L2 Notes: Semiclassical transport

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Lecture notes by Ethan Minot, visiting from Oregon State University
ethan.minot@aalto.fi
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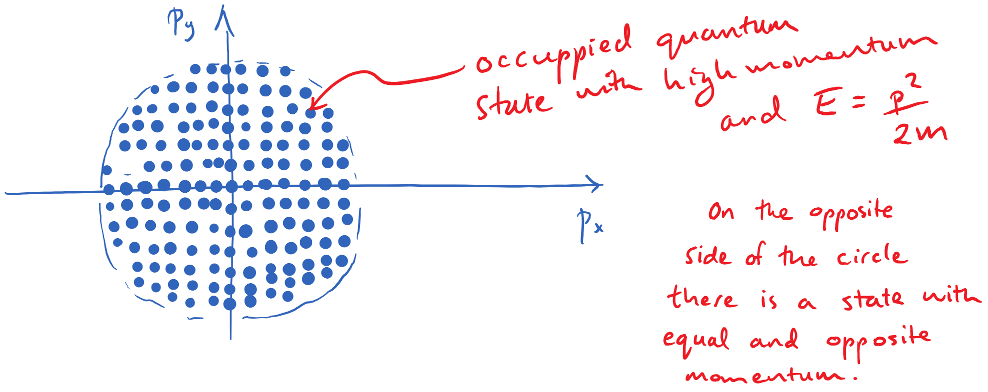
Only one electron in each quantum state. In metals, this means that quantum states with high kinetic energy are occupied. There are always fast moving electrons in the metal. In equilibrium, left movers are balanced with right movers. Semiclassical transport models capture this idea. There are limitations to semiclassical transport models, but it is a useful description for many situations.



occuppied quantum state with high momentum and $E = \frac{p^2}{2m}$

On the opposite side of the circle there is a state with equal and opposite momentum.

There is an even simpler model that doesn't even account for the distribution of filled quantum states. This simplest transport model is called the Drude model, we'll compare some semiclassical and quantum predictions to Drude prediction. Surprisingly, in some cases they are identical. For developing intuition and ability to do quick calculations, it's important to know the simplest model that is adequate for your system.

Least refined ↓ Most refined

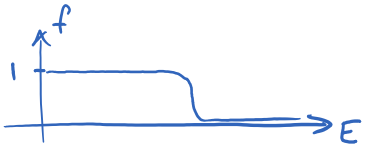
Drude model

Semiclassical transport (Boltzmann transport) ← Extract some information/insight from quantum mechanics and then treat electrons more like classical particles.

Landauer-Büttiker formalism

Both the semiclassical and Landauer pictures make use of the Fermi-Dirac distribution to describe the occupation of quantum states at finite temperature.

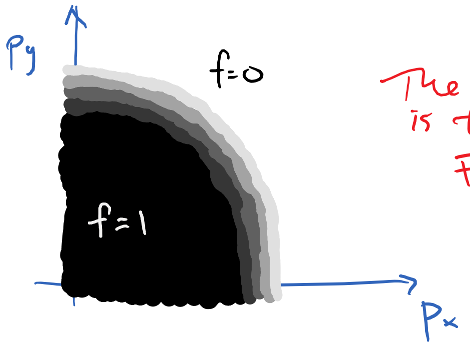
$$f(E) = \frac{1}{e^{(E-\mu)/k_BT} + 1}$$



occupation
function

Where E is the energy of the quantum state, which depends on p.

We can make a color plot of *f* in momentum space.



The effect of temperature is to blur the edge of the Fermi surface.

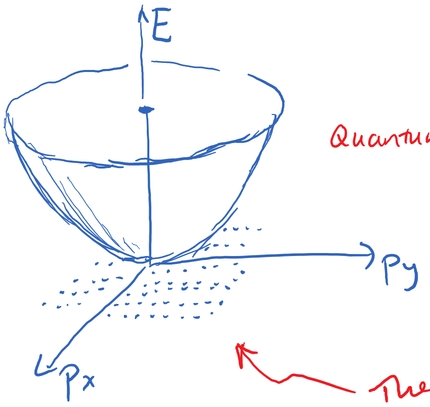
(only showing the positive quadrant of momentum space, not showing the full sphere)

Exercise to do with your neighbor:
If E = p^2/2m, and the radius of the Fermi surface is p_F, and E_F << k_BT, what is the width of the "blurred" region in momentum space?

The philosophy of this course is to make the simplest assumption for *E*(*p*).
In general, different metals and doped semiconductors can have interesting variation on *E*(*p*), but most ideas can be explained if we assume

$$E(p) = \frac{p^2}{2 m_{eff}}$$

effective mass,
can be larger or
smaller than electron mass

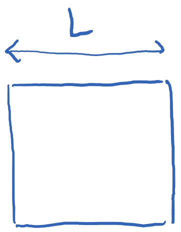


Quantum states lie on this parabolic bowl.

There is a uniform density of quantum states in momentum space

To find the density of state in momentum space, remember deBroglie relation, and apply periodic boundary conditions

$p = \hbar k$ $\qquad \left(p = \frac{h}{\lambda}\right)$ ← electron wavelength



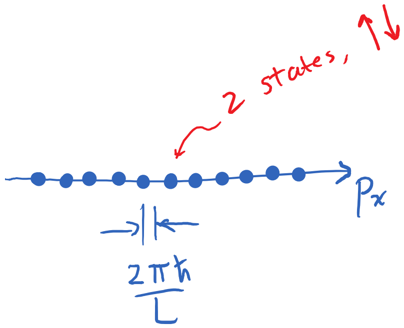
Size of sample in real space

Periodic B.C.

$k_x L = n_x 2\pi$ where n is integer

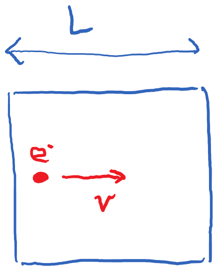
$k_x = \frac{2\pi}{L} n_x$

$p_x = \frac{2\pi\hbar}{L} n_x$



We'll need to know this spacing between states (which depends on the size of the sample) when we do integrals in momentum space.

We like to use momentum eigenstates for the electron wavefunctions. But, in quantum mechanics, when momentum is exactly known, position is completely delocalized. Philosophical question: Can we invent a semiclassical transport theory that treats electrons like particles? If yes, how do we extract useful information from the band structure (energy of the momentum eigenstates)?



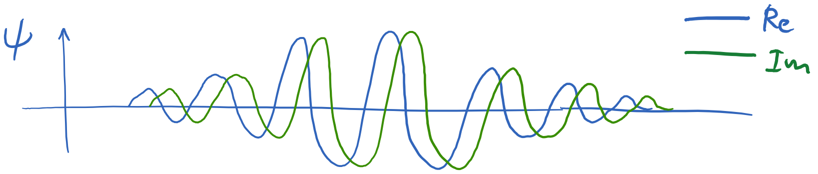
Size of sample in real space

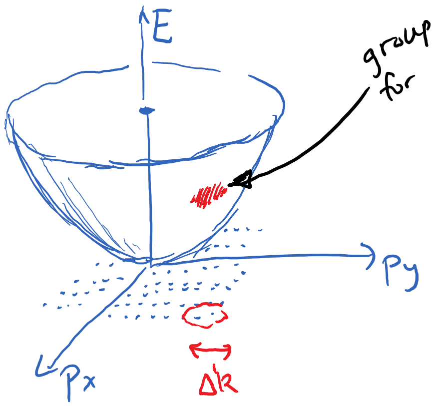
For a semiclassical theory can we think of a point-like particle being transported across the sample ?

