5. Scattering Theory & Transport

So far we have discussed how to solve the Schrödinger equation for a single electron and obtain the wave functions and bands $E(k)$ as a function of the wave vector $2k_x (v) = e^{ik \cdot r} u_x (v)$ which represents the phase of the Bloch wave. We also obtained the equations of motion which told us how the expected values of the position and momentum operators evolve in a crystal structure. It turns out they behave analogously to a free particle or a classical particle with some of the terms like velocity being re-defined to include the bandstructure.

Eqns. of motion: $\vec{v} = \frac{d\vec{x}}{dt} = \frac{1}{\hbar} \frac{\partial}{\partial k} E(k)$

$$\frac{d\vec{p}}{dt} = e \vec{F}$$

where $\vec{F}$ is the electric field acting on the electron ($\vec{F} = -\nabla V$).

 Armed with these equations, we now wish to move on to consider the motion of the electrons in a crystal.
Let us consider a simple crystal with a bandstructure given by

$$ E(k) = E_0 \left[ 1 + \cos \left( \frac{k \cdot a + \pi}{k} \right) \right] $$

which is typical of a tight-binding bandstructure of a 1D solid or a simple cubic crystal in 2/3D.

The group velocity is then given by

$$ \vec{v} = \frac{1}{\hbar} \frac{dE}{dk} = -E_0 \alpha \sin \left( \frac{k \cdot a + \pi}{k} \right) $$

and the wavevector changes according to

$$ k = -\frac{eE_t}{\hbar} + k_0 $$

assume $k(0) = 0$.

Now we combine these two into an expression for the velocity:

$$ \vec{v} = E_0 \alpha \sin \left( \frac{eE_t}{\hbar} \alpha + \pi \right) $$

Finally, if all the electrons are moving at this speed, the current density is simply

$$ \vec{j} = e \vec{n} \vec{v} $$
Therefore, our semiconductor crystal becomes an excellent high-frequency generator with \( \omega = \varepsilon F a / h \) even at DC field \( F \).

These oscillations, sometimes called Bloch oscillations, can be tuned by the lattice constant, which spurred on the development of very pure semiconductor superlattices (layered structures made up of two alternating layers of semiconductor materials) but the promised high-frequency generation never really took place.

A more general view of these Bloch oscillations valid for any band structure is the following: under a constant electric field, the electrons constantly accelerate at a rate \( eF / \hbar \). Regardless of their starting position and wavevector \( \mathbf{k} \), they will eventually reach the end of the Brillouin zone and simply enter into the next BZ. Doing so is equivalent to being mapped back to the opposite end of the 1st BZ.

Therefore, leaving the BZ has the effect of “flipping” the wavevector \( \mathbf{k} \) from \( \mathbf{k} \) to \( \mathbf{k} - 2\pi / a \). Flipping the wavevector \( \mathbf{k} \) also changes the velocity...
This very interesting consequence of the periodic lattice structure never really got realized, despite tremendous efforts. The reason is, of course, that there are other forces acting on the electrons, namely scattering, and scattering destroys this coherent process by changing the wave vector \( k \) of the electron. Another view is that the force acting on the electron causes it to gain energy and that energy gets lost in the collision process during scattering.
The most important source of scattering are phonons and electron-phonon scattering is often called inelastic because energy is transferred from electrons to the phonons during the collision. Phonons are lattice vibrations caused by collective motion of the atoms (not electrons!) in the crystal lattice (in the long wavelength limit, phonons carry sound, hence their name!). Phonons also carry thermal energy (and store it) in the lattice.

Electron-phonon scattering is therefore the primary source of dissipation of energy! Energy is supplied to the electrons from the external field, causing electrons to accelerate. Electrons undergo collisions with phonons and transfer their energy to them. Subsequently phonons carry the thermal energy out by diffusion:

\[ \text{Field} \rightarrow \text{electrons} \rightarrow \text{phonons} \rightarrow \text{heat dissipation} \]
Since electrons loose energy in the collision process, they must "return" to the region near the bottom of the conduction bend

\[ E(x) \]

When the force acting on the electron (\( eF/k \)) and the collisions equal each other, we have steady state and a DC current arises because the average velocity of the electrons is non-zero.

Drude proposed a simple model where the collisions were treated as a friction force \( F = m\dot{V}/\tau \) with \( \tau \) being the relaxation time constant. Then we could write (in the effective mass approximation)

\[ \frac{d\vec{k}}{dt} = m^* \vec{V} = F \] (force on the electron)
When friction is added, we get

\[ m^* \dot{v} = F_0 - F_F = F_0 - \frac{m v}{\tau} \]

If the force is removed, then we have

\[ \dot{v} = -\frac{v}{\tau} \quad \text{and} \quad \ddot{v} \leq 0 \]

hence \( \tau \) is the time constant at which the electrons "relax" back to their equilibrium state (often called the relaxation time).

