

Lecture notes on semiclassical transport

Contents

1	Classical Drude-Sommerfeld transport	2
2	Semiclassical Boltzmann transport	3
2.1	Boltzmann equation	3
2.2	Collision integral. Scattering from impurities.	5
2.3	Relaxation time approximation	7
2.4	Electrical conductivity	7

1 Classical Drude-Sommerfeld transport

In the most basic formulation of the Drude-Sommerfeld model, we consider the dynamics of single-particles in metals exposed to a static, homogeneous electric field. We represent the scattering from impurities in the crystalline lattice as a single phenomenological (i.e. not derived from a microscopic theory) parameter, the momentum relaxation time τ . This parameter represents the average time between scattering events. After each scattering event, we assume the momentum to be completely randomized, with a zero average. This is an approximate classical modeling of disorder that leaves much to be desired. However, it has the merit to lead to a correct identification of the particles mobility and conductivity. Furthermore, it will serve as a classical, intuitive backdrop as we make our way forward towards a more accurate quantum description.

If we assume the average time between scattering events to be τ , we infer the following relations:

$$\text{probability of scattering in a time interval } dt = \frac{dt}{\tau} \quad (1)$$

$$\text{probability of not scattering in a time interval } dt = 1 - \frac{dt}{\tau} \quad (2)$$

These allow us to write an equation of motion for the momentum \mathbf{p}

$$\mathbf{p}(t + dt) = \underbrace{\left(1 - \frac{dt}{\tau}\right)}_{\text{prob not scattering}} \times \underbrace{\left(\mathbf{p}(t) - e\mathbf{E}(t)dt\right)}_{\text{newtonian dynamics}} + \underbrace{\left(\frac{dt}{\tau}\right)}_{\text{prob scattering}} \times \underbrace{\left(\mathbf{0}\right)}_{\text{average p after scattering}} \quad (3)$$

which leads, up to linear order, to the following differential equation

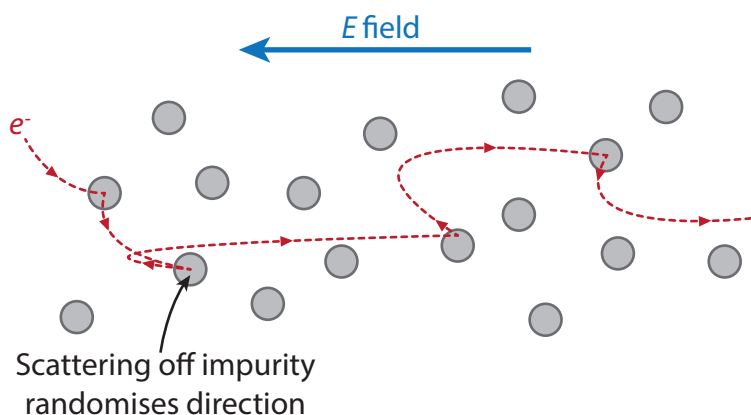
$$\mathbf{p}(t + dt) - \mathbf{p}(t) = -e\mathbf{E}(t)dt - \mathbf{p}(t)\frac{dt}{\tau} \quad (4)$$

$$\frac{d\mathbf{p}}{dt} = -e\mathbf{E}(t) - \frac{\mathbf{p}}{\tau} \quad (5)$$

For a time-independent homogeneous electric field $\mathbf{E}(t) = \mathbf{E}$, we find the following steady-state ($d\mathbf{p}/dt = 0$) solution:

$$\mathbf{p} = -e\tau\mathbf{E} \quad (6)$$

This steady-state corresponds to a drift of diffusing particles under a constant field (see figure).



These dynamics are characterised by a drift velocity

$$\mathbf{v} = \frac{\mathbf{p}}{m} = -\frac{e\tau}{m}\mathbf{E} = -\mu\mathbf{E} \quad (7)$$

The parameter μ is called the electron mobility. The drift velocity allows us to compute the current density

$$\mathbf{j} = -nev = ne\mu\mathbf{E} = \sigma\mathbf{E} \quad (8)$$

which leads us to identify the dc Drude-Sommerfeld conductivity

$$\sigma_{\text{dc}} = ne\mu = \frac{ne^2\tau}{m} \quad (9)$$

Despite the classical nature of this derivation, the relation we obtained for the conductivity holds up to more accurate scrutiny. We will develop two more advanced descriptions of the conductivity, the first based on a semiclassical model, the second fully quantum mechanical (during the lecture on correlation functions), and both approaches will lead to this result. The main intellectual gain from this extra effort will be a microscopic description of the momentum relaxation time τ . These more accurate models will also properly account for the presence of a crystal lattice (Bloch electrons dispersion) and can be extended to consider other sources of scattering in addition to impurities.