Rather than thinking of $\frac{1}{\sqrt{L^3}} e^{i\vec{k}\cdot\vec{r}}$ as basis states, I could construct a new basis of wavepacket states $\sum_{\text{nearby}} a_i \frac{1}{\sqrt{L^3}} e^{i\cdot\vec{k}_i\cdot\vec{r}}$ where a_i are weighting factors.

nearby
$\vec{k}$-states

Each wavepacket has a small spead in $\vec{k}$ (not too much)
and a small spread in position (not too much)





group velocity for this wave packet
$v_g = \frac{dE}{dp}$

Superposition of states to describe a wave packet

when $E = \frac{p^2}{2m}$, the group velocity is described by the familiar relationship $v_g = \frac{p}{m}$

For a wave packet with Δk

$\Delta x \Delta k \approx 1$

To make $\Delta x = 10\text{nm}$, need $\Delta k \approx 10^8\ \text{m}^{-1}$

In metals $k_F \approx 10^{10}\ \text{m}^{-1}$, therefore $\Delta k \approx 10^8\ \text{m}^{-1}$ is reasonably well defined.

In summary, for large samples (millimeter scale) we can use quantum mechanics to justify the semiclassical idea that electrons are travelling like particles with reasonably well defined position and momentum and a velocity given by dE/dp.

Now we can write a semiclassical equation for the charge current density moving through a material.

spin degeneracy

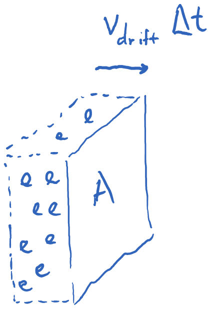
$$\vec{j}_c = -e\int d^3p \; \underbrace{\frac{\overset{\text{spin degeneracy}}{2}}{8\pi^3\hbar^3}}_{\text{number of states per unit volume, } L^3\text{, of the material, and per unit "volume" of momentum space.}} \; \frac{\vec{p}}{m} \; f(\vec{p})$$

velocity of a particular state

This is a more refined version of the Drude result

Drude transport $\vec{j}_c = ne\vec{v}_{drift}$

assume all electrons drifting at same velocity



charge crossing plane in time Δt is

$$e\,\underbrace{A v_{drift}\Delta t}_{\text{volume}}\;\underbrace{n}_{\text{charge density}}$$

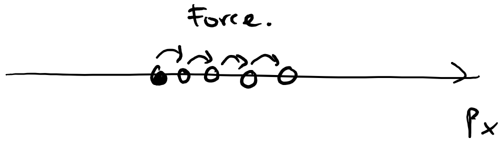
If we calculate this semiclassical transport integral for an equilibrium distribution of electrons…

$$\vec{j}_c = -e\int d^3p \; \frac{1}{4\pi^3\hbar^3}\,\frac{\vec{p}}{m}\,f(\vec{p}) = 0$$ when $f(\vec{p})$ is an equilibrium distribution

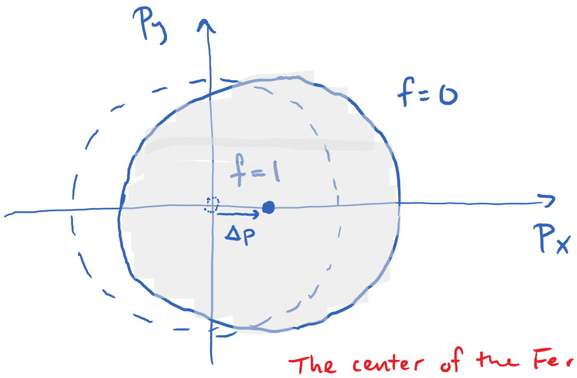
A net transport of charge occurs when there are forces on the electrons (electric or both electric and magnetic)

Classical result: $\Delta\vec{p} = \vec{F}\,\Delta t = e\vec{\mathcal{E}}\,\Delta t$

Quantum Mech: $\Delta\vec{p} = e\vec{\mathcal{E}}\,\Delta t$



The electric field causes incremental changes in the momentum state of an electron



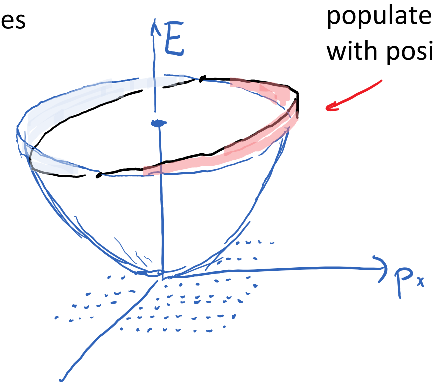
The $f(\vec{p})$ distribution changes.
No longer centered at $\vec{p}=0$.

The center of the Fermi sea has shifted by Δp.

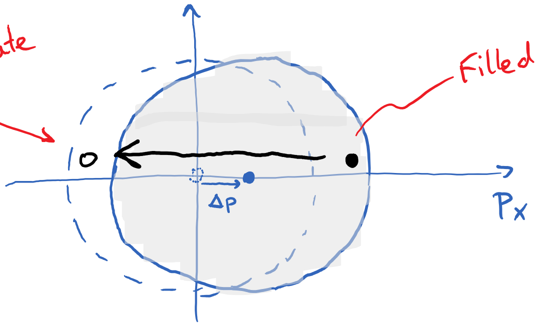
What stops Δp from increasing indefinitely?

Depopulate some states

populate some higher energy states with positive velocity



System will relax if there is a mechanism that scatters electrons between states.



Empty state

Filled state

Transition would reduce energy of the electron gas

Possible scattering mechanisms include phonon emission/absorption, e-e scattering (exchanging energy/momentum with other electrons) and scattering from defects in the crystal lattice.

If the typical time between scattering events is τ_{scat}

then $\Delta p = e\,\mathcal{E}\,\tau_{scat}$

single parameter to describe (approximately) all the physical processes.

Homework example: Given *f*(*p*) for a displaced Fermi sea, calculate the current density…

$$\vec{j}_c = \frac{-e}{4\pi^3\hbar^3 m}\int \vec{p}\, f(\vec{p})\, d^3p$$

With small adjustments, the formula can be adjusted for 2d or 1d systems - see the **old notes, page 4-6**.

There is a more elaborate and detailed formalism to describe the steady state occupation function: Boltzmann transport equation

Let f vary with $\vec{r}, \vec{p}$ and t

$$\frac{\partial f}{\partial t} = -\frac{\vec{p}}{m}\cdot\left(\frac{\partial f}{\partial x}\hat{x} + \frac{\partial f}{\partial y}\hat{y} + \frac{\partial f}{\partial y}\hat{z}\right) - \vec{F}\cdot\left(\frac{\partial f}{\partial p_x}\hat{x} + \frac{\partial f}{\partial p_y}\hat{y} + \frac{\partial f}{\partial p_z}\hat{z}\right) + I_{coll}[f]$$

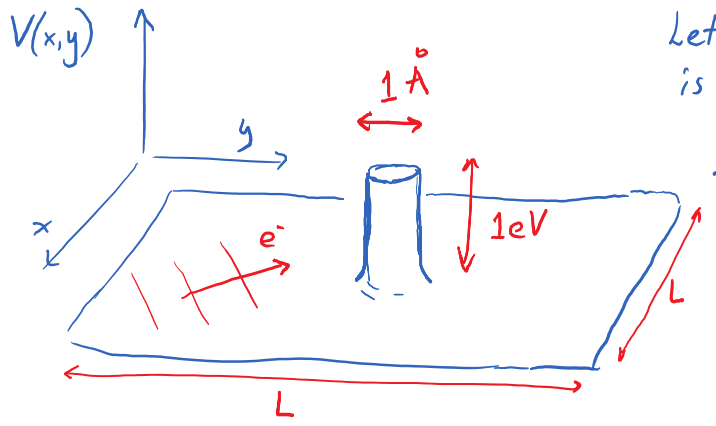
how the occupation of states with mom $\vec{p}$ and location $\vec{r}$ changes with t.

Collision integral: How fast occupation of states with mom $\vec{p}$ and position $\vec{r}$ are changing due to scattering. Requires an integral over the entire occupation function.

