NCN Summer School: July 2011

Near-equilibrium Transport:
Fundamentals and Applications

Lecture 5: Thermoelectric Effects: Mathematics

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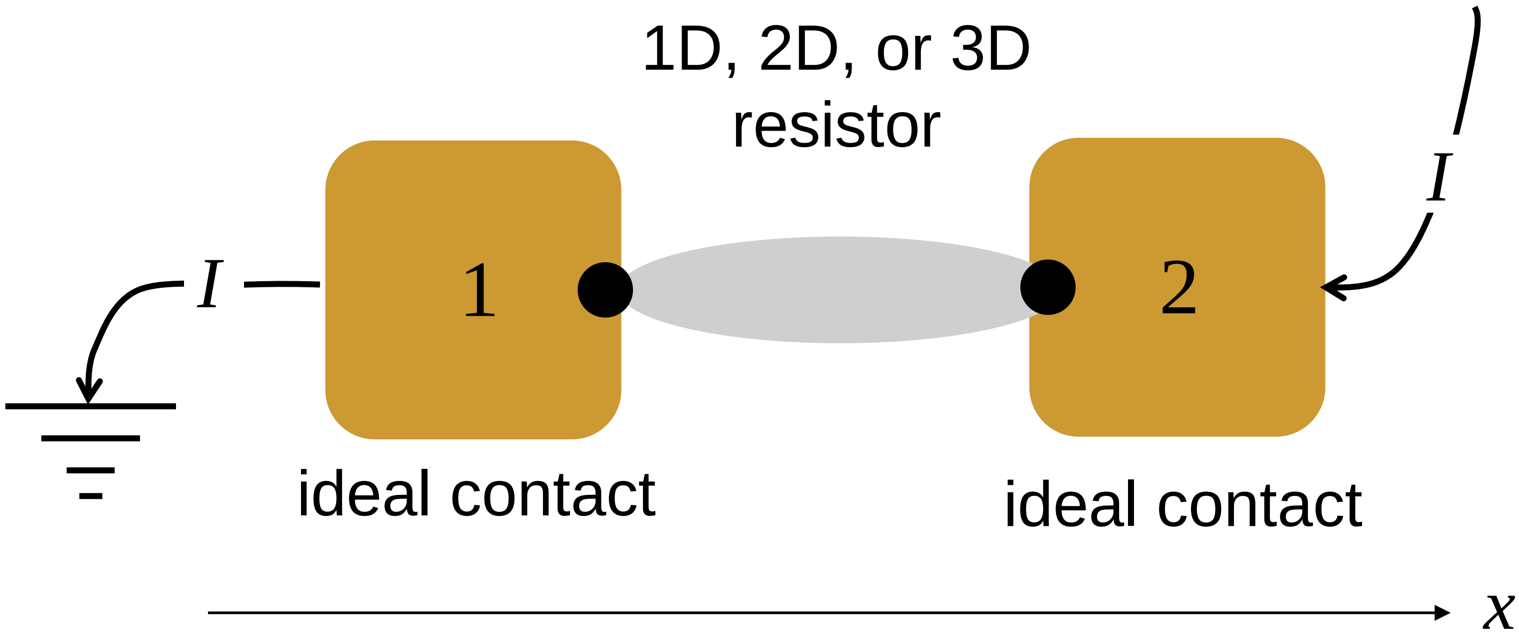
Landauer picture



Current is positive when it flows **into** contact 2 (i.e. positive current flows in the -*x* direction).

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

driving "forces" for transport

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

Differences in occupation, *f*, produce current.

$$(f_1 - f_2) \approx -\frac{\partial f_1}{\partial E}\Delta E_F$$

Assumes $T_{L1} = T_{L2}$.

but differences in temperature also produce differences in *f* and can, therefore, drive current (thermoelectric effects).

$$\Delta E_F = -q\Delta V = -q\left(V_2 - V_1\right)$$

$$\Delta T_L = T_{L2} - T_{L1}$$

review: constant temperature

$$I = GV \qquad G = \int G'(E)\,dE \qquad \left(T_{L1} = T_{L2}\right)$$

$$G'_{3D}(E) = \frac{2q^2}{h} T(E) M_{3D}(E) A\left(-\frac{\partial f_0}{\partial E}\right)$$

ballistic to diffusive

$$G'_{3D}(E) \equiv \sigma'(E)\frac{A}{L}$$

$$\sigma'(E) = \frac{2q^2}{h} M_{3D}(E)\lambda_{app}(E)\left(-\frac{\partial f_0}{\partial E}\right)$$

$$\lambda_{app}(E) = T(E)L = \frac{1}{1/\lambda + 1/L}$$

$$G_{3D} = \sigma\frac{A}{L}$$

$$\sigma = \frac{2q^2}{h}\int M_{3D}(E)\lambda_{app}(E)\left(-\frac{\partial f_0}{\partial E}\right)dE$$

questions

1) What electric current, *I*, flows when there is a difference in Fermi levels ***and*** temperature across a device?

