An outline of Drude theory

1 Static conductivity

According to classical mechanics, the motion of a free electron in a constant $\mathbf{E}$ field obeys the Newton equation

$$m\frac{d\mathbf{v}}{dt} = -e\mathbf{E}, \tag{1}$$

whose solution is $\mathbf{v}(t) = \mathbf{v}(0) - e\mathbf{E}t/m$; the electronic current density is $\mathbf{j}(t) = -en\mathbf{v}(t)$, where $n = N/V$ is the electron density. The macroscopic current obeys therefore the equation:

$$\frac{d\mathbf{j}}{dt} = (n/m)\, e^2\mathbf{E}. \tag{2}$$

Analogous results are retrieved in quantum mechanics (QM) and the macroscopic current obeys the equation:

$$\frac{d\mathbf{j}}{dt} = (n/m)_{\text{eff}}\, e^2\mathbf{E}. \tag{3}$$

The quantity $(n/m)_{\text{eff}}$ measures the density of free carriers and their (inverse) inertia. QM linear response theory provides indeed the value of $(n/m)_{\text{eff}}$; this is discussed below, Sec. 4.

In order to retrieve Ohm's law, Drude introduces "by hand"a phenomenological dissipation term in the equation of motion. In QM we *cannot* do the same; nonetheless a relaxation time τ can be inserted phenomenologically in the response functions. The classical equation of motion, including dissipation, is

$$\left(\frac{d\mathbf{j}}{dt} + \frac{\mathbf{j}}{\tau}\right) = (n/m)_{\text{eff}} e^2\mathbf{E}. \tag{4}$$

For any given initial conditions, $\mathbf{j}(t)$ has a transient which decays exponentially with lifetime τ. After this, the steady state solution is

$$\mathbf{j} = \sigma_{\text{Drude}}\mathbf{E} = (n/m)_{\text{eff}} e^2\tau\ \mathbf{E}, \tag{5}$$

where σ_{Drude} is the dc (i.e. static) conductivity in the Drude model. Notice that a dissipative system forgets its past, and the same steady state is reached independently of the initial conditions.

2 Drude theory (ω-dependent)

We now identify the input signal with a time-dependent electric field $\mathbf{E}(t)$ and the output one with the linearly induced current density $\mathbf{j}(t)$: the generalized susceptibility χ coincides in this case with the conductivity (scalar in isotropic systems). Switching then to the frequency domain, the conductivity $\sigma(\omega)$ measures the current linearly induced by an electric field at frequency ω

$$\mathbf{j}(\omega) = \sigma(\omega)\mathbf{E}(\omega). \tag{6}$$

We adopt our usual conventions about Fourier transforms; other conventions may change the sign of the imaginary parts in the response functions.

Inserting $\mathbf{E}(t) = \mathbf{E}(\omega)\mathrm{e}^{-i\omega t}$ in Eq. (4), we get

$$\left(-i\omega + \frac{1}{\tau}\right)\mathbf{j}(\omega) = (n/m)_{\text{eff}}e^2\mathbf{E}(\omega). \tag{7}$$

The Drude phenomenological formula is then

$$\sigma_{\text{Drude}}(\omega) = \frac{ie^2(n/m)_{\text{eff}}}{\omega + i/\tau}, \tag{8}$$

where $(n/m)_{\text{eff}}$ is the quantum analogue of the original n/m in the classical theory. The dc limit is purely dissipative:

$$\sigma_{\text{Drude}}(0) = e^2(n/m)_{\text{eff}}\tau. \tag{9}$$

We rewrite Eq. (8) as

$$\sigma_{\text{Drude}}(\omega) = \frac{i}{\pi}\frac{D}{\omega + i\eta}, \tag{10}$$

where $D = \pi e^2(n/m)_{\text{eff}}$ is the Drude weight and $\eta = 1/\tau$. Since $\eta > 0$ the conductivity has a pole in the complex ω plane at $\omega = -i\eta$ and is analytic in the upper half plane. This fact ensures a causal response and guarantees the Kramers-Kronig relationships.

The real and imaginary parts of σ denote in-phase (dissipative) and out-of-phase (reactive) response to the $\mathbf{E}$ field. Within the Drude model

$$\text{Re}\ \sigma_{\text{Drude}}(\omega) = \frac{1}{\pi}\frac{D\eta}{\omega^2 + \eta^2}\,; \qquad \text{Im}\ \sigma_{\text{Drude}}(\omega) = \frac{1}{\pi}\frac{D\omega}{\omega^2 + \eta^2}. \tag{11}$$

In the nondissipative ($\eta \to 0^+$), yet causal, limit we get

$$\text{Re}\ \sigma_{\text{Drude}}(\omega) = D\,\delta(\omega)\,; \qquad \text{Im}\ \sigma_{\text{Drude}}(\omega) = \frac{D}{\pi}\mathcal{P}\frac{1}{\omega}, \tag{12}$$

where $\mathcal{P}$ denotes the principal part. The dc ($\omega = 0$) in-phase conductivity has a δ-like divergence: this accounts for the obvious fact that free electrons in a constant field undergo free acceleration. The Drude weight measures, as said above, the inverse inertia of the many–electron system; it vanishes in insulators. For $\eta \to 0^+$ the current does not reach a steady state limit; equivalently, we may say that the system has an undamped normal mode at $\omega = 0$.

