

Physics of Quantum Devices

Kinetic Theory of Gases

The following section is notes from Kardar chapter 3. Prof. Kanti's notes start from BTE, so that's what I am going to revise. Missed Suddho's first lecture, which was supposedly a revision of Bloch's theorem

Kinetic theory is concerned with the macroscopic properties of large numbers of particles, starting from their classical equations of motion. This course then goes on to develop the semiclassical, and quantum pictures.

Phenomenological thermodynamics is fine and all, but there is a way of creating a much more satisfactory *emergent* theory. The following need to be outlined

- definition of "equilibrium" for moving particles
- whether all systems evolve towards equilibrium
- time evolution of non-equilibrium systems

Start with something like the ideal gas. N -particle system, generalized coordinates $\{\vec{q}_i(t), \vec{p}_i(t)\} \forall i \in N$. A microstate $\mu(t) \in \Gamma$, where Γ is the $6N$ -dimensional phase space, evolves according to

$$\begin{cases} \frac{d\vec{q}_i}{dt} = \frac{d\mathcal{H}}{d\vec{p}_i} \\ \frac{d\vec{p}_i}{dt} = -\frac{d\mathcal{H}}{d\vec{q}_i} \end{cases}, \quad (1)$$

An important fact to keep in mind is that the microscopic equations of motion 1 have *time reversal symmetry*, $\because \mathcal{H}$ is invariant under the transformation $T(\mathbf{p}, \mathbf{q}) \rightarrow (-\mathbf{p}, \mathbf{q})$

Representing macrostates requires the introduction of ensembles of a system.

Boltzmann Transport Equation

What exactly does it mean to describe a condensed matter system outside equilibrium? Reminding us of the Fermi-Dirac distro, in equilibrium

$$f(\varepsilon) = \frac{1}{1 + \exp((\varepsilon - \mu)/\beta)} \quad (2)$$

In equilibrium, $\mu(T=0)\varepsilon_F$, where μ is the electrochemical potential. ε_F reflects the carrier density. If your carrier density varies, then your electrochemical potential μ has spatiotemporal variation.

A non-equilibrium would look something like

$$f(k, \vec{r}, t) = \frac{1}{1 + \exp((\varepsilon(k) - \mu(\vec{r}, t)) \beta(\vec{r}, t))} \quad (3)$$

once we are assuming that there are temperature and carrier concentration gradients, you can at best define particle distribution in a small volume of the phase space. The form of the function remains the same, which is basically representative of us taking a local-equilibrium approximation (see de Groot, Mazur).

Local Equilibrium: No idea.

Now, how would you go about defining current density \vec{j} ? Consider Drude model

$$\vec{j} = nev_d.$$

A general non-equilibrium system would have spatiotemporally varying n , v_d and all. We can arrive at a current density expression using the density of states and the distribution function by filling up the bandstructure/energy levels. We consider the contribution of electrons from a small volume element of phase space d^3k

$$\vec{j} = (-e)2 \times \frac{1}{8\pi^3} \int f(k, \vec{r}, t) v_n(k) d^3k \quad (4)$$

Dynamics or something IDK

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \dot{\vec{r}} \cdot \nabla_{\vec{r}} f + \dot{\vec{k}} \cdot \nabla_{\vec{k}} f \quad (5)$$

$$\vec{v}(\vec{k}) = \frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon(\vec{k}) \quad (6)$$

$$\dot{\vec{r}} = \frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon(\vec{k}) \quad (7)$$

$$\hbar \dot{\vec{k}} = \vec{F} \quad (8)$$

$$\implies \frac{df}{dt} + \vec{v}(\vec{k}) \cdot \nabla_{\vec{r}} f + \frac{\vec{F}}{\hbar} \cdot \nabla_{\vec{k}} f \quad (9)$$

How does one define steady state? We would expect the distribution function to remain constant throughout the dynamics of the system, i.e.

$$\frac{df}{dt} = 0 \quad (10)$$

To account for collisions we define

$$\left. \frac{\partial f}{\partial t} + \vec{v}(\vec{k}) \cdot \nabla_{\vec{r}} f + \frac{\vec{F}}{\hbar} \cdot \nabla_{\vec{k}} f - \frac{\partial f}{\partial t} \right|_{\text{coll}} \quad (11)$$

Now, using 10

$$\left. \frac{\partial f}{\partial t} + \vec{v}(\vec{k}) \cdot \nabla_{\vec{r}} f + \frac{\vec{F}}{\hbar} \cdot \nabla_{\vec{k}} f \right|_{\text{coll}} = 0 \quad (12)$$

Now, recall that we did a problem that showed Bloch oscillations, why do we not really see oscillatory behaviour when we actually sit down to do some experiment? It has something to do with the scattering timescale versus the oscillation period.

We had the Bloch frequency

$$\omega_B = \left(\frac{eE}{\hbar} a \right) \quad (13)$$

For the parameters $E = 10\text{kV/cm}$, $a = 1\text{Angstrom}$, we get $\omega_B \sim 10^{12}\text{Hertz}$. So one would expect a condition like

$$\omega_B \tau \gg 1.$$

At room temperature, relaxation times are typically $\sim 10^{-15}$ or so. In the problem, we did not take into account scattering. How would one observe Bloch oscillations? You would have to measure some local volatages. How would you go about placing probes at a distance a apart?

