ECE 656: Electronic Transport in Semiconductors Fall 2017

(Electronic) Heat Current

Mark Lundstrom

Electrical and Computer Engineering
Purdue University
West Lafayette, IN USA

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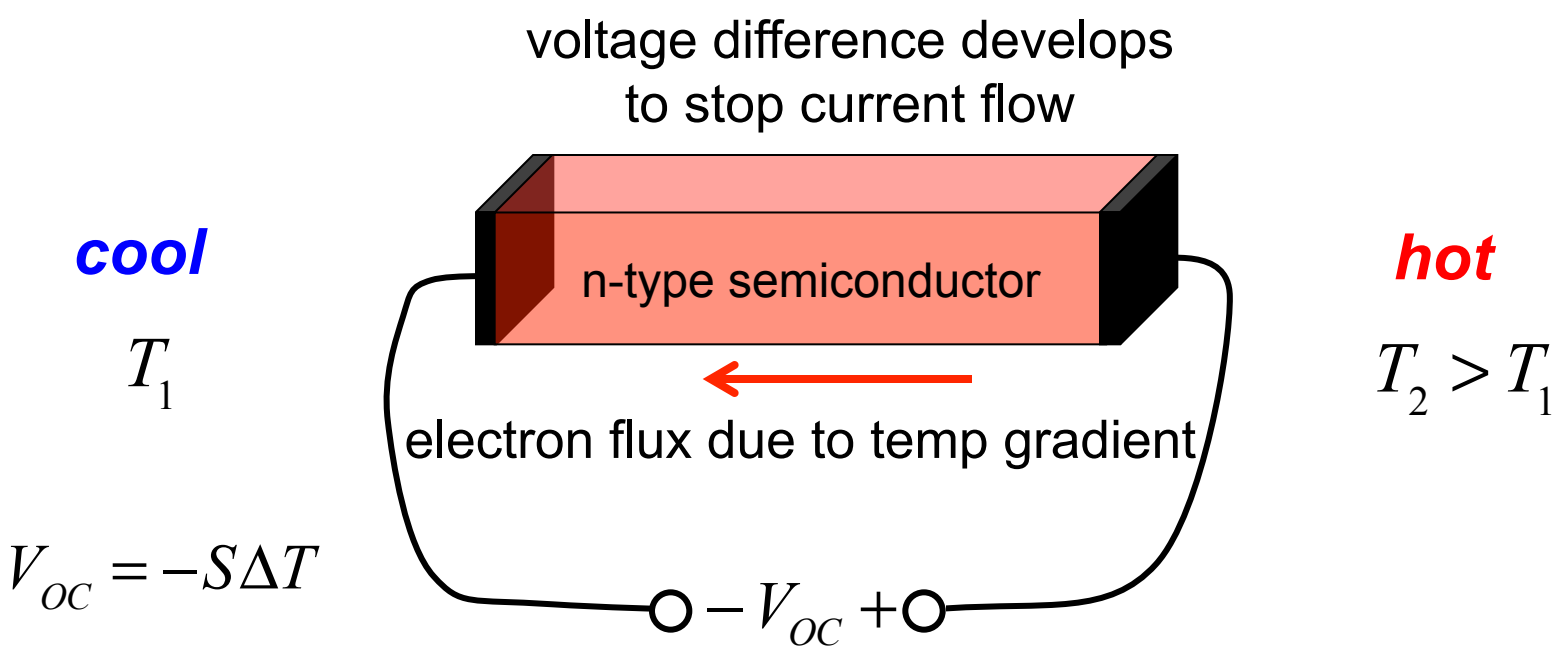
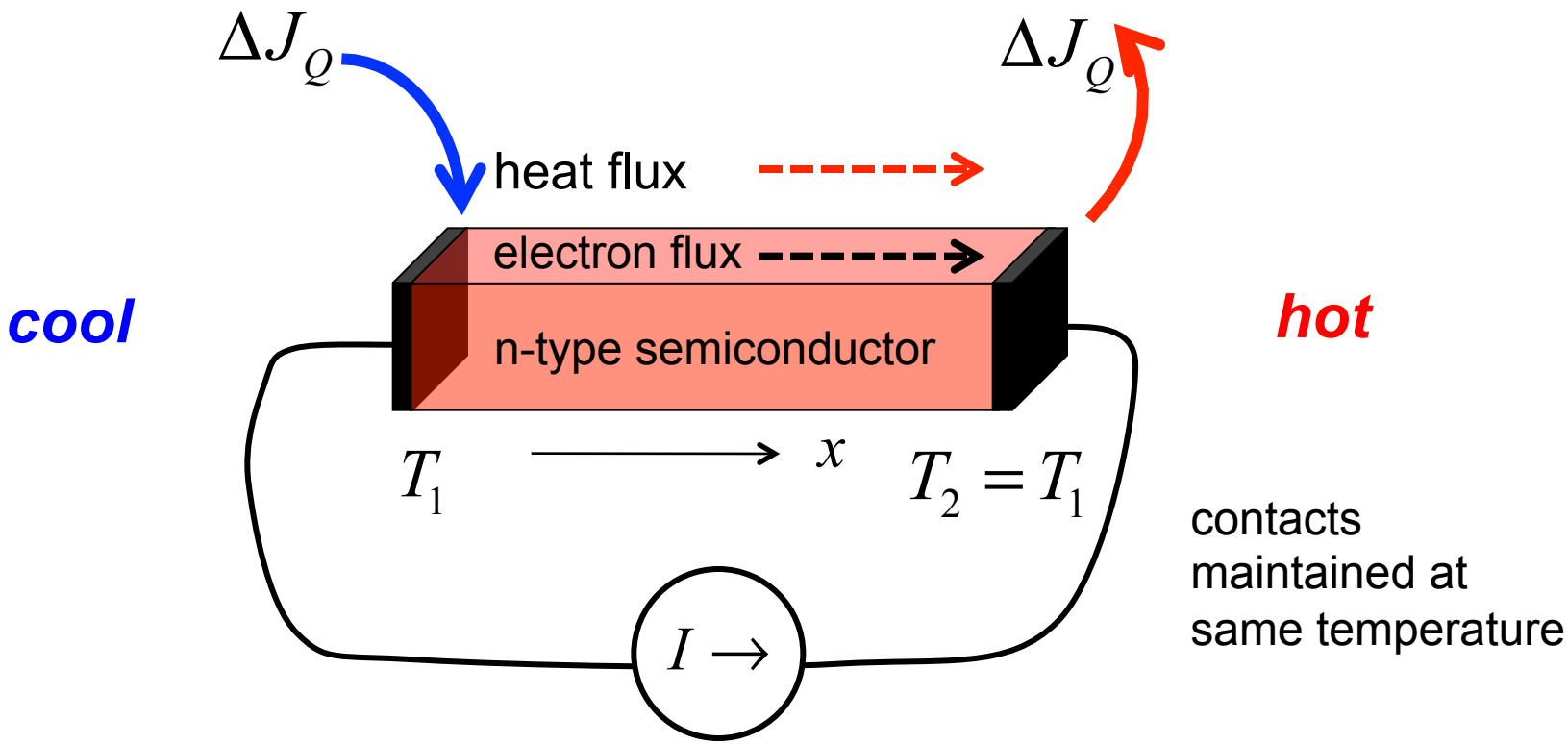
Seebeck effect