Homework will have "simple" example (i.e. can be solved without writing computational code) for finding a steady state solution of this PDE. There is more information in the **old notes page 2-4**.

i.e. what $f(\vec{r},\vec{p})$ will make $\frac{\partial f}{\partial t} \to 0$?

The collision integral depends on the scattering mechanism. I'll give on example. Imagine the crystal has one missing atom and that missing atom is the only source of scattering. We'll use Fermi's golden rule to find the rate for an electron in the crystal to transition from one quantum state to another.



Let's assume the potential is 1eV tall and 1 Å big.

Treat the vacancy like a delta fn

$$V(\vec{r}) = u\,\delta(\vec{r})$$

where $u = 1\ \text{eV}\cdot\text{Å}^3$

Eigenstates in this crystal are $\dfrac{e^{\frac{i}{\hbar}\vec{p}\cdot r}}{\sqrt{L^3}}$ ← volume = L^3

Transition matrix element due to $V(\vec{r})$ is

$$\langle p_f | V | p_i \rangle = \frac{u}{L^3}$$

This matrix element is the same for any k_f

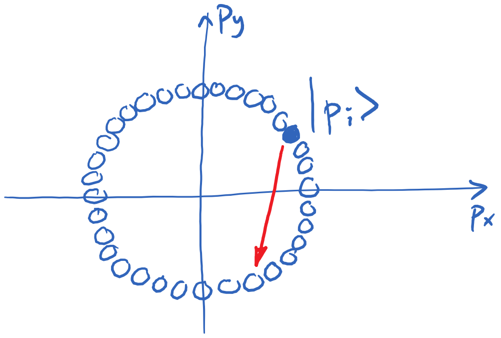
Fermi's golden rule for making a transition into a continuum of possible $|k_f\rangle$

I'll assume all $|k_f\rangle$ with correct energy are unoccupied.

energy of final state = energy of initial state

$$\Gamma = \frac{2\pi}{\hbar}\underbrace{\left(\frac{u}{L^3}\right)^2}_{\substack{\text{Matrix}\\\text{element}\\\text{squared}}}\underbrace{g(E)\cdot L^3}$$

$g(E)$ is DoS per unit volume, so I need to multiply by L^3



$1/\Gamma$ tells us the lifetime in the initial state.

(Scattering into any of these unoccupied states is equally likely.)

From this, we can now calculate the collision integral that goes into Boltzmann equation.

$\frac{\partial f}{\partial t}$ for a certain $\vec{r}, \vec{p}$ depends on its current value (whether it is occupied) and the occupation of all other states that have equal energy.

Diffusion:
If there is a gradient in carrier density, and no forces on the carriers, how much diffusion current do we expect?

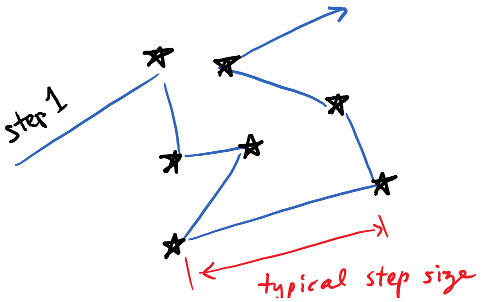
Fick's law

$$\vec{j} = -e\underbrace{D}_{\text{Diffusion coefficient}}\nabla \underbrace{n}_{\text{carrier density}}$$

$$\sqrt{\langle x^2 \rangle} = \sqrt{Dt}$$

D can formally be derived from the Boltzmann transport equation.
But it's also useful (for intuition and estimations) to know coarse-grained derivations for D.

If there is a well-defined Fermi surface, D can be derived by considering a random walk with step size $v_F \tau_{scat}$.



$|\leftarrow$ typical step size

$v_F \tau_{scat}$

If elapsed time is t, then the number of steps is $\frac{t}{\tau_{scat}}$

The rms displacement $\sqrt{\langle x^2 \rangle} = \sqrt{N_{step}}\, l_{step}$

If you don't remember this result, google "Random walks the mathematics in 1 dimension" - to find a very accessible webpage from an MIT professor.

$$= \sqrt{\frac{t}{\tau_{scat}}}\, v_F \tau_{scat} = \sqrt{v_F^2 \tau_{scat}\, t}$$

Compare with definition $\sqrt{\langle x^2 \rangle} = \sqrt{Dt}$

$$\Rightarrow \quad D \approx v_F^2 \tau_{scat}$$

(exact result is
$\frac{1}{3} v_F^2 \tau_{scat}$ in 3d
$\frac{1}{2} v_F^2 \tau_{scat}$ in 2d)

If the Fermi surface is not well defined, for example a low concentration of carriers in a room-temperature semiconductor, then the motion is driven by thermal energy.
(i.e. Situations where the occupation function looks more like a classical Boltzmann exponential rather than a step function).

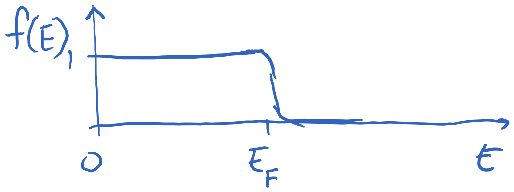
Einstein relation $D = \frac{\mu}{e} k_B T$ See **old notes page 7**

where μ is mobility. (not to be confused with chemical potential)

And μ in the constant of proportionality in the relationship

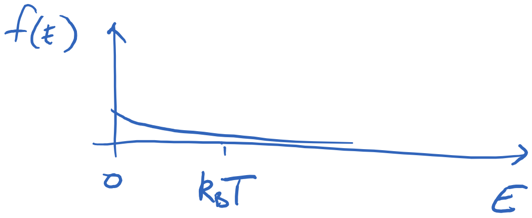
$$\vec{v}_{drift} = \mu \vec{\mathcal{E}}$$

SUMMARY OF DIFFUSION RESULTS



Low temperatures and/or high concentration of carriers

$$D \approx v_F^2 \tau_{scat}$$

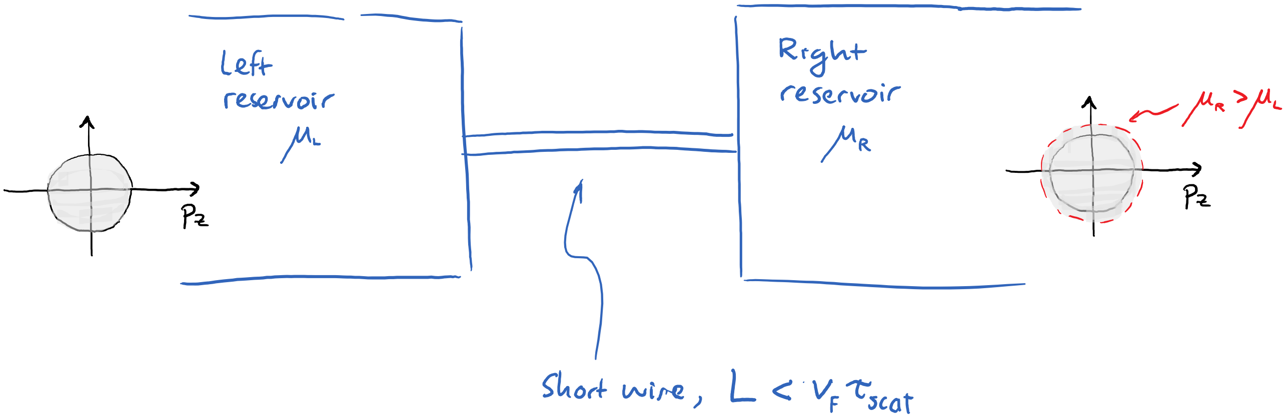


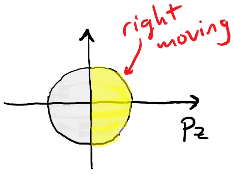
Increased temperature, f(E) is not a step function any more

$$D = \frac{\mu}{e} k_B T$$

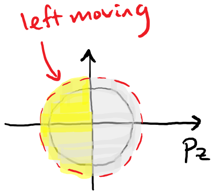
Transition to Nanoscale Systems

Imagine shrinking the length of a wire so it is shorter than the scattering length. What can we predict from semiclassical transport?





