Lecture XX VI
Fermi Surfaces and Metals

Yu-Jun Zhao
Department of Physics, SCUT

www.compphys.cn/~zhaoyj/lectures/
The Fermi surface is the surface of constant energy $\varepsilon_F$ in $k$ space.

The Fermi surface separates the unfilled orbitals from the filled orbitals at absolute zero $T = 0K$.

Few people would define a metal as ‘a solid with a Fermi surface.’ This may nevertheless be the most meaning definition of a metal one can give today; it represents a profound advance in the understanding of why metals behaves as they do.
An example of the Fermi surface of superconducting cuprates measured by ARPES.

How about Fermi surface for an insulator?

The large Fermi surface predicted by band theory is observed by ARPES and STS for overdoped copper oxides (bottom right).

doi:10.1038/nature14165
Reduced zone scheme

It is always possible to select the wavevector index $k$ of any Bloch function to lie within the first Brillouin zone.

Prove: suppose $\psi_{-k}^-(\vec{r})$ is a Bloch function, and

$$\psi_{-k}^-(\vec{r}) = e^{i\vec{k}' \cdot \vec{r}} u_{-k}^-(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} (e^{-i\vec{G} \cdot \vec{r}} u_{-k}^-(\vec{r}))$$

Define $u_{-k}^+'(\vec{r}) \equiv e^{-i\vec{G} \cdot \vec{r}} u_{-k-G}^-(\vec{r})$

$$u_{-k}^+'(\vec{r} + \vec{T}) = e^{-i\vec{G} \cdot (\vec{r} + \vec{T})} u_{-k-G}^-(\vec{r} + \vec{T}) = e^{-i\vec{G} \cdot \vec{T}} e^{-i\vec{G} \cdot \vec{r}} u_{-k-G}^-(\vec{r})$$
$$= e^{-i\vec{G} \cdot \vec{r}} u_{-k-G}^-(\vec{r}) = u_{-k}^+'(\vec{r})$$

Then

$$\psi_{-k}^-(\vec{r}) = u_{-k}^+'(\vec{r}) e^{i\vec{k} \cdot \vec{r}} = \psi_{-k}^-(\vec{r})$$

We can always mapping the band in the reduced zone scheme.
In the reduced zone scheme, one can find different energies at same value of wavevector. Each different energy characterizes a different band.

Two wavefunctions at same \( k \) but different energies will be independent of each other: the wavefunctions will be made up of different combination of the plane waves \( \exp[i(\vec{k} + \vec{G}) \cdot \vec{r}] \).
Periodic zone scheme

We can repeat a given Brillouin zone periodically through all wavevector space.

We can translate not only a band from other zones into the first zone, but also a band in first zone into every other zones in the periodic zone scheme.

\[ \varepsilon_{\bar{k} + \bar{G}} = \varepsilon_{\bar{k}} \]

Here \( \varepsilon_{k+G} \) is understood to refer to the same energy band as \( \varepsilon_k \).

Extended zone scheme
Extended zone scheme

Reduced zone scheme

Periodic zone scheme
Construction of Fermi surface

The equation of the zone boundaries is \(2k \cdot G + G^2 = 0\) and is satisfied if \(k\) terminates on the plane normal to \(G\) at the midpoint of \(G\).
The free electron Fermi gas in a square lattice

Mapping of the 1st, 2nd and 3rd Brillouin zone in the reduced zone scheme.

The free electron Fermi surface in the extended zone scheme.

The free electron Fermi surface in the reduced zone scheme.
The parts of the free electron Fermi surface in the third zone appear disconnected as drawn in the reduced zone scheme.

The free electron Fermi surface in the third zone as drawn in the periodic zone scheme.
Nearly free electrons

We can make approximate constructions freehand by the use of four facts:

- The interaction of the electron with the periodic potential of the crystal causes energy gaps at zone boundaries.

- Almost always the Fermi surface will intersect zone boundaries perpendicularly.

- The crystal potential will round out sharp corners in the Fermi surfaces.

- The total volume enclosed by the Fermi surface depends only on the electron concentration and is independent of the details of the lattice interaction.
Constant energy surface in the Brillouin zone of a simple square lattice with nearly free electron approximation.

Constant energy surface is **discontinuous** at Brillouin zone boundary.

The free electron Fermi surface at 2\textsuperscript{nd} and 3\textsuperscript{rd} zones.

The near free electron Fermi surface at 2\textsuperscript{nd} and 3\textsuperscript{rd} zones. (Hole like, Electron like)
A full filled band:
1) Plot the reciprocal lattice

2) Plot the free-electron Fermi spheres around each lattice point with the radius appropriate to the electron concentration.

For a given 1st BZ region:

Any point in $k$ space that lies within at least one sphere corresponds to an occupied state in 1st zone. Points within at least two spheres correspond to occupied states in 2nd zone, and similarly for points in three spheres in 3rd zone, and so on.
Alkali metals have weak interactions between the conduction electrons and the lattice. Because the alkali metals have only one valence electron per atom, the first Brillouin zone boundaries are distant from the approximately spherical Fermi surface that filled one-half of the volume of the zone.

The divalent metals, e.g. Be and Mg, also have weak lattice interactions and nearly spherical Fermi surface. But because they have two valence electrons each, the Fermi surface encloses twice the volume in $k$ space as for the alkalis, i.e. the volume enclosed by the Fermi surface is exactly equal to that of the a zone. But the Fermi surface is nearly spherical which extends out of the first zone and into the second zone.
The free electron Fermi surfaces for fcc cubic metals of valence 2 and 3.