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

$J_n < 0$ $\qquad$ $J_n/(-q) > 0$ $\qquad$ $J_Q = \pi_n J_n > 0$



Transport equations and coefficients

TE transport equations (inverted form)

$$J = \sigma \mathcal{E} - S\sigma \, dT/dx$$

$$J_Q = TS\sigma \mathcal{E} - \kappa_0 \, dT/dx$$

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

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

TE transport coefficients

$\rho = 1/\sigma$	S
π	κ_e

(diffusive transport)

$$R = \rho \, L/A$$

Transport equations and coefficients

$$J = \sigma \mathcal{E} - \sigma S \, dT/dx$$

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

(diffusive transport)

$$\sigma = \int \sigma'(E) dE$$

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

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

Outline

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

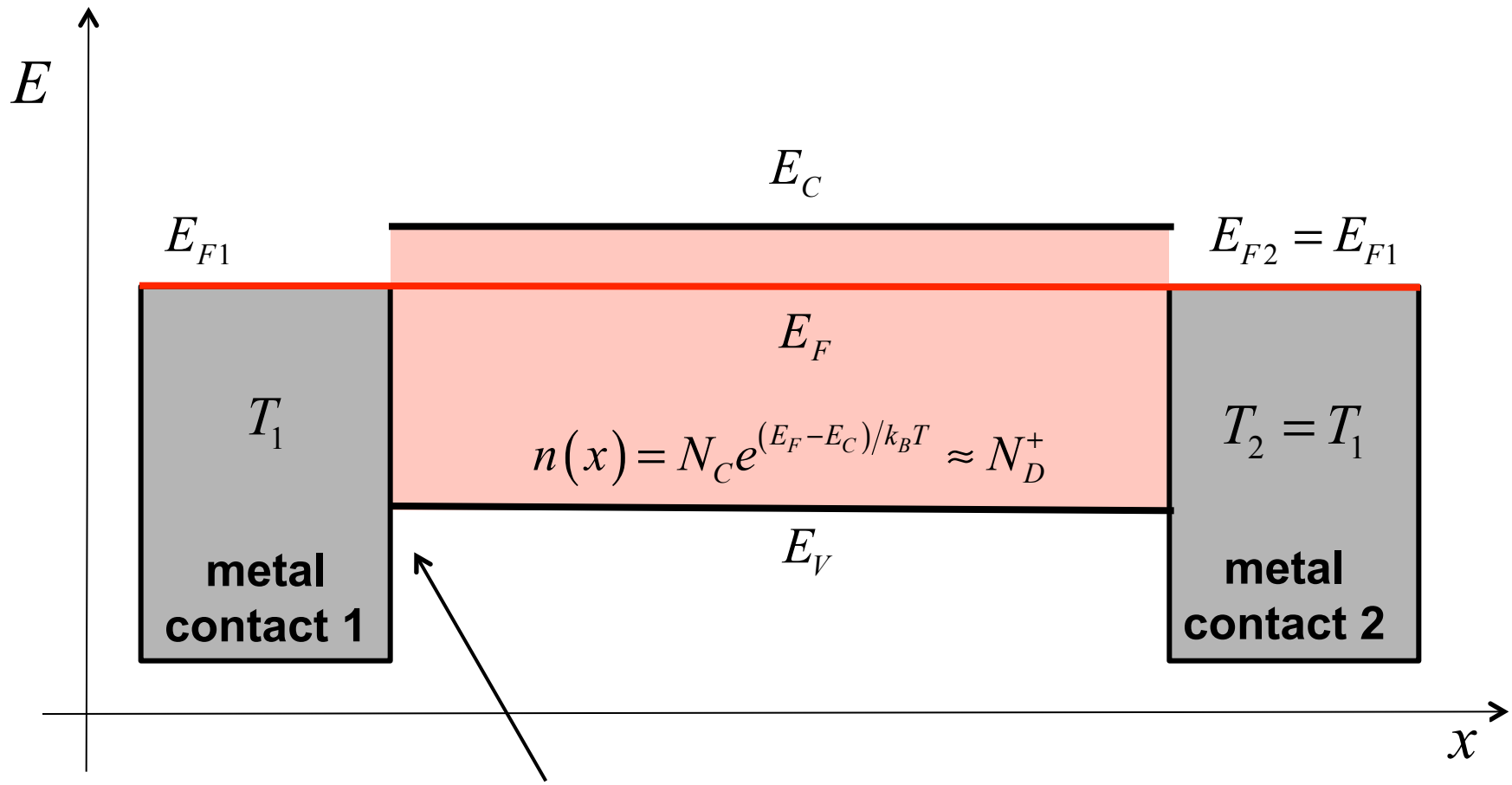
Questions:

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

What determines the Peltier coefficient, π_n ?

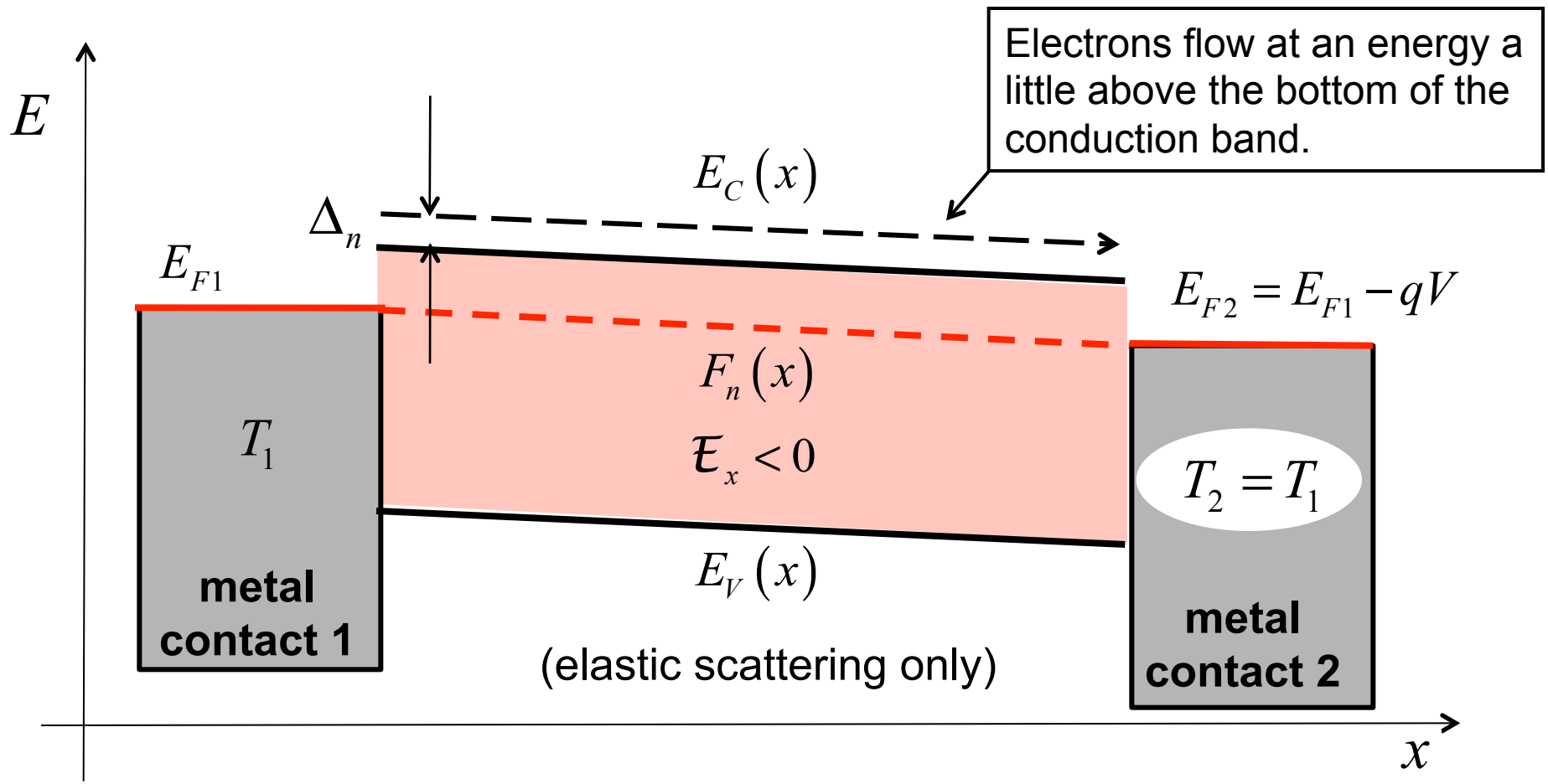
Answer: We should draw an energy band diagram.