2) What heat current, I_Q, flows for a given ΔE_F and ΔT ?

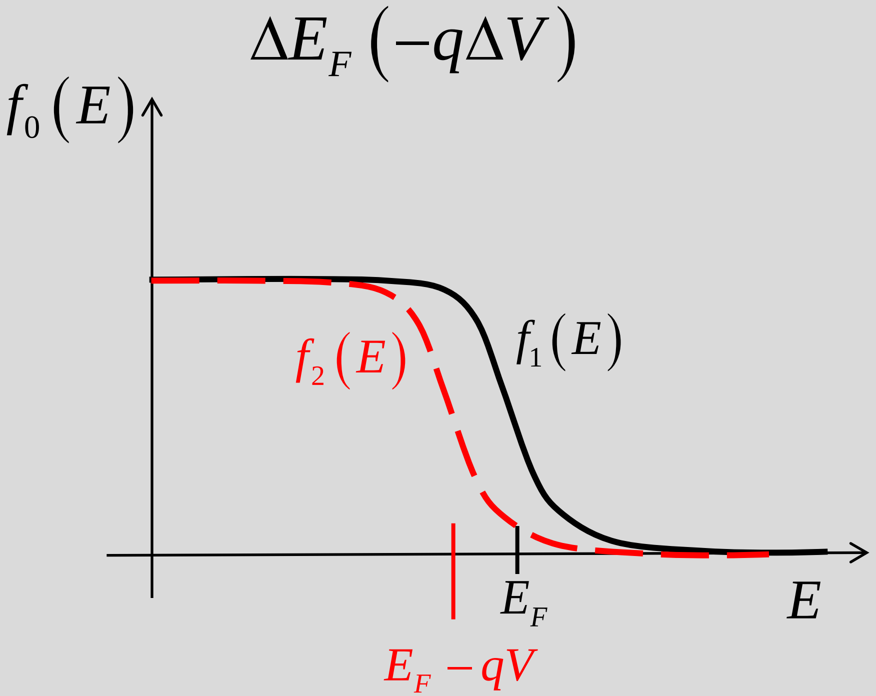
3) How are the electric and heat currents related?

4) What determines the sign and magnitude of *the* TE coefficients?

outline

1) Introduction
2) **Driving forces for current flow**
3) Charge current
4) Heat current
5) Discussion
6) Summary

when ⊗T = 0, the driving force is: ΔE_F



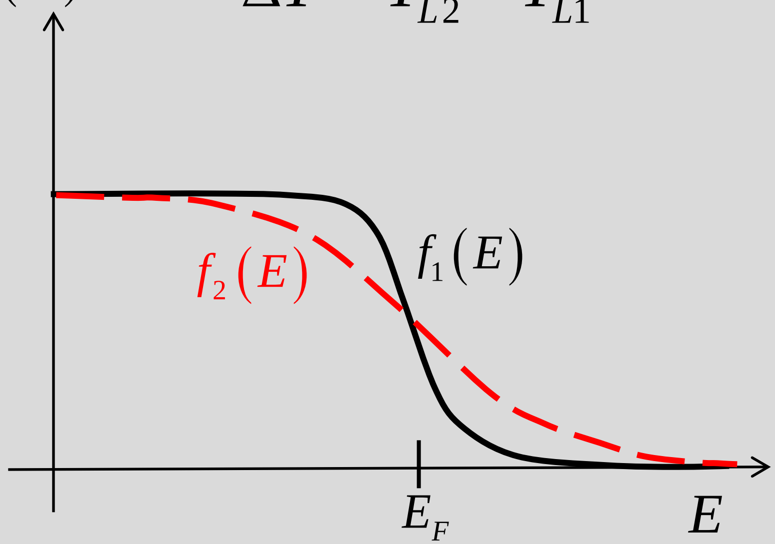
f_1 > *f_2* and current flows

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

$$\left(f_1 \approx f_2 \approx f_0\right)$$

driving force: differences in temperature

$$f_0(E) \qquad \Delta T = T_{L2} - T_{L1}$$



$|f_1 - f_2| > 0$ so current flows, but the sign depends on whether the states are located above or below E_F (n-type or p-type).

$$(f_1 - f_2) \approx f_1 - \left(f_1 + \frac{\partial f_1}{\partial T_L}\Delta T\right)$$

