Solving the BTE:

Metals

Mark Lundstrom

Electrical and Computer Engineering
Purdue University
West Lafayette, IN USA
Steady-state BTE for small E-fields

\[
\frac{\partial f}{\partial t} + \bar{v} \cdot \nabla_r f + \bar{F}_e \cdot \nabla_p f = - \frac{f - f_0}{\tau_m}
\]

Steady-state, 1D, spatially uniform, no B-field:

\[
-q\mathcal{E} \frac{\partial f}{\partial p_x} \approx -q\mathcal{E} \frac{\partial f_0}{\partial p_x} = - \frac{f - f_0}{\tau_m}
\]

\[
f = f_0 + q\tau_m \mathcal{E} \frac{\partial f_0}{\partial p_x}
\]

\[
n \approx n_0
\]

\[
F_n \approx E_F
\]
Steady-state BTE for small E-fields

\[ J_{nx} = \frac{1}{\Omega} \sum_{k} (-q) \nu_x f \]

\[ J_{nx} = \sigma_n \overline{E}_x \]

\[ \sigma_n = \frac{1}{\Omega} \sum_{k} q^2 \nu_x^2 \tau_m \left( -\frac{\partial f_0}{\partial E} \right) \]
Conductivity of a metal

Our solution to the BTE gave:

\[ \sigma_n = \frac{1}{\Omega} \sum_k q^2 v^2_x \tau_m \left( -\frac{\partial f_0}{\partial E} \right) \]

For a non-degenerate semiconductor, we simplified this to:

\[ \sigma_n = nq\mu_n \]

Metals have a very high density of electrons in the conduction band. What is the conductivity of a metal?
Conductivity of a metal

Our solution to the BTE gave: \[ \sigma_n = \frac{1}{\Omega} \sum_k q^2 \nu_x^2 \tau_m \left( -\frac{\partial f_0}{\partial E} \right) \]

Make the replacement (valid near equilibrium): \( \nu_x^2 \rightarrow \nu^2/3 \)

Convert the sum over k to an integral over k, then convert the integral over k to an integral over energy assuming parabolic bands. \( E = \hbar^2 k^2/2m^* \)

Result...
Conductivity of a metal

Result...

\[ \sigma_n = q^2 \int_0^\infty \frac{v^2 \tau_m}{3} \left( \frac{m^* \sqrt{2m^*E}}{\pi^2 \hbar^3} \right) \left( -\frac{\partial f_0}{\partial E} \right) dE \]

Recall:

\[ D_{3D}(E) = \left( \frac{m^* \sqrt{2m^*E}}{\pi^2 \hbar^3} \right) \]

Recognize:

\[ D_n(E) = \frac{v^2 \tau_m}{3} \]

\[ \sigma_n = q^2 \int_0^\infty D_n(E) D_{3D}(E) \left( -\frac{\partial f_0}{\partial E} \right) dE \]
Conductivity of a metal

Our solution to the BTE gave:

\[ \sigma_n = q^2 \int_0^\infty D_n(E)D_{3D}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE \]

In a metal, the Fermi level is very high in the band. The width of the Fermi window is small in comparison to the variation of the DOS.

\[ \left(-\frac{\partial f_0}{\partial E}\right) \approx \delta(E_F) \]
Conductivity of a metal

\[ \sigma_n = q^2 \int_0^\infty D_n(E) D_{3D}(E) \delta(E_F) \, dE \]

\[ J_{nx} = \sigma_n \mathcal{E}_x \]

\[ \sigma_n = q^2 D_n(E_F) D_{3D}(E_F) \]
Recap:

\[-q \mathcal{E}_x \frac{\partial f_0}{\partial p_x} = -\frac{f - f_0}{\tau_m} \rightarrow J_{nx} = \sigma_n \mathcal{E}_x\]

s.s. BTE with spatially uniform conditions.

non-degenerate semiconductor

\[
\sigma_n = n q \mu_n
\]
\[
\mu_n = \frac{q \langle \langle \tau_m \rangle \rangle}{m^*}
\]
\[
\langle \langle \tau_m \rangle \rangle \equiv \frac{\langle E \tau_m \rangle}{\langle E \rangle}
\]

degenerate metal or semiconductor

\[
\sigma_n = q^2 D_n(E_F) D_{3D}(E_F)
\]
\[
D_n(E_F) = \frac{\nu_F^2 \tau_m(E_F)}{3}
\]
\[
D_{3D}(E_F) = \left( \frac{m^* \sqrt{2m^* E_F}}{\pi^2 \hbar^3} \right)
\]
Now to confuse matters...

