Week 8 Summary:

Coupled Current Equations

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nano to macro device

\[ I = \frac{2q}{h} \int \mathcal{T}(E) M(E) (f_1 - f_2) dE \]

\[ f_1(E) = \frac{1}{1 + e^{(E - E_{F1})/k_B T_1}} \]

\[ f_2(E) = \frac{1}{1 + e^{(E - E_{F2})/k_B T_2}} \]

\[ M_{3D}(E) A = A \frac{\hbar}{4} \langle \psi^* \rangle D_{3D}(E) \]

\[ \mathcal{T}(E) = \frac{\lambda(E)}{\lambda(E) + L} \]
the current equation

In Week 7 we saw that the electrical current in the bulk is:

\[ J_{nx} = \sigma_n \frac{d}{dx} \left( \frac{F_n}{q} \right) \]

\[ \sigma_n = \text{conductivity} = \frac{1}{\rho_n} \quad (1/\Omega\cdot\text{m}) \]

Alternatively, we could write this equation in the inverted form as:

\[ \frac{d}{dx} \left( \frac{F_n}{q} \right) = \rho_n J_{nx} \]

How do these equations change when there is a temperature gradient?
Current in the presence of a temp gradient

The answer is:

\[ J_{\alpha x} = \sigma \frac{d(F_n/q)}{dx} - S_n \sigma \frac{dT}{dx} \]

\( S_n \) is the Seebeck coefficient in V/K.

Alternatively, we can write this equation as:

\[ \frac{d(F_n/q)}{dx} = \rho_n J_{\alpha x} + S_n \frac{dT}{dx} \]

(inverted form of the equations)
driving forces for current flow

\[ I = \frac{2q}{h} \int T(E) M(E)(f_i - f_z) dE \]

Differences in occupation, \( f \), produce current.
when $\Delta T = 0$, the driving force is: $\Delta E_F$

\[
\begin{align*}
(f_i - f_z) & \approx \left( - \frac{\partial f_0}{\partial E} \right) q \Delta V \\
(f_i = f_z = f_0)
\end{align*}
\]
driving force: differences in temperature

\[ \Delta T = T_2 - T_1 \]

\[ f_1 - f_2 = f_1 - f_1 - \left( f_1 + \frac{\partial f_1}{\partial T} \Delta T \right) \]

\[ = -\frac{\partial f_1}{\partial T} \Delta T \]

\[ \frac{\partial f_1}{\partial T_L} = -\left( \frac{E - E_F}{T_L} \right) \frac{\partial f_0}{\partial E} \]

\[ f_1 - f_2 \approx -\left( \frac{\partial f_0}{\partial E} \right) \frac{(E - E_F)}{T} \Delta T \]

\[ (f_i = f_2 \approx f_0) \]

|f_1 - f_2| > 0 so current flows.
transport in the bulk

\[ J = \frac{2q}{h} \int T(E) M(E) (f_i - f_2) \]

\[ (f_i - f_2) \approx -\left( \frac{\partial f_0}{\partial E} \right) q \Delta V \left( -\frac{\partial f_0}{\partial E} \right) \frac{(E - E_F)}{T} \Delta T \]

\[ T(E) = \frac{\lambda(E)}{L} \]

\[ J_{nx} = \sigma_n \frac{dF_n}{dx} - s_T \frac{dT}{dx} \]

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two forms of the current equation

\[
J_{nx} = \sigma_n \frac{dF_n}{dx} - s_f \frac{dT}{dx}
\]

\[
\frac{dF_n}{dx} = \rho_n J_{nx} + \rho_n s_f \frac{dT}{dx}
\]

\[
S_n = \frac{s_f}{\sigma_n}
\]

\[
S_n = \left( -\frac{1}{qT} \right) \int \left( E - E_F \right) \sigma'(E) dE \]

\[
S_n = \left( -\frac{(E_j - E_F)}{qT} \right)
\]

\[
= \left( \frac{k_B}{q} \right) \left( E_j - E_F \right)
\]

\[
= \left( \frac{k_B}{q} \right) \left( \frac{E_j - E_F}{k_B T} \right)
\]
hot point probe

\[ \tilde{V}(F_n/q) = \rho_n \tilde{j}_n + S_n \tilde{V}T \]

doped silicon wafer

hot!
more on the Seebeck coefficient

\[ S_n(T) = -\frac{1}{qT} (E_J - E_F) \]

\[ S_n(T) = -\frac{1}{qT} (E_C + \Delta_n - E_F) \]

\[ \Delta_n = \frac{\int (E - E_c) \sigma_n'(E) dE}{\int \sigma_n'(E) dE} \]

The parameter, \( \Delta_n \), depends on bandstructure and scattering.

\[ S_n(T) = \left( \frac{k_B}{q} \right) \left( \frac{E_c - E_L}{k_B T} + \delta_n \right) \]

\[ \left( \frac{k_B}{q} \right) = 86 \ \mu V/K \]

\[ \delta_n = \frac{E_F - E_c}{k_B T} \]

\[ \delta_n = 2 \] (3D, non-degenerate parabolic bands, energy-independent mfp)
understanding $S$

$$S = \frac{E_c - E_F}{qT}$$

1) $|S|$ is large for a non-degenerate semiconductor because the current carrying channels are way above (below) the Fermi level.