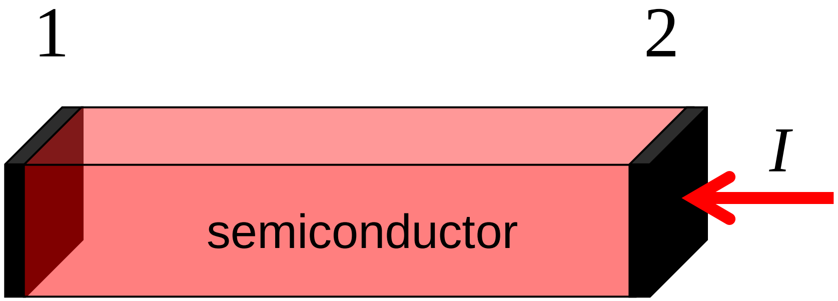
$$= -\frac{\partial f_1}{\partial T_L}\Delta T$$

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

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

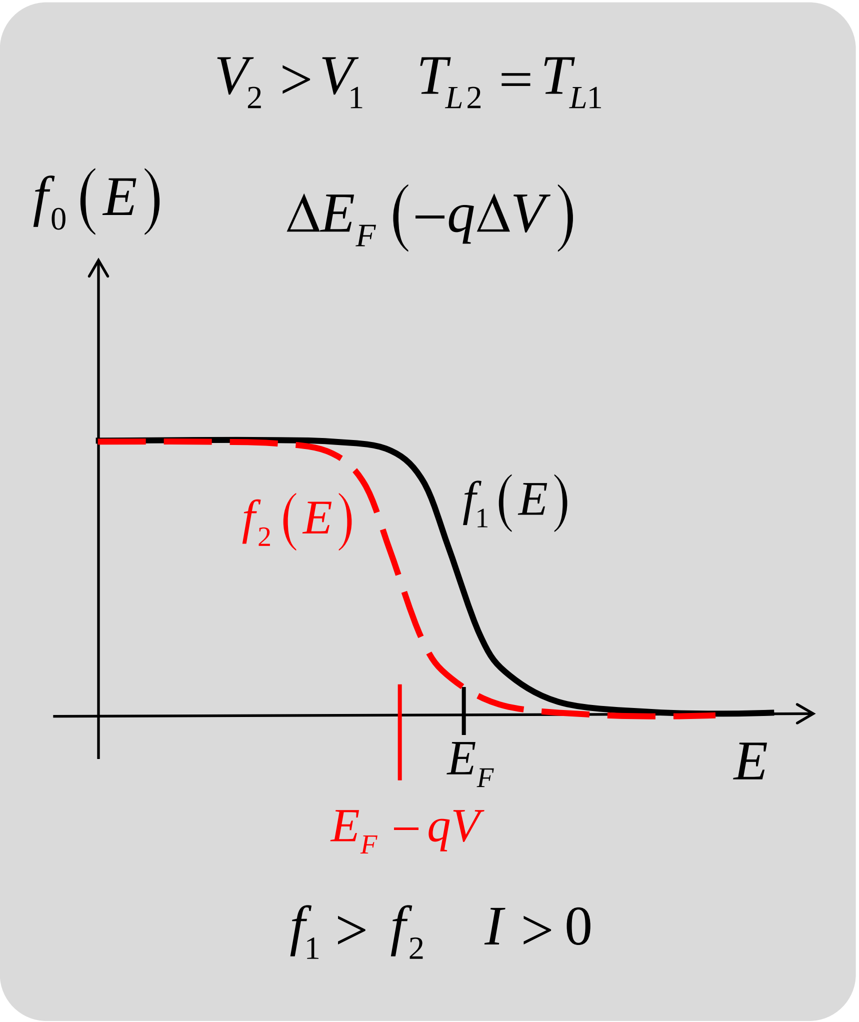
$$(f_1 \approx f_2 \approx f_0)$$

n-type vs. p-type…

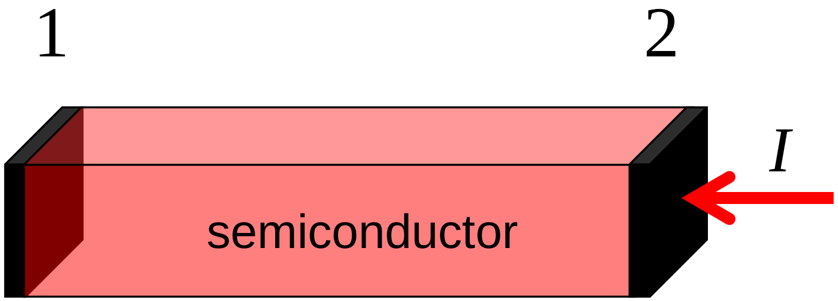


$$I = \frac{2q^2}{h}\int T(E)M(E)(f_1 - f_2)\,dE$$

The same answer for both n-type and p-type semiconductors!



