(Electronic) Heat Current

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Temperature gradients give rise to an open circuit voltage, which is known as the Seebeck effect. We expect a **positive** voltage for an n-type semiconductor (and **negative** voltage for a p-type semiconductor.)
Peltier effect

\[ J_n < 0 \quad J_n/(-q) > 0 \quad J_Q = \pi_n J_n > 0 \]

contacts maintained at same temperature
Transport equations and coefficients

**TE transport equations (inverted form)**

\[ J = \sigma \mathcal{E} - S \sigma \frac{dT}{dx} \]

\[ J_Q = TS \sigma \mathcal{E} - \kappa_0 \frac{dT}{dx} \]

\[ \mathcal{E} = \rho J + S \frac{dT}{dx} \]

\[ J_Q = \pi J - \kappa_e \frac{dT}{dx} \]

**TE transport coefficients**

<table>
<thead>
<tr>
<th>( \rho )</th>
<th>( S )</th>
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<td>( 1/\sigma )</td>
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<table>
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<th>( \pi )</th>
<th>( \kappa_e )</th>
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(diffusive transport)

\[ R = \rho L/A \]

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Transport equations and coefficients

\[ J = \sigma \mathcal{E} - \sigma S \frac{dT}{dx} \]

\[ \mathcal{E} = \rho J + S \frac{dT}{dx} \]

(diffusive transport)

\[ \sigma = \int \sigma'(E) dE \]

\[ \sigma'(E) = \frac{2q^2}{h} \lambda(E) \frac{M(E)}{A} \left( -\frac{\partial f_0}{\partial E} \right) \]

\[ S = -\frac{k_B}{q} \int \left( \frac{E - E_F}{k_B T} \right) \sigma'(E) dE \]

\[ \int \sigma'(E) dE \]
1) Introduction
2) **Physics of Peltier Effect**
3) Mathematics of Peltier Effect
4) Wiedemann-Franz Law and Lorenz Number
5) Example: Transport coefficients of Ge
6) Discussion
7) Summary
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.
N-type semiconductor: equilibrium, $V = 0$

$$n(x) = N_C e^{(E_F - E_C)/k_B T} \approx N_D$$

- Metal contact 1
- Metal contact 2
- Ideal contacts (no band bending)
N-type semiconductor: isothermal, $V > 0$

Electrons flow at an energy a little above the bottom of the conduction band.

$E_{F2} = E_{F1} - qV$

$T_2 = T_1$

(elastic scattering only)
N-type semiconductor: isothermal, $V > 0$

Energy absorbed per electron

$$Q = E_C(0) + \Delta_n - E_{F1}$$

Energy dissipated

$$Q = E_C(L) + \Delta_n(L) - E_{F2}$$

Heat is absorbed (emitted) when the average energy at which the heat current flows increases (decreases)
Peltier coefficient

1) Electrons flow from left to right when $V_2 > V_1$.

2) The flux of electrons from left to right is $J_{nx}/(-q)$

3) Each electron absorbs and then carries an amount of heat: $Q = E_C(0) + \Delta_n - E_{F1}$

4) So the heat flux from left to right is:

\[
J_{Q1} = \left[ E_C(0) + \Delta_n - E_{F1} \right] \times J_{nx}/(-q) = \pi_n J_{nx}
\]

\[
\pi_n = -\frac{\left[ E_C(0) + \Delta_n - E_{F1} \right]}{q}
\]

(less than zero for an n-type semiconductor)
A remarkable result

\[ \pi_n = -\frac{(E_C + \Delta_n - E_F)}{q} \]

\[ \pi_n = -\frac{(E_J - E_F)}{q} \]

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

\[ \pi_n = TS_n \quad \text{“Kelvin relation”} \]

The Peltier coefficient is proportional to the difference between the energy at which current flows and the Fermi energy – just as the Seebeck coefficient was.
The physics of Peltier cooling involves the transfer of energy by the movement of electrons across a temperature gradient. When electrons absorb thermal energy, $E - E_{F1}$, they enter contact 1 at the Fermi energy, $E_{F1}$. In the energy channel, the electrons dissipate energy, $E - E_{F2}$, as they leave contact 2 at the Fermi energy, $E_{F2}$.