N-type semiconductor: equilibrium, $V = 0$

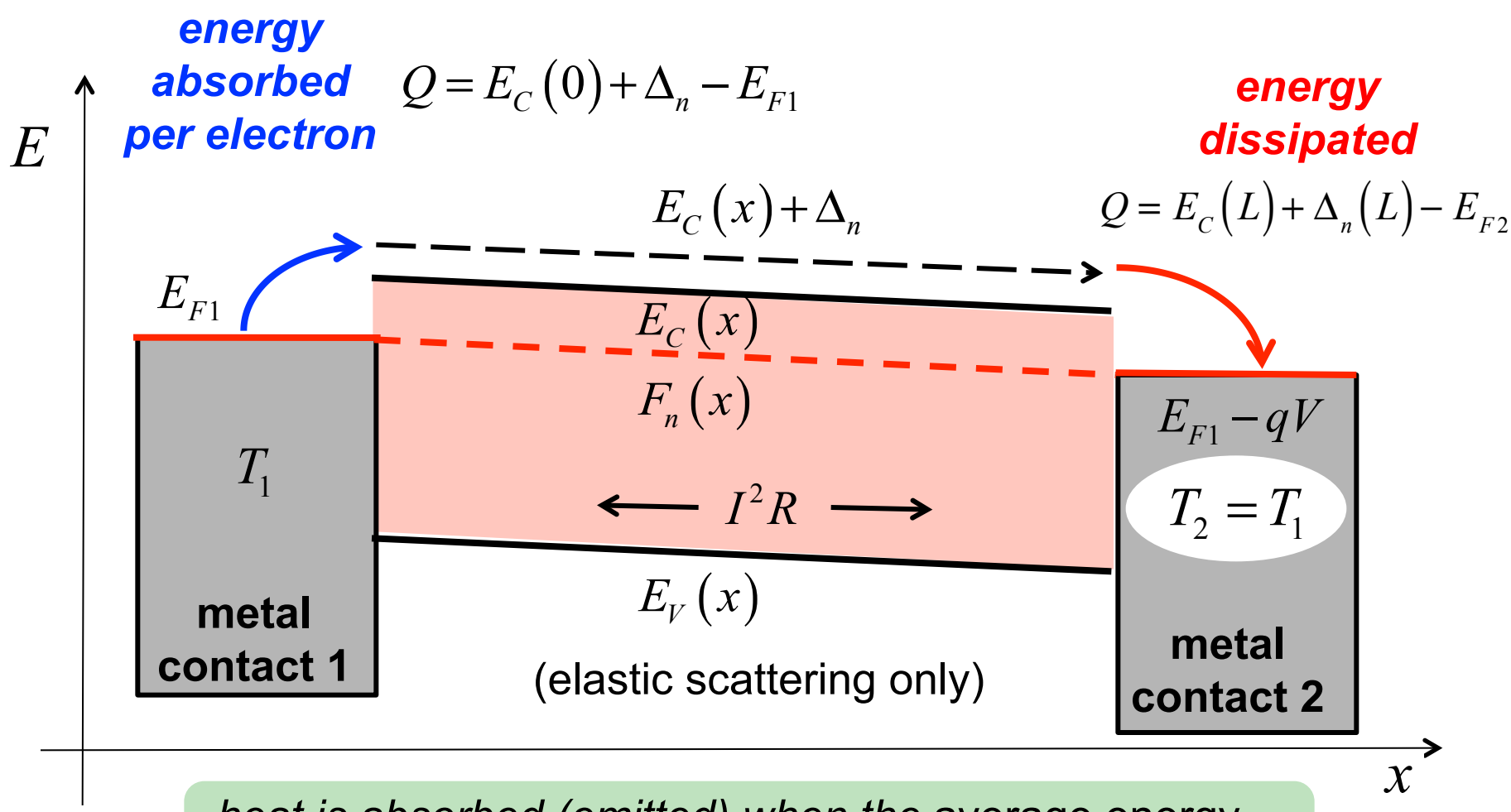


ideal contacts (no band bending)

N-type semiconductor: isothermal, $V > 0$



N-type semiconductor: isothermal, $V > 0$



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

$$\pi_n = -\frac{\left(E_C + \Delta_n - E_F\right)}{q}$$

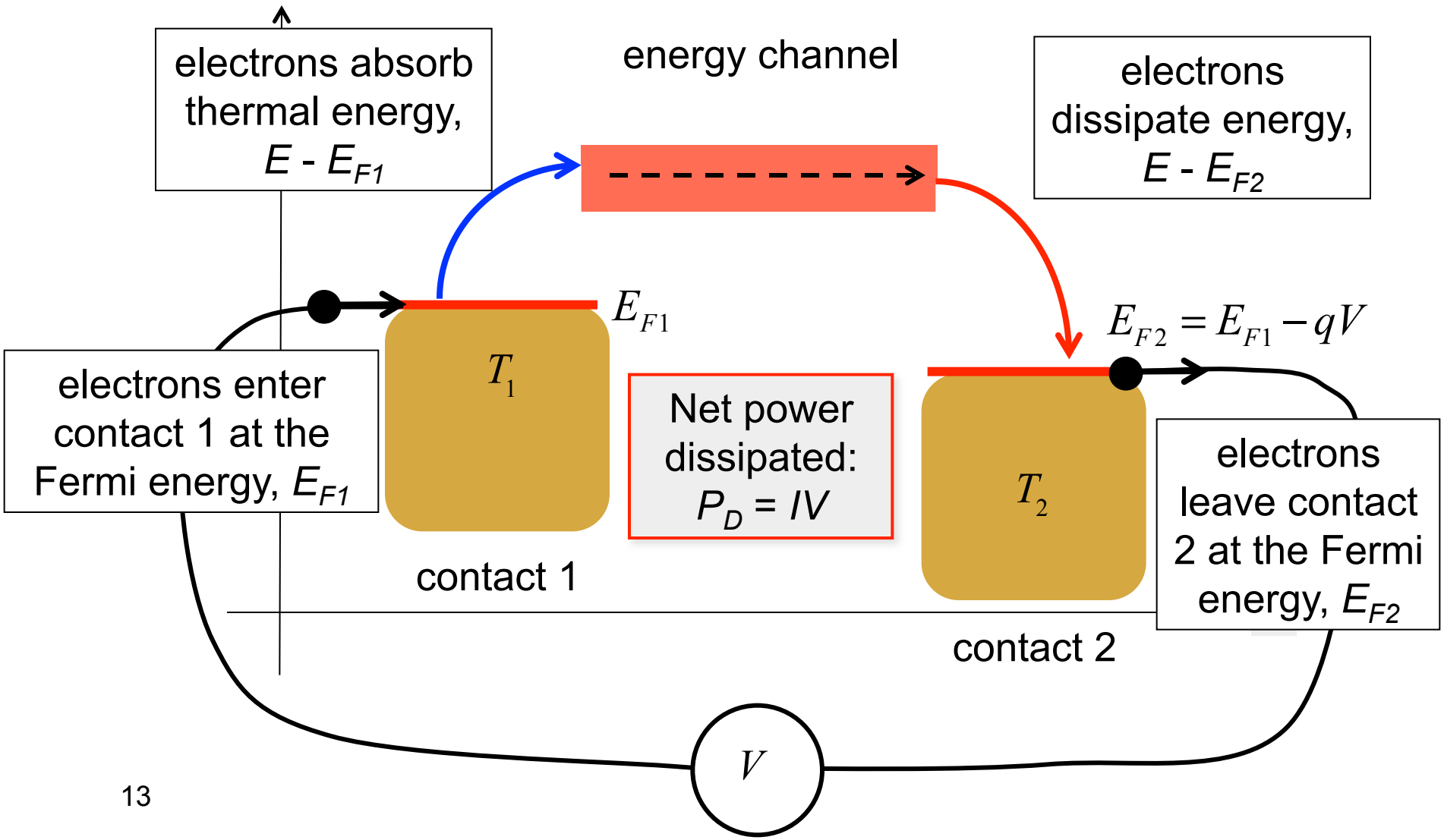
$$\pi_n = -\frac{\left(E_J - E_F\right)}{q}$$

$$S_n = -\frac{\left(E_J - E_F\right)}{qT}$$

$$\pi_n = TS_n$$ "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.