2 Semiclassical Boltzmann transport

2.1 Boltzmann equation

The Boltzmann semiclassical theory of transport is based on finding a distribution function that describes the electron system under some non-equilibrium conditions created by stimulating the solid with electromagnetic fields or thermal loads. We find an out of equilibrium distribution function by solving an equation generalised from the kinetic theory of diluted gases, the Boltzmann equation.

In the context of a transport theory of metals, the Boltzmann equation captures some elements of the quantum dynamics of electrons by describing them as wavepackets with a Fourier spectrum. However, we should be aware that this approach will not account for all quantum mechanical effects. As we will see, a notable limitation is that multiple scattering paths will be simply added up. Consequently, the description of quantum interference between different paths leading to the same final state will require a different formalism, summarised later in the course.

A (semiclassical) distribution function f describes the probability of a (quantum) particle to be in a position \mathbf{r} , with momentum \mathbf{p} , at time t , (within the constraints of the Heisenberg inequality).

$$\text{Number of electrons in an element of phase space} = \underbrace{\left(f(\mathbf{r}, \mathbf{p}, t) \right)}_{\text{distribution}} \underbrace{\left(2 \frac{d^3 \mathbf{r} d^3 \mathbf{p}}{(2\pi\hbar)^3} \right)}_{\text{density}} \quad (10)$$

In thermodynamic equilibrium, the distribution function is given by the Fermi-Dirac distribution f^{FD}

$$f(\mathbf{r}, \mathbf{p}, t) = f^{\text{FD}}(\mathbf{p}) = \frac{1}{e^{\epsilon(\mathbf{p}) - \mu} / k_B T} + 1 \quad (11)$$

The function $\epsilon(\mathbf{p})$ represents the electron dispersion.

The presence of external fields will introduce variations in the space, momentum and time dependence of the distribution function, creating some non-equilibrium conditions. The response of the system, by means of a redistribution of electrons in state $i = (\mathbf{r}, \mathbf{p})$, is described by the Boltzmann equation for f_i ,

$$\frac{d}{dt} f_i = I[f_i] \quad (12)$$

$$\frac{d}{dt} f(\mathbf{r}, \mathbf{p}, t) = \frac{\partial f}{\partial t} + \left(\frac{\partial f}{\partial x} \frac{dx}{dt} + \frac{\partial f}{\partial y} \frac{dy}{dt} + \frac{\partial f}{\partial z} \frac{dz}{dt} \right) + \left(\frac{\partial f}{\partial p_x} \frac{dp_x}{dt} + \frac{\partial f}{\partial p_y} \frac{dp_y}{dt} + \frac{\partial f}{\partial p_z} \frac{dp_z}{dt} \right) \quad (13)$$

$$= \underbrace{\left(\frac{\partial f}{\partial t} \right)}_{\text{time-dependent fields}} + \underbrace{\left(\nabla f \cdot \dot{\mathbf{r}} \right)}_{\text{inhomogeneous fields}} + \underbrace{\left(\frac{\partial f}{\partial \mathbf{p}} \cdot \dot{\mathbf{p}} \right)}_{\text{external forces}} = I[f(\mathbf{r}, \mathbf{p}, t)] \quad (14)$$

The action of external fields is described on the left hand side of the equation, where time-dependent, inhomogeneous fields and external forces modify the space, momentum and time dependence of the distribution function. The redistribution of electrons in state i , caused by scattering processes, (the probability of changing the occupation of state i through scattering) are described by a functional of the distribution $I[f_i]$, called the collision integral, on the right hand side of the equation.

