Nearly Free Electron Fermi Gas

1. Strengths and weaknesses of the free electron Fermi gas

The free electron Fermi gas was good for explaining the heat capacity of metals and the thermal and electrical conduction of metals. The Fermi nature of the gas (obeying the Pauli Exclusion Principle) created many closely spaced energy levels ($\varepsilon_n=\hbar^2k_n^2/2m$, $k_n = n2\pi/L$) that we will now start calling the **energy band**.

It was not able to distinguish insulators from semiconductors from metals, nor was it able to explain why some materials had Hall coefficients that were positive. It also predicted only one energy band for any material.

2. Nearly Free Electron Fermi Gas: a semi-quantitative argument

This model assumes that the free electron Fermi gas we dealt with previously is **perturbed only slightly by the periodic potential of the ion cores**. The wavefunction, ψ, for the electrons is assumed to be essentially the same: that is, $\psi(x,t) = X(x)T(t)$ where $X(x) = A\sin(kx+\theta)$ [or alternately, $X(x) = \boldsymbol{A}e^{ikx}$ where the complex constant, $\boldsymbol{A}$, contains the phase constant, θ: $\boldsymbol{A} = A_{real}e^{i\theta}$].

The influence of the ion cores comes in just as it did for x-ray diffraction (Bragg diffraction): when $\mathbf{k} = \frac{1}{2}\mathbf{G}$ we get standing waves set up and the (this time electron instead of EM [x-ray]) wave does not propagate through the material. Recall that a standing wave is one in which there are actually two waves of the same wavelength and approximately the same amplitude going in opposite directions - a condition often due to the reflection of a wave such as what happens in a guitar string when the string is plucked.

The two waves of approximately the same amplitude and the same wavelength going in opposite directions can be had two ways:

$$\psi(+) = Ae^{ikx} + Ae^{-ikx} \quad , \quad \text{or} \quad \psi(-) = Ae^{ikx} - Ae^{-ikx} \, ,$$

where k here is considered positive and the ± on the k indicates the forward and reverse directions for the wave.

Now since

$$e^{ikx} = \cos(kx) + i\sin(kx) \, , \quad \text{and} \quad e^{-ikx} = \cos(kx) - i\sin(kx)$$

we have:

$$\psi(+) = 2A\cos(kx) \qquad \text{and} \qquad \psi(-) = i2A\sin(kx) \, .$$

Recall that the probability is equal to $\psi^*\psi$ so that we have:

$$\text{Prob}(+) = 4A^2\cos^2(kx) \qquad \text{and} \qquad \text{Prob}(-) = 4A^2\sin^2(kx) \, .$$

Thus the electrons having the $\psi(+)$ state will tend to be at the positions $kx=n\pi$ [since $\cos(n\pi)=\pm1$], or $x=n\pi/k$, but since $k_x = \frac{1}{2}G_x = \frac{1}{2}(2\pi/a) = \pi/a$, the electrons tend to be at the positions $x = n\pi/(\pi/a) = na$. But these are the positions of the ions. On the other hand, the electrons having the $\psi(-)$ will tend to be at the positions $kx = (n+\frac{1}{2})\pi$ [since $\sin(n\pi+\frac{1}{2}\pi)=\pm1$], or $x = (n+\frac{1}{2})a$. These are the inbetween positions of the ions.

Now the electrons near the ions (the $\psi(+)$ electrons) will have a lower potential energy than the electrons further away (the $\psi(-)$ electrons).

Thus at the zone boundary (**k** ≈ ½**G**), there will be a shifting of the electron energies in such a way that we have an **energy "gap"**. The **k values remain evenly spaced**, but due to the different potential energies, the **total energies of the electrons do not remain evenly spaced**. To restate: **the potential energies due to the ion cores will create an energy gap in the energies of the otherwise free electrons near the Brillouin zone boundary.** Since there are now gaps in the one originally big energy band, we now will talk about several energy bands, each separated from the next one by **an energy gap at the Brillouin zone boundaries** (**k** ≈ ½**G**).

3. Importance of the energy gap

The existence of an energy gap allows us to explain the difference between insulators, semiconductors and conductors!

If all the available "free" electrons fill up a band, and the next unfilled levels are in the next band which contains an appreciable band gap (energy jump), then the electrons in the filled (valence) band will not be able to make the jump unless there is a large amount of energy available (such as in lightning!). This type of material will then be an **insulator**.

If on the other hand, the available "free" electrons do not fill up a band, or if another unfilled band is at the same energy, then electrons near the Fermi energy will be able to make a jump to a higher level (and absorb energy) with ease. These materials then can easily carry current with the addition of only a little energy and so are conductors. These materials are obviously **metals**.

The inbetween case, where the band gap is between a filled and an unfilled band but the gap itself is small, this case is the one of **semiconductors**!

4. Where do we go from here?

Although this allows us to differentiate insulators, conductors (metals), and semiconductors, it does not tell us much about the properties of different semiconductors. To do this, we will need to take a deeper (and more complicated) look at the potential energy due to the ion cores and try to solve Schrodinger's Equation for this case.

After we have done this, we will then have the tools available to consider semiconductors in more detail - which we will do in part 4 of the course.