Electrons entering the wire from the left come from one reservoir (described by µ_L).



Electrons entering the wire from the right come from another reservoir (described by µ_R).

Occupation function inside the wire

$$\begin{cases} \frac{1}{e^{(E-\mu_L)/kT_L}+1} & p_z > 0 \end{cases}$$

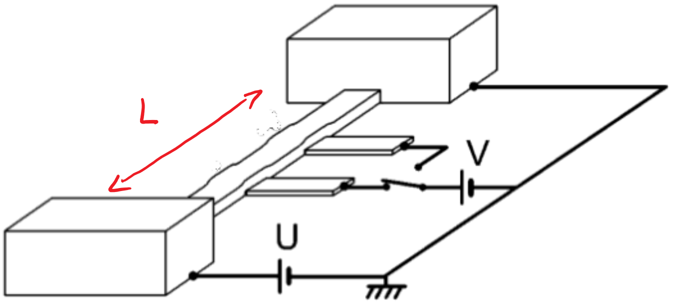
$$f_{wire}(p) = \begin{cases} \dfrac{1}{e^{(E-\mu_L)/k_B T_L}+1} & p_z > 0 \\[2ex] \dfrac{1}{e^{(E-\mu_R)/k_B T_R}+1} & p_z < 0 \end{cases}$$

where $E = \dfrac{p^2}{2m_{eff}}$

The function describing left-movers is decoupled from the function describing right-movers because there is no scattering in the wire. This is an example of unusual phenomena that can happen in nanoelectronics (this wouldn't happen in a macroscopic wire).

Experiment showing this phenomena:

"Energy distribution function of quasiparticles in mesoscopic wires" PRL **79**, 3490 (1997)

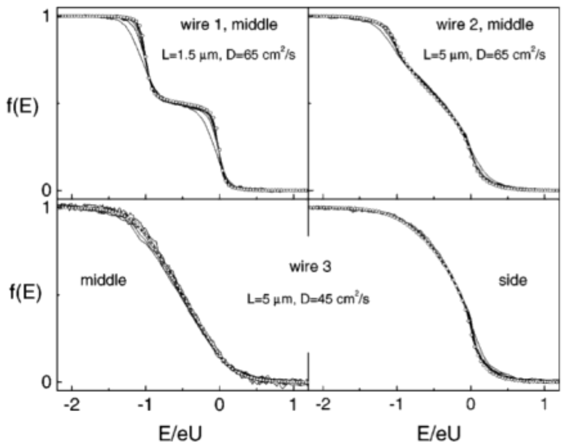


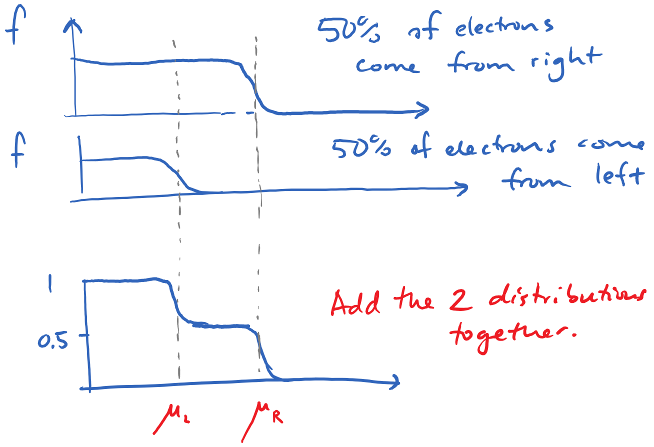
Copper wires,
110 nm wide
45 nm thick
Vary the length, L
$T = 25\,mK$
$U = 0.2\,mV$

Exercise to do with your neighbor:

a) When L is very long (so the electrons thermalize in the wire) , sketch f(E) in the center of the wire (calculate k_BT for 25 mK).
b) When L is very short (so the electrons have memory of which reservoir they originated), sketch f(E) in the center of the wire.

ANSWER FROM THE EXPERIMENT





50% of electrons come from right

50% of electrons come from left

Add the 2 distributions together.

The are many more exotic effects, but well need to move beyond the semiclassical transport model.

Next lecture introduces the Landauer-Buttiker formalism.

The semiclassical theory of transport

G. S. Paraoanu

O. V. Lounasmaa Laboratory, School of Science,

Aalto University, P.O. Box 15100, FI-00076 AALTO,Finland

Abstract

PHYS-E0551 Low Temperature Physics: Nanoelectronics

I. INTRODUCTION

This lecture deals with an approach to transport in nanostructures based on the Boltzmann equation and known as the semiclassical theory. The general approach (which we will use over and over again in this course) is to extract the truly essential feature from the problem of transport at nanoscale, and attempt to incorporate all the unknown features in a small number of parameters. Transport is a nonequilibrium phenomenon, therefore electrons cannot be assumed to be described by equilibrium distribution functions such as the Fermi function. However, because the devices we will study are very small, the transfer of electrons will not perturb too much the electrodes to which it is coupled. These electrodes are usually referred to as *reservoirs* and the electrons are assumed to populate the reservoirs' energy states according to the (equilibrium) Fermi-Dirac distribution $f_{\mathrm{FD}}(E;\mu,T)$,

$$f_{\mathrm{FD}}(E;\mu,T)=\frac{1}{e^{(E-\mu)/k_{\mathrm{B}}T}+1}, \tag{1}$$

where μ is the chemical potential and T is the temperature.

II. BOLTZMANN EQUATION

In quantum physics the position and momentum cannot be simultaneously well-defined. However, in the semiclassical approximation we can define a *distribution function* $f(\vec{r},\vec{p})$ (also called *filling factor*) such that the number of electrons in a volume $d\vec{r}d\vec{p}$ in the position-momentum phase space is

$$2\times f(\vec{r},\vec{p})\times\frac{d^3\vec{r}d^3\vec{p}}{(2\pi\hbar)^3}, \tag{2}$$

where as usual the factor of 2 comes from the spin. For simplicity, for the moment we will consider only the 3D case; the results in lower dimensions can be derived in a similar way. This type of coarse-grained approach is suitable if the scale of the interval $d\vec{r}$ is larger than the typical scale of the electronic wavepacket, which is of the order of the electron Fermi wavelength (the wavelength of an electron at the Fermi surface) λ_{F}. For example in metals λ_{F} is of the order of 0.1 - 1 nm.

