SCPY 371: Solid State Physics **1st Semester 2021**

Lecture 9: Metals and Fermi surfaces

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In this chapter, we will learn about another group of materials, that is, metals. From the previous chapter, we know that metals are a group of materials with the unfilled top-most band. However, we do not know what this unfilled band looks like. Therefore, here we will focus on how to determine the shape of this band or what we will call **Fermi surface** in metals.

9.1 Fermi surfaces

For simplicity, we will first start with again the free electron model in one dimension. Then we will add electron-lattice interaction and generalize to the three-dimensional case later. For the free electron model, the dispersion relation can be described by a simple quadratic equation. Now let us imagine that we add electrons to this dispersion. The first electron will go the lowest state and when the number of electrons increases, so does the maximum energy. This maximum energy is what we called the **Fermi level**. The Fermi surface indicates the surface with energy equal to the Fermi level. Note that the Fermi surface in one dimension is a lone segment.

Now if we include a weak interaction between electrons and lattice, we will find that the dispersion can be mapped into the first Brillouin zone as we have discussed before. That means, if we keep adding electrons and the Fermi level keeps rising, then at some point the energy will be beyond the first Brillouin zone and we have to map it back to the first Brillouin zone. This is in fact the origin of the band structure that you are now all familiar. Therefore, the Fermi level is now on the second band. We can now imagine that if we keep adding electrons more bands will be filled and Fermi level keeps rising. Hence, the shape of the Fermi surface will also change depending the shape of the band and hoe high the Fermi level in that band. In two dimensions, we will have to think of the Fermi level as a radius of a circle and in three dimensional as a radius of a sphere. In particular, in the free-electron model in three dimensions, the Fermi surface is constructed from a sphere of radius $\vec{k}_F$, which depends on the value of electron concentrations or the number of electrons in a unit cell. Below will learn how to construct the fermi surface but first we will remind ourselves how to think of or draw the dispersion relation. There are three schemes to think of the dispersion relation.

1. **Extended zone scheme**: In this case, we will divide the dispersion into different zone and the different bands belong to the different zone. Therefore, in this case, there are the second, third, forth, and so on Brillouin zones beyond the first Brillouin zone.

2. **Reduced zone scheme**: In this case, we will only draw all bands in one zone by mapping the dispersion at high energy back to the first Brillouin zone.

3. **Periodic zone scheme**: In this case, the first Brillouin zone of the reduced zone scheme is drawn repeatedly for every zone.

The next question that we have to answer is that how we can divide the momentum space into different Brillouin zones.

Construction of Brillouin zones At the beginning of this course, we have already learned how to construct the first Brillouin zone and may have touch on the construction of higher-order zone. However, let us again see how the construction goes.

1. Draw a straight line from the origin to nearest, second nearest, third nearest and so forth neighbors.
2. Draw a line bisecting and perpendicular to the the line in drawn in No. 1.
3. The inner most enclosed area is called the first Brillouin zone. The next layer of surfaces is the second Brillouin zone and so on.

The Fermi surface is defined to be the outer most Brillouin zone with states occupied by electrons assumed that the Fermi level is a sphere for a three-dimensional lattice.

In Kittel, there is an example of a square lattice. Once the Brillouin zones are constructed, we then draw a Fermi level, in this case, we will assume that the Fermi level is a sphere. Note that this is only the case for the free electron model. The overlapping area of the sphere and the Brillouin zones indicate the area of occupied states. Therefore, the boundary between the occupied states and unoccupied states indicates the Fermi surfaces. We will have to use the reduced zone scheme to map those occupies are or states back to the first Brillouin zone.

There is another construction of Fermi surfaces, which is credited to Harrison. In this construction, the spheres of radius $|\vec{k}_F|$ are draw at all centers of the first Brillouin zone. The occupied states in the first Brillouin zone are indicated by the area which is enclosed by at least one sphere. Those in the second Brillouin zone are indicated by the area which is enclosed by at at least two sphere and so on. I think you get the idea. At the end, these two methods of constructing the Fermi surfaces yield the same result.

Nearly free electrons Now we will go beyond the free electron model and include the electron-lattice interaction. However, we will assume that this interaction is still quite small. Once the interaction between electrons and lattice is included, we can redraw the Fermi surfaces keeping in mind the following facts:

1. The interaction cause the opening of energy gaps at the zone boundaries.
2. The Fermi surface *almost always* is normal to the zone boundaries.
3. The periodic potential from nucleuses will make the sharp corners of the Fermi surface smooth.
4. The total area enclosed by the sphere of the Fermi level does not depend on the electron-lattice interaction. It only depends on the number of electron in a unit cell or electron concentration.