The Boltzmann equation describes a transfer of electrons from state i to the others and vice-versa, governed by the collision integral. The collision integral accounts for the probability of loss (increase) of particles from (into) state i associated with the scattering mechanisms that we consider. We will assume the limit of weak deviations from equilibrium, in which the collision integral is a linear functional. A typical form for calculating this functional from the probability per unit of time of having a transition from state \mathbf{p} to state \mathbf{p}' (encoded by the scattering rate $u_{\mathbf{p}'\mathbf{p}}$) is:

$$I[f_i] = \text{Probability of changing the occupation of state } \mathbf{p} = \quad (15)$$

$$= \underbrace{\int 2_s \frac{d^3\mathbf{r}d^3\mathbf{p}}{(2\pi\hbar)^3}}_{\text{sum over all possible states}} \left[\underbrace{\left(-u_{\mathbf{p}'\mathbf{p}}f_{\mathbf{p}}(1-f_{\mathbf{p}'}) \right)}_{\text{loss of particles from p to p}'} + \underbrace{\left(u_{\mathbf{p}\mathbf{p}'}f_{\mathbf{p}'}(1-f_{\mathbf{p}}) \right)}_{\text{gain of particles from p' to p}} \right] \quad (16)$$

In a Boltzmann transport calculation we: 1) identify the relevant scattering processes, 2) write the associated collision integral, a functional of the distribution function 3) solve the Boltzmann equation for the distribution function f and 4) using the solution f , calculate the electrical conductivity or other transport quantities of interest (e.g. thermal transport).

2.2 Collision integral. Scattering from impurities.

The next step is to describe the collision integral (probability of loss (increase) of particles from (into) state i) associated with scattering from impurities using Fermi's golden rule, a basic formulation of perturbation theory (a perturbative analysis of impurity scattering is also known as the Born approximation). In this description, the probability per unit of time (scattering rate) to have a transition from state \mathbf{p} to state \mathbf{p}' is

$$w_{\mathbf{p}'\mathbf{p}} = \frac{2\pi}{\hbar} |V_{\mathbf{p}'\mathbf{p}}|^2 \delta[\epsilon(\mathbf{p}) - \epsilon(\mathbf{p}')] \quad (17)$$

where $V_{\mathbf{p}\mathbf{p}'}$ is the matrix element of the total impurity potential $V(\mathbf{r})$. This potential is the sum of all the potentials associated with the individual impurities $v(\mathbf{r} - \mathbf{r}_n)$ (indexed by their positions \mathbf{r}_n on the lattice sites):

$$V(\mathbf{r}) = \sum_n v(\mathbf{r} - \mathbf{r}_n) \quad (18)$$

We compute the matrix elements using the Bloch's states

$$\psi_{\mathbf{p}}(\mathbf{r}) = \frac{1}{\sqrt{\mathcal{V}}} u_{\mathbf{p}}(\mathbf{r}) e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \quad (19)$$

remembering that $u_{\mathbf{p}}(\mathbf{r}) = u_{\mathbf{p}}(\mathbf{r} + \mathbf{r}_n)$. We define the matrix elements of the individual impurity potential as

$$v_{\mathbf{p}'\mathbf{p}} = \int e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}/\hbar} u_{\mathbf{p}'}^*(\mathbf{r}) v(\mathbf{r}) u_{\mathbf{p}}(\mathbf{r}) d^3\mathbf{r} \quad (20)$$

Therefore we find for the matrix elements of the whole impurity potential

$$V_{\mathbf{p}'\mathbf{p}} = \int \psi_{\mathbf{p}'}^*(\mathbf{r})V(\mathbf{r})\psi_{\mathbf{p}}(\mathbf{r})d^3\mathbf{r} = \quad (21)$$

$$= \frac{1}{\mathcal{V}} \sum_n \int e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}/\hbar} u_{\mathbf{p}'}^*(\mathbf{r})v(\mathbf{r}-\mathbf{r}_n)u_{\mathbf{p}}(\mathbf{r})d^3\mathbf{r} = \quad (22)$$

$$= \frac{1}{\mathcal{V}} \sum_n \int e^{i(\mathbf{p}-\mathbf{p}')\cdot(\mathbf{r}+\mathbf{r}_n)/\hbar} u_{\mathbf{p}'}^*(\mathbf{r}+\mathbf{r}_n)v(\mathbf{r})u_{\mathbf{p}}(\mathbf{r}+\mathbf{r}_n)d^3\mathbf{r} = \quad (23)$$

$$= \frac{1}{\mathcal{V}} \sum_n e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}_n/\hbar} \int e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}/\hbar} u_{\mathbf{p}'}^*(\mathbf{r})v(\mathbf{r})u_{\mathbf{p}}(\mathbf{r})d^3\mathbf{r} = \quad (24)$$

$$V_{\mathbf{p}'\mathbf{p}} = \frac{1}{\mathcal{V}} \sum_n e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}_n/\hbar} v_{\mathbf{p}'\mathbf{p}} \quad (25)$$

