Solid State Physics: Midterm Review

October 3, 2018

1 Drude Theory

1.1 Basic Model

- Theory of metallic conduction proposed by Paul Drude.

- Considers metal a "gas" of electrons on which the kinetic theory of gases may be applied.

- Assumption of kinetic theory of gases: molecules, or electrons, are identical constituents that move in straight lines until they encounter a collision.

- Assumption of metallic "gases": when atoms of a metallic element form a metal, the valence (or "conduction") electrons move freely while the positively charged ions remain stationary.

- Reality: metals have a much higher density than gas and include very strong electron-electron and electron-ion interactions.

The *charge carrier density n* may be written as

$$n = \frac{N}{V} = N_A Z \frac{\rho}{A}$$

where N is the total number of conduction electrons, V is the sample volume, N_A is Avogradro's number, Z is the number of valence electrons per atom, ρ is the mass density of the metal, and A is the atomic mass (mass per mole of the metal). A typical charge carrier density is on the order of n $10^{22} cm^{-3}$ for metals.

Another useful way to characterize the charge carrier density is by specifying r_s, the radius of the spherical volume containing one charge carrier.

$$\frac{V}{N} = \frac{1}{n} = \frac{4}{3}\pi r_s^3 \rightarrow r_s = (\frac{3}{4\pi n})^{1/3}$$

The basic assumption of the Drude theory are:

- *Indepedent electron approximation*: electrons do not interact with one another (between collisions).

- *Free electron approximation*: electrons do not interact with positively charged ions (between collisions).

- Collisions are instantaneous events that abruptly alter the electron velocity. The mechanism of scattering is not well-defined. Drude assumed it was only due to electron-ion scattering, but the reality is much more complicated.

- Electrons experience a collision with probability $1/\tau$ per unit time. The probability of a collision in time dt is dt/τ. τ is the *mean free time*, or *relaxation time*.

- Electrons achieve thermal equilibrium only through collision. After each collision, an electron emerges with a randomly oriented velocity proportional to the local temperature T.

1.2   DC Conductivity

Ohm's Law:
$$V = IR$$

where V is the voltage drop, I is the current, and R is the resistance. Using $\rho = RA/L$, where L is the distance over which the voltage drop occurs, and A is the cross-sectional area of the sample,

$$\mathbf{E} = \rho\mathbf{j}$$

where $\mathbf{j}$ is the current density - the amount of charge flowing through a unit area per unit time. For n electrons moving with velocity $\mathbf{v}$,

$$\mathbf{j} = nq\mathbf{v} = n(-e)\mathbf{v}$$

- When $\mathbf{E} = 0$, there is no preferred direction so $\langle \mathbf{v} \rangle = 0$ and therefore $\mathbf{j} = 0$.

- When $\mathbf{E} \neq 0$, the velocity of an electron is given by

$$\mathbf{v} = \mathbf{v}_0 + \frac{(-e)\mathbf{E}t}{m}$$

So,
$$\langle \mathbf{v} \rangle = \langle \mathbf{v}_0 \rangle + \frac{(-e)\mathbf{E}\tau}{m} = \frac{(-e)\mathbf{E}\tau}{m}$$

Where the velocity acquired over time t due to a constant acceleration of $\mathbf{a} = \frac{-e\mathbf{E}}{m}$ is given by $\mathbf{a}t$.

We can therefore generally write the current density as

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

where the *conductivity* σ is given by $ne^2\tau/m$. If we consider the *mean free path*, $l = \langle v \rangle \tau$, Drude's predictions for $\langle v \rangle$ based on kinetic theory of gases estimate l 5angstroms. This is consistent with Drude's view that electron-ion collisions dominated. In reality, the mean free path is at least an order of magnitude larger. At low temperatures, the mean free path is underestimated by a factor of 10^3.