In this class, we will not attempt to calculate the detailed band structure and will not be interested in the quantitive detail of the Fermi surfaces. Therefore, we will only try to get a qualitative description of the Fermi surface in order to understand physics of metals in general.

9.2 Measurements of Fermi surfaces

In this section, we will learn how we can measure the Fermi surfaces in metals. The shape of Fermi surfaces affect many physical properties of metals. Therefore, there are several methods of measuring the Fermi surfaces. These methods include magnetoresistance, anomalous skin effect, cyclotron resonance, magneto-acoustic geometric effects, the Subnikov-de Haas effect, and the de Haas-van Alphen effect. In this class, we will not consider all of these effects but will focus on only one, that is, the de Haas-van Alphen effect. This method relies on the fact that the electron orbit is quantized in magnetic field. We will learn about the basic theory behind this effect.

Quantization of electron orbit in magnetic field In the presence of magnetic field, electron momentum can be written as

$$\vec{p} = \vec{p}_{\text{kin}} + \vec{p}_{\text{m}} = \hbar\vec{k} + q\vec{A},$$

where the last term refers to the momentum due to the magnetic field. Next, we will apply the Bohr-Sommerfeld relation to express the quantization of the orbits in the magnetic field:

$$\oint \vec{p} \cdot d\vec{r} = (n+\gamma)2\pi\hbar,$$

where γ is the phase correction factor and equal to $\frac{1}{2}$ for free electrons. From the expression of momentum, we obtain

$$\oint \vec{p} \cdot d\vec{r} = \oint \hbar\vec{k} \cdot d\vec{r} + q \oint \vec{A} \cdot d\vec{r}$$

From the equation of motion for electron, we have

$$\begin{aligned} \frac{d\vec{p}}{dt} &= q\vec{v} \times \vec{B} \\ \Rightarrow \quad \hbar\frac{d\vec{k}}{dt} &= q\frac{d\vec{r}}{dt} \times \vec{B} \\ \Rightarrow \quad \hbar\vec{k} &= q\vec{r} \times \vec{B}. \end{aligned}$$

Therefore, we can write

$$\oint \hbar\vec{k} \cdot d\vec{r} = q \oint \vec{r} \times \vec{B} \cdot d\vec{r} = -q\vec{B} \cdot \oint \vec{r} \times d\vec{r} = -2q\Phi,$$

where $\oint \vec{r} \times d\vec{r} = 2A$ where A is the area enclosed by the orbit. For the other term, we can apply the Stokes theorem to obtain

$$q \oint \vec{A} \cdot d\vec{r} = q \int \nabla \times \vec{A} \cdot d\sigma = q\Phi.$$

Therefore, at the end, we have the following relation for the quantization of the orbits

$$\oint \vec{p} \cdot d\vec{r} = -q\Phi = (n+\gamma)2\pi\hbar.$$

This equation imply that the magnetic flux of electrons in the orbits is quantized, that is,

$$\Phi_n = (n+\gamma)\frac{2\pi\hbar}{e},$$

where we have replaced q by $-e$ for electron charge. The unit of the quantization of flux is equal to $\frac{2\pi\hbar}{e}$. Now we have to find the relation between the quantization of magnetic flux with the area in the reciprocal space. First we note that from the equation of motion

$$\Delta r = \frac{\hbar}{eB}\Delta k,$$

that is,

$$A_n = \left(\frac{\hbar}{eB}\right)^2 S_n$$

where A_n and S_n are the areas in the real and reciprocal space, respectively. Since $\Phi_n = BA_n$, it follows that

$$\Phi_n = BA_n = \left(\frac{\hbar}{e}\right)^2 \frac{1}{B} S_n = (n+\gamma)\frac{2\pi\hbar}{e},$$

that is

$$S_n = (n+\gamma)\frac{2\pi e}{\hbar}B.$$

From this equation, we can see that the area in the reciprocal space is proportional to the magnetic field. Therefore, by increasing B from orbits n to $n+1$, we can see the change in the area of the Fermi surface in the reciprocal space by a unit of $\frac{2\pi e}{\hbar}$, that is,

$$S\left(\frac{1}{B_{n+1}}-\frac{1}{B_n}\right)=\frac{2\pi e}{\hbar}$$

This periodic change in the Fermi surface with respect to the magnetic field give rise to the oscillation of other physical measurable properties. If the oscillation is measured in the magnetic moment, then we will call that phenomenon the **de Hass-van Alphen** effect. But if the oscillation is measured in the electrical resistivity, the we will call the phenomenon the **Shubnikov-de Haas** effect. In this class, we will only consider the de Haas-van Alphen effect. However, the physics of the the Shubnikov-de Haas effect is the same.

de Haas-van Alphen Effect Now we will try to explain the oscillation of the measured magnetic moment in magnetic field. The de Haas-van Alphen is the result of the quantization of the magnetic flux which we discussed above. In the measurement, we can observe this effect in a pure sample where the collision with impurity is kept at minimal and the measurement should be done at as low temperature as possible to decrease the thermal population of the higher Landau levels.