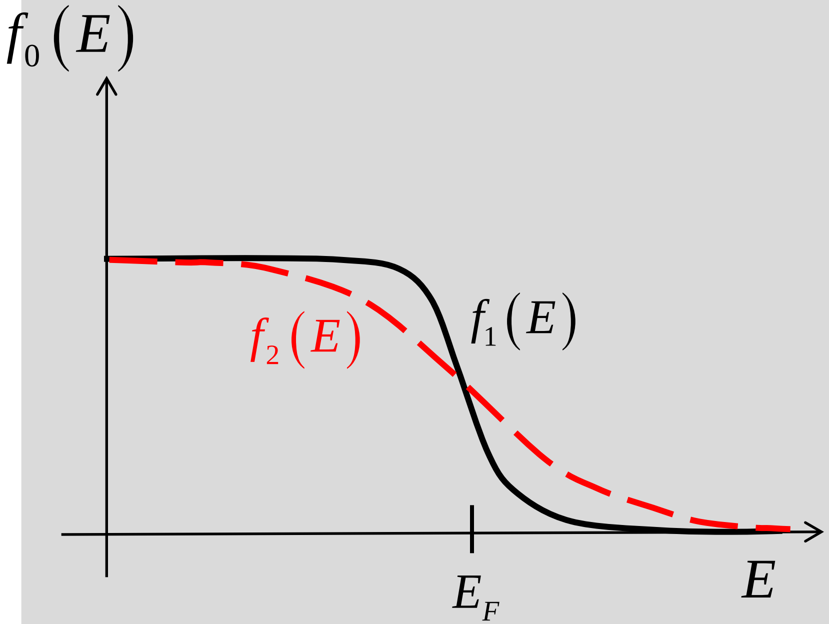
n-type vs. p-type (ii)…



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

n-type: I < 0
p-type: I > 0

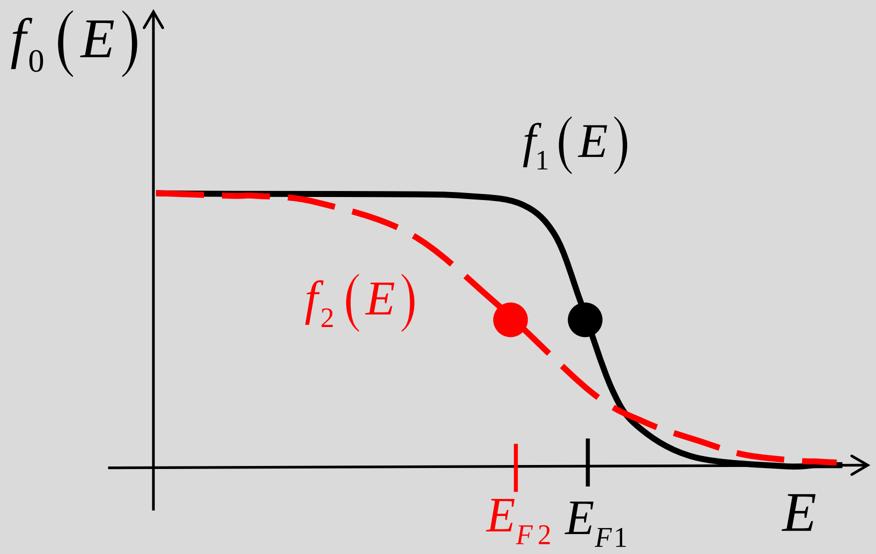
$V_2 = V_1 \quad T_{L2} > T_{L1}$



n-type: $E > E_F: \quad f_2 > f_1$

p-type: $E < E_F: \quad f_1 > f_2$

finally: differences in **both** E_F **and** T



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

outline

1) Introduction
2) Driving forces for current flow
3) **Charge current**
4) Heat Current
5) Discussion
6) Summary

the math…

$$I'(E)=\frac{2q}{h}T(E)M(E)(f_1-f_2) \qquad I=\int I'(E)\,dE$$

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

$$I'(E)=G'(E)\Delta V+S_T'(E)\Delta T$$

S_T is related to the “Soret coefficient” for electro-thermal diffusion

the math…

$$I'(E) = G'(E)\Delta V + S_T'(E)\Delta T$$

$$S_T'(E) = -\frac{2q}{h} T(E) M(E) \left(-\frac{\partial f_0}{\partial E}\right) \frac{(E - E_F)}{T_L}$$

$$S_T'(E) = -G'(E) \frac{(E - E_F)}{qT_L}$$

$$S_T = \int S_T'(E)\, dE = -\int \frac{(E - E_F)}{qT_L} G'(E)\, dE$$

S_T is negative for n-type and positive for p-type.

re-cap

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

$$G = \frac{2q^2}{h}\int T(E)M(E)\left(-\frac{\partial f_0}{\partial E}\right)dE = \frac{2q^2}{h}\int G'(E)dE$$

$$S_T = -\int \frac{(E - E_F)}{qT_L} G'(E)dE$$

Valid near equilibrium for 1D, 2D, or 3D and from ballistic to diffusive transport.