The net power dissipated, $P_D$, can be calculated as $IV$. The equation for $E_{F2}$ is $E_{F2} = E_{F1} - qV$, where $q$ is the charge of an electron and $V$ is the voltage applied.

This process is a fundamental aspect of thermoelectric devices, where energy is converted into a temperature difference, leading to cooling effects.
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Nano to macro device

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

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

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

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

\[ \mathcal{T}(E) = \frac{\lambda(E)}{\lambda(E) + L} \]
Charge current $\rightarrow$ heat current

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

$$q \rightarrow (E - E_F)$$

$$I_Q = \frac{2}{h} \int (E - E_F)\mathcal{T}(E)M(E)(f_1 - f_2)\,dE$$

Note: if $E_C > E_{F1}$, then electrons in the contact must absorb energy to flow in one of the energy channels in the device.
Heat current

\[ I'_{Q_1}(E) = \frac{2(E - E_{F_1})}{h} \mathcal{T}(E) M(E) (f_1 - f_2) \]

\[ I'_{Q_2}(E) = \frac{2(E - E_{F_2})}{h} \mathcal{T}(E) M(E) (f_1 - f_2) \]
the math

\[ I'_Q(E) = \frac{2(E - E_{F1})}{h} \mathcal{T}(E) M(E) (f_1 - f_2) \]

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

\[ I'_Q(E) = - TS(E) \sigma(E) \Delta V - K'_0 (E) \Delta T \]

\[ K'_0 (E) = \frac{2 \left( E - E_F \right)^2}{h} \mathcal{T}(E) M(E) \left( - \frac{\partial f_0}{\partial E} \right) \]

\[ I_Q = \int I'_Q(E) dE \]

\[ K_0 = \int K'_0 (E) dE \]
The result

\[ I = G \Delta V + SG \Delta T \]
\[ I_Q = -TSG \Delta V - K_0 \Delta T \]
\[ \Delta V = RI - S \Delta T \]
\[ I_Q = -\Pi - K_e \Delta T \]

\[ G = \frac{2q^2}{h} \int \mathcal{T}(E) M(E) \left( -\frac{\partial f_0}{\partial E} \right) dE \]
\[ S = -\int \frac{(E - E_F)}{qT} G'(E) dE / \int G'(E) dE \]
\[ K_0 = \int \frac{(E - E_F)^2}{q^2T} G'(E) dE \]
\[ K_e = K_0 - \Pi SG \]
\[ \Pi = TS \]
3D bulk semiconductors

\[ J = \sigma \mathcal{E} - S\sigma \frac{dT}{dx} \]
\[ J_Q = TS_T \mathcal{E} - \kappa_0 \frac{dT}{dx} \]
\[ \mathcal{E} = \rho J + S \frac{dT}{dx} \]
\[ J_Q = \pi J - \kappa_e \frac{dT}{dx} \]

(diffusive transport)

\[ \sigma = \int \sigma'(E) dE \]
\[ \sigma'(E) = \frac{2q^2}{h} \lambda(E) \frac{M(E)}{A} \left( -\frac{\partial f_0}{\partial E} \right) \]
\[ S = -\int \frac{(E - E_F)}{qT} \sigma'(E) dE \left/ \int \sigma'(E) dE \right. \]
\[ \kappa_0 = \int \frac{(E - E_F)^2}{q^2T} \sigma'(E) dE \]
\[ \pi = TS \]
\[ \kappa_e = \kappa_0 - \pi S\sigma \]
Both electrons and lattice vibrations carry heat – we have been discussing the electronic part.