For simplicity, we will only consider the case at $T=0$ K. The area in the $\vec{k}$ space for each Landua level is equal to

$$\Delta S = S_{n+1}-S_n=\frac{2\pi e}{\hbar}B.$$

But we know that the area of one state is equal to $(2\pi/L)^2$, where L is the size of the sample. Note that we ignore the spin degree of freedom. Therefore, the number of states for each Landau level is equal to

$$D(B)=\frac{2\pi eB}{\hbar}\left(\frac{L}{2\pi}\right)^2\propto B.$$

As we can see that as B increases, each Landau level can also affords more electrons. Now we will consider the consequence of this result. Suppose that there are N electrons in the system. Let B_s be a critical field at which all levels are completely filled up to the $s+1^{th}$ level and the next level is empty. Then we have to following relation

$$N=sD(B_s)$$

Now suppose that we increase the magnetic field. Since D for each level increases, more electrons can be in the lower levels. Therefore, the s^{th} becomes partially filled. And the number of electrons in this level is equal to

$$n_s=N-sD(B).$$

where $B>B_s$ The total energy for the filled level is equal to

$$\sum_{n=1}^{s}D\hbar\omega_c\left(n-\frac{1}{2}\right)=\frac{1}{2}D\hbar\omega_c s^2,$$

where $\omega_c=eB/m^\star$. And for the partially filled level that lies on top of the filled level, the energy of that level is equal to

$$\left(s+\frac{1}{2}\right)\hbar\omega_c(N-sD).$$

Therefore, the total energy is the sum of the above two terms and plotted as a function of $1/B$.

In order to calculate the magnetization, we first need to calculate the total energy of the electrons and the magnetization can be calculated using $\mu = -\frac{\partial U}{\partial B}$. The oscillation of μ occurs as the Landau level change from being filled to partially filled and back to being filled again. And the period of this oscillation is equal to

$$\Delta\left(\frac{1}{B}\right) = \frac{2\pi e}{\hbar S},$$

where is the extremal area which will contribute the most to the response.

Example of Fermi surface in Cu Copper is the fcc lattice and the shortest distance across the first Brillouin zone is

$$\frac{2\pi}{a}3^{1/2} = \frac{10.88}{a}.$$

For the monovalent metal, the concentration of electron per unit cell is equal to

$$n = \frac{4}{a^3},$$

where there are four Cu in the unit cell for the fcc lattice. Hence, the radius of the Fermi level extends to

$$k_F = \left(3\pi^2 n\right)^{1/3} = \frac{4.90}{a}.$$

Hence, the diameter of the Fermi sphere is equal to $\frac{9.80}{a}$, which is the Fermi sphere is contained within the first Brillouin zone. However, since there are energy gaps at the boundaries that tend to lower the energy near the zone boundaries. Therefore, the Fermi level is not spherical and can stick out from the first Brillouin zone.

Measuring Fermi surface of gold In this example, we will try to calculate the extremal area of the Fermi surface given the period of the magnetization oscillation. Suppose that the period of the magnetization oscillation for gold measured along the [111] direction is 2×10^{-9} gauss^{-1} which corresponds to

$$S = \frac{2\pi e}{\hbar}\frac{1}{\Delta(1/B)} = 4.8 \times 10^{16} \quad \text{cm}^{-2}$$

In addition, the second strong oscillation is also observed at the period of 6×10^{-8} gauss^{-1}, which corresponds to the area of 1.6×10^{15} gauss^{-2}. This smaller area indicate the neck area at the zone boundaries. Another extremal orbit is the 'dog's bone' see Fig. 9.2.

References

[1] Kittel, C.: Introduction to Solid State Physics 7$^{\text{th}}$ Edition (Chapter 3), John Wiley & Sons, Inc. (1996).

[2] Ashcroft, N. W. and Mermin, N. D.: Solid State Physics (Chapter 20), Thomson Learning, Inc. (1976).