exercise

Develop a diffusive transport equation that describes bulk transport in the presence of gradients in the electrochemical potential ***and*** temperature.

$$J_{nx} = \sigma_n \frac{dF_n/q}{dx} \rightarrow ?$$

$$J_{nx} = \sigma_n \frac{dF_n/q}{dx} - s_T \frac{dT_L}{dx}$$

$$I = -I_x = G\Delta V + S_T \Delta T$$

$$I_x = J_{nx} A = -G\Delta V - S_T \Delta T$$

$$J_{nx} = -\frac{G}{A}\Delta V - \frac{S_T}{A}\Delta T$$

$$J_{nx} = -G\frac{L}{A}\frac{\Delta V}{L} - S_T \frac{L}{A}\frac{\Delta T}{L}$$

$$G = \sigma_n A/L \qquad \Delta V = -\Delta F_n/q$$

$$S_T = s_T A/L$$

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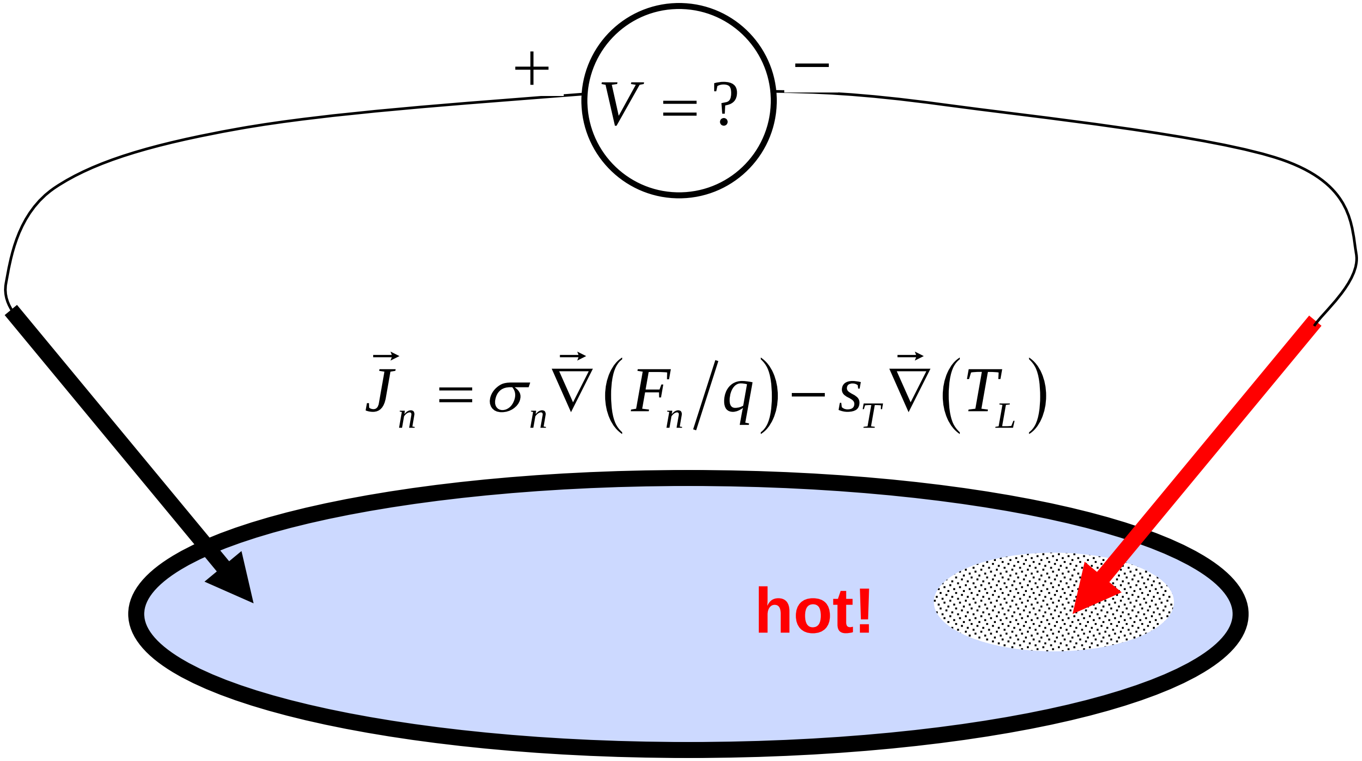
hot point probe



$$\vec{J}_n = \sigma_n \vec{\nabla}\left(F_n/q\right) - s_T \vec{\nabla}\left(T_L\right)$$