2) $|S|$ is small for a degenerate semiconductor (or metal) because the current flows near the Fermi energy.
heat current

Thermoelectricity involves the flow of charge and heat, so in addition to the equation for the charge current, we need an equation for the heat current:

\[ J_{Q\times} = -\kappa_0 \frac{dT}{dx} \quad W/m^3 \quad E_x = 0 \]

1) How is \( \kappa_0 \) related to the properties of the material?

2) How does this equation change when there is a current flow?
The answer is:

\[ J_{\dot{Q}e} = \left( S_a \sigma_a T \right) \frac{d\left( F_a/q \right)}{dx} - \kappa_0 \frac{dT}{dx} \quad W/m^2 \]

Alternatively, we can write this equation as:

\[ J_{\dot{Q}e} = \pi_a J_{\dot{Q}e} - \kappa_e \frac{dT}{dx} \]

\[ \pi_a = S_a \frac{T}{T} \]

\[ \kappa_e = \kappa_0 - S_a \sigma_a T \]

\( \pi \) is the Peltier coefficient in W/A

**Important point:** Both electrons and the lattice (phonons) carry heat. These equations refer only to the portion of the heat carried by the electrons.
understanding the Peltier effect

Questions:

Why does $J_Q = \pi_n J_n$?
(when the two contacts are at the same temperature)

What determines the Peltier coefficient, $\pi_n$?

Answer: We should draw an energy band diagram.
physics of Peltier cooling

- Electrons absorb thermal energy, $E - E_{F1}$
- Energy channel
- Electrons dissipate energy, $E - E_{F2}$

Electrons enter contact 1 at the Fermi energy, $E_{F1}$

Net power dissipated: $P_D = IV$

Electrons leave contact 2 at the Fermi energy, $E_{F2}$

$E_{F2} = E_{F1} - qV$
closer look at contact 1

energy channel

“evaporation” of the electron liquid
relations between parameters

\[ \pi = TS \quad \text{Kelvin relation} \]

\[ \frac{\kappa}{\sigma} = \left( \frac{k_B}{q} \right)^2 \left[ \left( \frac{E - E_F}{k_B T} \right)^2 \right] - \left( \frac{E - E_F}{k_B T} \right)^2 \] \[ T = \mathcal{L} T \quad \text{Wiedeman-Franz “Law”} \]
bulk, 3D semiconductors

\[ \kappa_n = \sigma_n T L \]

\( L \) is the “Lorenz number”

The Lorenz number depends on details of bandstructure, scattering, dimensionality, and degree of degeneracy, but for a constant mfp and parabolic energy bands, it is useful to remember:

\[ L \approx \frac{2}{\left( \frac{k_B}{q} \right)^2} \quad \frac{\pi}{3} \left( \frac{k_B}{q} \right)^2 \]

non-degenerate, 3D semiconductors

fully degenerate e.g. 3D metals

a “rule of thumb” not a “law of nature”

TE power generation

1) How much heat can be converted into electricity? (what determines the efficiency?)

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TE cooling

1) What determines the maximum temperature difference?
2) How much heat can be pumped?
3) What is the coefficient of performance?
figure of merit

\[ Z = \frac{S^2 \sigma_n}{\kappa} \text{ K}^{-1} \]

\[ ZT = \frac{S^2 \sigma_n T}{\kappa} \]

dimensionless figure of merit

The higher the ZT figure of merit, the more efficient a TE device.

1) What material properties are needed for a high ZT?
2) Given a material, how can we optimize ZT?
PF vs. Fermi level

\[ ZT = \frac{S_n^2 \sigma_n T_L}{\kappa} \]
The peak PF occurs when $E_F$ is near the band edge.

$$ZT = \frac{S^2 \sigma T}{\kappa}$$

$$PF = S_n^2 \sigma_n$$
TE coefficients (3D, bulk)

\( J_x = \sigma E_x - \sigma S \frac{dT}{dx} \)
\( J_x^0 = T \sigma S E_x - \kappa_0 \frac{dT}{dx} \)

\[ E_x = \rho J_x + S \frac{dT}{dx} \]
\[ J_x^0 = \pi J_x - \kappa_x^0 \frac{dT}{dx} \]

(diffusive transport)

\[ \sigma = \int \sigma'(E) dE \]
\[ \sigma'(E) = \frac{2q^2}{h} \lambda(E) \frac{M(E)}{A} \left( - \frac{\partial f_0}{\partial E} \right) \]
\[ S = -\frac{k_B}{q} \int \left( \frac{E - E_F}{k_B T} \right) \sigma'(E) dE / \int \sigma'(E) dE \]
\[ \pi = TS \]
\[ \kappa_0 = T \left( \frac{k_B}{q} \right)^2 \int \left( \frac{E - E_F}{k_B T} \right)^2 \sigma'(E) dE \]
\[ \kappa_x^0 = \kappa_0 - \pi S \sigma \]