physics of Peltier cooling



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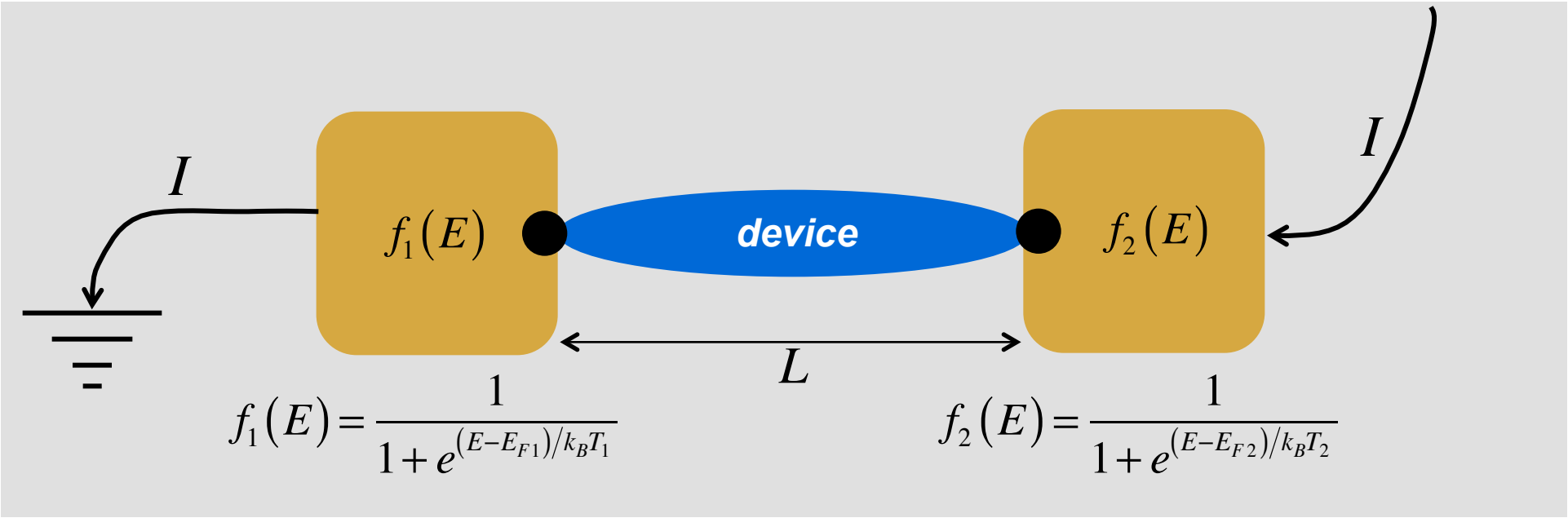
Nano to macro device

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



$$M(E) = M_{3D}(E)A = A\frac{h}{4}\langle \upsilon_x^+ \rangle D_{3D}(E) \qquad \mathcal{T}(E) = \frac{\lambda(E)}{\lambda(E)+L}$$

Charge current → heat current

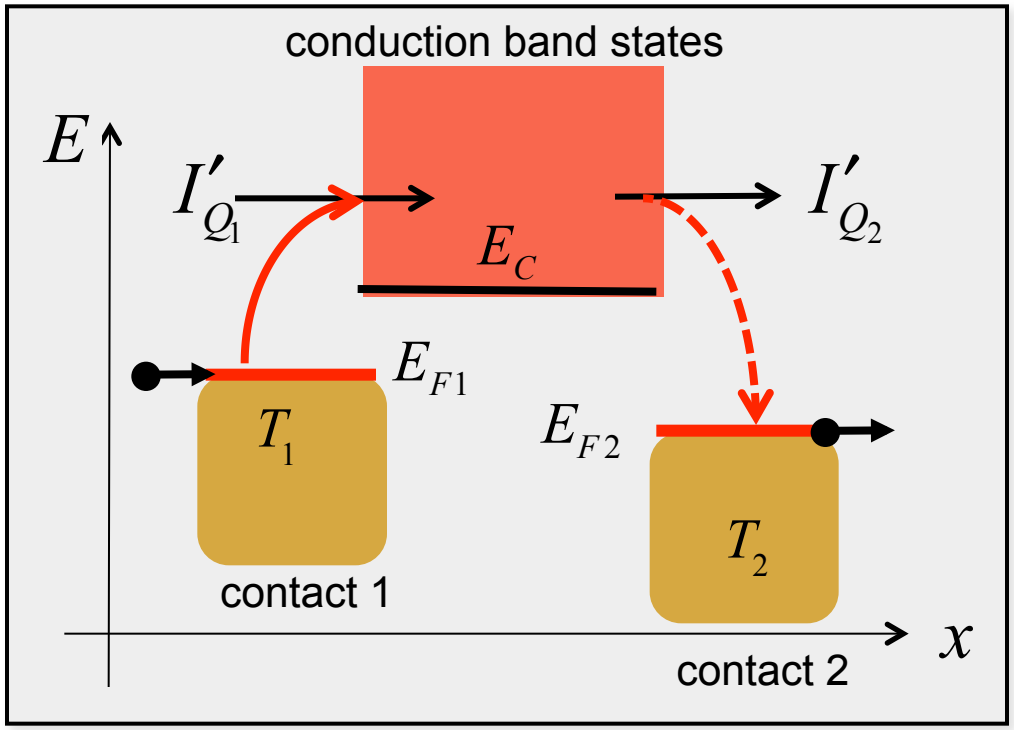
$$I = \frac{2q}{h}\int \mathcal{T}(E)M(E)(f_1 - f_2)dE$$

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

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

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



$$I'_{Q_1}(E) = \frac{2(E - E_{F1})}{h} \mathcal{T}(E) M(E)(f_1 - f_2)$$

$$I'_{Q_2}(E) = \frac{2(E - E_{F2})}{h} \mathcal{T}(E) M(E)(f_1 - f_2)$$

the math

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

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

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

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

$$I_Q = \int I'_Q(E)\, dE$$

$$K_0 = \int K_0(E)\, dE$$

The result

$$I = G\Delta V + SG\Delta T$$

$$I_Q = -TSG\Delta V - K_0\Delta T$$

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$$\Delta V = RI - S\Delta T$$

$$I_Q = -\Pi I - K_e\Delta T$$

$$G = \frac{2q^2}{h}\int \mathcal{T}(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

$$S = -\int \frac{(E-E_F)}{qT}G'(E)dE \Big/ \int G'(E)dE$$

$$K_0 = \int \frac{(E-E_F)^2}{q^2T}G'(E)dE$$

$$K_e = K_0 - \Pi SG$$

$$\Pi = TS$$

3D bulk semiconductors

$$J = \sigma \mathcal{E} - S\sigma \, dT/dx$$

$$J_Q = TS_T \mathcal{E} - \kappa_0 \, dT/dx$$

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

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

(diffusive transport)

$$\sigma = \int \sigma'(E)\,dE$$

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

$$S = -\int \frac{(E - E_F)}{qT}\sigma'(E)\,dE \Big/ \int \sigma'(E)\,dE$$

$$\kappa_0 = \int \frac{(E - E_F)^2}{q^2 T}\sigma'(E)\,dE$$

$$\pi = TS$$

$$\kappa_e = \kappa_0 - \pi S \sigma$$

Lattice thermal conductivity

$$J_Q = \pi J - \kappa \frac{dT}{dx} \qquad \kappa = \kappa_e + \kappa_L$$

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

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

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

Kelvin relation

$$\pi = TS$$

(fundamental)

"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 material details.