doped silicon wafer

outline

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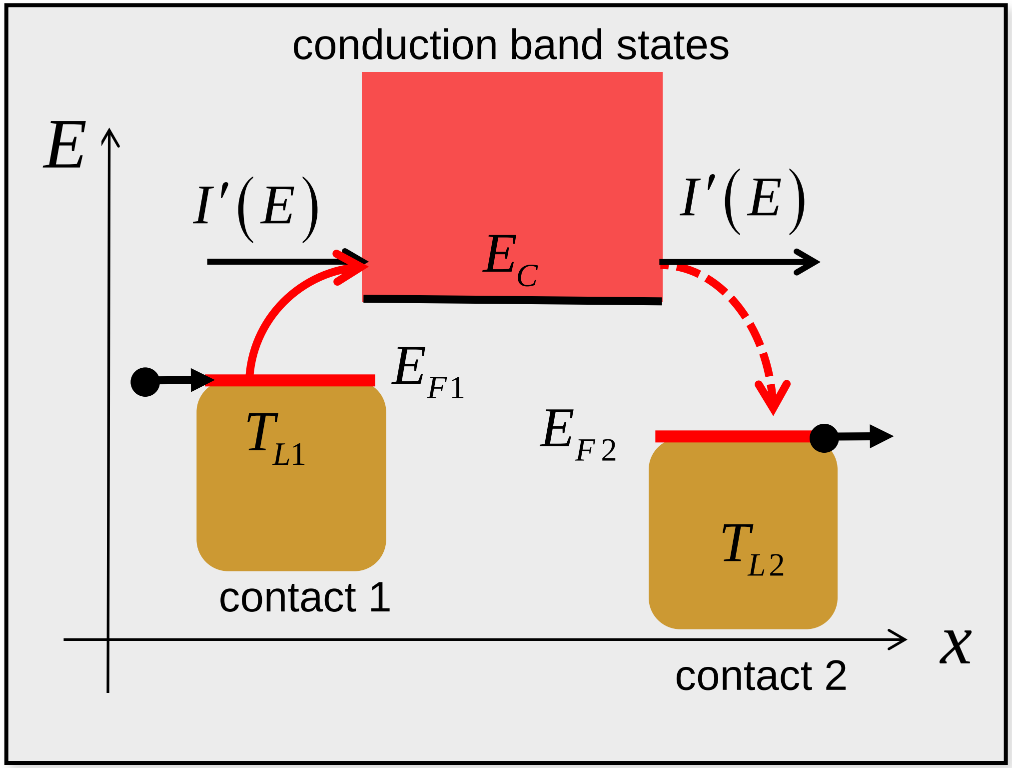
electric current



Electrons carry **charge**, so there is an electrical current.

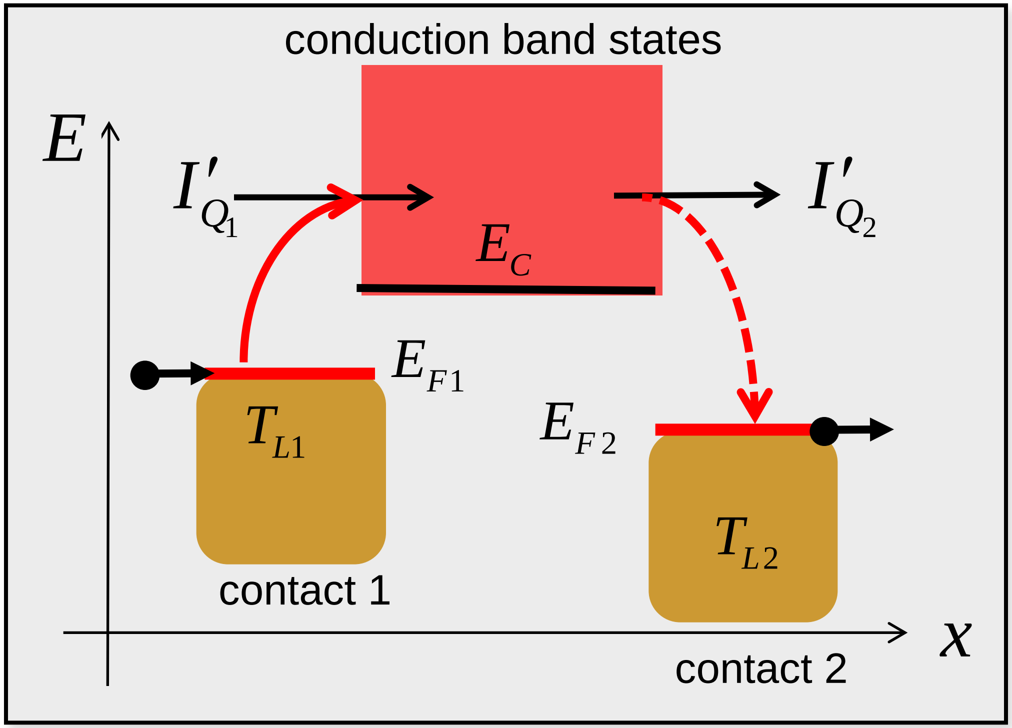
$$I'(E) = \frac{2q}{h} T(E) M(E) (f_1 - f_2)$$

But electrons also carry **heat** (thermal energy), so there is a heat current too.

