Lecture 13: Solving the BTE: equilibrium and ballistic
outline

1) Quick review

2) Equilibrium BTE

3) Ballistic BTE

4) Discussion

5) Summary
equilibrium distribution function

\[ f_0 = \frac{1}{1 + e^{(E - E_F)/k_BT}} \]

\[ f_0 \approx e^{-(E - E_F)/k_BT} \ll 1 \]

\( E >> E_F \) (nondegenerate)
chemical potential and Fermi level

\[ f_0 = \frac{1}{1 + e^{(E - E_F)/k_B T}} \]

\[ f_0 = \frac{1}{1 + e^{(E - \mu)/k_B T}} \]

\( \mu \) is the chemical (or electrochemical) potential.

\( \mu(T = 0) \) is the Fermi level

We will use \( E_F \)
$f_0$ in $k$-space

$f_0 \approx e^{-(E - E_F)/k_BT}$

$E = E_C + E(k) \approx E_C + \frac{\hbar^2 k^2}{2m^*}$

$f_0 \approx e^{(E_F - E_C)/k_BT} e^{-\hbar^2 k^2/2m^* k_BT}$

Maxwellian distribution
(spread is related to $T$)
\[ f_0 = \frac{1}{1 + e^{(E - E_F)/k_B T}} \]

\[ E = E_C + E(k) \approx E_C + \frac{\hbar^2 k^2}{2m^*} \]

\[ E_F = E_C + \frac{\hbar^2 k_F^2}{2m^*} \]

\[ f_0 = \frac{1}{1 + e^{\hbar^2 (k^2 - k_F^2)/2m^* k_B T}} \]

Fermi-Dirac distribution
To find $f$ out of equilibrium, solve the BTE.

\[
\frac{d(hk_x)}{dt} = -q\mathcal{E}_x
\]
BTE

\[ f(r, p, t) \]

\[ \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_r f + \mathbf{F}_e \cdot \nabla_p f = \hat{C}f \]

\[ \hat{C}f(r, p, t) = \sum_{p'} S(r', p) f(p') [1 - f(p)] \]

\[ - \sum_{p'} S(r, p') f(p) [1 - f(p')] \]
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BTE in equilibrium

\[ \frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_r f + \mathbf{r} \cdot \nabla_p f = \hat{C} f \]

\( \hat{C} f = 0 \) in two cases:

- equilibrium
- ballistic transport

Consider equilibrium first and solve:

\[ \mathbf{v} \cdot \nabla_r f + \mathbf{F}_e \cdot \nabla_p f = 0 \]
detailed balance

\[ \hat{C}f = 0 \]

\[ \hat{C}f = \sum_{p'} S(p', p) f(p') \left[ 1 - f(p) \right] \]

\[ - \sum_{p'} S(p, p') f(p) \left[ 1 - f(p') \right] = 0 \]

\[ S(p', p) f_0(p') \left[ 1 - f_0(p) \right] = S(p, p') f_0(p) \left[ 1 - f_0(p') \right] \]

(holds for any pair of \( p \) and \( p' \))
BTE in equilibrium

\[ \vec{v} \bullet \nabla_r f_0 + \dot{F}_e \bullet \nabla_p f_0 = 0 \]

assume:

\[ f_0 = g(E_{TOT}) = g\left[ E_C(r) + E(hk) \right] \]

\[ \vec{v} \bullet \frac{dg}{dE_{TOT}} \nabla_r E_{TOT} + F_e \bullet \frac{dg}{dE_{TOT}} \nabla_p E_{TOT} = 0 \]

\[ \vec{v} \bullet \nabla_r E_C(r) + \dot{F}_e \bullet \nabla_p E(hk) = 0 \]

\[ \vec{v} \bullet \left( -\dot{F}_e \right) + \dot{F}_e \bullet \vec{v} = 0 \]

Any function of total energy satisfies the equilibrium BTE!
from EE-606, we know:

\[ f_0 = \frac{1}{1 + e^{(E - E_F)/k_BT}} = \frac{1}{1 + e^{\Theta}} \]

\[ \Theta = \frac{E_C(r) + E(k) - E_F}{k_BT} \]

\[ \vec{v} \cdot \nabla_r f_0 + \vec{F}_e \cdot \nabla_p f_0 = 0 \]

equilibrium BTE

\[ \vec{v} \cdot \frac{\partial f_0}{\partial \Theta} \nabla_r \Theta + \vec{F}_e \cdot \frac{\partial f_0}{\partial \Theta} \nabla_p \Theta = 0 \]

\[ \vec{v} \cdot \left\{ \frac{\nabla E_C - \nabla E_F}{k_BT} + \frac{(E - E_F)}{k_B} \nabla_r \left( \frac{1}{T} \right) \right\} + \vec{F}_e \cdot \frac{\nu}{k_BT} = 0 \]
equilibrium

$$\vec{v} \cdot \left\{ -\nabla E_F + \left( \frac{E - E_F}{k_B T} \right) \left( -\frac{\nabla_r T}{T} \right) \right\} = 0$$

to satisfy this equation for any energy, $E_{TOT}$, $\nabla E_F = \nabla T = 0$

the Fermi level and temperature are constant in equilibrium.
but…

T.E. Humphrey and H. Linke argue that in a nanostructured material, it is possible to have Fermi level and temperature gradients in equilibrium.

what determines $f_0$, the equilibrium $f$?

\[ \nu \cdot \nabla r f_0 + F_e \cdot \nabla p f_0 = \hat{C} f_0 = 0 \]

satisfied by any function of total energy

must ensure detailed balance in equilibrium.