Electronic thermal conductivity

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

$$\kappa_e = \kappa_0 - T\sigma S^2$$

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

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

Wiedemann-Franz “Law”

W-F "law"

$\kappa_e = T\sigma\mathcal{L}$ $\mathcal{L}$ 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:

$$\mathcal{L} \approx 2\left(\frac{k_B}{q}\right)^2$$

non-degenerate,
3D semiconductors

$$\mathcal{L} \approx \frac{\pi^2}{3}\left(\frac{k_B}{q}\right)^2$$

fully degenerate
e.g. 3D metals

a "rule of thumb" not a "law of nature"

(G.D. Mahan and M. Bartkowiak, *Appl. Phys. Lett.*, **74**, 953, 1999)

Lorenz number for a single channel

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

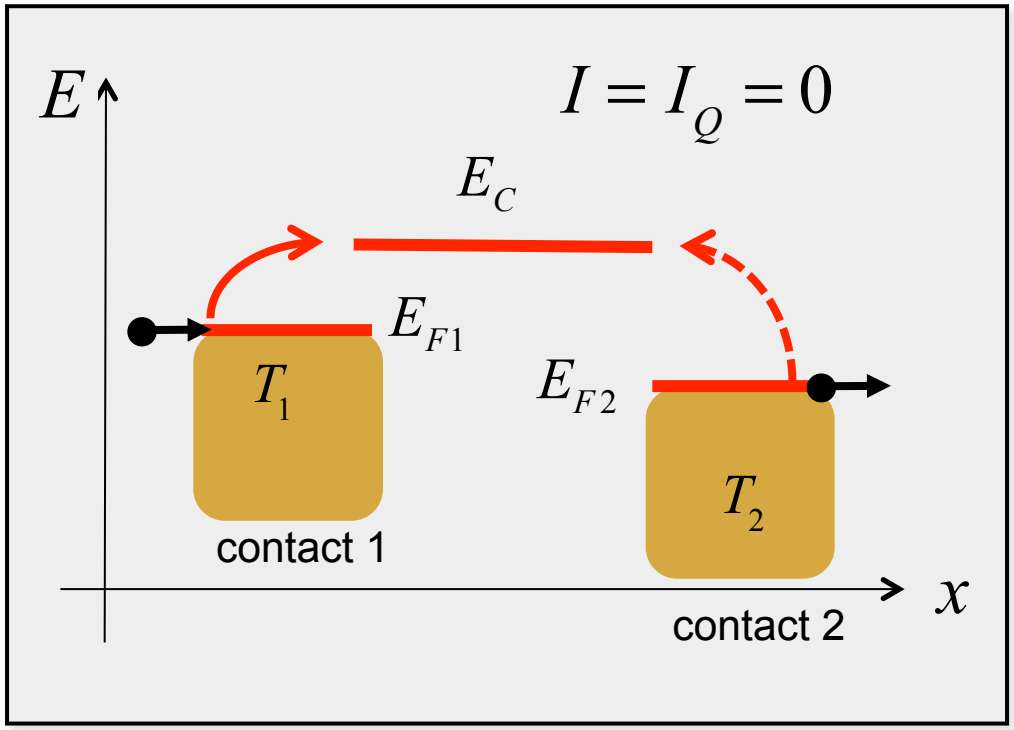
$$M(E)=M_0\delta(E-E_C)$$

$$\left\langle\left(\frac{E-E_F}{k_BT}\right)^2\right\rangle=\left\langle\left(\frac{E-E_F}{k_BT}\right)\right\rangle^2$$

$$\boxed{\mathcal{L}=0}$$

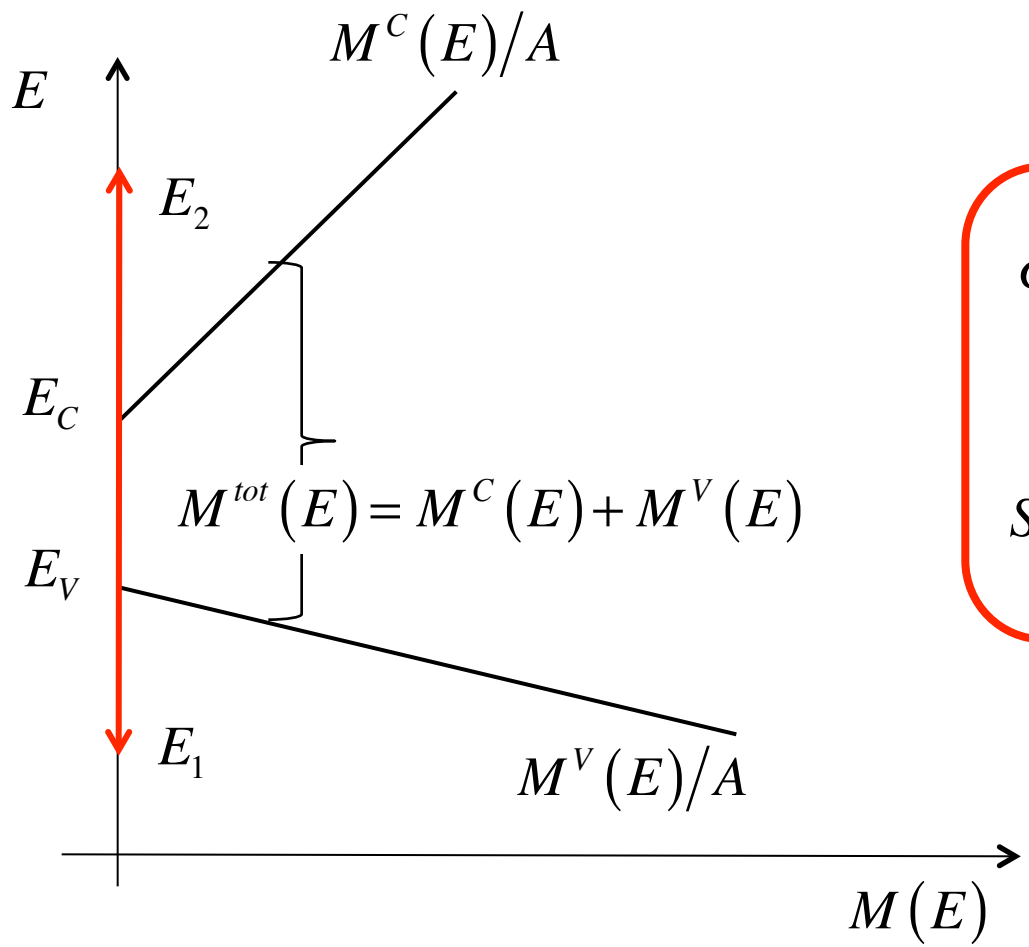
How can we understand this result physically?