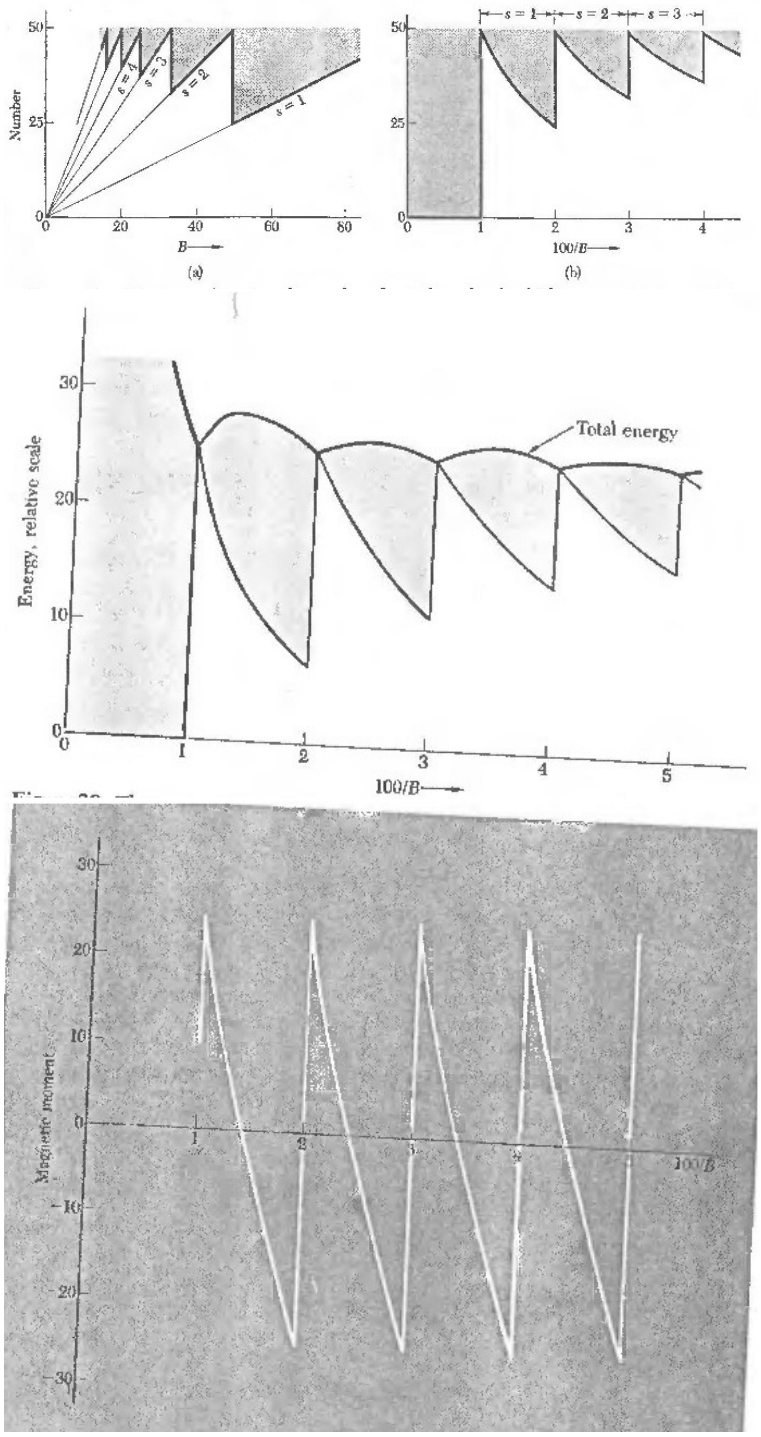

Figure 9.1: Landau levels. The figures are taken from Kittel.

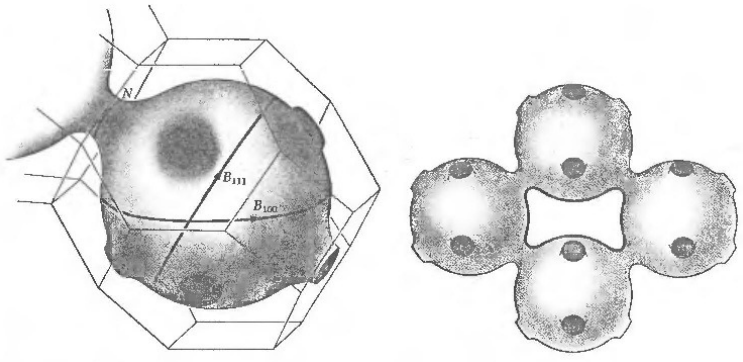

Figure 9.2: Fermi surfaces of copper show the 'neck' and 'dog's bone' orbits. The figure is taken from Kittel.