- Boltzmann Transport Equation

We have previously discussed the equilibrium distribution function, given for electrons, by the Fermi–Dirac distribution. We know that if we remove all external forces and wait a long time, the system (composed of the electrons in our crystal) will reach equilibrium and take on the FD distribution which will tell us how many electrons (on average) are occupying a given state. From the distribution function we can now evaluate all the desired properties of our system, such as velocity, current, etc. So we have for our current

$$ j = -2e \frac{\partial}{(2\pi)^3} \int d\mathbf{k} \ n(\mathbf{k}) \ f(\mathbf{k}) $$

And similar expressions for other averages like density

$$ n = \frac{1}{(2\pi)^3} \int d\mathbf{k} \ f(\mathbf{k}) $$

$$ \langle \mathbf{v} \rangle = \frac{1}{(2\pi)^3} \int d\mathbf{k} \ \mathbf{v}(\mathbf{k}) \ f(\mathbf{k}) $$
If we were to evaluate the velocity from this expression, we would of course get zero because \( \dot{V}(t) = -\ddot{V}(t) \) so \( \dot{V}(t) \) is an odd function of \( t \) while \( f(E(t)) = f(E(t)) = f(E(t)) = f(t) \) is an even function of \( E \) because of \( E(t) \) being even. The only way to get \( <u> \neq 0 \) and \( j \neq 0 \) is to push the distribution function out of equilibrium by applying a force (such as an electric field) or a temperature gradient. The field will cause electrons to accelerate and the temperature gradient will cause them to diffuse from the region having higher \( T \) (and therefore higher \( f(E) \)) to a region of lower \( T \) and smaller \( f(E) \).

In order to understand this process, we want to pose a general expression for the evolution of the distribution function over time so that we know how \( f(E) \) approaches steady state. First, we give \( f(E) \) additional arguments at position \( \vec{r} \) and time \( t \) to get \( f(\vec{r}, E, t) \).
Next we ask how \( f(q^1, \vec{q}, t) \) evolves over time by taking a derivative

\[
\frac{df}{dt} = \frac{df}{d\vec{q}} + \frac{df}{dt} \frac{d\vec{q}}{dt} + \frac{df}{d\vec{r}} \frac{d\vec{r}}{dt}
\]

simply by applying the chain rule.

Next, we recognize that our equations of motion have already told us what \( \frac{d\vec{q}}{dt} \) and \( \frac{d\vec{r}}{dt} \) should be:

\[
\frac{d\vec{q}}{dt} = \vec{v}(\vec{r}) = \frac{1}{\hbar} \nabla \hbar \cdot \nabla F(\vec{r})
\]

and

\[
\frac{d\vec{r}}{dt} = \frac{1}{\hbar} \frac{d\vec{p}}{dt} = \frac{1}{\hbar} e \vec{F}
\]

With these two substitutions, we arrive at the Boltzmann transport equation, or at least one half of it:

\[
\frac{df}{dt} = \frac{df}{d\vec{q}} + \frac{df}{d\vec{r}} \cdot \vec{v}(\vec{r}) + \left( -\frac{eF}{\hbar} \right) \cdot \nabla f
\]

Of course, we already know that this is only one half of the story: The other half is scattering. Time-dependent perturbation theory tells us that electrons can change their \( \vec{r} \) by scattering with plasma imperfections, etc. and that we can write this scattering rate from
Fermi's Golden Rule (\#2) as
\[
S(k, k') = \frac{2\pi}{\hbar} |<k' | H | k>|^2 \delta(E(k') - E(k))
\]

Previously, we computed the total scattering rate simply as a sum
\[
\Gamma(k) = \sum_{k'} S(k, k')
\]

meaning that we equated the rate of loss of electrons out of a state \( k \) to the total out scattering. This is, of course, not the entire picture: if we have \( f(k) \) electrons in \( k \) and they leave at a rate \( S(k, k') \) for state \( k' \) then our total rate of change of \( f(k) \) will be
\[
\frac{df}{dt}_{\text{out}} = \sum_{k'} f(k') S(k, k') = f(k)\Gamma(k)
\]