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

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



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

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

the math

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

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

$$I'_Q(E) = -T_L S_T(E) \Delta V - K_0(E) \Delta T$$

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

the result

$$I'_Q(E) = -T_L S_T(E)\Delta V - K_0(E)\Delta T$$

(First minus sign because positive electric current is in the negative x-direction but positive heat current is in the positive x-direction.)

$$K'_0(E) = \frac{(E-E_F)^2}{q^2 T_L} G'(E)$$

$$I_Q = \int I'_Q(E)\,dE = -T_L S_T \Delta V - K_0 \Delta T$$

$$K_0 = \int \frac{(E-E_F)^2}{q^2 T_L} G'(E)\,dE$$

K_0 is the short circuit thermal conductance.

outline

1) Introduction
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re-cap

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

$$I_Q = -T_L S_T \Delta V - K_0 \Delta T$$

Coupled current equations: temperature differences cause electric current to flow and voltage differences cause heat current to flow.

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

$$S_T = -\int \frac{(E-E_F)}{qT_L} G'(E)\,dE$$

$$K_0 = \int \frac{(E-E_F)^2}{q^2 T_L} G'(E)\,dE$$

(Thermal conductivity only refer to electrons - not lattice.)

exercise

Derive the corresponding **coupled current** equations for 3D, diffusive transport.

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

$$I_Q = -T_L S_T \Delta V - K_0 \Delta T$$

$$J_{nx} = \sigma \frac{d\left(F_n/q\right)}{dx} - s_T \frac{dT_L}{dx}$$

$$J_{Qx} = T_L s_T \frac{d\left(F_n/q\right)}{dx} - \kappa_0 \frac{dT_L}{dx}$$

inverting the equations

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

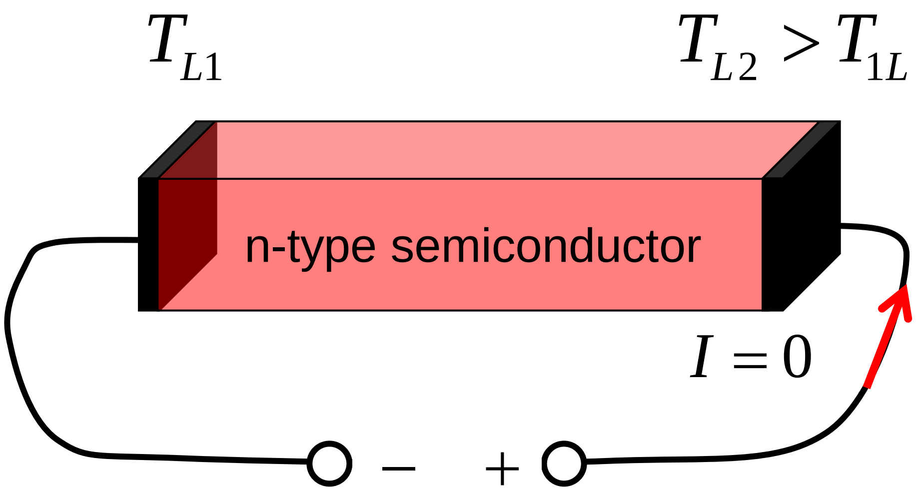
$$I_Q = -T_L S_T \Delta V - K_0 \Delta T$$

$$\Delta V = \frac{1}{G} I - \frac{S_T}{G} \Delta T$$

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

$$S = \frac{S_T}{G}$$ (Seebeck coefficient)