In metals, heat conduction by electrons dominates: $\kappa_e >> \kappa_L$

In semiconductors, lattice vibrations dominate: $\kappa_L >> \kappa_e$
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Coupled current equations

\[ \mathcal{E} = \rho J + S \frac{dT}{dx} \]

\[ J_{\varphi} = \pi J - \kappa_e \frac{dT}{dx} \]

Kelvin relation

\[ \pi = TS \]

("Onsager relations" for coupled flows)

We expect a relation between the electrical conductivity and the electronic thermal conductivity, but it is not fundamental; it depends on material details.
Electronic thermal conductivity

\[
\kappa_0 = \int_{-\infty}^{+\infty} \frac{(E - E_F)^2}{q^2 T} \sigma'(E) dE = \frac{2q^2}{h} \frac{\lambda(E)}{M(E) / A} \left( -\frac{\partial f_0}{\partial E} \right)
\]

\[
\kappa_e = \kappa_0 - T\sigma S^2
\]

\[
\kappa_0 = T \left( \frac{k_B}{q} \right)^2 \left\langle \left( \frac{E - E_F}{k_B T} \right)^2 \right\rangle \sigma
\]

\[
S^2 = \left( \frac{k_B}{q} \right)^2 \left\langle \left( \frac{E - E_F}{k_B T} \right)^2 \right\rangle
\]

\[
\kappa_e = T\sigma \left( \frac{k_B}{q} \right)^2 \left\{ \left\langle \left( \frac{E - E_F}{k_B T} \right)^2 \right\rangle - \left\langle \left( \frac{E - E_F}{k_B T} \right) \right\rangle^2 \right\} = T\sigma \mathcal{L}
\]

Wiedemann-Franz “Law”
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:

\[
\mathcal{L} \approx 2 \left( \frac{k_B}{q} \right)^2 \quad \text{non-degenerate, 3D semiconductors}
\]

\[
\mathcal{L} \approx \frac{\pi^2}{3} \left( \frac{k_B}{q} \right)^2 \quad \text{fully degenerate e.g. 3D metals}
\]

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

Lorenz number for a single channel

\[ \kappa_e = T \sigma \left( \frac{k_B}{q} \right)^2 \left\{ \left\langle \left( \frac{E - E_F}{k_B T} \right)^2 \right\rangle - \left\langle \left( \frac{E - E_F}{k_B T} \right) \right\rangle^2 \right\} = T \sigma \mathcal{L} \]

\[ M(E) = M_0 \delta(E - E_C) \]

\[ \left\langle \left( \frac{E - E_F}{k_B T} \right)^2 \right\rangle = \left\langle \left( \frac{E - E_F}{k_B T} \right) \right\rangle^2 \]

\[ \mathcal{L} = 0 \]

How can we understand this result physically?
If there is only a single channel, then if it is open-circuited, no electrons can flow. There is no charge transport and no heat transport.
Bipolar conduction

\[ M^{\text{tot}}(E) = M^{C}(E) + M^{V}(E) \]

\[ \sigma_{\text{tot}} = \sigma_n + \sigma_p \]

\[ S_{\text{tot}} = \frac{S_n \sigma_n + S_p \sigma_p}{\sigma_{\text{tot}}} \]
Bipolar conduction

\[ \sigma_{tot} = \sigma_n + \sigma_p \]

\[ S_{tot} = \frac{S_n \sigma_n + S_p \sigma_p}{\sigma_{tot}} \]

\[ \kappa_e = \kappa_{en} + \kappa_{ep} + T \left( \frac{\sigma_n \sigma_p}{(\sigma_n + \sigma_p)} \right) \left( S_p - S_n \right)^2 \]

\[ \mathcal{L} = \frac{\kappa_e}{\sigma_{tot} T} \]

\[ \mathcal{L} = \frac{\kappa_{en}}{\sigma_n T (\sigma_n + \sigma_p)} + \frac{\kappa_{ep}}{\sigma_p T (\sigma_n + \sigma_p)} + \sigma_n \sigma_p \left( \frac{S_p - S_n}{\sigma_n + \sigma_p} \right)^2 \]
Lorenz number vs. Fermi level at 300 K

Silicon ($E_G = 1.1 \text{ eV}$)

Bi$_2$Te$_3$ ($E_G = 0.15 \text{ eV}$)

(Computation by Dr. Xufeng Wang, Purdue University, Oct. 2017.)
Physics (unipolar)

Holes flowing down the temperature gradient

Holes flowing up the QFL gradient

\[ T_1 > T_0 \]

\[ I = 0 \]
Holes and electrons flow at the same rate to the left contact, where they recombine. An energy of $E_G$ has been transported by the e-h pair to the contact.