Lorenz number for a single channel



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



$$\sigma_{tot} = \sigma_n + \sigma_p$$

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

Bipolar conduction

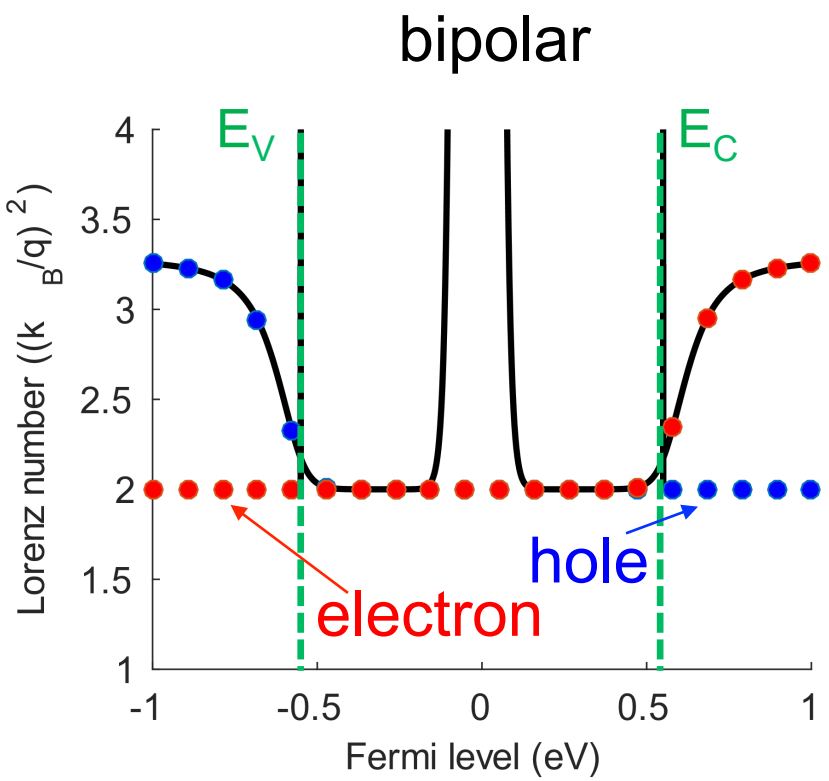
$$\sigma_{tot} = \sigma_n + \sigma_p \qquad S_{tot} = \frac{S_n\sigma_n + S_p\sigma_p}{\sigma_{tot}}$$

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

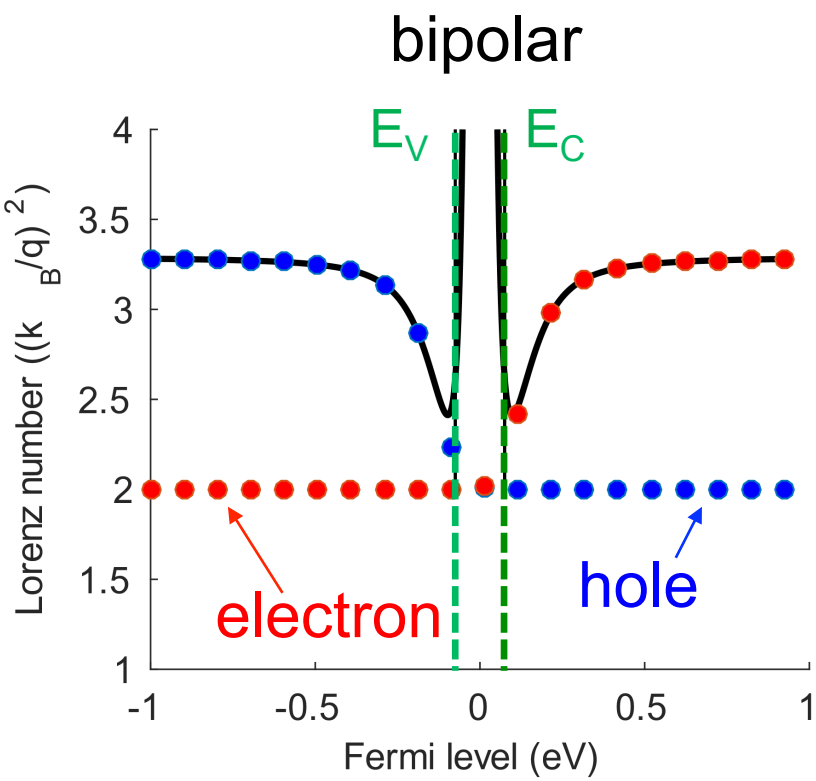
$$\mathcal{L} = \frac{\kappa_e}{\sigma_{tot}T}$$

$$\mathcal{L} = \frac{\kappa_{en}}{\sigma_n T}\frac{\sigma_n}{\left(\sigma_n + \sigma_p\right)} + \frac{\kappa_{ep}}{\sigma_p T}\frac{\sigma_p}{\left(\sigma_n + \sigma_p\right)} + \sigma_n\sigma_p\left(\frac{S_p - S_n}{\sigma_n + \sigma_p}\right)^2$$

Lorenz number vs. Fermi level at 300 K



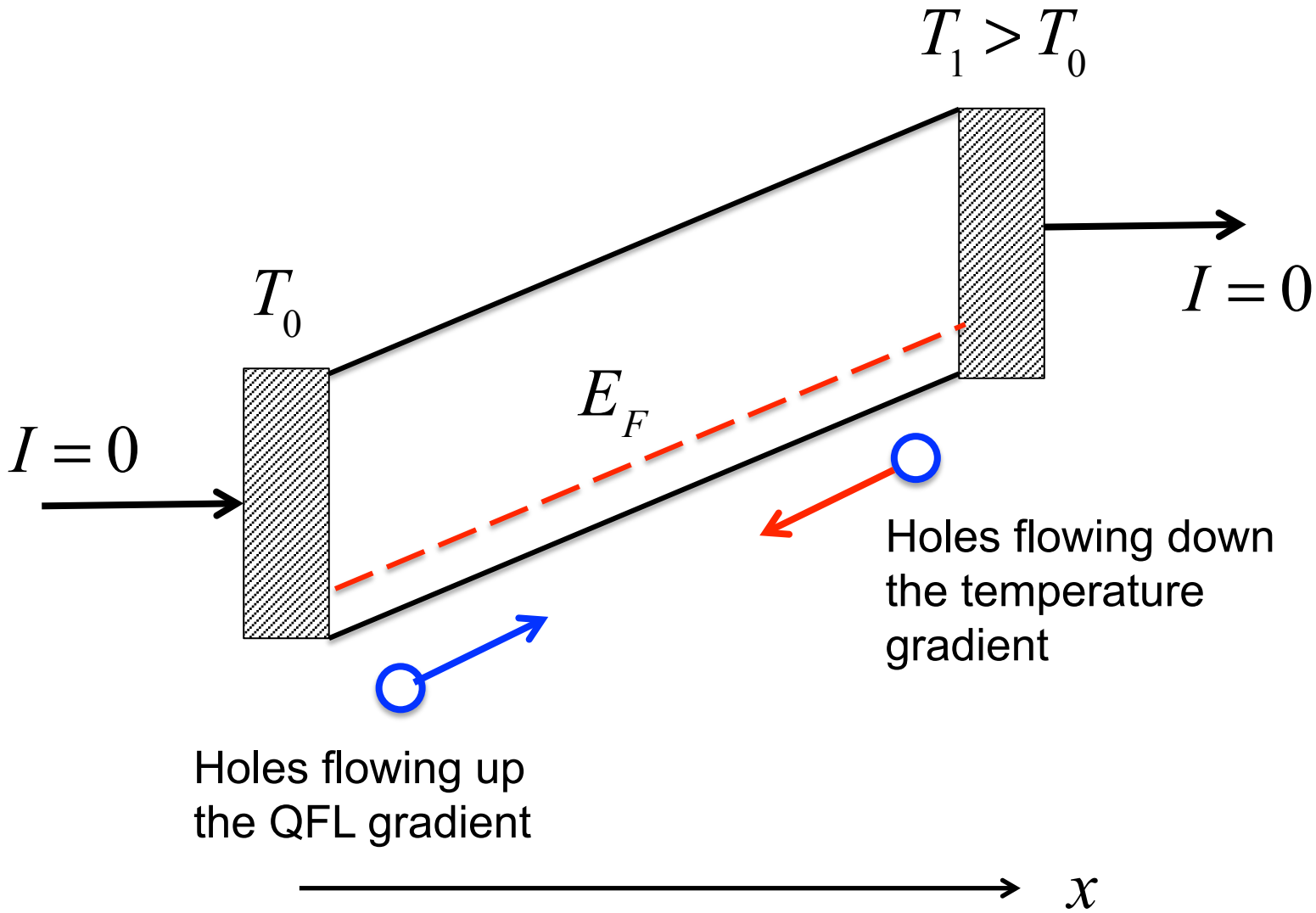
Silicon (E_G = 1.1 eV)