Our result for metals is: \[ \sigma_n = q^2 D_n(E_F) D_{3D}(E_F) \]

Let’s see if we can express this in terms of the electron density,

\[
\begin{align*}
  n &= \int_0^{E_F} D_{3D}(E) dE = \int_0^{E_F} \left( \frac{m^* \sqrt{2m^*E}}{\pi^2 \hbar^3} \right) dE = \left( \frac{m^* \sqrt{2m^*}}{\pi^2 \hbar^3} \right) \int_0^{E_F} \sqrt{E} \, dE \\
  n &= \left( \frac{m^* \sqrt{2m^*}}{\pi^2 \hbar^3} \right) \frac{2}{3} E_F^{2/3} = D_{3D}(E_F) \frac{2}{3} E_F \\
  D_{3D}(E_F) &= \frac{3}{2} \frac{n}{E_F}
\end{align*}
\]
Now to confuse matters...

\[ \sigma_n = q^2 D_n(E_F) D_{3D}(E_F) \quad D_{3D}(E_F) = \frac{3}{2} \frac{n}{E_F} \]

\[ \sigma_n = q^2 D_n(E_F) \frac{n}{2} \frac{3}{E_F} = nq \left( \frac{D_n(E_F)}{2} \frac{3}{E_F/q} \right) \]

\[ \mu_n = \left( \frac{D_n(E_F)}{2} \frac{3}{E_F/q} \right) = \left( \frac{\nu_F^2 \tau_m(E_F)}{2} \frac{3}{E_F/q} \right) = \frac{q \tau_m(E)}{m^*} \]

\[ \frac{D_n}{k_B T / q} = \mu_n \]

nondegenerate Einstein relation

\[ \frac{1}{2} m^* \nu_F^2 = E_F \]
Second Recap:

\[ -q \mathcal{E}_x \frac{\partial f_0}{\partial p_x} = -\frac{f - f_0}{\tau_m} \rightarrow J_{nx} = \sigma_n \mathcal{E}_x \]

s.s. BTE with spatially uniform conditions.

**non-degenerate semiconductor**

\[ \sigma_n = nq\mu_n \]

\[ \mu_n = \frac{q\langle \langle \tau_m \rangle \rangle}{m^*} \]

\[ \langle \langle \tau_m \rangle \rangle \equiv \frac{\langle E \tau_m \rangle}{\langle E \rangle} \]

**degenerate metal or semiconductor**

\[ \sigma_n = nq\mu_n \]

\[ \mu_n = \frac{q \tau_m (E_F)}{m^*} \]

But only a tiny fraction of the electrons contribute to conduction!
Take away

For conductivity, remember this:

\[ \sigma_n = \frac{1}{\Omega} \sum_k q^2 v_x^2 \tau_m \left( -\frac{\partial f_0}{\partial E} \right) \]

Not this:

\[ \sigma_n = n q \mu_n \quad \mu_n = \frac{q \tau}{m^*} \]
Questions?

\[ \frac{\partial f}{\partial t} + \bar{v} \cdot \nabla_r f + \vec{F}_e \cdot \nabla_p f = -\frac{f - f_s}{\tau_m} \]

general case:

\[ \sigma_n = \frac{1}{\Omega} \sum_k q^2 v_x^2 \tau_m \left( -\frac{\partial f_0}{\partial E} \right) \]

for a metal:

\[ \sigma_n = q^2 D_n(E_F) D_{3D}(E_F) \]