This quantity depends explicitly on the position of each individual impurity, which renders its calculation impossible in any realistic scenario. In order to continue, we need to perform an operation called impurity averaging, which consists in averaging the calculation of the matrix element over all possible realisations of disorder. This is possible whenever the mean root square deviations of a quantity are much smaller than its average, which is the case for macroscopic solids. In this case disorder is said to be self-averaging. For mesoscopic solids this condition is not satisfied. Impurity averaging consists in summing over all possible impurity positions in the following way:

$$\langle |V_{\mathbf{p}'\mathbf{p}}|^2 \rangle = \frac{1}{\mathcal{V}^2} \left\langle \sum_{n,k} e^{i(\mathbf{p}-\mathbf{p}')\cdot(\mathbf{r}_n-\mathbf{r}_k)/\hbar} \right\rangle |v_{\mathbf{p}'\mathbf{p}}|^2 \quad (26)$$

The terms $n \neq k$ will return a collection of randomly and evenly distributed phases. They will average out to zero. The terms $n = k$ will instead sum up to the number of impurities N_i . Therefore we obtain

$$\langle |V_{\mathbf{p}'\mathbf{p}}|^2 \rangle = \frac{n_i}{\mathcal{V}} |v_{\mathbf{p}'\mathbf{p}}|^2 \quad (27)$$

where $n_i = N_i/\mathcal{V}$ denotes the density of impurities. Under this assumption, Fermi's golden rule returns the following approximation for the scattering rate (probability per unit of time)

$$w_{\mathbf{p}'\mathbf{p}} = \frac{2\pi n_i}{\hbar \mathcal{V}} |v_{\mathbf{p}'\mathbf{p}}|^2 \delta[\epsilon(\mathbf{p}) - \epsilon(\mathbf{p}')] \quad (28)$$

We are now in a position to write an expression for the collision integral (probability of loss (increase) of particles from (into) state i) associated with scattering from impurities:

$$I[f_i] = \int 2_s \frac{d^3\mathbf{r}d^3\mathbf{p}}{(2\pi\hbar)^3} [(-w_{\mathbf{p}'\mathbf{p}}f_{\mathbf{p}}(1-f_{\mathbf{p}'}) + (w_{\mathbf{p}\mathbf{p}'}f_{\mathbf{p}'}(1-f_{\mathbf{p}}))] \quad (29)$$

2.3 Relaxation time approximation

We now make some further simplifying assumptions on the nature of scattering from impurities. We will assume an isotropic electron dispersion and isotropic scattering described by a matrix element w_0 . In this case the scattering rate is

$$w_{\mathbf{p}'\mathbf{p}} = w_{\mathbf{p}\mathbf{p}'} = w_0 \delta[\epsilon(\mathbf{p}) - \epsilon(\mathbf{p}')] \quad (30)$$

and the collision integral becomes

$$I[f_{\mathbf{p}}] = -w_0 \mathcal{V} \int 2_s \frac{d^3 \mathbf{p}'}{(2\pi\hbar)^3} \delta[\epsilon(\mathbf{p}) - \epsilon(\mathbf{p}')] (f_{\mathbf{p}} - f_{\mathbf{p}'}) = \quad (31)$$

$$= -w_0 \mathcal{V} g[\epsilon(\mathbf{p})] \int \frac{d\Omega'}{4\pi} (f_{\mathbf{p}} - f_{\mathbf{p}'}) \quad (32)$$

The integral over the solid angle Ω' is performed over the orientations of the states \mathbf{p}' having the same norm as state \mathbf{p} (isotropic elastic scattering). The scattering rate is defined as $1/\tau = w_0 \mathcal{V} g[\epsilon(\mathbf{p})]$, where $g[\epsilon(\mathbf{p})]$ is the density of states at energy $\epsilon(\mathbf{p})$:

$$I[f_{\mathbf{p}}] = -\frac{1}{\tau} f_{\mathbf{p}} + \frac{1}{\tau} \int \frac{d\Omega'}{4\pi} f_{\mathbf{p}'} \quad (33)$$