1.3 Drude Equation of Motion

The time-dependent current density may be written in terms of the momentum $\mathbf{p}(t)$ as

$$\mathbf{j}(t) = n(-e)\mathbf{v}(t) = -\frac{ne}{m}\mathbf{p}(t)$$

At an infinitesimal time dt later, the momentum will be given by

$$\mathbf{p}(t + dt) = \left(1 - \frac{dt}{\tau}\right)[\mathbf{p}(t) + \mathbf{F}dt] + \left(\frac{dt}{\tau}\right)\mathcal{O}(\mathbf{F}dt)$$

The first term comes from the fact that, with probability $1 - dt/\tau$, the electron will not collide during time dt and will therefore acquire the impulse $\mathbf{F}dt$ in addition to its original momentum, $\mathbf{p}(t)$. The second term comes from the case that the electron does collide, which happens with probability dt/τ, in which case its contribution to the momentum is $\mathcal{O}(\mathbf{F}dt)$ since its velocity after collision averages over all directions to zero. Therefore,

$$\mathbf{p}(t + dt) = \mathbf{p}(t) - \frac{\mathbf{p}(t)dt}{\tau} + \mathbf{F}dt + \mathcal{O}(dt^2)$$

Ignoring the higher-order terms in dt, we obtain:

$$\frac{\mathbf{p}(t + dt) - \mathbf{p}(t)}{dt} = \frac{d\mathbf{p}(t)}{dt} = -\frac{\mathbf{p}(t)}{\tau} + \mathbf{F}$$

1.4 Hall Effect and Magnetoresistance

E.H. Hall predicted that the force experienced by a current due to a magnetic field would manifest as an observable transverse voltage, today known as the Hall voltage. The experimental setup is an applied electric field E_x driving current in the $+\hat{x}$ direction along a sample. An applied magnetic field is also present, $\mathbf{B} = B\hat{z}$ perpendicular to the sample. Charge carriers experience a Lorentz force given by

$$qE_x\hat{x} + q(\mathbf{v} \times \mathbf{B})$$

In the case of electrons, $q = -e$, and the second term gives rise to a deflection in the $-\hat{y}$ direction. As electrons build up on the sample surface along the $-\hat{y}$ edge, a transverse electric field E_y is created in the $-\hat{y}$ direction. This field will grow in magnitude until is opposes the magnetic force term. Therefore,

$$qE_y\hat{y} + q(\mathbf{v} \times \mathbf{B}) = 0$$

In the case of electrons,
$$-eE_y + -ev_x B = 0$$

Therefore, the transverse electric field has magnitude $E_y = -v_x B$.

There are two quantities of interest:

- *Magnetoresistance* $\rho(B) = \frac{E_x}{j_x}$. This quantity is field independent.

- *Hall coefficient* $R_H = \frac{E_y}{j_x B}$. This value is negative for negative charge carriers and positive for positive charge carriers. Measurement of the Hall coefficient, or Hall field E_y, gives information about the charge carriers.

Starting with the Drude equation of motion, we can derive equations for the magnetoresistance and Hall coefficient.

$$\frac{d\mathbf{p}(t)}{dt} = -\frac{\mathbf{p}(t)}{\tau} + \mathbf{F} = \frac{\mathbf{p}(t)}{\tau} + (-e\mathbf{E} + \frac{-e}{m})(\mathbf{p} \times \mathbf{B})$$

In the steady state, $\frac{d\mathbf{p}}{dt} = 0$, so we obtain

$$0 = -\frac{p_x}{\tau} + (-eE_x + \frac{-e}{m} p_y B) = -eE_x - \omega p_y - \frac{p_x}{\tau}$$

$$0 = -\frac{p_y}{\tau} + (-eE_y - \frac{-e}{m} p_x B) = -eE_y + \omega p_x - \frac{p_y}{\tau}$$

where $\omega = eB/m$, the cyclotron frequency. The quantity $\omega\tau$ is a good measure of the strength of the magnetic field. For example, if $\omega\tau$ is very small, the current is very nearly parallel to E_x. From these we obtain

$$\sigma_0 E_x = \omega j_y \tau + j_x$$

$$\sigma_0 E_y = -\omega j_x \tau + j_y$$

The Hall voltage is obtained in the limit when $j_y = 0$. Therefore, the steady state transverse field is given by

$$E_y = \frac{-\omega j_x \tau}{\sigma_0} = -\frac{B}{ne} j_x$$

So the Hall coefficient is given by

$$R_H = \frac{E_y}{j_x B} = -\frac{1}{ne}$$

This result predicts that the Hall coefficient is dependent only on the number of charge carriers. However, the actual value is temperature and field-dependent. But the limiting value, in the case of very low temperature and very high fields, is the Drude result.