Holes flowing down the temperature gradient

Net electron flow

Net hole flow

Holes flowing up the QFL gradient

$T_1 > T_0$

$I = 0$

$I = 0$

$E_F$

$\chi$
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Example: TE transport parameters of n-Ge

\[ \rho_n \quad \Omega \cdot m \]
\[ S_n \quad V/K \]
\[ \pi_n \quad W/A = V \]
\[ \kappa_n \quad W/m \cdot K \]

\[ E = \rho_n J_n + S_n \frac{dT}{dx} \left( \frac{V}{m} \right) \]
\[ J_Q = \pi_n J_n - \kappa_n \frac{dT}{dx} \left( W \right) \]

\[ N_D = 10^{15} \text{ cm}^{-3} \]
\[ T = 300 \text{ K} \]
\[ \mu_n = 3200 \text{ cm}^2/\text{V-s} \]

\[ n_0 = N_C e^{(E_F-E_c)/k_BT} \approx N_D \]
\[ N_C = 1.04 \times 10^{19} \text{ cm}^{-3} \]

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### TE transport parameters of n-Ge: resistivity

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<th>Unit</th>
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<tr>
<td>$\rho_n$</td>
<td>$\Omega\cdot\text{cm}$</td>
</tr>
<tr>
<td>$S_n$</td>
<td>$\text{V/K}$</td>
</tr>
<tr>
<td>$\pi_n$</td>
<td>$\text{W/A} = \text{V}$</td>
</tr>
<tr>
<td>$\kappa_n$</td>
<td>$\text{W/m-K}$</td>
</tr>
</tbody>
</table>

\[
\mathcal{E} = \rho_n J_n + S_n \frac{dT}{dx} \left(\frac{\text{V}}{\text{m}}\right)
\]

\[
J_Q = \pi_n J_n - \kappa_n \frac{dT}{dx} \left(\text{W}\right)
\]

\[
N_D = 10^{15} \text{ cm}^{-3} \approx n_0
\]

\[
\mu_n = 3200 \text{ cm}^2/\text{V-s}
\]

\[
\sigma_n = n_0 q \mu_n \quad \text{S/cm}
\]

\[
\rho_n = \frac{1}{n_0 q \mu_n} \approx 2 \text{ } \Omega\cdot\text{cm}
\]
TE transport parameters of n-Ge: Seebeck coeff.

\[ \rho_n = 2 \text{ } \Omega \text{-cm} \]
\[ S_n = \text{V/K} \]
\[ \pi_n = \text{W/A} = \text{V} \]
\[ \kappa_n = \text{W/m-K} \]

\[ E = \rho_n J_n + S_n \frac{dT}{dx} \left( \frac{\text{V}}{\text{m}} \right) \]
\[ J_Q = \pi_n J_n - \kappa_n \frac{dT}{dx} \left( \text{W} \right) \]

\[ N_D = 10^{15} \text{ } \text{cm}^{-3} \approx n_0 \]
\[ n_0 = N_C e^{(E_F - E_c)/k_B T} \]
\[ N_C = 1.04 \times 10^{19} \text{ } \text{cm}^{-3} \]
\[ T = 300 \text{ K} \]

\[ \left( E_c - E_F \right)/k_B T \approx \ln \left( N_C / n_0 \right) \approx 9.3 \]
\[ \delta_n \approx 2 \text{ (non-degenerate, 3D)} \]

\[ S_n = \left( \frac{k_B}{-q} \right) \left\{ \frac{\left( E_c - E_F \right)}{k_B T} + \delta_n \right\} \approx -970 \text{ } \mu \text{V/K} \]
TE transport parameters of n-Ge: Peltier coeff.