Bi_2Te_3 (E_G = 0.15 eV)

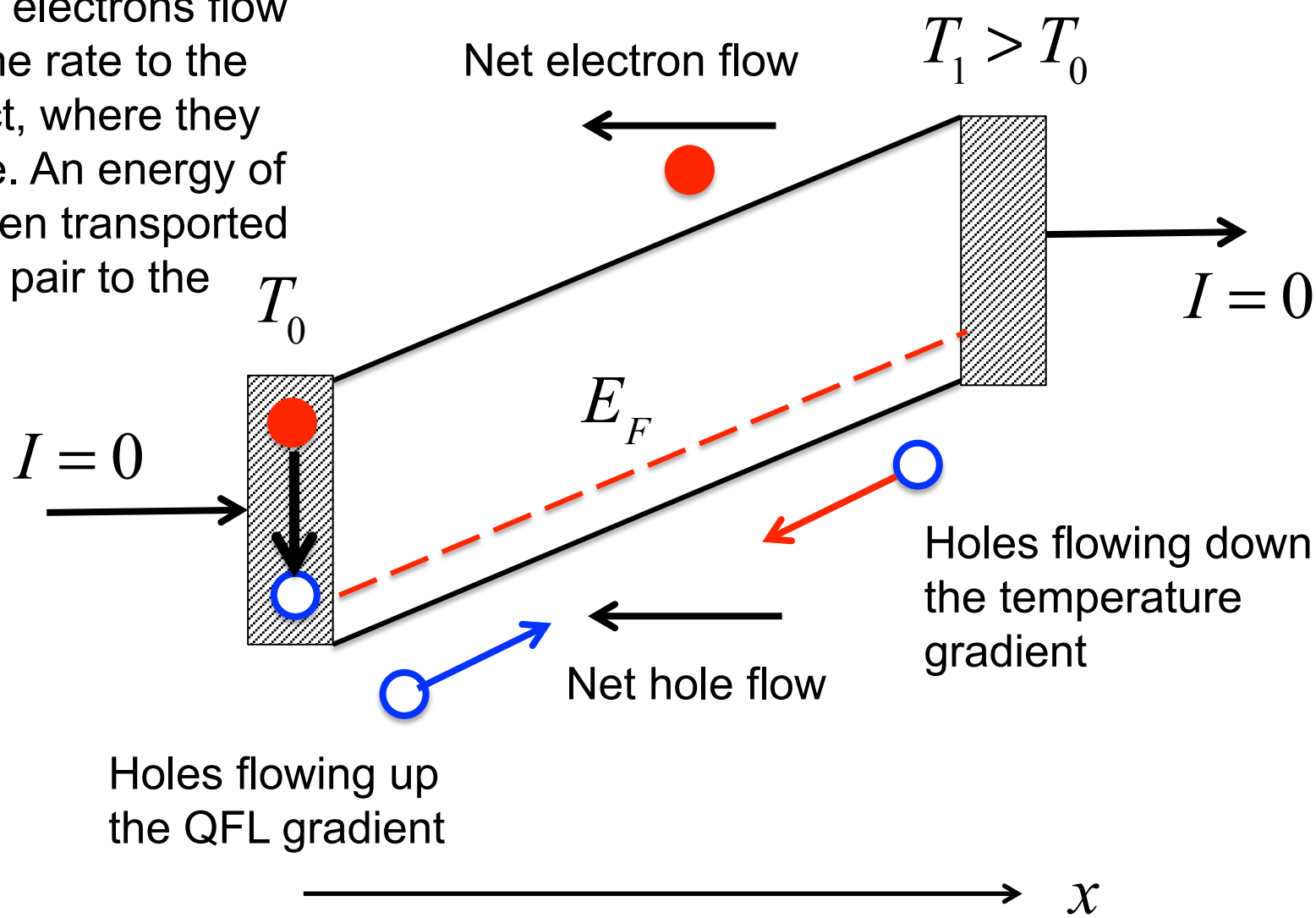
(Computation by Dr. Xufeng Wang, Purdue University, Oct. 2017.

Physics (unipolar)



Physics (bipolar)

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.



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Example: TE transport parameters of n-Ge

ρ_n Ω-m

S_n V/K

π_n $\mathrm{W/A = V}$

κ_n W/m-K

$$\mathcal{E} = \rho_n J_n + S_n \frac{dT}{dx} \quad \left(\frac{\mathrm{V}}{\mathrm{m}}\right)$$

$$J_Q = \pi_n J_n - \kappa_n \frac{dT}{dx} \quad (\mathrm{W})$$

$N_D = 10^{15}\ \mathrm{cm}^{-3}$

$T = 300\ \mathrm{K}$

$\mu_n = 3200\ \mathrm{cm}^2/\mathrm{V\text{-}s}$

$$n_0 = N_C e^{(E_F - E_c)/k_B T_L} \approx N_D$$

$$N_C = 1.04 \times 10^{19} \quad \mathrm{cm}^{-3}$$

TE transport parameters of n-Ge: resistivity

ρ_n Ω-cm

S_n V/K

π_n W/A = V

κ_n W/m-K

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

$$J_Q = \pi_n J_n - \kappa_n \frac{dT}{dx} \quad (\text{W})$$

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

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

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

$$\rho_n = 1/n_0 q \mu_n \approx 2\ \Omega\text{-cm}$$

TE transport parameters of n-Ge: Seebeck coeff.

$\rho_n = 2 \quad \Omega\text{-cm}$

$S_n \quad \text{V/K}$

$\pi_n \quad \text{W/A} = \text{V}$

$\kappa_n \quad \text{W/m-K}$

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

$$J_Q = \pi_n J_n - \kappa_n \frac{dT}{dx} \quad (\text{W})$$

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

$n_0 = N_C e^{(E_F - E_c)/k_B T}$

$N_C = 1.04 \times 10^{19} \quad \text{cm}^{-3}$

$T = 300\ \text{K}$

$$(E_c - E_F)/k_B T \approx \ln(N_C/n_0) \approx 9.3$$

$\delta_n \approx 2$ (non-degenerate, 3D)

$$S_n = \left(\frac{k_B}{-q}\right)\left\{\frac{(E_c - E_F)}{k_B T} + \delta_n\right\} \approx -970\ \mu\text{V/K}$$

TE transport parameters of n-Ge: Peltier coeff.

$\rho_n = 2 \quad \Omega\text{-cm}$

$S_n = -970 \text{ V/K}$

$\pi_n \quad \text{W/A} = \text{V}$

$\kappa_n \quad \text{W/m-K}$

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

$$J_Q = \pi_n J_n - \kappa_n \frac{dT}{dx} \quad (\text{W})$$

$$\pi_n = TS_n \approx -0.3 \text{ V}$$

TE transport parameters of n-Ge: Peltier coeff.

