

Lecture notes in Solid State 3

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Classical free electron model for metals: The Drude model

Recommended reading:

- Chapter 1, Ashcroft & Mermin.

The conductivity of metals is described very well by the classical Drude formula,

$$\sigma_D = \frac{ne^2\tau}{m} \quad (1.1)$$

where m is the electronic mass (as decided by the band-structure) and e is the electronic charge. The conductivity is directly proportional to the electronic density n ; and, to τ , the mean free time between collisions of the conducting electrons with defects that are generically present in the system:

- Static defects that scatter the electron elastically, including: static impurities and structural defects. One can define the elastic mean free time τ_e .
- Dynamical defects which scatter the electron inelastically (as they can carry off energy) including: photons, other electrons, other excitations (such as plasmons). One can accordingly define the inelastic mean free time τ_φ .

The efficiency of the latter processes depends on the temperature T : we expect it to increase as T is increased. At very low temperatures the dominant scattering is elastic, and then τ does not depend strongly on temperature but instead it depends on the amount of disorder (realized as random static impurities). We expect τ to decrease as the temperature or the amount of disorder in the system are increased.

The Drude model

1897 - discovery of the electron (J. J. Thomson). 1900 - only three years later, Drude applied the kinetic theory of gases to a metal - considering it to be a “gas of electrons”. Assumptions:

1. Electrons are classical objects: solid spheres of identical shape.
2. There is a compensating positive charge attached to immobile particles, to ensure overall charge neutrality:

- (a) Each isolated atom of the metallic element has a nucleus of charge eZ_a ($0 < e = 1.60 \times 10^{-19}\text{C}$, Z_a is the atomic number).
- (b) Surrounding the nucleus are Z_a electrons of total charge $-eZ_a$, composed of Z weakly bound valence electrons, and $Z_a - Z$ tightly bound electrons, the core electrons. In a metal, the core electrons remain bound to the nucleus and form the (immobile, positively charged) metallic ion, while the (mobile, negatively charged) valence electrons are allowed to wander far away from the parent atom. In this context they are called the conduction electrons.
3. Electrons are almost free (no forces act between electrons), except electrons can collide with ions (more generally, and more correctly, we need only assume that there is some scattering mechanism, as modern theories show that static ions on a perfectly ordered lattice do not lead to scattering. We will see that later when we discuss Bloch theorem). Between collisions they move as dictated by Newton's laws of motion. Electron-electron interactions are neglected between collisions (independent electron approximation). Electron-ion interactions are neglected as well (free electron approximation).

Many of the properties of metals can be described using the classical Drude theory, including

- Conductivity,
- Conductivity at finite magnetic field and Hall conductivity,
- Thermal conductivity (and the historic explanation of the Wiedemann-Franz law which agrees with experimental results: only about a factor of 2 too small compared to them),
- Thermoelectric effects (Seebeck effect),
- AC conductivity,
- Interaction with the electromagnetic field (reflection below the plasma frequency, transmission above the plasma frequency, plasma oscillations at the plasma frequency).

While many of the results turn out to be inaccurate and the mechanism for scattering remains unexplained, the basic assumption of a free electrons gas that undergoes scattering remains essentially the same in modern theories.

The modified Newton-like equation describing the average momentum for an electron can be derived in the following way. An electron experiences a collision with a probability per unit time of $1/\tau$, where τ is known as the relaxation time or the mean free time. So the probability for a collision in a time interval dt is dt/τ , and this is also the fraction of electrons that collided during that time. For a macroscopic number of electrons that have collided, the average momentum immediately following the collision is zero. The average momentum for the electrons at time $t + dt$ is therefore

$$\mathbf{p}(t + dt) = \underbrace{\frac{dt}{\tau} [0 + \mathbf{F}(t)dt]}_{\text{electrons that collided}} + \underbrace{\left(1 - \frac{dt}{\tau}\right) [\mathbf{p}(t) + \mathbf{F}(t)dt]}_{\text{electrons that did not collide}}, \quad (1.2)$$

where $\mathbf{p}(t)$ is the momentum per electron, $\mathbf{F}(t)$ is the external force per electron. Therefore,

$$\mathbf{p}(t + dt) - \mathbf{p}(t) = \mathbf{F}(t)dt - \frac{\mathbf{p}(t)}{\tau}dt + O(dt)^2, \quad (1.3)$$

and we get the central equation of motion for the Drude model

$$\frac{d\mathbf{p}}{dt} = -\frac{\mathbf{p}(t)}{\tau} + \mathbf{F}(t). \quad (1.4)$$

Hence the effect of individual electron collisions is to introduce a frictional damping term to the equation of motion.

