# Lecture 11

Tuesday, February 08, 2011

## Free electrons

This childish-sounding theory turns out to be not only very useful but also very deep.

In Kittel, some discussions are made with the fixed boundary condition (p. 134, 137). This is useful, but we will stick with the Born-von Karman boundary condition. Kittel chooses to work with the following free-particle wave function without any normalization factor.

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}$$

An alternative choice would be to normalize this function with $\psi_{\vec{k}}(\vec{r}) = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}}$ where $V$ is the volume. In this lecture note, we will follow Kittel, and will not worry about the normalization (until we have to, if ever, that is).

This wave function is an eigenstate in free space, with the energy eigenvalue:

$$\epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$$

Here, $m$ is the electron mass. Let us recall that the above wave function shows only the spatial part. Including the spin part, the wave function needs to be written as:

$$\psi_{\vec{k},s}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, \chi_s$$

where $\chi_s$ can be $\chi_{1/2}$ ("up" spin) or $\chi_{-1/2}$ ("down" spin).

Following our discussion of any general form of wave in crystal, $P(\vec{r})e^{i\vec{k}\cdot\vec{r}}$, where $P(\vec{r})$ is the lattice periodic function, which in this case is simply a constant (number one), we should have

$$k_a = \frac{2\pi}{L_a} l, \qquad k_b = \frac{2\pi}{L_b} m, \qquad k_c = \frac{2\pi}{L_c} n$$

where $l, m, n =$ integers, $k_a, k_b, k_c$ are the components of $\vec{k}$ along the $\vec{a}^*, \vec{b}^*, \vec{c}^*$ axes respectively, and $L_a, L_b, L_c$ are the dimensions of the crystal along the $\vec{a}, \vec{b}, \vec{c}$ axes respectively. The volume per $\vec{k}$ value is $\frac{(2\pi)^3}{V}$ as in the previous lectures.

Thus, the periodic boundary condition "quantizes" $\vec{k}$, which in free space is proportional to the momentum $\vec{p} = \hbar\vec{k}$.

## Fermi surface, and all other Fermi quantities ($\epsilon_F, T_F, k_F, p_F, v_F$)

In a cubic cm of a common metal such as Na, Ag, Au, Al, there are typically $10^{22}\sim 10^{23}$ conduction electrons, which are described as free electrons to a good approximation.

Consider $T = 0$. What is the ground state of this collection of free electrons? Recall that the electron is a spin 1/2 particle, which means that it is a Fermion. Thus, the ground state is formed by putting electrons one by one at the lowest energy level, as given by $\vec{k}$, $\epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$ and spin "up" or "down."

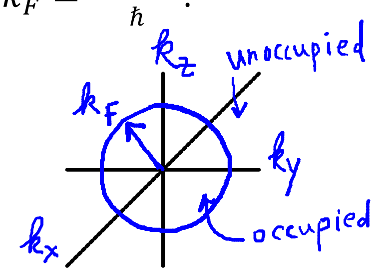
Filling electrons to the energy levels available, it is then obvious that there must be the maximum energy occupied. This energy is the **Fermi energy** $\epsilon_F$. Now, here are a bunch of definitions. These definitions are given in general form (applicable even if the electron dispersion is not a free electron dispersion), and then the expression appropriate for the free electron dispersion is given.

The **Fermi temperature**: $T_F = \epsilon_F / k_B$.

The **Fermi wave vector**: $\vec{k}_F$ defined by $\epsilon_F = \epsilon_{\vec{k}=\vec{k}_F}$. Thus, $k_F = \frac{\sqrt{2m\epsilon_F}}{\hbar}$.

The **Fermi momentum**: $\vec{p}_F = \hbar\vec{k}_F$.

The **Fermi velocity**: $\vec{v}_F = \frac{1}{\hbar}\frac{\partial \epsilon_{\vec{k}}}{\partial \vec{k}}\Big|_{\vec{k}=\vec{k}_F}$. Thus, $v_F = \frac{\hbar k_F}{m}$.




Let $N$ be the total number of electrons. $k_F$ is determined from

→ volume in $\vec{k}$ space

Spin up and down

$$2\frac{\frac{4}{3}\pi k_F^3}{\frac{(2\pi)^3}{V}} = N$$

volume in $\vec{k}$ space

volume per $\vec{k}$ point

$$k_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3} = (3\pi^2 n)^{1/3}$$

electron # density

$$\epsilon_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

The typical number density is $10^{-22} \sim 10^{-23}\ \mathrm{cm}^{-3}$. And, thus **the typical Fermi energy is a few eV**. Converting this to temperature, **the typical Fermi temperature is 10,000 to 100,000 K**. $k_F \sim O(1)\ \text{Å}^{-1}$. $v_F \sim \frac{\hbar k_F}{m} = \frac{\hbar c}{mc^2} k_F c \sim \frac{1}{100} c$ (thus, the non-relativistic mechanics). [Note that the speed of sound is about 100 times smaller than $v_F$.]

Given the dispersion relation $\epsilon_{\vec{k}}$, the DOS is easily obtained as in the phonon problem.

spin up and down

$$\text{number of states in } d^3\vec{k} = 2\frac{d^3\vec{k}}{\frac{(2\pi)^3}{V}} = \frac{V}{4\pi^3} k^2 dk d\Omega$$

$dN$, the number of states between $\epsilon$ and $\epsilon + d\epsilon$ is obtained by integrating over the solid angle, since the dispersion relation $\epsilon$ is a function of $k$. [Note that here we use the energy variable $\epsilon$, which is equivalent to $\omega$, up to $\hbar$, in the phonon problem.]

$$dN = D(\epsilon)d\epsilon = \frac{V}{4\pi^3} k^2 dk 4\pi = \frac{V}{\pi^2} k^2 dk = \frac{V}{\pi^2} k \frac{m}{\hbar^2} d\epsilon = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon^{1/2} d\epsilon$$

$$D(\epsilon) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon^{1/2}$$

Density of states at $\epsilon_F$ is very important. By noting that $N \propto k_F^3 \propto \epsilon_F^{3/2}$, we get

$$\frac{dN}{d\epsilon_F} = D(\epsilon_F) = \frac{3}{2}\frac{N}{\epsilon_F}$$

Electrons and phonons -- different scales

The electronic energy scale ($1 \sim 10$ eV) is much higher, 100 to 1000 times higher than the phonon energy scale ($10 \sim 100$ meV). Equivalently, the Fermi temperature is much higher than the Debye temperature ($\sim O(100)$ K).

Thus, electrons are in a quantum mechanical state at room temperature, while phonons are more or less classical. It is often said that the electron gas is **degenerate**. What this means is that the system is in a quantum regime so that the identical nature of electrons is important. The density is high enough so that the mean distance between electrons $r_s$, defined through $\frac{V}{N} = \frac{4\pi}{3} r_s^3$, is much shorter than the thermal De Broglie wave length, about ten times as large as $r_s$ at room temperature (calculation left for your exercise).

Another thing to take notice of is the difference in speeds. Ions vibrate with roughly the speed of sound while the electrons zip around 100 to 1000 times faster.