1.5 AC Electrical Conductivity

We wish to calculate the current induced by a time-dependent electric field. The field can be written in the form

$$\mathbf{E}(t) = Re(\mathbf{E}(\omega)e^{-i\omega t})$$

In the absence of a magnetic field, the equation of motion becomes

$$\frac{d\mathbf{p}(t)}{dt} = -\frac{\mathbf{p}(t)}{\tau} + \mathbf{F} = \frac{\mathbf{p}(t)}{\tau} + -e\mathbf{E}$$

And the solution we seek is therefore of the form

$$\mathbf{p}(t) = Re(\mathbf{p}(\omega)e^{-i\omega t})$$

The equation of motion gives us

$$-i\omega\mathbf{p}(\omega) = -\frac{\mathbf{p}(\omega)}{\tau} - e\mathbf{E}(\omega)$$

And we can use the fact that $\mathbf{j} = -ne\mathbf{p}/m$ to write

$$\mathbf{j}(t) = Re(\mathbf{j}(\omega)e^{-i\omega t})$$

and then rewrite the equation of motion as

$$i\frac{m\omega}{ne}\mathbf{j}(\omega) = \frac{m\mathbf{j}(\omega)}{ne\tau} - e\mathbf{E}(\omega)$$

$$\left[i\frac{m\omega}{ne} - \frac{m}{ne\tau}\right]\mathbf{j}(\omega) = -e\mathbf{E}(\omega)$$

$$\mathbf{j}(\omega) = \frac{-ne^2}{m(i\omega - \frac{1}{\tau})}\mathbf{E}(\omega)$$

We finally obtain the expression for the frequency-dependent AC conductivity $\sigma(\omega)$:

$$\mathbf{j}(\omega) = \sigma(\omega)\mathbf{E}(\omega)$$

where

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau}$$

In the case of $\omega = 0$, this reduces to the DC conductivity. There are two complications addressed in Ashcroft/Mermin:

- Neglecting the $\mathbf{B}$ counterpart: this is acceptable because the term is technically scaled by a factor of v/c. In most cases, it is roughly 10^{-10} of the $\mathbf{E}$-field term and may safely be ignored.

- We have assumed spatial uniformity, but the $\mathbf{E}$-field actually varies in time and space. However, as long as the field does not vary much over a few mean free path lengths, we may safely assume spatial invariance.

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1.6 Thermal Conductivity

The Wiedemann-Franz law states that the ratio of the thermal to the electrical conductance, κ/σ, is directly proportional to the temperature.

The Drude model assumes the bulk of thermal conductance is performed by conduction electrons.

2 Sommerfeld Theory

Sommerfeld combined Fermi-Dirac statistics with the Drude model.

2.1 Basic Fermi-Dirac Statistics

Given a system of free electrons with chemical potential μ, the probability of an eigenstate of energy E bring occupied is given by the Fermi factor

$$n_F(\beta(E - \mu)) = \frac{1}{e^{\beta(E-\mu)} + 1}$$

At very low temperature, $n_F \approx 1$ for $E < \mu$ and $n_F \approx 0$ for $E > \mu$. So, n_F is a step function at low T. At higher T, it becomes more spread out.

