

Physics 0551 Lecture #17

Title: Drude continued and the Free Electron Gas

As was stated last Drude's theory arrives at the empirical laws of Ohm for DC fields

$$\vec{j} = \frac{ne^2\tau}{m}\vec{E} \quad \sigma = \frac{ne^2\tau}{m}$$

This formalism can be extended to encompass AC fields.

Let

$$\begin{aligned} \vec{E}(t) &= \vec{E}e^{i\omega t} & q = -e = \text{unit of charge} \\ m\vec{a} &= -e\vec{E}\exp(i\omega t) - \frac{m}{\tau}v \end{aligned}$$

Assume a solution

$$\begin{aligned} \vec{v} &= \vec{v}_0e^{i\omega t} \\ \vec{a} &= +i\omega\vec{v}_0e^{i\omega t} \end{aligned}$$

and

$$\begin{aligned} im\omega\vec{v}_0 &= -e\vec{E} - \frac{m}{\tau}\vec{v}_0 \\ \vec{v}_0 &= -e\vec{E}/m(1/\tau + i\omega) \end{aligned}$$

Now multiply by $-ne$:

$$\begin{aligned} -nev_0 &= \vec{j} = \frac{\tau ne^2\vec{E}/m}{(1 + i\omega\tau)} \\ \vec{j} &= \sigma\vec{E} = \frac{\sigma_0\vec{E}}{(1 + i\omega\tau)} \end{aligned}$$

If $\omega \rightarrow 0$ then we reduce back to the DC field expression. If $\omega \gg \frac{1}{\tau}$ then the response is out of phase with the applied field, no net current. (Electrons do not get a chance to scatter.) This implies that at some frequency, the electric field can propagate *through* the electron "gas". For alkali metals (Na, K, etc.) this occurs in the UV. Thus, another success for Drude's model.

Failures of the Drude theory:

1. The expected $\frac{3}{2}k_B T$ contribution for each electron in the classical gas is not observed.
2. There is no fundamental method to determine the relaxation time τ .
 $v_{\text{electron}}\tau \gg \text{lattice constant.}$
3. Measured magnetic susceptibility, χ (to be presented later), is much too small.

4. Experimentally some materials have *positive* Hall coefficients.

The solution to all above shortcomings was with the introduction of the Quantum Mechanical theory of Sommerfeld.

Thus we must replace classical electron gas Boltzmann distribution with Fermi-Dirac statistics which are appropriate for spin 1/2 particles.

$$\begin{aligned} \text{Boltzmann: } f(\vec{v}) &= n \left(\frac{m}{2\pi k_B T} \right)^{3/2} e^{-mv^2/2k_B T} \\ \text{F-D: } f(\vec{v}) &= \frac{\left(\frac{m}{\hbar}\right)^3}{4\pi^3} \frac{1}{\exp\left[\left(\frac{1}{2}mv^2 - k_B T_0\right)/k_B T\right] + 1} \end{aligned}$$

or more conventionally

$$f(\epsilon_s) = \text{occupancy of a state, } s = \frac{1}{\exp[(\epsilon_s - \mu)/k_B T] + 1}$$

ϵ_s is the energy of an allowed electron state

μ is the chemical potential (i.e., just the energy required to add an additional particle to the system.)

The explicit calculation for F-D statistics appears in myriad of thermodynamics texts.

This is my *crude* “*intuitive*” approach:

Examine a particular state, ϵ_s , for a single electron	Energy
F-D statistics implies two possibilities \rightarrow unoccupied	0
occupied	ϵ_s

The Boltzmann occupancy factor

$$\langle n_s \rangle \equiv f(\epsilon_s) = \frac{0e^{-0/k_B T} + 1e^{-\epsilon_s/k_B T}}{e^{-0/k_B T} + e^{-\epsilon_s/k_B T}} = \frac{1}{e^{\epsilon_s/k_B T} + 1}$$

In actuality, there are many electrons and many states which can be occupied. Consequently we must modify the previous expression with an appropriate weighting factor. Hence a factor λ is multiplied by $e^{-\epsilon_s/k_B T}$.

$\lambda \equiv$ activity coefficient $= e^{\mu/k_B T}$ where $\mu \equiv$ chemical potential.

This gives the familiar form of Fermi-Dirac statistics.

Another important aspect of the Sommerfeld model is to treat electrons as waves, not ballistic particles, which satisfy the Schrödinger wave equation:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\Psi_k(\vec{r}) = \epsilon_k\Psi_k(\vec{r})$$

If $V(\vec{r}) = 0$ then $\Psi_k = Ae^{i\vec{k}\cdot\vec{r}}$ and $E_k = \frac{\hbar^2 k^2}{2m}$ $\vec{p} = \hbar\vec{k}$ $\vec{p} = -i\hbar\nabla$

subject to the normalization condition

$$\int \Psi^*\Psi dV = 1 \quad A^2 = \text{Volume} = V \quad \Psi_k = \frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{r}}$$

Since we will be considering electrons in a crystal, we once again invoke periodic boundary conditions $\Psi_k(x, y, z) = \Psi_k(x + L, y, z)$ and so on.