NB: value of $k_F$
Electron orbits, hole orbits, and open orbits

In a static magnetic field, electrons move on a curve of constant energy on a plane normal to $\mathbf{B}$. An electron on the Fermi surface will move in a curve on the Fermi surface. Three types of orbits:

Orbits that enclose filled states are electron orbits.
Orbits that enclose empty states are hole orbits.
Orbits that move from zone to zone without closing are open orbits.

\[ \hbar \frac{dk}{dt} = -\frac{e}{c} \mathbf{v} \times \mathbf{B} = -\frac{e}{\hbar^2 c} \nabla \mathbf{v} \times \mathbf{B} \]
Figure 15 Constant energy surface in the Brillouin zone of a simple cubic lattice, for the assumed energy band $\varepsilon_k = -\alpha - 2\gamma(\cos k_x a + \cos k_y a + \cos k_z a)$. (a) Constant energy surface $\varepsilon = -\alpha$. The filled volume contains one electron per primitive cell. (b) The same surface exhibited in the periodic zone scheme. The connectivity of the orbits is clearly shown. Can you find electron, hole, and open orbits for motion in a magnetic field $B\hat{z}$? (A. Sommerfeld and H. A. Bethe.)
Calculation of energy bands

- Tight binding method for energy bands

The tight binding approximation or LCAO (linear combination of atomic orbitals) approximation starts out from the wavefunctions of the free atoms.

The tight binding approximation is quite good for the inner electrons of atoms, but it is not a good description of the conduction electrons.

Suppose that the ground state of an electron moving in the potential $U(r)$ of an isolated atom is $\varphi(r)$. If the influence of one atom on another atom is small, we obtain an approximate wavefunction for one electron in the whole crystal by

$$\psi_{k}(\vec{r}) = \sum_{j}^{N} C_{kj} \varphi(\vec{r} - \vec{r}_j)$$

Atomic orbital wavefunction
This function is of the Bloch form if \( C_{kj} = N^{-1/2} e^{i\vec{k} \cdot \vec{r}_j} \)

Then

\[
\psi_k(\vec{r}) = N^{-1/2} \sum_j \exp(i\vec{k} \cdot \vec{r}_j) \phi(\vec{r} - \vec{r}_j)
\]

Prove:

\[
\psi_k(\vec{r} + \vec{T}) = N^{-1/2} \sum_j \exp[i\vec{k} \cdot (\vec{r}_j)] \phi(\vec{r} + \vec{T} - \vec{r}_j)
\]

\[
= \exp(i\vec{k} \cdot \vec{T}) N^{-1/2} \sum_j \exp[i\vec{k} \cdot (\vec{r}_j - \vec{T})] \phi[\vec{r} - (\vec{r}_j - \vec{T})]
\]

\[
= \exp(i\vec{k} \cdot \vec{T}) \psi_k(\vec{r})
\]
The first-order energy

\[ \varepsilon_k = \langle \vec{k} | H | \vec{k} \rangle = N^{-1} \sum_j \sum_m \exp[i\vec{k} \cdot (\vec{r}_j - \vec{r}_m)] \langle \varphi_m | H | \varphi_j \rangle \]

where \( \varphi_m \equiv \varphi(\vec{r} \cdots \vec{r}_m) \).

Set \( \vec{\rho}_m = \vec{r}_m - \vec{r}_j \),

\[ \langle \vec{k} | H | \vec{k} \rangle = \sum_m \exp(i\vec{k} \cdot \vec{\rho}_m) \int dV \varphi^* (\vec{r} - \vec{\rho}_m) H \varphi(\vec{r}) \]

Neglect all integrals except those on the same atom and those between nearest neighbors. We write:

\[ \int dV \varphi^* (\vec{r}) H \varphi(\vec{r}) = -\alpha; \quad \int dV \varphi^* (\vec{r} - \vec{\rho}_m) H \varphi(\vec{r}) = -\gamma. \]

Then

\[ \varepsilon_k = \langle \vec{k} | H | \vec{k} \rangle = -\alpha - \gamma \sum_m \exp(-i\vec{k} \cdot \vec{\rho}_m) \]
For a **simple cubic structure**, the nearest-neighbor atoms are

$$\vec{\rho}_m = (\pm a, 0, 0); \ (0, \pm a, 0); \ (0, 0, \pm a).$$

Then

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

The energies are confined to a band of width $12\gamma$.

In the limit $ka \ll 1$, $\varepsilon_k \approx -\alpha - 6\gamma + \gamma k^2 a^2$. The effective mass is

$$m^* = \hbar^2 / 2\gamma a^2$$
For the **bcc structure** with eight nearest neighbors,

\[ \varepsilon_k = -\alpha - 8\gamma \cos \frac{k_x a}{2} \cos \frac{k_y a}{2} \cos \frac{k_z a}{2} \]

For the **fcc structure** with twelve nearest neighbors,

\[ \varepsilon_k = -\alpha - 4\gamma \left( \cos \frac{k_y a}{2} \cos \frac{k_z a}{2} + \cos \frac{k_z a}{2} \cos \frac{k_x a}{2} + \cos \frac{k_x a}{2} \cos \frac{k_y a}{2} \right) \]

\( \gamma \) is the overlap integral. The weaker the overlap, the narrower is the energy band, and the higher is the effective mass.