for bands that are naturally periodic, such as those considered in the tight-binding approximation. For example, for a simple cubic lattice, we had $\epsilon_k = -\alpha - 2\gamma\left(\cos(k_x a)+\cos(k_y a)+\cos(k_z a)\right)$.

So, we have three zone schemes:

1. Extended zone scheme;
2. Reduced zone scheme;
3. Periodic zone scheme.

All three can be seen in Fig. 10.1 below:

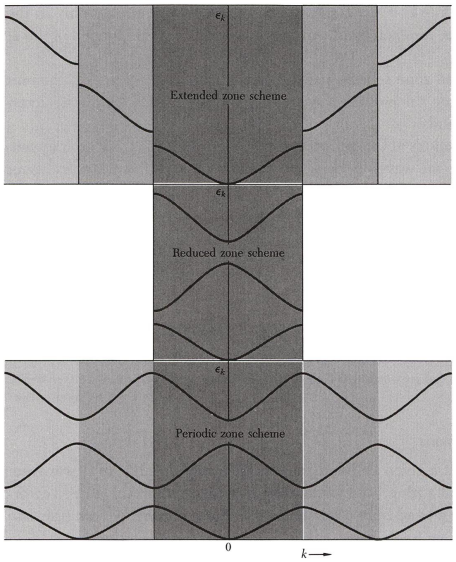

Figure 10.1: Three energy bands plotted in (a) extended (Brillouin) (b) reduced, and (c) periodic zone schemes.