In more technical terms, following a collision, we will use the Boltzmann distribution to generate a velocity for the electrons

$$f(\mathbf{v}) = \left(\frac{m}{2\pi k_B T} \right)^{3/2} \exp \left[-\frac{m\mathbf{v}^2}{2k_B T} \right] \quad (1.5)$$

so the electrons have an average speed which is controlled by the (local) temperature, but the average velocity is zero due to the angular averaging.

Conductivity

Ohm's law: the current I flowing in a wire is proportional to the potential drop V along the wire

$$V = IR, \quad (1.6)$$

where R is the resistance (measured in Ohms) which depends on the shape of the wire. One can define the resistivity ρ according to

$$\mathbf{E} = \rho \mathbf{j}, \quad (1.7)$$

where $\mathbf{E}$ is the electric field and $\mathbf{j}$ is the current density. The quantities are related in the following way. For a current flowing in a wire of length L and cross-sectional area A the current density along the wire is $j = I/A$. Since $V = EL$, we get $V = (\rho I/A)L$ hence

$$R = \rho L/A. \quad (1.8)$$

All the dependence of R on the dimensions of the wire is now explicit, hence ρ is a material property. The inverse resistivity is the conductivity $\sigma = \rho^{-1}$. The inverse resistance is the conductance G (measured in 1/Ohms).

In the framework of the Drude model, we can solve explicitly the differential equation with $\mathbf{F} = -e\mathbf{E}$, to get

$$\mathbf{p}(t) = -e\tau\mathbf{E} + (\mathbf{p}_0 + e\tau\mathbf{E})e^{-t/\tau} \quad (1.9)$$

when $t \rightarrow \infty$ we reach steady state, for which we get a drift velocity

$$\mathbf{v} = -\frac{e\mathbf{E}\tau}{m}, \quad (1.10)$$

and a corresponding current density is

$$\mathbf{j} = -nev = \frac{ne^2\tau}{m}\mathbf{E}, \quad \sigma_D = \frac{ne^2\tau}{m}, \quad (1.11)$$

justifying Eq. (1.1).

Thermal conductivity

The Drude model was able to give an explanation to the empirical law of Wiedemann and Franz (1853), that the ratio of the thermal to electrical conductivity is directly proportional to the temperature, with a proportionality constant which is more or less the same for all metals. Hence, one defines the ratio $\kappa/\sigma T$, known as the Lorenz number. To estimate the thermal conductivity of electrons one considers a metal bar along which the temperature varies slowly. Fourier's law states that

$$\mathbf{j}_q = -\kappa \nabla T \quad (1.12)$$

where $\mathbf{j}^q$ is the thermal current density (its magnitude is the thermal energy per unit time crossing a unit area perpendicular to the flow). Electrons arriving at point $\mathbf{r}$ with velocity $\mathbf{v}$ have on average underwent a collision at $\mathbf{r} - \mathbf{v}\tau$ and will carry thermal energy $E[T(\mathbf{r} - \mathbf{v}\tau)]$, hence

$$\mathbf{j}_q = -\frac{1}{2}n\mathbf{v} \{E[T(\mathbf{x} - \mathbf{v}\tau)] - E[T(\mathbf{x} + \mathbf{v}\tau)]\} \quad (1.13)$$

$$\simeq -\tau n \frac{\partial E}{\partial T} \mathbf{v} \cdot (\nabla T) \quad (1.14)$$

Averaging, we get

$$\langle \mathbf{v}\mathbf{v} \rangle = \frac{1}{3} \langle v^2 \rangle I \quad (1.15)$$

and defining

$$c_V = n \frac{dE}{dT} = \frac{3}{2} n k_B \quad (1.16)$$

we arrive at the result

$$\kappa = \frac{1}{3} c_V \tau \langle v^2 \rangle \quad (1.17)$$

The Lorenz number is

$$L = \frac{\kappa}{\sigma T} = \frac{1}{3} \frac{c_V \langle mv^2 \rangle}{ne^2 T} \quad (1.18)$$

with $\langle mv^2 \rangle = 3k_B T$ one gets

$$L = \frac{3}{2} \left(\frac{k_B}{e} \right)^2 = 1.11 \times 10^{-8} \text{ (J/CK)}^2 \quad (1.19)$$

Quantum free electron model for metals: The Sommerfeld model

Recommended reading:

- Chapter 2, Ashcroft & Mermin.