\[ \rho_n = 2 \, \Omega \cdot \text{cm} \]
\[ S_n = -970 \, \text{V/K} \]
\[ \pi_n = \frac{\text{W}}{\text{A}} = \text{V} \]
\[ \kappa_n = \frac{\text{W}}{\text{m} \cdot \text{K}} \]

\[ \mathcal{E} = \rho_n J_n + S_n \frac{dT}{dx} \left( \frac{\text{V}}{\text{m}} \right) \]

\[ J_Q = \pi_n J_n - \kappa_n \frac{dT}{dx} \left( \text{W} \right) \]

\[ \pi_n = TS_n \approx -0.3 \, \text{V} \]
TE transport parameters of n-Ge: Peltier coeff.

\[ \rho_n = 2 \ \Omega \text{-cm} \]
\[ S_n = -970 \ \text{V/K} \]
\[ \pi_n = -0.3 \ \text{W/A} = \text{V} \]
\[ \kappa_n = \text{W/m-K} \]

\[ \mathcal{E} = \rho_n J_n + S_n \frac{dT}{dx} \left( \frac{\text{V}}{\text{m}} \right) \]
\[ J_Q = \pi_n J_n - \kappa_n \frac{dT}{dx} \left( \text{W} \right) \]

\[ \frac{\kappa_n}{T \sigma_n} = L \] (Lorenz number)
\[ L \approx 2 \left( \frac{k_B}{q} \right)^2 \] (non-degenerate, 3D)
\[ \sigma_n = 1/\rho_n \]

\[ \kappa_n = 2.2 \times 10^{-4} \ \text{W/m-K} \]
TE transport parameters of n-Ge:

\( \rho_n = 2 \ \Omega\text{-cm} \)

\( S_n = -970 \ \text{V/K} \)

\( \pi_n = -0.3 \ \text{W/A = V} \)

\( \kappa_n = 2.2 \times 10^{-4} \ \text{W/m-K} \)

\[ \mathcal{E} = \rho_n J_n + S_n \frac{dT}{dx} \left( \frac{\text{V}}{\text{m}} \right) \]

\[ J_Q = \pi_n J_n - \kappa_n \frac{dT}{dx} \left( \text{W} \right) \]

All of these parameters depend on the temperature and carrier concentration (Fermi level).

Note also:

\( \kappa_L = 58 \ \text{W/m-K} \gg \kappa_n \)
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Origin of Peltier cooling

$E_{F1}$

$T_{L1}$

$E$

$\lambda_E$

energy channel

"evaporation" of the electron liquid

$f_0$

$x$
“It is interesting that the thermoelectric cooling and heating regions are contained in the highly doped contact layers.”

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The TE transport equations

\[ J = \sigma \mathcal{E} - \sigma S \frac{dT}{dx} \]

\[ J_Q = T \sigma S \mathcal{E} - \kappa_0 \frac{dT}{dx} \]

\[ \mathcal{E} = \rho J + S \frac{dT}{dx} \]

\[ J_Q = \pi J - \kappa_e \frac{dT}{dx} \]

(diffusive transport)

\[ \sigma = \int \sigma'(E) dE \]

\[ \sigma'(E) = \frac{2q^2}{h} \lambda(E) \frac{M(E)}{A} \left( - \frac{\partial f_0}{\partial E} \right) \]

\[ S = -\frac{k_B}{q} \int \left( \frac{E - E_F}{k_B T} \right) \sigma'(E) dE \left/ \int \sigma'(E) dE \right. \]

\[ \pi = TS \]

\[ \kappa_0 = T \left( \frac{k_B}{q} \right)^2 \int \left( \frac{E - E_F}{k_B T} \right)^2 \sigma'(E) dE \]

\[ \kappa_e = \kappa_0 - \pi S \sigma \]
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