Let us now assume that at a time t the electrons are indeed described by such a distribution function $f(\vec{r},\vec{p},t)$. After a time dt, the distribution will be $f(\vec{r}+\vec{v}dt,\vec{p}+\vec{F}dt,t+dt)$, where $\vec{v}=\vec{p}/m$ is the electron velocity and $\vec{F}$ is the force (typically due to and electric or magnetic field applied). In the absence of collisions, the distribution $f(\vec{r}+\vec{v}dt, \vec{p}+\vec{F}dt, t+dt)$ at $t+dt$ should be identical to the initial one. In other words, as the volume element $d^3\vec{r}d^3\vec{p}$ moves in the 6-dimensional phase space from $(\vec{r},\vec{p})$ to $(\vec{r}+\vec{v}dt, \vec{p}+\vec{F}dt)$, the number of particles it contains remains unchanged. In the presence of collisions (scattering from impurities, from other electrons, or from phonons), there will be a difference between the two, due to scattering events in the time interval dt, and we write

$$f(\vec{r}+\vec{v}dt, \vec{p}+\vec{F}dt, t+dt) - f(\vec{r},\vec{p},t) = I_{\rm coll}[f]dt, \tag{3}$$

where $I_{\rm coll}[f]$ is called *collision integral.* Note that $I_{\rm coll}[f]$ still depends on the vectors $\vec{r}$ and $\vec{p}$. Expand now Eq. (3) in dt and keep only the first-order terms,

$$(\partial_t + \vec{v}\cdot\partial_{\vec{r}} + \vec{F}\cdot\partial_{\vec{p}})f(\vec{r},\vec{p},t) = I_{\rm coll}[f]. \tag{4}$$

Eq. (4) above is called *the Boltzmann equation.* In general, this is a nonlinear equation: the collision integral itself depends on the distribution of electrons. However, it it is possible to find solutions by linearizing the equation, an example of which we will see below when we discuss the diffusion limit. Note also that $\vec{v}$ contains an intrinsic momentum-dependence via $\vec{v} = \vec{p}/m$, and also $\vec{F}$ can depend in general on momentum. For example for electrons in both an electric field $\vec{\mathcal{E}}$ and a magnetic field $\vec{B}$, $\vec{F}$ is given by

$$\vec{F} = -e(\vec{\mathcal{E}} + \vec{v}\times\vec{B}). \tag{5}$$

Boltzmann equation in zero magnetic field

If no magnetic field is applied, then a more compact formula can be derived. The electrons will be subjected only to an electric-field force $\vec{F} = -e\vec{\mathcal{E}} = \partial_{\vec{r}}\mu(\vec{r})$, where $\mu(\vec{r})$ is the scalar potential associated with the electric field. The energy of the electrons can be written as $E(\vec{r}) = \epsilon_{\rm F} + \mu(\vec{r})$, where the energy at the Fermi level is taken momentum-independent, which is the case for metals where the Fermi surface has spherical symmetry. Therefore

$$\vec{F} = \partial_{\vec{r}}\mu(\vec{r}) = \partial_{\vec{r}}E(\vec{r}), \tag{6}$$

and also we can separate the momentum-dependence of f into a dependence on the direction $\hat{\vec{p}}$ and one on absolute value of $\vec{p}$, which in turn can be replaced by an energy-dependence. With these notations, we have

$$\vec{v}\cdot\partial_{\vec{r}}f(\vec{r},\vec{p}) + \vec{F}\cdot\partial_{\vec{p}}f(\vec{r},\vec{p}) = \tag{7}$$

$$= \vec{v} \cdot \partial_{\vec{r}} f(\vec{r}, \hat{\vec{p}}) + (\partial_{\vec{r}} E) \cdot (\partial_{\vec{p}} E) \partial_E f(\vec{r}, \hat{\vec{p}}, E) \tag{8}$$

$$= \vec{v}[\partial_{\vec{r}} + (\partial_{\vec{r}} E)\partial_E] f(\vec{r}, \hat{\vec{p}}, E) = \vec{v} \cdot \vec{\nabla} f(\vec{r}, \hat{\vec{p}}, E), \tag{9}$$

where $\vec{\nabla}$ is the total derivative with respect to position (which includes the dependence via E) and we also used $\vec{v} = \partial_{\vec{p}} E$. Thus we write the Boltzmann equation in the form

$$(\partial_t + \vec{v} \cdot \vec{\nabla}) f(\vec{r}, \hat{\vec{p}}, E) = I_{\mathrm{coll}}[f]. \tag{10}$$

Eq. (10) is referred to as the Boltzmann equation in the ballistic limit.

Observables in the semiclassical approach

To establish the connection between a law of dynamical evolution and the results of the experiment, we need to define the observables. Let us consider the three-dimensional case and quadratic energy dispersion. For example, in quantum mechanics we have a law of evolution (Schrödinger's equation, Dirac equation, etc.) and a clear prescription for the observables, which have to be unitary operators. We can define [1] the charge current density at $\vec{r}$

$$\begin{aligned} \vec{j}_{\mathrm{e}}(\vec{r}) &= -e \int \frac{d^3\vec{p}}{4\pi^3\hbar^3} \vec{v} f(\vec{r}, \vec{p}) & (11) \\ &= -e \int dp p^2 \frac{1}{\pi^2\hbar^3} \int \frac{d\hat{\vec{p}}}{4\pi} \vec{v} f(\vec{r}, \vec{p}) & (12) \\ &= -e \int dE \mathcal{N}_{3\mathrm{D}}(E) \int \frac{d\hat{\vec{p}}}{4\pi} \vec{v} f(\vec{r}, \hat{\vec{p}}, E), & (13) \end{aligned}$$

where $\hat{\vec{p}} = \vec{p}/p$ (with $p = |\vec{p}|$) is the direction of the momentum vector and $d\hat{\vec{p}}$ is the solid-angle element. In spherical coordinates $\hat{\vec{p}} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ and $d\hat{\vec{p}} = d\varphi d\theta \sin\theta$. In the first equation we used the fact that the number of electrons in the volume element $d^3\vec{p}$ is

$$2 \times f(\vec{p}) \frac{d^3\vec{p}}{(2\pi\hbar)^3}. \tag{14}$$

To get the third equality we employ the quadratic dispersion relation

$$E(p) = \frac{p^2}{2m}, \tag{15}$$

and the density of states derived in the previous lecture,

$$\mathcal{N}_{3\mathrm{D}}(E) dE = \frac{k^2 dk}{\pi^2} = \frac{p^2 dp}{\pi^2\hbar^3} = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} dE. \tag{16}$$

A useful formula in this context, allowing us to break the integral over momenta into an integral over energies and another one over solid angle is

$$\int \frac{d^3\vec{p}}{(2\pi\hbar)^3} \dots = \int dp \frac{p^2}{2\pi^2\hbar^3} \int \frac{d\hat{\vec{p}}}{4\pi} \dots = \frac{1}{2} \int dE \mathcal{N}_{3\mathrm{D}}(E) \int \frac{d\hat{\vec{p}}}{4\pi} \dots, \tag{17}$$

where the origin of the factor of 1/2 if front of the last expression is the fact that we include the electron spin in the definition of the density of states. The result Eq. (13) is easy to interpret: had the speed not been present there, the result would have been just the total charge - obtained by summing over all energies with the corresponding density of states and occupation factors. Note that the factor of 4π is the total solid angle of the sphere, $\int d\hat{\vec{p}} = 4\pi$. With the speed present, one gets the total current.

Similarly, for the heat current we can use the thermodynamic relation $dQ = dU - \mu dN$ and get

$$\vec{j}_{\mathrm{Q}}(\vec{r}) = \int dE \mathcal{N}_{3\mathrm{D}}(E)(E-\mu) \int \frac{d\hat{\vec{p}}}{4\pi} \vec{v} f(\vec{r}, \hat{p}, E). \tag{18}$$

Limits of interest

There are several regimes in which the Boltzmann equation can be further written up in a more explicit form and solved. These regimes can be defined by comparing the size of the sample L with the scattering lengths l_{el}, $l_{\mathrm{e-e}}$, and $l_{\mathrm{e-ph}}$ (elastic, electron-electron, and electron-phonon).

The ballistic regime is defined by $L \ll l_{\mathrm{el}}, l_{\mathrm{e-e}}, l_{\mathrm{e-ph}}$. In this case the electron does not interact with anything except external potentials. The current for each momentum state is conserved.

The diffusive nonequilibrium regime is defined by $l_{\mathrm{el}} \ll L \ll l_{\mathrm{e-e}}, l_{\mathrm{e-ph}}$. In this case the elastic scattering will change the direction of the electron's momentum while keeping their energy constant.

Two other regimes (which will not be discussed in these lectures) can be defined as well:

The quasi-equilibrium regime is defined by $l_{\mathrm{el}}, l_{\mathrm{e-e}} \ll L \ll l_{\mathrm{e-ph}}$. In this case the e-e scattering mixes different energies.