A quantum model: a free electron gas. At thermal equilibrium, the number of electrons having energy E is given by the Fermi distribution

$$f(E) = \frac{1}{e^{\beta(E-\mu)} + 1}, \quad (1.20)$$

in which $\beta = 1/(k_B T)$ is the inverse temperature (k_B is the Boltzmann constant) and μ is the chemical potential. At zero temperature ($\beta \rightarrow \infty$) the chemical

potential is equal to the Fermi energy, E_F , and the Fermi function describes a step-function, such that all states with energy $E \leq E_F$ are full and all states with energy about E_F are empty. In the grand-canonical ensemble, where the chemical potential is fixed, the number of electrons is temperature-dependent. The electronic density (number of electrons per unit volume) is given by

$$n = \int_{-\infty}^{\infty} dE \mathcal{N}(E) f(E), \quad (1.21)$$

where $\mathcal{N}(E)$ is the density of states (number of states having energy E per unit volume).

We can straightforwardly adopt the results of the Drude model for this case, however, we need to correct the following points:

- The typical velocity squared for the electrons, $\langle v^2 \rangle$, is set by the Fermi energy and not by the temperature

$$\left\langle \frac{mv^2}{2} \right\rangle = E_F, \quad (1.22)$$

(compare with $\left\langle \frac{mv^2}{2} \right\rangle = \frac{3}{2} k_B T$ for the Boltzmann distribution).

- The electronic heat capacity is proportional to the temperature and is not a constant. The reason is that at finite temperature T there are $\sim \Omega(E_F) k_B T$ electrons which become excited (here $\Omega(E_F) \sim n/E_F$ is the density of states at the Fermi energy), and they each typically carry additional energy $k_B T$, leading to an increase in energy of about $E \sim \Omega(E_F) (k_B T)^2$ compared to the ground state; Hence $c_V \propto \frac{dE}{dT} \propto T$.

By using equilibrium results to calculate the various physical quantities, one can adopt the results from the Drude theory after the following corrections:

- $c_V \rightarrow c_V \left(\frac{k_B T}{E_F} \right)$,
- $\left\langle \frac{mv^2}{2} \right\rangle \rightarrow \left\langle \frac{mv^2}{2} \right\rangle \left(\frac{E_F}{k_B T} \right)$.

Hence, since L is proportional to the product, it remains about the same, while Q gets reduced by a factor of $k_B T/E_F$ to about 1% of its classical value. An exact calculation within the Sommerfeld model (using a Sommerfeld expansion, see chapter 2 Ashcroft & Mermin) leads to

$$L = \frac{\pi^2}{3} \left(\frac{k_B}{e} \right)^2 = 2.44 \times 10^{-8} \text{ (J/CK)}^2, \quad (1.23)$$

which is an excellent match with the typical experimental value of L .

A semiclassical way to calculate directly transport coefficients in the Sommerfeld model is provided by the Boltzmann equation, that extends Sommerfeld's equilibrium theory to nonequilibrium cases.

Introduction to Localization

Plan

- Single spatially separated atoms: electrons are localized near atoms.
- Clean crystal: tunneling between perfectly ordered atoms $\rightarrow$ Bloch theorem $\rightarrow$ extended electronic eigenstates.
- What happens if we add disorder?

The Anderson model

Tight-binding in the presence of on-site disorder

$$H = \sum_i \epsilon_i |i\rangle\langle i| + t \sum_{\langle ij \rangle} |i\rangle\langle j| \quad (1.24)$$

and

$$\epsilon_i \in [-W/2, W/2] \quad (1.25)$$

randomly and uniformly chosen, where W is the disorder strength,

$$\overline{\epsilon_i} = 0 \quad (1.26)$$

$$\overline{\epsilon_i \epsilon_j} = \frac{W^2}{12} \delta_{ij} \quad (1.27)$$

In the presence of magnetic field

$$H = \sum_i \epsilon_i |i\rangle\langle i| + t \sum_{\langle ij \rangle} e^{i\theta_{ij}} |i\rangle\langle j| \quad (1.28)$$

where $\theta_{ij} = -\frac{e}{\hbar c} \int_i^j A \cdot d\ell$, known as the Peierls substitution.

The Anderson model - implications for transport

Localized states decay away from their center, i.e. behave asymptotically like

$$\psi(\mathbf{r}) = A(\mathbf{r}) e^{-|\mathbf{r}|/\lambda} \quad (1.29)$$

where λ is the localization length, and $\lambda \rightarrow \infty$ corresponds to an extended state.