For electrons in a box of size $V = L^3$, the wavefunctions of the free electron particles are given by

$$\Psi = e^{i\mathbf{k}\cdot\mathbf{r}}$$

Imposing PBC, we find that $\mathbf{k} = (2\pi/L)(n_1, n_2, n_3)$ where n_i are integers. The corresponding energies of the plane waves are

$$\epsilon(\mathbf{k}) = \frac{\hbar|\mathbf{k}|^2}{2m}$$

The total number of electrons in the system, N, is given by the sum of all possible states times the probability of each state being occupied. Therefore,

$$N = 2\sum_{\mathbf{k}} n_F(\beta(\epsilon(\mathbf{k}) - \mu))$$

where the factor of 2 comes from each state allowing two possible spin configurations. In the continuous limit, we can make use of the following:

$$\int f(x)dx = \sum f(x)\delta x$$

Therefore, N can be written

$$N = 2\frac{L^3}{(2\pi)^3}\int d\mathbf{k}\, n_F(\beta(\epsilon(\mathbf{k}) - \mu))$$

Some definitions:

- The *Fermi energy*, E_F, is the chemical potential at $T = 0$. Sometimes also called the *Fermi Level*. In the case of a continuum of states, the Fermi energy is the energy of the most energetic occupied electron state. In the case of a discrete set of states, the Fermi energy is the energy halfway between the highest occupied and lowest unoccupied states.

- The *Fermi sea* is the set of states filled at $T = 0$.

- The *Fermi temperature*, T_F, is given by $T_F = E_F/k_B$.

- The *Fermi wavevector*, k_F, satisfies

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

- The *Fermi momentum* $p_F = \hbar k_F$.

- The *Fermi velocity* $v_F = p_F/m = \hbar k_F/m$.

2.2 Fermi Energy at T = 0

Consider a 3-dimensional metal with N electrons at $T = 0$. The total number of electrons can be written as

$$N = 2\frac{L^3}{(2\pi)^3} \int d\mathbf{k} \, n_F(\beta(\epsilon(\mathbf{k}) - \mu))$$

At $T = 0$, the Fermi function n_F becomes a step function that switches at E_F such that

$$n_F = \Theta(E_F - \epsilon(\mathbf{k}))$$

Therefore,

$$N = 2\frac{L^3}{(2\pi)^3} \int d\mathbf{k}\,\Theta(E_F - \epsilon(\mathbf{k})) = 2\frac{L^3}{(2\pi)^3} \int^{|k|<k_F} d\mathbf{k}$$

The final integral simply yields the volume of a ball of radius k_F. Therefore,

$$N = 2\frac{L^3}{(2\pi)^3} \left(\frac{4}{3}\pi k_F^3\right)$$

The surface of this ball is known as the *Fermi surface* - it is the surface dividing filled from unfilled states at $T = 0$.

This result gives us equations for the Fermi wavevector and Fermi energy:

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

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

For a typical metal, we can estimate the number of free electrons, and therefore calculate the Fermi energy. The Fermi energies and corresponding Fermi temperatures are extremely large (7 eV, 80000K for copper). This indicates that only electrons that are very close to the Fermi surface have any hope of receiving enough energy to exceed the Fermi energy. All other electrons would require an insane amount of energy to move, as no unoccupied states are nearby.

2.3 Heat Capacity

The heat capacity C is given generally by

$$C = \frac{\partial E}{\partial T}$$

To calculate the heat capacity, we need an equation for the total energy of the system. The expectation value of the total energy of the system is given by

$$E_{total} = 2\frac{L^3}{(2\pi)^3}\int d\mathbf{k}\epsilon(\mathbf{k})n_F(\beta(\epsilon(\mathbf{k})-\mu))$$

Integrating out the *theta* and *phi* contributions, we obtain the one-dimensional integral

$$E_{total} = 2\frac{L^3}{(2\pi)^3}\int 4\pi k^2 dk\epsilon(\mathbf{k})n_F(\beta(\epsilon(\mathbf{k})-\mu))$$

Using the relationships

$$k = \sqrt{\frac{2\epsilon m}{\hbar^2}}$$

$$dk = \sqrt{\frac{m}{2\epsilon\hbar^2}}d\epsilon$$

The total energy may be written as

$$E_{total} = (L^3)\int_0^\infty \epsilon g(\epsilon)n_F(\beta(\epsilon-\mu))d\epsilon$$

where $g(\epsilon)d\epsilon$ is the *density of states per unit volume* - the total number of eigenstates with energies between ϵ and $\epsilon + d\epsilon$.