In a constant electric field \( F_0 = -eF \)

and we have

\[ m^* \dot{v} = -eF - \frac{m^* v}{\tau} \]

In steady-state \( \dot{v} = 0 \) (no time derivatives) and the solution is simply

\[ v = -\frac{eF}{m^*} \]

The DC current is then proportional to \( F \)

\[ j = -e v = \frac{e^2}{m^*} n F = \sigma F \]

Defining conductivity as \( \sigma = en \mu \Rightarrow \mu = \frac{e \tau}{m^*} \)
Next we turn to this simple Drude theory of transport to examine more general cases when there is an ac electric field or a magnetic field present. We will consider these cases separately:

1) Ac electric field $F = F_0 e^{i \omega t}$

We need to solve the equation

$$m \ddot{v} = -eF - m v / r$$

We can try to guess that the response will also have a harmonic component at frequency $\omega$

$$v = v_0 (e^{i \omega t} + e^{-i \omega t})$$

Then we have $\dot{v} = v_0 (i \omega e^{i \omega t} - i \omega e^{-i \omega t})$

Plugging this into the above equation gives us

$$m i \omega v_0 (e^{i \omega t} - e^{-i \omega t}) = -eF_0 (e^{i \omega t} + e^{-i \omega t}) - m \ddot{v} v_0 (e^{i \omega t} + e^{-i \omega t})$$
We can separate this into two similar equations for the two complex conjugates

\[ m^* \omega v_o e^{\text{int}} = -eF_e e^{\text{int}} - m^* v_o e^{\text{int}} \]

and

\[ -m^* \omega v_o e^{\text{int}} = -eF_e e^{\text{int}} - m^* v_o e^{\text{int}} \]

both of which satisfy the original equation

\[ m^* v = -eF - m^* v/\tau \]

Finally, we write the expression for velocity as a function of mobility by solving for \( v_o \)

\[ v_o = \frac{eF_e}{imw + m^*/\tau} = \frac{\mu F_e}{1 + imw} \]

In other words, the response is modified from the DC case by a factor of \( 1/(1 + imw) \) which implies an inductive response at frequencies greater than \( f = 1/(2\pi\tau) \). The Drude model captures the frequency dependent behavior of semiconductors quite well at low doping densities, but has to be modified slightly...
at high (degenerate) dopings where the simple theory of a single effective \( t \) starts to fail.

2) \( \vec{F} \) is constant, \( \vec{B} \neq 0 \)

Let us consider the case when a magnetic field is turned on and, for simplicity, assume that it points in the \( z \) direction so that \( \vec{B} = (0, 0, B_z) \) while \( \vec{F} = (F_x, F_y, 0) \).

The total force on each electron will be the so-called Lorentz force, which is a combination of \( \vec{F} \) and \( \vec{B} \)

\[
\text{Force} = -e (\vec{F} + \vec{v} \times \vec{B})
\]

so that our equation in steady state becomes

\[
-e (\vec{F} + \vec{v} \times \vec{B}) = \frac{m^* \vec{v}}{\gamma}
\]

We can break it up into components as

\[
-e \left[ (F_x, F_y, 0) - (0, -v \times B_z, 0) \right] = \frac{m^* (v_x, v_y, 0)}{\gamma}
\]
which is solved by $-V_x = \mu F_x$

and $E_y = V_x B_z$

This occurrence of electric field $E_y$ is often called the Hall effect; even if we do not apply an electric field in the $y$ direction $E_y$, it arises out of the magnetic field $B_z$ due to the $V_x B_z$ term.

The reason $F_y$ arises is the accumulation of electrons at the ends of a finite sample which is necessary to prevent a flow of current.

The magnetic field will deflect electrons in the $y$ direction and they will accumulate at the ends of the sample.

When $B_z$ is large, the electrons are forced to go in circular orbits, sometimes called cyclotron orbits, whose radius depends on $B_z$ and $V_x$. 
In that case, if temperature is low enough to avoid scattering and \( B_z \) is high enough, electrons inside the sample will start to go in completely circular orbits.

\[
\text{In order to have a circular orbit, the force on the particle } eVxR = e\Phi B_z \text{ has to equal the centrifugal force of acceleration } m^* a_{cent} = \frac{m^* v_x^2}{r}.
\]

So \( eVxB_z = \frac{m^* v_x^2}{r} \text{ or } v = \frac{m^* v_x}{eB_z} \)

The time to complete the circle is \( t = \frac{2\pi v}{v_x} = \frac{2\pi m^*}{eB_z} \)

or we can think of this as an angular frequency \( \omega = \frac{2\pi}{t} = \frac{eB_z}{m^*} \)

This is called the cyclotron frequency. When electrons are forced to move in cyclotron orbits, their energies become quantized as \( E_n = \hbar \omega (n + \frac{1}{2}) \). These energy levels are now equal to
the standard quantum harmonic oscillator. These levels \( E_n \) are called Landau levels and each level can be occupied by many electrons. When this quantization occurs, even scattering becomes restricted since the states before and after scattering are restricted to be one of the Landau levels; restricting scattering this way causes the resistance to decrease to its minimum value and we obtain a quantum conductance \( G = \frac{I}{V} = n \frac{e^2}{V_{\text{Hall}}} \).

This quantization of the Hall effect is called the integer quantum Hall effect.