The following results apply for the Anderson model: If the dimensionality of the system $d \leq 2$, then all eigenstates are localized (no matter how weak the disorder is). For $d = 3$:

- Density of states forms tails of the band consisting of localized states
- Interior of the band corresponds to extended states
- Critical energies E_c , E'_c separating localized from extended states are called the mobility edges

Implications for transport:

- Only extended states contribute to transport/conductivity significantly

- Position of mobility edge depends on the magnitude of disorder
- At critical magnitude of disorder: metal-insulator phase transition, i.e. all states become localized (Anderson transition).

Current transport is by electrons with energy $E \simeq E_F$. For $E_F < E_c$ (within the hopping regime):

- Current transport by localized electrons, electrons tunnel/hop from one localized state to the other
- Tunneling probability between localized wavefunctions $\alpha \rightarrow \beta$: $p(r_{\alpha\beta}, E_\beta, E_\alpha) \propto e^{-\alpha r_{\alpha\beta}} e^{-(E_\beta - E_\alpha)/k_B T}$, leading to Mott's law for conductivity: $\sigma(T) \propto e^{-(T_0/T)^{1/4}}$ (but at $T \rightarrow 0$ the system is insulating).

For $E_F > E_c$: Fermi-energy within region of extended states: metallic regime

- Disorder leads to positive interference of certain terms in perturbation expansion of conductivity: enhanced backscattering (weak localization) leads to reduced conductivity.
- Externally applied magnetic field destroys positive interference and weak localization (negative magnetoresistance, i.e. the decrease of resistance with magnetic field).

Dirac materials: weak anti-localisation

- Backscattering is forbidden due to a Berry phase effect in k -space (leading in the presence of magnetic field to positive magnetoresistance, i.e. the increase of resistance with magnetic field).

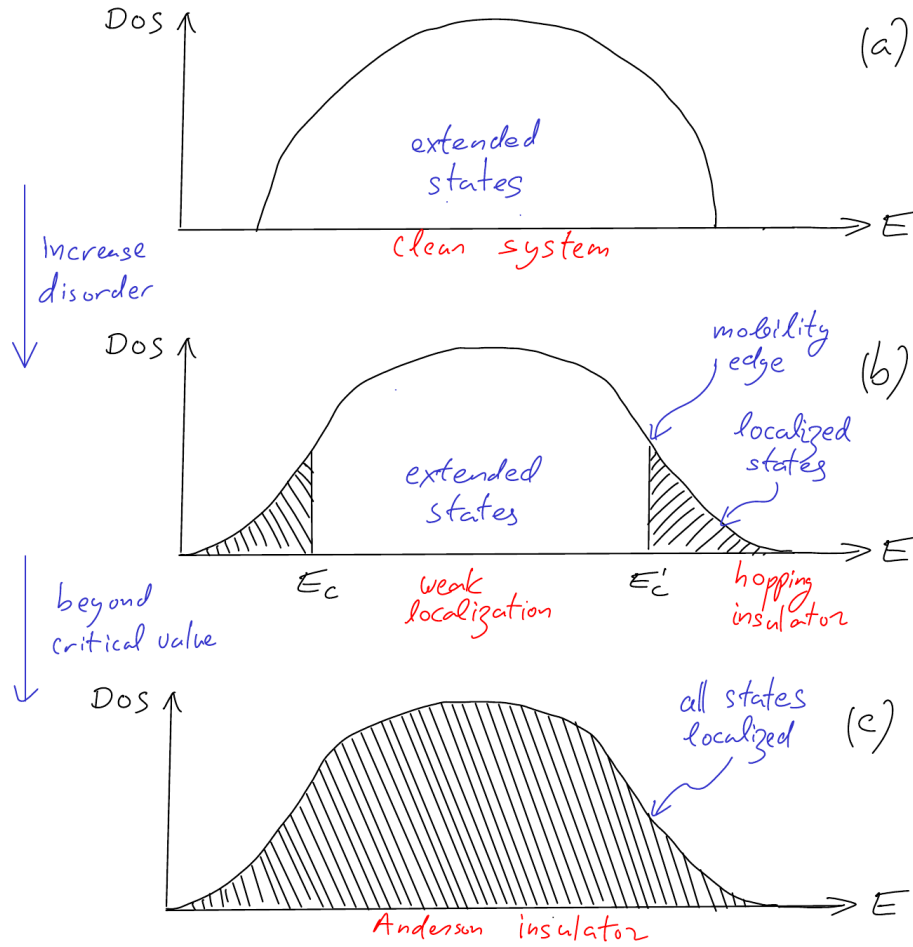


Fig. 1.1: Anderson metal-insulator transition: (a) Clean limit, all states in the band are extended. (b) Disorder is turned on. Tails of localized states appear, separated by the mobility edge from the region of extended states. (c) Beyond a threshold, all states become localized.