The local equilibrium regime defined by $l_{\mathrm{el}}, l_{\mathrm{e-e}}, l_{\mathrm{e-ph}} \ll L$. In this case the e-ph scattering and e-e scattering ensures that locally the electrons are in equilibrium with their environment.

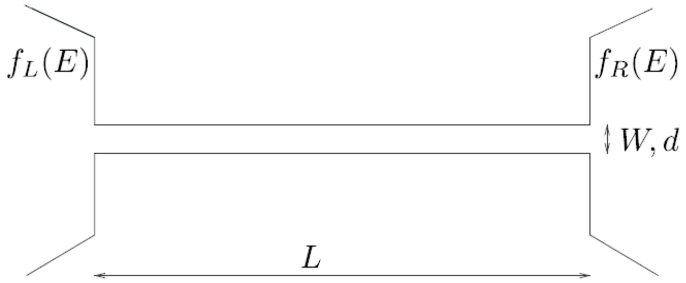


FIG. 1: A one-dimensional wire connected to two reservoirs, left (L) and right (R). Figure from Ref. [1].

III. BOLTZMANN EQUATION IN THE BALLISTIC REGIME

In the ballistic regime we have $I_{\mathrm{coll}}[f] = 0$ therefore the Boltzmann equation is simplified considerably. Let us study it though the example below.

Application: one-dimensional ballistic wire. A simple and useful example is the case of the quasi- one dimensional ballistic wire of length L without impurities, see Fig. 1. Neglecting any other collisions, we get for the Boltzmann equation

$$v_z \frac{d}{dz} f(\vec{r}, \hat{\vec{p}}, E) = 0. \tag{19}$$

Clearly the general solution is that f is a constant function of z - but which value it takes depends on the boundary conditions. The boundary conditions for f are

$$f(z, \hat{\vec{p}}, E)|_{z=0} = f_L(E), \tag{20}$$

$$f(z, \hat{\vec{p}}, E)|_{z=L} = f_R(E). \tag{21}$$

This yields the following solution

$$f(\vec{r}, \hat{\vec{p}}, E) = \begin{cases} f_L(E), & \hat{\vec{p}}_z > 0, \\ f_R(E), & \hat{\vec{p}}_z < 0 \end{cases} \tag{22}$$

Thus f depends on $\hat{\vec{p}}$: the "right-moving" carriers with $\hat{\vec{p}}_z < 0$ carry the distribution of the left lead, $f_L(E)$, while the "left-moving" carriers with $\hat{\vec{p}}_z > 0$ carry the distribution of the right lead, $f_R(E)$.

IV. BOLTZMANN EQUATION IN THE DIFFUSIVE REGIME

For elastic processes (for example electrons scattered on impurities) the collision integral $I_{\rm el}[f(\vec{r},\vec{p},t)]$ can be written as the difference between the rate of scattering from all the states with momentum $\vec{p\prime}$ to the momentum state $\vec{p}$ and the rate of scattering from the state $\vec{p}$ to all the states with momentum $\vec{p\prime}$,

$$I_{\rm el}[f](\vec{r},\vec{p},t) = \int \frac{d^3\vec{p\prime}}{(2\pi\hbar)^3} V \left[J_{\vec{p\prime},\vec{p}}(\vec{r},t) - J_{\vec{p},\vec{p\prime}}(\vec{r},t)\right], \tag{23}$$

where $J_{\vec{p\prime},\vec{p}}$ and $J_{\vec{p},\vec{p\prime}}$ are scattering rates (units: s^{-1}) from $\vec{p\prime} \to \vec{p}$ and $\vec{p} \to \vec{p\prime}$ respectively, and V is the volume. Note that you can also write this as a sum over discrete states [3],

$$I_{\rm el}[f](\vec{r},\vec{p},t) = \sum_{\vec{p\prime}} \left[J_{\vec{p\prime},\vec{p}}(\vec{r},t) - J_{\vec{p},\vec{p\prime}}(\vec{r},t)\right], \tag{24}$$

which follows from the usual discrete-to-continuous formula

$$\frac{1}{V}\sum_{\vec{p\prime}} = \int \frac{d^3\vec{p\prime}}{(2\pi\hbar)^3}. \tag{25}$$

Further, $J_{\vec{p},\vec{p\prime}}(\vec{r},t)$ must be proportional to the number of states from which the scattering occurs, which is $f(\vec{r},\vec{p},t)$ and to the number of states available for scattering into, $1 - f(\vec{r},\vec{p\prime},t)$, that is

$$J_{\vec{p\prime},\vec{p}}(\vec{r},t) = W_{\vec{p\prime},\vec{p}} f(\vec{r},\vec{p\prime},t)\left[1 - f(\vec{r},\vec{p},t)\right]. \tag{26}$$

Now, $W_{\vec{p},\vec{p\prime}}$ can be calculated by applying the Fermi golden rule with a certain scattering potential $U_{\rm imp}$ corresponding to a single impurity as a perturbation and summing over all impurities. This is known in scattering theory as the Born approximation. Using the momentum states

$$\langle \vec{r}|\vec{p}\rangle = \frac{1}{\sqrt{V}} e^{\frac{i}{\hbar}\vec{p}\vec{r}} \tag{27}$$

as incoming and outgoing states, we can write

$$\begin{aligned} W_{\vec{p},\vec{p\prime}} &= \frac{2\pi}{\hbar} |\langle \vec{p\prime}| \sum_{\rm imp} \hat{U}_{\rm imp} |\vec{p}\rangle|^2 \delta(E_p - E_{p'}) & (28) \\ &\approx \frac{2\pi}{\hbar} \sum_{\rm imp} |\langle \vec{p\prime}|\hat{U}_{\rm imp}|\vec{p}\rangle|^2 \delta(E_p - E_{p'}). & (29) \end{aligned}$$

From the formula above it is clear that this formalism does not capture the interference effects of electrons as they travel between two scatterers. Indeed, the mixed (interference) terms between different scatterers that contain phase information are dropped. This is another reason why this formalism is **semiclassical**: the wave properties of the electron are completely neglected.

Typically the impurity potential is isotropic and the matrix element calculated with the Golden Rule does not depend on the value of the momentum (energy) or on the direction of the incoming/outgoing electrons. In this case the quantity $w = (2\pi/\hbar)\sum_{\text{imp}} |\langle \vec{p\prime}|\hat{U}_{\text{imp}}|\vec{p}\rangle|^2$ (dimensions: J/s) is a constant.

Then, putting all these together, we find

$$\begin{aligned} I_{\text{el}}[f](\vec{r},\vec{p},t) &= \int \frac{d^3\vec{p\prime}}{(2\pi\hbar)^3} V\left[J_{\vec{p\prime},\vec{p}}(\vec{r},t) - J_{\vec{p},\vec{p\prime}}(\vec{r},t)\right] & (30) \\ &= \frac{1}{2} wV \int dE' \mathcal{N}_{3\text{D}}(E')\delta(E'-E) \int \frac{d\hat{\vec{p\prime}}}{4\pi}[f(\vec{r},\hat{\vec{p\prime}},E',t) - f(\vec{r},\hat{\vec{p}},E,t)] & (31) \\ &\approx \frac{1}{2} wV\mathcal{N}_{3\text{D}}(E) \int \frac{d\hat{\vec{p\prime}}}{4\pi}[f(\vec{r},\hat{\vec{p\prime}},E,t) - f(\vec{r},\hat{\vec{p}},E,t)]. & (32) \end{aligned}$$

Next, let us introduce the *scattering time* τ by

$$\frac{1}{\tau(E)} = \frac{1}{2} wV\mathcal{N}_{3\text{D}}(E). \tag{33}$$

Note that $\tau(E)$ depends on the total number of states per energy interval available in the volume of the sample at the energy E of the incoming/outgoing electron (because these processes are elastic, the energy before and after collision is the same), that is, $V\mathcal{N}_{3\text{D}}(E)$. Also w contains the information about the number/concentration of impurities (scattering centers). Another useful definition for the scattering time is

$$\frac{1}{\tau_p} = \sum_{\vec{p\prime}} W_{\vec{p\prime},\vec{p}}, \tag{34}$$

and you can verify that it yields Eq. (33) when Eq. (17) and the definition of w is used. In many cases of interest, $\tau(E)$ can be taken as energy-independent and approximated by its value at the Fermi level, $\tau(E) \approx \tau(E_{\text{F}}) = \tau$. The time τ comes up with the correct dimensionality (seconds) as you can readily verify from the formula above.