$$g(\epsilon)d\epsilon = \frac{2}{(2\pi)^3}4\pi k^2 dk = \frac{(2m)^{3/2}}{2\pi^2\hbar^3}\epsilon^{1/2}d\epsilon$$

Using the expression for the Fermi energy for a 3D metal at $T = 0$, we can further write

$$g(\epsilon) = \frac{3n}{2E_F}\left(\frac{\epsilon}{E_F}\right)^{1/2}$$

Once the chemical potential is fixed by the number of electrons in the system, the total energy may be calculated as above. The partial derivative with respect to temperature will yield the heat capacity.

When $T = 0$, the Fermi function is a step function and the chemical potential is simply $\mu = E_F$. For non-zero, but low, temperature the chemical potential is given by

$$\mu = E_F + \mathcal{O}(T/T_F)^2$$

Let $E[T = 0]$ be the kinetic energy of the system at $T = 0$. For a finite temperature, the spread of the step function is roughly $\approx k_B T$. That is, only electrons within a range of $k_B T$ of μ can be excited and they are excited within a range $k_B T$ above μ. The energy is then given by

$$E[T] \approx E[T = 0] + \frac{\alpha}{2}[Vg(E_F)k_B T](k_B T) = E[T = 0] + \frac{\alpha}{2}D(E_F)(k_B T)^2$$

Therefore,

$$C = \frac{\partial E}{\partial T} = \alpha D(E_F)k_B^2 T$$

Using

$$Vg(\epsilon) = D(\epsilon) = \frac{3N}{2E_F}\left(\frac{\epsilon}{E_F}\right)^{1/2}$$

2.4 Density of States

2.4.1 Method 1

The density of states $D(\epsilon)$ can be calculated from the following expression for the total energy

$$E_{total} = \int \epsilon D(\epsilon) n_F(\beta(\epsilon - \mu)) d\epsilon$$

In one dimension, the expectation value of the total energy is

$$E_{total} = 2\frac{L}{2\pi} \int d\mathbf{k}\epsilon(\mathbf{k}) n_F(\beta(\epsilon - \mu))$$

We now make use of

$$k = \sqrt{\frac{2m\epsilon}{\hbar^2}}$$

$$\frac{dk}{d\epsilon} = \frac{1}{2}\left(\frac{2m\epsilon}{\hbar^2}\right)^{-1/2}\frac{2m}{\hbar^2} = \sqrt{\frac{m}{2\hbar^2\epsilon}}$$

to obtain the following integral over $d\epsilon$

$$E_{total} = 2\frac{L}{2\pi} \int \sqrt{\frac{m}{2\hbar^2\epsilon}}\epsilon(\mathbf{k}) n_F(\beta(\epsilon - \mu)) d\epsilon$$

Therefore,

$$D(\epsilon) = \frac{L}{\pi}\sqrt{\frac{m}{2\hbar^2\epsilon}}$$

Likewise, for two dimensions:

$$D(\epsilon) = \frac{L^2 m}{\pi \hbar^2}$$

and for three dimensions:

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

2.4.2 Method 2

To derive the same result for $D(\epsilon)$, we may first consider the total number of states $\mathcal{N}$ where, for 3 dimensions,

$$\mathcal{N} = 2 \left(\frac{1}{\delta k} \right)^3 \left(\frac{4\pi k^3}{3} \right) = 2 \left(\frac{L}{2\pi} \right)^3 \left(\frac{4\pi (2m\epsilon)^{3/2}}{3\hbar^3} \right) = \frac{L^3}{3\pi^2} \frac{(2m\epsilon)^{3/2}}{\hbar^3}$$

The density of states $D(\epsilon)$ is then given by

$$D(\epsilon) = \frac{\partial \mathcal{N}}{\partial \epsilon} = \frac{L^3}{2\pi^2} \frac{(2m)^{3/2} (\epsilon)^{1/2}}{\hbar^3}$$