It is possible to increase a can be increased artificially, something- something multilayer systems. You can artifically tweak the product $\omega_B \tau$ to your liking.

Relaxation time approximation

$$\left. \frac{\partial f}{\partial t} \right|_{\text{collisions}} = -\frac{\delta f}{\tau} \quad (14)$$

where $\delta f = f - f^0$, is the difference between noneq. and eq. disros. Basically we are introducing an empirical restoring force. $\tau(\varepsilon) \rightarrow$ Relaxation time

We are not at equilibrium at $t = 0$ and we want to look at the transient response of the system/distribution.

$$\frac{df}{dt} = \left(-\frac{\delta f}{\tau} + (0) + (0) + (0) \right). \quad (15)$$

As $t \rightarrow \infty$, $f \rightarrow f^0$.

$$f(t) = f_0 + C \exp\left(-\frac{t}{\tau}\right) \quad (16)$$

Back to the current problem at hand

We have the dynamical equation for $f(\vec{r}, k, t)$ within the relaxation time approximation

$$\frac{\partial f}{\partial t} + \vec{v}_k \cdot \nabla_r f + \frac{\vec{F}}{\hbar} \cdot \nabla_k f = -\frac{\delta f}{\tau} \quad (17)$$

Case 1: $\vec{E} \neq 0$

No gradients anywhere, steady state

$$\frac{q\vec{E}}{\hbar} \cdot \nabla_k f = -\frac{\delta f}{\tau} \quad (18)$$

$$\vec{j}_q = \sigma \vec{E} \quad (\text{sigma tensor}) \quad (19)$$

From 18

$$\begin{aligned} \frac{q\vec{E}}{\hbar} \cdot \nabla_k (f^0 + \delta f) 0 &= -\frac{\delta f}{\tau} \\ \Rightarrow \frac{q\vec{E}}{\hbar} \cdot \nabla_k & \\ \text{or } \delta f^0 - \frac{q\tau}{\hbar} \vec{E} \cdot \nabla_k f^0 & \end{aligned} \quad (20)$$

$$\therefore f = f^0 - \frac{q\tau}{\hbar} \cdot \nabla_k f^0 \quad (21)$$

f does not need to be the FD distro. In the next class, we will focus more on the FD distro and see what kind of properties and behaviour is observed.

BTW

$$-\frac{q\vec{E}t}{\hbar} = \delta \vec{k} = \dot{\vec{k}} \delta t \quad (22)$$

if we consider $\delta t = \tau$ so that

$$\begin{aligned} f &= f^0 + \delta \vec{k} \cdot \nabla_k f^0 \\ &= f^0(\vec{k} + \delta \vec{k}) \end{aligned} \quad (23)$$

i.e. the distribution shifted from the origin in the presence of a static electric field. Basically

$$f^0(k + \delta k) = f^0(k) + \delta \vec{k} \cdot \nabla_k f^0 \quad (24)$$

So, if we plot the Fermi sphere, it's going to be shifted along the +x direction if an electric field is applied along \hat{x} .

Current Density

This is what we had set out to do. Recall from 4

$$\vec{j} = \frac{q}{4\pi^3} \int d^3k \vec{v}_k (f^0 + \delta f^0) \quad (25)$$

TODO: SUBSTITUTE

So, we started from Bloch electrons, applied an electric field on those electrons. If we plug in f as the FD distro, we should be able to derive Ohm's law.

Also, even if you didn't have a very nice Fermi sphere, the same procedure holds for calculating the current density for a more general Fermi sphere.

One of my colleagues asked whether Ohm's law is a manifestation of Fermionic carriers.

We have the FD distro

Remember what $f_{\text{FD}}(1 - f_{\text{FD}})$ looks like?

We want to recover Drude conductivity

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m} \quad (26)$$

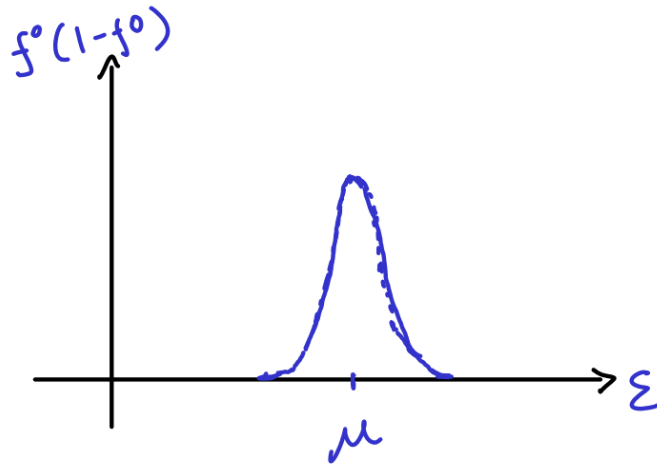


Figure 1: Derivative of the Fermi-Dirac distribution

$$\vec{v}_k = \frac{\hbar k}{m} \quad (27)$$

((((Couldn't keep up today.)))) Plug in $g(\varepsilon)$ for free electrons/Sommerfeld metal ($g(\varepsilon) \sim \sqrt{\varepsilon}$)

$$\sigma_{xx} = \sigma_{yy} = \sigma_{zz} = \frac{ne^2\tau}{m} \quad (28)$$

Nice. We started with Bloch electrons and were able to derive Drude conductivity. Getting a feel for the power of this method? The generality?