Finally, if we assume that the distribution of states \mathbf{p}' , averaged over all possible directions of this vector, is the same as the equilibrium distribution, that is

$$\int \frac{d\Omega'}{4\pi} f_{\mathbf{p}'} = f_{\mathbf{p}}^{\text{FD}} \quad (34)$$

we find

$$\boxed{I[f_{\mathbf{p}}] = -\frac{1}{\tau} (f_{\mathbf{p}} - f_{\mathbf{p}}^{\text{FD}})} \quad (35)$$

We have reduced the collision integral into a form known as the relaxation time approximation. If the set of idealised conditions outlined here are realised, this form of the collision integral is exact. However, it is often used in many practical calculations even if these ideal conditions are not present. The relaxation-time approximation is often the first approach used to describe transport, disregarding the complexities introduced by anisotropic electronic structures, scattering centres with asymmetric cross section, etc.

2.4 Electrical conductivity

For a time-independent, homogeneous electric field \mathbf{E} , the Boltzmann equation reduces to

$$\frac{\partial f}{\partial \mathbf{p}} \cdot \dot{\mathbf{p}} = I[f_{\mathbf{p}}] \quad (36)$$

$$-\frac{\partial f}{\partial \mathbf{p}} \cdot e\mathbf{E} = I[f_{\mathbf{p}}] \quad (37)$$

In the relaxation-time approximation

$$-\frac{\partial f}{\partial \mathbf{p}} \cdot e\mathbf{E} = -\frac{1}{\tau}(f_{\mathbf{p}} - f_{\mathbf{p}}^{\text{FD}}) \quad (38)$$

we need to solve this equation for $f_{\mathbf{p}}$. Our strategy will focus on expanding the solution $f_{\mathbf{p}}$ in powers of the electric field \mathbf{E} :

$$f_{\mathbf{p}} = f_{\mathbf{p}}^{\text{FD}} + f_{\mathbf{p}}^1 + \text{higher order terms in } \mathbf{E} \quad (39)$$

with $f_{\mathbf{p}}^1 \propto \mathbf{E}$ and the zero-order term is identified as the Fermi-Dirac distribution. In the linear response regime, we retain only the linear terms in the electric field:

$$e\mathbf{E} \cdot \frac{\partial}{\partial \mathbf{p}} [f_{\mathbf{p}}^{\text{FD}} + f_{\mathbf{p}}^1] = \frac{1}{\tau} (f_{\mathbf{p}}^{\text{FD}} + f_{\mathbf{p}}^1 - f_{\mathbf{p}}^{\text{FD}}) \quad (40)$$

Since $f_{\mathbf{p}}^1 \propto \mathbf{E}$ we can solve this expression in the linear response regime:

$$f_{\mathbf{p}}^1 = e\tau \mathbf{E} \cdot \frac{\partial}{\partial \mathbf{p}} f_{\mathbf{p}}^{\text{FD}} = \quad (41)$$

$$= e\tau \mathbf{E} \cdot \frac{d}{d\epsilon} f_{\mathbf{p}}^{\text{FD}} \frac{\partial \epsilon}{\partial \mathbf{p}} = \quad (42)$$

$$= \left(\frac{d}{d\epsilon} f_{\mathbf{p}}^{\text{FD}} \right) e\tau \mathbf{E} \cdot \mathbf{v} = \quad (43)$$

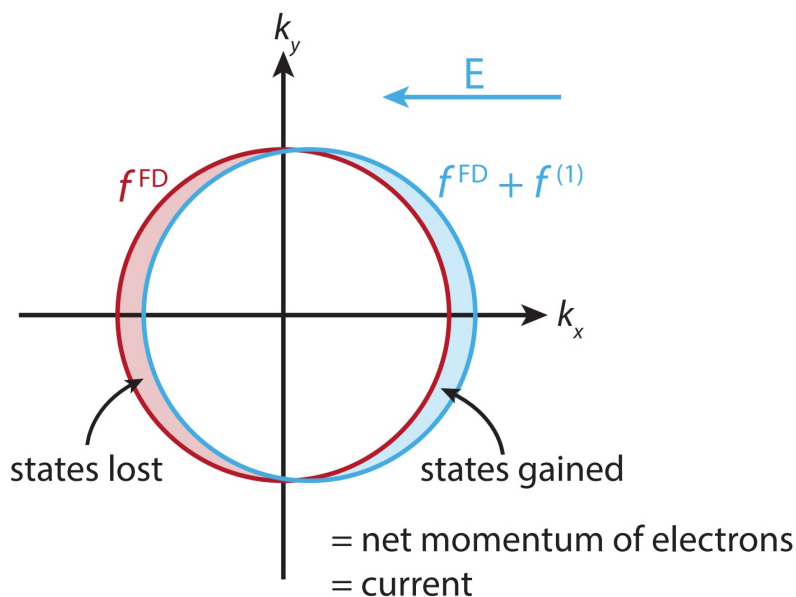
where $\mathbf{v} = \frac{\partial \epsilon}{\partial \mathbf{p}}$ is the group velocity of the wavepacket.