3 Classical theory in the vector-potential gauge

As explained below, the vector-potential gauge is mandatory within QM. It is therefore instructive to alternatively derive the same results as above in the vector potential gauge. The classical current is then

$$j = -\frac{e\,n}{m}\left(p + \frac{e}{c}A\right), \tag{13}$$

where the vector potential is time-dependent, but the dc limit is implicitly understood. The Drude conductivity is

$$\sigma_{\text{Drude}}(\omega) = \frac{d\,j(\omega)}{dE(\omega)} = \frac{d\,j(\omega)}{dA(\omega)}\frac{dA(\omega)}{dE(\omega)}. \tag{14}$$

Given that $\mathbf{E}(\omega) = i\omega\mathbf{A}(\omega)/c$, causal inversion yields

$$\frac{dA(\omega)}{dE(\omega)} = -\lim_{\eta\to 0^+}\frac{ic}{\omega + i\eta} = -c\left[\pi\delta(\omega) + \frac{i}{\omega}\right]. \tag{15}$$

Since we are interested in the dc limit only, it will be enough to derive Eq. (13) with respect to a *static* vector potential, hence

$$\frac{d\,j}{dA} = -\frac{e^2 n}{mc}, \tag{16}$$

$$\text{Re}\ \sigma_{\text{Drude}}(\omega) = \frac{e^2\pi n}{m}\,\delta(\omega)\ : \tag{17}$$

as expected, this is the same result as found above.

4 Quantum mechanics

The conductivity tensor in QM is defined via linear-response theory; its expression belongs to the family of Kubo formulas, thoroughly discussed in the Lecture Notes.

In general longitudinal conductivity is a symmetric Cartesian tensor $\sigma_{\alpha\beta}$, and is the sum of a regular term and a Drude (δ-like) term:

$$\text{Re}\ \sigma_{\alpha\beta}(\omega) = D_{\alpha\beta}\,\delta(\omega) + \sigma^{(\text{regular})}_{\alpha\beta}(\omega). \tag{18}$$

The Drude term accounts for free acceleration, in analogy to the classical case. Recalling our previous definition $D = \pi e^2 (n/m)_{\text{eff}}$, linear-response theory provides the QM expression for $(n/m)_{\text{eff}}$. The Kubo formula for conductivity can be formally written even for correlated systems, and even for finite temperature.

In order to deal with dc currents within Born-von-Kàrmàn periodic boundary conditions it is mandatory to adopt the vector-potential gauge (no steady current may flow in a bounded sample); ergo

$$\sigma_{\alpha\beta}(\omega) = \frac{\partial j_\alpha(\omega)}{\partial E_\beta(\omega)} = \frac{\partial j_\alpha(\omega)}{\partial A_\beta(\omega)} \frac{dA(\omega)}{dE(\omega)} = -c \frac{\partial j_\alpha(\omega)}{\partial A_\beta(\omega)} \left[\pi \delta(\omega) + \frac{i}{\omega} \right], \tag{19}$$

where the factor $\partial j_\alpha(\omega)/\partial E_\beta(\omega)$ requires in general time-dependent perturbation theory (i.e. a sum-over-states Kubo formula).

However, if we are interested in the dc response only, it will be enough to insert into Eq. (19) the response of the many-electron system to a *static* vector potential $\mathbf{A}$ (constant in space):

$$\sigma^{(\mathrm{D})}_{\alpha\beta}(\omega) = -c \frac{\partial j_\alpha}{\partial A_\beta} \left[\pi \delta(\omega) + \frac{i}{\omega} \right]. \tag{20}$$

The QM expression for Drude weight is then

$$D_{\alpha\beta} = -c\pi \frac{\partial j_\alpha}{\partial A_\beta}. \tag{21}$$

In the special case of noninteracting electrons in a periodic (mean-field) potential we define the α component of the electron velocity in the n-th band as