only satisfied by:

\[ f_0 = \frac{1}{1 + e^{(E-E_F)/k_BT}} \]
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generic ballistic device

\[ f(E) = f_0(E_F) \]

\[ f(E) \neq f_0(E) \]

\[ f(E) = f_0(E_{F2}) \]
solution for a ballistic device

**Steady-state ballistic BTE:**

\[ \nu_x \cdot \nabla f(x, p_x) - qE_x \frac{\partial f(x, p_x)}{\partial p_x} = 0 \]

**Solution:**

\[ f(x, p_x) = g(E) = g[E_C(x) + E(hk_x)] \]

**Boundary conditions:**

First-order equation in space --> one boundary condition, but we have two contacts!
**boundary conditions**

**Solution:** Apply one-half of the boundary condition to each contact.

\[ f(0, p_x > 0) \]

\[ f(0, p_x < 0) \]

incoming flux
boundary conditions for the BTE

**Solution:** Specify incoming flux.

What about the exiting flux?

*determined by the device*
solution to the s.s. ballistic BTE

\[
E
\]

\[
E_{F1}
\]

contact 1

ballistic device

contact 2

\[
E_C(x)
\]

\[
E_{F2} = E_{F1} - qV_A
\]

\[
\nu_x \cdot \frac{\partial f(x, p_x)}{\partial x} - qE_x \frac{\partial f(x, p_x)}{\partial p_x} = 0
\]

\[
f(0, p_x > 0) = \frac{1}{1 + e^{(E-E_{F1})/k_BT}}
\]

\[
f(W, p_x < 0) = \frac{1}{1 + e^{(E-E_{F2})/k_BT}}
\]

\[
f(x, p_x) = g\left[ E_C(x) + E(hk_x) \right]
\]

\[
f(x, p_x) = \frac{1}{1 + e^{(E-E_F)/k_BT}}
\]

but what Fermi level do we use?
follow trajectories in phase space

\[ E_{F2} = E_{F1} - qV_A \]
importance of reflection-less contacts

Contact 1: ‘reflection-less’ or ‘absorbing’ contacts

Contact 2: ‘reflection-less’ or ‘absorbing’ contacts

\[ E_{F2} = E_{F1} - qV_A \]
to determine the appropriate Fermi level

Within a ballistic device, the probability that a $k$-state is occupied is given by an equilibrium Fermi function.

For a given state at a given location, the Fermi level to use is the one from the contact that populated the $k$-state.

Within a ballistic device, each $k$-state is in equilibrium with one contact or the other.

The overall distribution, however, is as far from equilibrium as it can be.
example

\[ E_{F2} = E_{F1} - qV_A \]
\[ n_L(0) = n_L^1(0) + n_L^2(0) \]

\[ n_L^1(0) = n_L^+(0) = \frac{1}{L} \sum_{k_x > 0} f_0(E_{F1}) \]

\[ n_L^2(0) = n_L^-(0) = \frac{1}{L} \sum_{k_x < 0} f_0(E_{F2}) \]

\[ n_L^1(0) = \int D_{1D}^1(0, E) f_0(E_{F1}) dE \]

\[ n_L^2(0) = \int D_{1D}^2(0, E) f_0(E_{F2}) dE \]
\[ n_L(0) = \frac{1}{L} \sum_{k_x > 0} f_0(E_{F1}) + \frac{1}{L} \sum_{k_x < 0} f_0(E_{F2}) = \int D_{1D}(0, E) f_0(E_{F1}) + D_{1D}^2(0, E) f_0(E_{F2}) dE \]

\[ D_{1D}^1(0, E) = D_{1D}^2(0, E) = D_{1D}(E)/2 \]
another example

\[\begin{align*}
E_F &= E_{F1} - qV_A \\
D_{1D}^1(x_1, E) + D_{1D}^2(x_1, E) &\neq D_{1D}(E) / 2
\end{align*}\]

"local density of states"

\[n_L(x_1) = \int D_{1D}^1(x_1, E) f_0(E_{F1}) + D_{1D}^2(x_1, E) f_0(E_{F2}) dE\]
distribution function

suggested exercise

\[ E_F^2 = E_F^1 - qV_A \]
solution to the ballistic BTE: summary

1) states divide into two parts, fillable by each of the contacts

\[ n_L(x) = \int D_{1D}^1(x, E) f_0(E_{F1}) + D_{1D}^2(x, E) f_0(E_{F2}) dE \]

2) but....
Bound states can occur. They may be difficult (or impossible to fill from the contacts). In practice, they could be filled by scattering.
diffusive transport

\[ n_L(x) = \int D_{1D}(x, E) f\left[ F_n(x) \right] dE \]

\[ f(x, E) = \frac{1}{1 + e^{[E - F_n(x)]/k_BT}} \]

\[ D_{1D}(x, E) = \frac{1}{\pi \hbar} \sqrt{\frac{2m^*}{(E - E_C(x))}} \]
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\[ I = \frac{1}{L} \sum_{k<0} q \nu_x f_0(E_{F2}) \]

\[ I^+ = \frac{1}{L} \sum_{k>0} q \nu_x f_0(E_{F1}) \]

\[ I = I^+ - I^- \]
\[ I = q \left[ \frac{D_{1D}(E_F)}{2L} (E_{F_1} - E_{F_2}) \right] \nu_F \]

\[ I = q^2 \left[ \frac{D_{1D}(E_F)}{2L} \nu_F \right] V \]

\[ M(E_F) = \gamma(E_F) \pi \frac{D_{1D}(E_F)}{2} \]

\[ \gamma(E_F) = \frac{h}{\tau} = \frac{h}{L/\nu_F} \]

\[ M(E_F) = \frac{h}{2} \frac{D_{1D}(E_F)}{2L} \nu_F \]
questions

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