We have now solved the Boltzmann equation in the relaxation time approximation and we are equipped with an out of equilibrium distribution function induced by a weak electric field (see figure):

$$\boxed{f_{\mathbf{p}}^{\text{linear response}} = f_{\mathbf{p}}^{\text{FD}} + \left(\frac{d}{d\epsilon} f_{\mathbf{p}}^{\text{FD}} \right) e\tau \mathbf{E} \cdot \mathbf{v}} \quad (44)$$

We can use this knowledge to calculate the current induced by an external electric field and therefore infer the conductivity. The current density is given by the product of the charge $-e$, the group velocity \mathbf{v} associated with the state at \mathbf{p} , the density of states per unit volume $D_{\mathbf{p}} = 2/(2\pi\hbar)^3$ and the probability density function $f_{\mathbf{p}}$ summed over all states.

$$\mathbf{j} = -nev = -e \int \mathbf{v} D_{\mathbf{p}} f_{\mathbf{p}} d^3\mathbf{p} = -2e \int \mathbf{v} f_{\mathbf{p}} \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} \quad (45)$$



Since there is no current at equilibrium, for an isotropic medium we find

$$\mathbf{j} = -2e^2 \int \left(\frac{d}{d\epsilon} f^{\text{FD}} \right) \tau \mathbf{v} (\mathbf{E} \cdot \mathbf{v}) \frac{d^3 \mathbf{p}}{(2\pi\hbar)^3} \quad (46)$$

For $k_B T \ll \epsilon_F$, we have $\frac{d}{d\epsilon} f^{\text{FD}} = -\delta(\epsilon - \mu)$. In other words, the conductivity is determined by electronic states sharply located at the Fermi surface.

We can then change the integration over all momenta, to an integration over just the Fermi surface. For an isotropic Fermi Surface

$$2 \int \left(-\frac{d}{d\epsilon} f^{\text{FD}} \right) \frac{d^3 \mathbf{p}}{(2\pi\hbar)^3} = g(\mu) \int_{\text{FS}} dS \quad (47)$$

where the surface integral is normalised $\int_{\text{FS}} dS = 1$ and the density of states $g(\mu)$ has absorbed the factor 2 for spin degeneracy. For a spherical Fermi surface, the current can be written

$$\mathbf{j} = e^2 \int \frac{\sin \theta d\theta d\phi}{4\pi} g(\mu) \tau \mathbf{v} (\mathbf{E} \cdot \mathbf{v}) \simeq \frac{1}{3} e^2 \left(g v^2 \tau \right)_{\epsilon=\mu} \mathbf{E} \quad (48)$$

where the factor of 1/3 appears from the integration over the sphere of $\mathbf{v} (\mathbf{E} \cdot \mathbf{v})$, remembering that in this case \mathbf{v} is always normal to the surface.

Remembering that

$$\mathbf{j} = -nev = ne\mu \mathbf{E} = \sigma \mathbf{E} \quad (49)$$

we identify the conductivity

$$\sigma = \frac{1}{3} e^2 \left(g v^2 \tau \right)_{\epsilon=\mu} \quad (50)$$

This relation can be used to calculate the conductivity within the relaxation-time approximation of isotropic solids with a known dispersion relation. Using a parabolic dispersion with effective mass m^* , we find

$$\sigma_{\text{dc}} = \frac{n e^2 \tau}{m^*} \quad (51)$$

which coincides with the Drude-Sommerfeld result for $m^* = m$.