Next, we expand the distribution f into a spherically-symmetric component f_0 and a direction-dependent component,

$$f(\vec{r},\hat{\vec{p}},E,t) \approx f_0(\vec{r},E,t) + \delta\vec{f}(\vec{r},E,t)\cdot\hat{\vec{p}}. \tag{35}$$

Inserting this into Eq. (32) we find

$$I_{\text{el}}[f](\vec{r},\vec{p},t) = \frac{1}{\tau}\int \frac{d\hat{\vec{p}}'}{4\pi}[f(\vec{r},\hat{\vec{p}}',t)-f(\vec{r},\hat{\vec{p}},t)] \approx \frac{1}{\tau}\delta\vec{f}(\vec{r},E,t)\int \frac{d\hat{\vec{p}}'}{4\pi}(\hat{\vec{p}}'-\hat{\vec{p}}) = -\frac{1}{\tau}\delta\vec{f}(\vec{r},E,t)\cdot\hat{\vec{p}}. \tag{36}$$

Note that here we used $\int \frac{d\hat{\vec{p}}'}{4\pi}\hat{\vec{p}}' = 0$, because the average of a vector over a sphere is zero. With these assumptions we can now write the Boltzmann equation,

$$(\partial_t + \vec{v}\cdot\vec{\nabla})[f_0(\vec{r},E,t) + \delta\vec{f}(\vec{r},E,t)\cdot\hat{\vec{p}}] = -\frac{1}{\tau}\delta\vec{f}(\vec{r},E,t)\cdot\hat{\vec{p}}. \tag{37}$$

For spherical Fermi surfaces, we now have $\vec{v} = \vec{p}/m = p\hat{\vec{p}}/m = v\hat{\vec{p}}$. We write $\hat{\vec{p}}$ in spherical coordinates, such that

$$\hat{\vec{p}} = (\hat{\vec{p}}_x, \hat{\vec{p}}_y, \hat{\vec{p}}_z) = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta). \tag{38}$$

Next, we integrate Eq. (37) over the directions of $\hat{\vec{p}}$, calculating for example $(1/4\pi)\int d\hat{\vec{p}}$, where the integration measure is the solid angle $d\hat{\vec{p}} = d\varphi d\theta\sin\theta$, and we find

$$\left(\partial_t f_0 + \frac{1}{3}v\vec{\nabla}\cdot\delta\vec{f}\right) = 0, \tag{39}$$

and then we multiply Eq. (37) by any of the components $\hat{\vec{p}}_x, \hat{\vec{p}}_y, \hat{\vec{p}}_z$ and then we integrate again over $\hat{\vec{p}}$ to obtain

$$\frac{1}{3}\left[v\vec{\nabla}f_0 + \partial_t(\delta\vec{f})\right] = -\frac{1}{3\tau}\delta\vec{f}. \tag{40}$$

A useful integral for obtaining these two expressions is

$$\frac{1}{4\pi}\int_0^{2\pi} d\varphi\int_0^{\pi} d\theta\sin(\theta)\cos^n(\theta) = \begin{cases} \frac{1}{n+1} & \text{if } n = \text{even;} \\ 0 & \text{if } n = \text{odd.} \end{cases} \tag{41}$$

Also, you will easily notice that

$$\int d\hat{\vec{p}}\hat{\vec{p}}_x = \int d\hat{\vec{p}}\hat{\vec{p}}_y = \int d\hat{\vec{p}}\hat{\vec{p}}_z = \int d\hat{\vec{p}}\hat{\vec{p}}_x\hat{\vec{p}}_y = \int d\hat{\vec{p}}\hat{\vec{p}}_y\hat{\vec{p}}_z = \int d\hat{\vec{p}}\hat{\vec{p}}_x\hat{\vec{p}}_z = 0. \tag{42}$$

Now, in Eq. (40) we will neglect the term $\partial_t(\delta\vec{f})$ with respect to the first term which depends on f_0, and get as a result

$$\delta\vec{f} \approx -v\tau\vec{\nabla}f_0. \tag{43}$$

Then, using this result in Eq. (39) we obtain the Boltzmann equation in the diffusion limit,

$$\left(\partial_t - D\nabla^2\right) f_0(\vec{r},E,t) = 0, \tag{44}$$

where the quantity

$$D = \frac{1}{3}v^2\tau \tag{45}$$

is called **diffusion constant**. From the Boltzmann equation in the diffusive limit one can also notice that the length scale of the electron distribution variation corresponding to a time τ is $\sqrt{D\tau}$.

One can generalize the form Eq. (44) to allow for the presence of inelastic processes, described by a collision integral I_{inel}; then the diffusion Boltzmann equation can be written as

$$\left(\partial_t - D\nabla^2\right) f_0(\vec{r}, E, t) = I_{\mathrm{inel}}[f_0]. \tag{46}$$

We can also identify, directly from the Boltzmann equation, the probability current corresponding to the energy E as $-D\vec{\nabla} f_0(\vec{r}, E, t)$: indeed, you can see that $\partial_t f_0(\vec{r}, E, t) + \vec{\nabla}(-D\vec{\nabla} f_0(\vec{r}, E, t)) = 0$, thus the diffusive Boltzmann equation takes the form of a continuity equation. To get the electrical current, we have to multiply the probability current by the charge and by the density of states then integrate over energies. Typically the density of states is constant (near the Fermi energy) but in general D can be energy-dependent, due to either the energy dependence of v or of τ. Thus we write the rather general form of the total current density,

$$\vec{j}_{\mathrm{e}}(\vec{r}, t) = e\mathcal{N}_{\mathrm{F}} \int dE D(E) \vec{\nabla} f_0(\vec{r}, E, t). \tag{47}$$

Similarly, the heat current is

$$\vec{j}_{\mathrm{Q}}(\vec{r}, t) = -\mathcal{N}_{\mathrm{F}} \int dE (E-\mu) D(E) \vec{\nabla} f_0(\vec{r}, E, t). \tag{48}$$

Application I: The conductivity of a wire in the diffusive limit

A standard problem that illustrates the power of the Boltzmann formalism is obtaining the distribution f_0 in a wire in the stationary case. In one dimensions, the Boltzmann equation becomes

$$D\frac{d^2}{dz^2} f_0(z, E) = 0. \tag{49}$$

This is a second-order differential equation that can be solved by direct integration. Taking into account the boundary conditions $f_0(z=0, E) = f_{\mathrm{L}}(E)$ and $f_0(z=L, E) = f_{\mathrm{R}}(E)$ we get immediately the solution

$$f_0(z, E) = f_L(E)\frac{L-z}{L} + f_R(E)\frac{z}{L}. \tag{50}$$

Assuming now D independent on energy, we get for the charge current

$$j_e = e\mathcal{N}_F D \int_{-\infty}^{\infty} dE \frac{d}{dz} f(z,E) = \frac{e\mathcal{N}_F D}{L} \int_{-\infty}^{\infty} dz [f_R(E) - f_L(E)] = \tag{51}$$

$$= \frac{e\mathcal{N}_F D}{L}(\mu_R - \mu_L) = \frac{e\mathcal{N}_F D}{L} eV = \sigma_D \frac{V}{L}, \tag{52}$$

where $\sigma_D = e^2\mathcal{N}_F D$ is the electrical conductivity. This relation between electrical conductivity and diffusion is called the **Einstein relation**.