Thus

$$\begin{aligned} k_x L &= n_x 2\pi \rightarrow k_x = n_x \frac{2\pi}{L} \\ k_y L &= n_y 2\pi \rightarrow k_y = n_y \frac{2\pi}{L} \\ k_z L &= n_z 1\pi \rightarrow k_z = n_z \frac{2\pi}{L} \end{aligned} \quad (\text{This should look familiar})$$

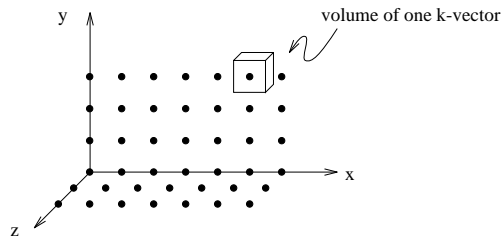
So we have once again “digitized” reciprocal space.

Since

$$\begin{aligned} \vec{k} &= n_x \frac{2\pi}{L} \hat{x} + n_y \frac{2\pi}{L} \hat{y} + n_z \frac{2\pi}{L} \hat{z} \\ k^2 &= \left(\frac{2\pi}{L}\right)^2 n^2 \quad \text{and} \quad n^2 = n_x^2 + n_y^2 + n_z^2 \\ E &= \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{2\pi}{L}\right)^2 n^2 \end{aligned}$$

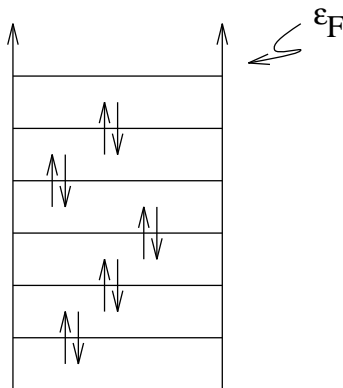
	n_x	n_y	n_z	n^2
6	± 1	± 1	± 1	3
12	± 1	± 1	0	2
6	0	0	± 1	1
	± 1	0	0	

In reciprocal space each allowed k -vector occupies $\left(\frac{2\pi}{L}\right)^3$ volume in k -space



$$\mathcal{D}(\vec{k}) d^3k = \frac{V}{(2\pi)^3} d^3k$$

To find the ground state (lowest energy state) at $T=0$, one fills all the lowest energy levels subject to the constraints of the Pauli exclusion principle. The last state's energy is the Fermi Energy, ϵ_F , (or equivalently, the chemical potential at zero temperature).



Recall that the chemical potential, $\mu(T)$, is just the change in free energy, F , with changes in number of particles.

$$\mu = \left(\frac{\partial F}{\partial N}\right)_{T,V}$$

If there are N total free electrons in a system,

$$2 \int_0^{k_F} \mathcal{D}(\vec{k}) d^3 k = N \quad \text{factor of 2 for spin degeneracy } (\uparrow \text{ or } \downarrow)$$

$$\text{or } \frac{\frac{4}{3}\pi k_F^3}{\left(\frac{2\pi}{L}\right)^3} = \frac{N}{2} \qquad k_F = \left(3\pi^2 \frac{N}{V}\right)^{1/3}$$

k_F is just the wave vector of an electron at the Fermi energy.

A sphere of radius k_F is called the Fermi sphere. At $T = 0$, all states $k \leq k_F$ are occupied, and all states $k > k_F$ are unoccupied.

Since

$$E = \hbar^2 k^2 / 2m$$

$$\epsilon_F = \hbar^2 k_F^2 / 2m = \frac{\hbar^2}{2m} \left(3\pi^2 \frac{N}{V}\right)^{2/3}$$

Typical values for ϵ_F range from 2-10 eV

$$\frac{1}{2} m v_F^2 = \epsilon_F \quad v_F \approx 10^6 \text{ m/sec or about 1\% of } c \text{ (the speed of light)}$$

Rather focusing on $\mathcal{D}(k)$, we can obtain $\mathcal{D}(\epsilon)$ or $\mathcal{D}(\hbar\omega)$.

$$\mathcal{D}(\epsilon) = \frac{dN(\epsilon)}{d\epsilon} \qquad E = \frac{\hbar^2}{2m} \left(3\pi^2 \frac{N}{V}\right)^{2/3}$$

$$N = \frac{V}{3\pi^2} \left(\frac{2mE}{\hbar^2}\right)^{3/2}$$

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

$$\mathcal{D}(\varepsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} E^{1/2} \quad \text{in 3 dimensions}$$

In 1D $\mathcal{D}(\varepsilon) \propto E^{-1/2}$

2D $\mathcal{D}(\varepsilon)$ is constant

Note: $E = \frac{\hbar^2 k^2}{2m} = \hbar\omega$