We need to add the reverse process from \( k' \) back to \( k \) as
\[
\frac{df}{dt}_{\text{in}} = \sum_{k'} f(k') S(k', k)
\]
Then we get the total rate of change
\[
\frac{df}{dt} = \frac{df}{dt} \left[ \frac{1}{n} - \frac{1}{n_{\text{out}}} \right]
\]

\[
= \sum_{\ell'} \left[ S(k', k) f(k') - S(k, k') f(k) \right]
\]

We can add the Pauli Exclusion Principle which says that there can be no more than one electron in a state by writing the probability that a state is occupied as \( \sum 1 - f(k) \) and \( \sum 1 - f(k') \) and including these probabilities in the collision integral above to get

\[
\frac{df}{dt} \left[ \text{local} \right] = \sum_{\ell'} \left[ S(k', \ell) f(k') \left[ 1 - f(k) \right] \right.
\]

\[
- S(k, \ell') f(k) \left[ 1 - f(k') \right] \]

All of these considerations make the BTE a complicated non-linear integro-differential equation which is nearly impossible to solve in general. However, solutions are possible for a few special cases, including low-dimensional systems (1-D), systems possessing spherical symmetry, or...
systems which are spatially homogeneous. In the latter case, we can eliminate the spatial gradient \( \nabla f = 0 \) due to the homogeneity; often we also assume steady-state because we are only interested in the solution a long time after the stimulus (field or temperature) has been applied. Then we also set \( \frac{df}{dt} = 0 \) and get

\[
\frac{df}{dt} \mid \text{momentum} = -e F \cdot \frac{\nabla f}{\hbar}
\]

The collision integral is often simplified by assuming a Relaxation Time Approximation where the out-of-equilibrium portion of the distribution function \( f = f_f - f_0 \) goes to zero at a decay constant \( \Gamma(k) = \frac{\hbar}{\tau(k)} \), \( \tau(k) \) being the inverse of the scattering rate \( \Gamma(k) \). Then we have

\[
-\frac{e F}{\hbar} \cdot \nabla f(k) = -\frac{f_f - f_0}{\tau(k)}
\]

Since \( f(k) \) is not too different from the equilibrium Fermi-Dirac distribution

\[
f_0(E) = \frac{\exp \left( \frac{E - E_F}{k_B T} \right) + 1}{\exp \left( \frac{E - E_F}{k_B T} \right) - 1}
\]
we can write \( q_k f = \partial_k \frac{f_0}{\partial E} (k) \) = 
\[
\frac{2f}{\partial E} \frac{\partial E}{\partial E} \bar{v}_y(k) = e \frac{\partial}{\partial E} \frac{f_0}{f_0} \bar{v}_y(k)
\]
Finally \( e \bar{F} = \bar{v}_y(k) \frac{\partial f_0}{\partial E} = \frac{f - f_0}{f_1(k)} \)
and we can solve directly as
\[
f(k) = f_0(k) - e \bar{I}(k) \bar{v}_y(k) \bar{F} \left( \frac{\partial f_0}{\partial E} \right)
\]
The equilibrium part, given by \( f_0(k) \)
does not contribute to the current because of symmetry, so we only get a current from
\[
j = -e^2 \sum k \bar{v}_y(k) \bar{v}_y(k) \bar{F} \left( \frac{\partial f_0}{\partial E} \right)
\]
Using the fact that the average component of \( \bar{v}_y(k) \) in the direction of \( \bar{F} \) is \( \bar{v}_z \), we can also simplify to
\[
j = -\frac{e}{3} \sum k \bar{v}_z(k) \bar{v}_z(k) \bar{F} \left( \frac{\partial f_0}{\partial E} \right)
\]
We see that \( j \) is proportional to \( \bar{F} \)
and Ohm's law holds. We write
Conductivity as $j = -\sigma \vec{E}$ with

$$\sigma = \frac{e^2}{3} \sum_{\vec{k}} \frac{v_{g}^2(\vec{k}) \gamma(\vec{k})}{k} \frac{\partial f_0}{\partial E}$$

and mobility as $\sigma = e n \mu$ so that

$$\mu = e \frac{1}{3} \sum_{\vec{k}} \frac{v_{g}^2(\vec{k}) \gamma(\vec{k})}{k} \frac{\partial f_0}{\partial E} \sum_{\vec{k}} f_0$$