Similarly one can calculate the heat current density

$$j_Q = -D\mathcal{N}_F \int_{-\infty}^{\infty} dE (E-\mu) \frac{d}{dz} f(z,E) \tag{53}$$

$$= \frac{D\mathcal{N}_F}{L} \int_{-\infty}^{\infty} dE (E-\mu)[f_L(E) - f_R(E)] \tag{54}$$

$$= \frac{D\mathcal{N}_F}{L} \frac{\pi^2 k_B^2}{6} [T_L^2 - T_R^2] \tag{55}$$

$$\approx \frac{\pi^2 T k_B^2 \sigma}{3e^2 L}(T_L - T_R) \tag{56}$$

$$= \kappa_{\text{th}}(T_L - T_R)/L. \tag{57}$$

This is called the Wiedemann-Franz law. Here we assumed that $|T_L - T_R| << T_R \approx T_L \approx T$, therefore $T_L^2 - T_R^2 \approx 2T(T_L - T_R)$, and also we used some useful integrals (see [1] A. 7.)

$$\int_{-\infty}^{\infty} (f_0(E;\mu_1,T_1) - f_0(E;\mu_2,T_2))\, dE = \mu_1 - \mu_2, \tag{58}$$

and

$$\int_{-\infty}^{\infty} E\,(f_0(E;\mu_1,T_1) - f_0(E;\mu_2,T_2))\, dE = \frac{\pi^2 k_{\mathrm{B}}^2}{6}(T_1^2 - T_2^2) + \frac{1}{2}(\mu_1^2 - \mu_2^2). \tag{59}$$

Note that κ_{th} is proportional with the temperature via a combination of universal constants.

Application II: Diffusion of dopants in semiconductors

The applications of the diffusion equation are not limited to transport of electrons. In the technology of semiconductors, an important problem is understading how dopant atoms diffuse in the semiconductor from regions of high consentration to regions with low concentration. Let $C(z,t)$ be the concentration of dopants along the direction z which goes perpendicular to the surface of the material. This quantity satisfies and equation similar to the Boltzmann equation in the diffusion limit,

$$\frac{\partial C(z,t)}{\partial t} - D\frac{\partial^2 C(z,t)}{\partial z^2} = 0, \tag{60}$$

which is called **Fick's equation**.

This equation can be solved exactly with two types of boundary conditions, corresponding to

a) **inexhaustible diffusion.** In this case the dopant is assumed to be present with a constant concentration $C(0,t) = C_S$ at one of the surfaces of the semiconductor, $z = 0$. At large depths, we assume that the dopant is never present, $C(\infty, t) = 0$. The solution with these boundary conditions is

$$C(z,t) = C_S \mathrm{erfc}\left[\frac{z}{2\sqrt{Dt}}\right], \tag{61}$$

where *erfc* is a special function called the complementarity error function and is given by

$$\mathrm{erfc} = 1 - \frac{2}{\sqrt{\pi}} \int_0^x e^{-y^2} dy. \tag{62}$$

The quantity $2\sqrt{Dt}$ is called diffusion length.

b) **exhaustible diffusion.** In this case the total amount of dopant is fixed to a value S. We can write this as

$$\int_0^\infty dz C(z,t) = S \tag{63}$$

The other boundary condition is the same as before, $C(\infty, t) = 0$. The solution with these boundary conditions is a Gaussian distribution

$$C(z,t) = \frac{S}{\sqrt{\pi D t}} \exp\left[-\frac{z^2}{4Dt}\right]. \tag{64}$$

This time the concentration at the surface ($z = 0$) is not constant: as the dopant diffuses in the semiconductor, it decreases as $C(z,t) = S/\sqrt{\pi D t}$.

Application III: Connection with the Drude formula for conductivity in a metal

Using the semiclassical analysis based on the Boltzmann equation we have derived a formula for the conductivity,

$$\sigma_D = e^2 \mathcal{N}_{\mathrm{F}} D = e^2 \mathcal{N}_{\mathrm{F}} \frac{v_{\mathrm{F}}^2 \tau}{3}. \tag{65}$$

Here $\mathcal{N}_{\mathrm{F}}$ is the density of states at the Fermi level, D is the diffusion constant, and v_{F} is the Fermi velocity. This formula resembles (up to a numerical factor) the result found by

Drude,

$$\sigma_{\text{Drude}} = \frac{ne^2\tau}{m}, \tag{66}$$

if we identify the electron density $n \approx \mathcal{N}_{\text{F}} m v_{\text{F}}^2$.

For completeness, let us remind here how this formula is derived. The Drude model regards the solid as a pinball machine, with electrons bouncing off ions fixed at their position in the lattice. If $\vec{v}_0$ is the speed of the electron after one collision, then in a time t before the next collision the electron will be accelerated to

$$\vec{v}_0 - \frac{e\vec{E}t}{m}. \tag{67}$$

Now, the angular distribution of speeds immediately after collision $\vec{v}_0$ is random, therefore when averaged over an ensemble of electrons, $\langle \vec{v}_0 \rangle = 0$. As a result, the average velocity of the electrons is $\langle v \rangle = -\frac{e\vec{E}\tau}{m}$ where τ is the average time between collisions. The current is $\vec{j} = -en\langle v \rangle$, with n the electron density. As a result, from Ohm's law $\vec{j} = \sigma_{\text{Drude}}\vec{E}$ we obtain the result Eq. (66).

Application IV: Drude model for the Hall effect

Finally, as a bonus to the Drude formula, let us consider the situation when a two-dimensional sample in the (x, y)-plane is in a magnetic field B oriented perpendicular to the sample, that is, $\vec{B} = B\hat{\vec{z}}$. So far we have not included magnetic fields in the formalism, but, using similar considerations as above, wit is rathre straightforward to do it. In the steady state the change in the momentum due to scattering should equal the change in the momentum due to the applied fields, that is

$$\frac{m\vec{v}}{\tau} = -e[\vec{E} + \vec{v} \times \vec{B}]. \tag{68}$$

In terms of the in-plane components, the equation above can be put in the matrix form

$$\begin{pmatrix} \frac{m}{e\tau} & B \\ -B & \frac{m}{e\tau} \end{pmatrix} \begin{pmatrix} v_x \\ v_y \end{pmatrix} = - \begin{pmatrix} E_x \\ E_y \end{pmatrix}. \tag{69}$$

Next, the current is $\vec{J} = -evn$, with the corresponding components $J_x = -env_x$ and $J_y = -env_y$. As a result we get

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ \rho_{yx} & \rho_{yy} \end{pmatrix} \begin{pmatrix} J_x \\ J_y \end{pmatrix}, \tag{70}$$

where

$$\rho_{xx} = \frac{1}{\sigma_{\text{Drude}}}, \tag{71}$$

and

$$\rho_{xy} = -\rho_{yx} = \frac{\mu B}{\sigma_{\text{Drude}}} = \frac{B}{en}, \tag{72}$$

where $\mu = \frac{e\tau}{m}$ is the mobility. Eq. (70) predicts that by applying a magnetic field, a Hall (transversal) resistance will appear, which increases linearly with the applied magnetic field B.

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[1] Tero T. Heikkilä, The physics of nanoelectronics, Oxford University Press (2013), Chapter 2.

[2] Yuli. V. Nazarov and Yaroslav M. Blanter, Quantum Transport - Introduction to Nanoscience, Cambridge University Press, Cambridge (2009), Chapter 1.

[3] Here is a subtle point that is often glossed over very easily: it is indeed the case that Eq. (24) turns out to be identical to Eq. (23) when using for example $\sum_{\vec{p}'} \to [V/(2\pi\hbar)^3] \int d^3\vec{p}'$. However, the concepts behind these two equations are quite different. Eq. (23) views the electrons as localized in small volume elements in phase space, while Eq. (24) uses extended states, resulting from box quantization.