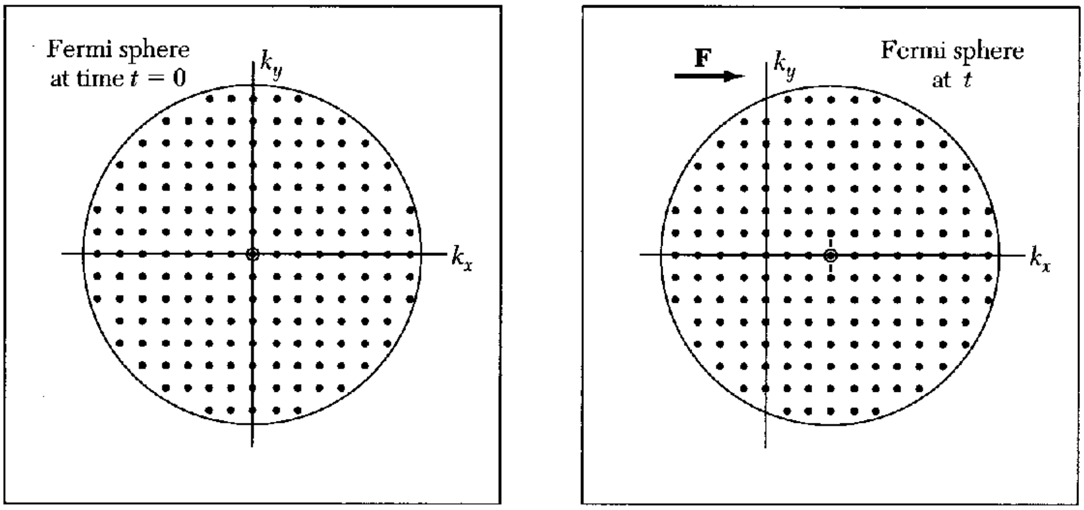
$$v_{n\alpha}(\mathbf{k}) = \frac{1}{\hbar} \frac{\partial \varepsilon_n(\mathbf{k})}{\partial k_\alpha}; \tag{22}$$

the Drude weight can be cast as

$$D_{\alpha\beta} = -\frac{2\pi e^2}{(2\pi)^3} \sum_n \int d\mathbf{k} \; \frac{\partial f_\epsilon}{\partial \varepsilon_n(\mathbf{k})} \; v_{n\alpha}(\mathbf{k}) v_{n\beta}(\mathbf{k}), \tag{23}$$

where f_ϵ is the Fermi distribution function. At zero temperature D is a pure Fermi-surface property, i.e. D depends only on the shape of the Fermi surface and on the $\mathbf{k}$-derivatives of the band structure $\varepsilon_n(\mathbf{k})$ at the Fermi surface. Clearly, these are the only ingredients which can account for free acceleration in a crystalline system.

Eq. (23) is derived at the semiclassical level in Chap. 13 of the Ashcroft-Mermin textbook. We remind that a full QM approach requires dealing with the vector potential, while the semiclassical approximation allows dealing with the field $\mathbf{E}$: this makes life easier. The general QM theory of the Drude weight can be found in the Lecture Notes.



(a) (b)

Figure 10 (a) The Fermi sphere encloses the occupied electron orbitals in **k** space in the ground state of the electron gas. The net momentum is zero, because for every orbital **k** there is an occupied orbital at $-\mathbf{k}$. (b) Under the influence of a constant force **F** acting for a time interval t every orbital has its **k** vector increased by $\delta\mathbf{k} = \mathbf{F}t/\hbar$. This is equivalent to a displacement of the whole Fermi sphere by $\delta\mathbf{k}$. The total momentum is $N\hbar\delta\mathbf{k}$, if there are N electrons present. The application of the force increases the energy of the system by $N(\hbar\delta\mathbf{k})^2/2m$.

It is a simple exercise to apply Eq. (23) to the simple case of noninteracting electrons in zero potential (free electron gas), and at zero temperature. In this case we have:

$$f_\epsilon = \theta(\epsilon_{\mathrm{F}} - \epsilon), \qquad \varepsilon(k) = \frac{\hbar^2}{2m}k^2; \tag{24}$$

$$f'_{\epsilon(\mathbf{k})} = -\,\delta(\varepsilon_{\mathrm{F}} - \frac{\hbar^2}{2m}k^2) = -\frac{m}{\hbar^2 k_{\mathrm{F}}}\delta(k_{\mathrm{F}} - k); \qquad \frac{1}{3}v^2 = \frac{\hbar^2 k_{\mathrm{F}}^2}{3m^2}. \tag{25}$$

$$D = -\frac{2\pi e^2}{(2\pi)^3}\left(-\frac{m}{\hbar^2 k_{\mathrm{F}}}\right) 4\pi k_{\mathrm{F}}^2\,\frac{\hbar^2 k_{\mathrm{F}}^2}{3m^2} = \pi e^2 \frac{k_{\mathrm{F}}^3}{3\pi^2 m} = \pi e^2 \frac{n}{m}. \tag{26}$$

It is remarkable that for noninteracting electrons in zero potential we get precisely $(n/m)_{\mathrm{eff}} = n/m$, i.e. the QM result coincides with the classical one, obtained by Drude in 1900. In other words Schrödinger equation, Pauli principle, and Fermi-Dirac statistics do not provide any correction to the original Drude result in this simple case. The reasons why this happens are pretty clear from a figure in Kittel, reproduced here.