$\rho_n = 2 \quad \Omega\text{-cm}$

$S_n = -970 \text{ V/K}$

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

$\kappa_n \quad \text{W/m-K}$

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

$$J_Q = \pi_n J_n - \kappa_n \frac{dT}{dx} \quad (\text{W})$$

$$\frac{\kappa_n}{T\sigma_n} = L$$ (Lorenz number)

$L \approx 2\left(k_B/q\right)^2$ (non-degenerate, 3D)

$\sigma_n = 1/\rho_n$

$\kappa_n = 2.2\times10^{-4} \quad \text{W/m-K}$

TE transport parameters of n-Ge:

$$\rho_n = 2 \quad \Omega\text{-cm}$$

$$S_n = -970 \quad \text{V/K}$$

$$\pi_n = -0.3 \quad \text{W/A} = \text{V}$$

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

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

$$J_Q = \pi_n J_n - \kappa_n \frac{dT}{dx} \quad (\text{W})$$

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

Note also:

$$\kappa_L = 58 \text{ W/m-K} >> \kappa_n$$

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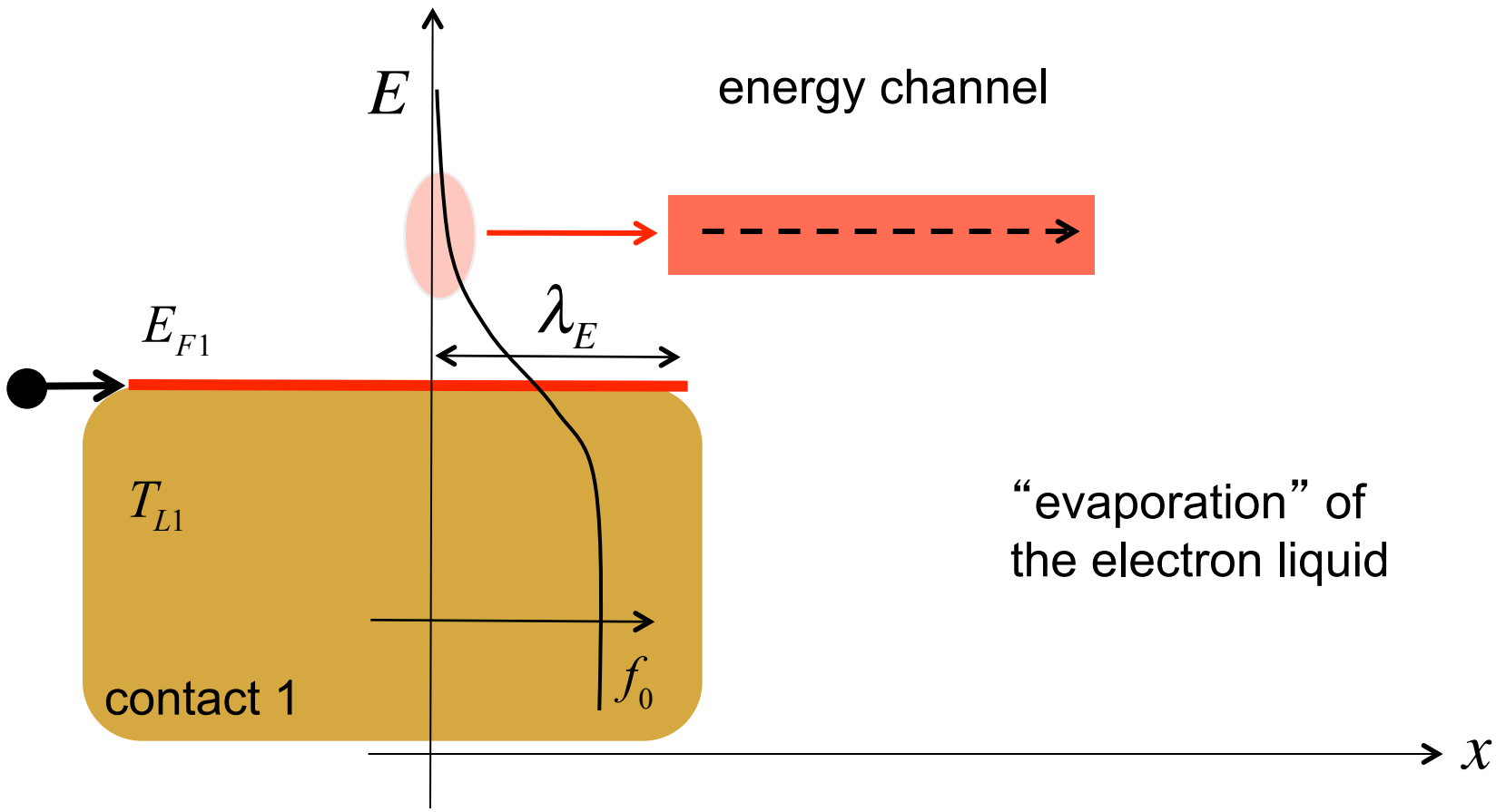
Origin of Peltier cooling



"evaporation" of
the electron liquid

Monte Carlo simulation

"It is interesting that the thermoelectric cooling and heating regions are contained in the highly doped contact layers."

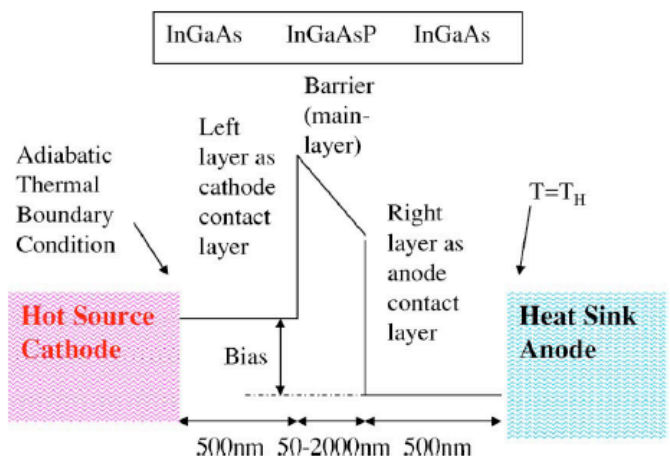


FIG. 1. (Color online) Schematic of the heterostructure.

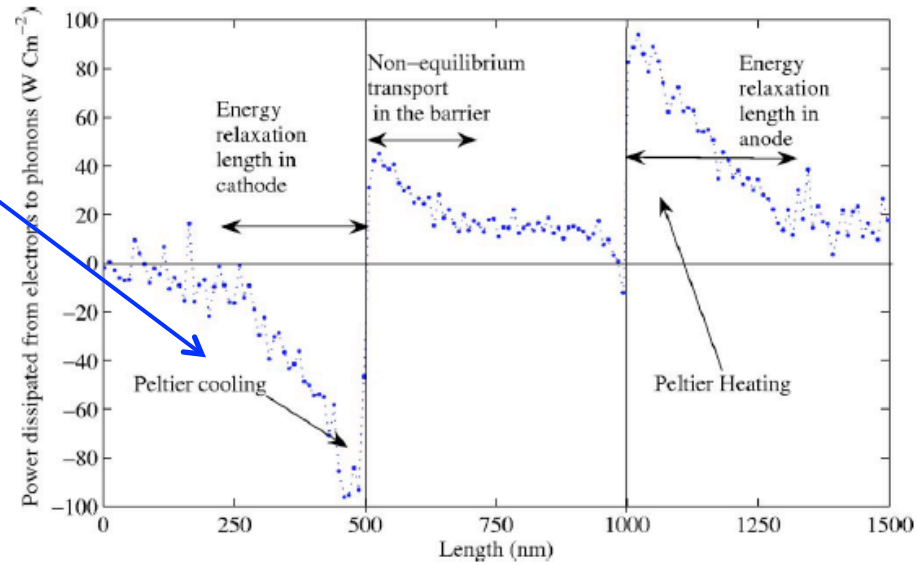


FIG. 3. (Color online) Source term (electron-phonon energy exchange) along the heterostructure obtained from MC simulation. The applied bias is 40 mV. Nonequilibrium regions at the ends of the contacts are disregarded as explained before. Peltier cooling at the cathode-barrier junction and Peltier heating at the anode-barrier junction can be observed.

Mona Zebarjadi, Ali Shakouri, and Keivan Esfarjani, "Thermoelectric transport perpendicular to thin-film heterostructures calculated using the Monte Carlo technique," *Phys. Rev. B*, **74**, 195331 (2006).

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The TE transport equations

$$J = \sigma \mathcal{E} - \sigma S \, dT/dx$$

$$J_Q = T\sigma S \mathcal{E} - \kappa_0 \, dT/dx$$

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

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

(diffusive transport)

$$\sigma = \int \sigma'(E) dE$$

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

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

$$\pi = TS$$

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

$$\kappa_e = \kappa_0 - \pi S \sigma$$

Questions?

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