Seebeck coefficient



$$\Delta V = ?$$

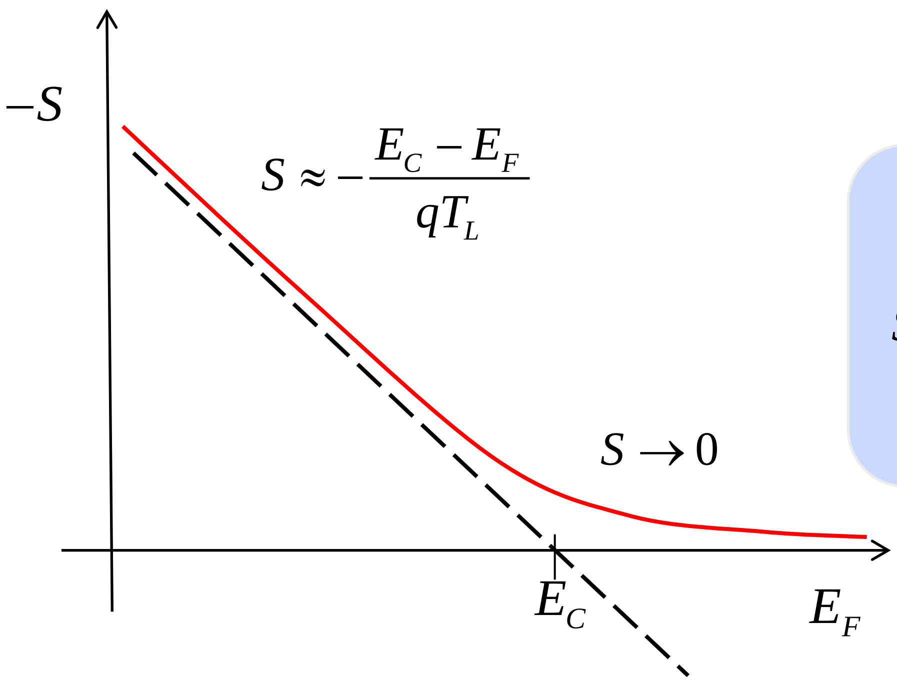
$$\Delta V = RI - S\Delta T$$

$$S = \frac{S_T}{G}$$

$$S = \frac{-\int \frac{(E - E_F)}{qT_L} G'(E)\, dE}{\int G'(E)\, dE}$$

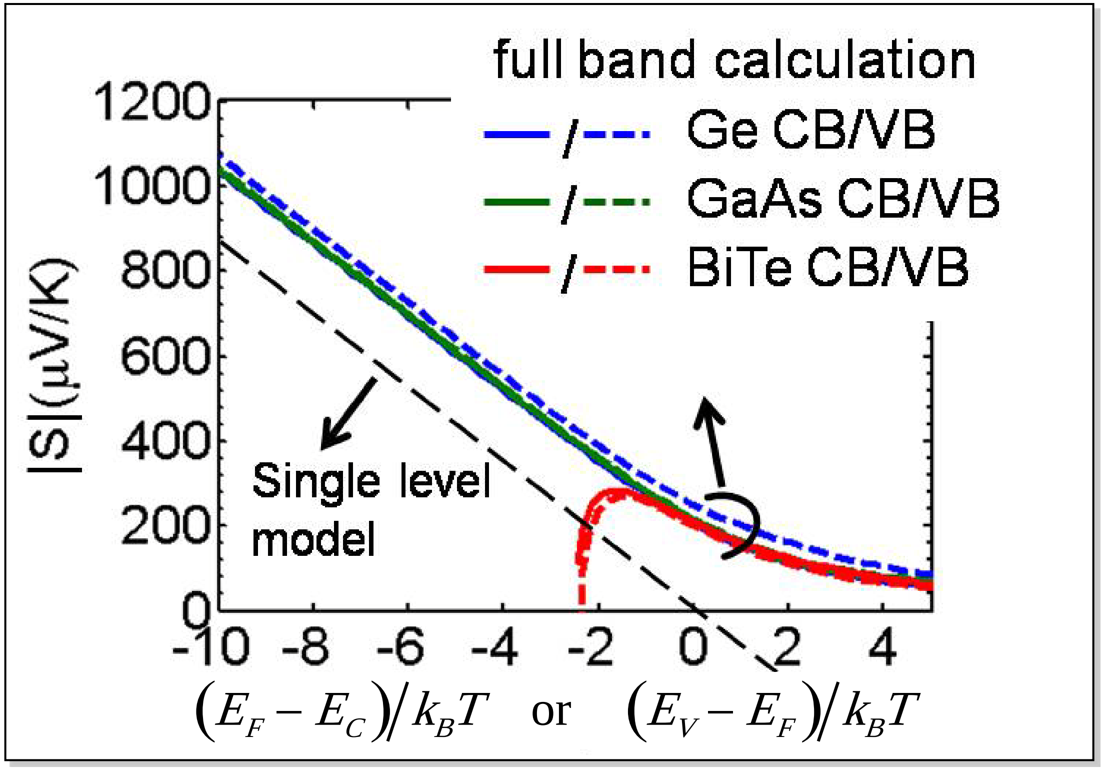
$S < 0$ for *n*-type
$S > 0$ for *p*-type

Seebeck coefficient of bulk semiconductors



$$S = \frac{-\int \frac{(E - E_F)}{qT_L} G'(E)\, dE}{\int G'(E)\, dE} = -\frac{E_J - E_F}{qT_L}$$

“full band” Seebeck coefficient



Changwook Jeong, et al., “On Landauer vs. Boltzmann and Full Band vs. Effective Mass Evaluation of Thermoelectric Transport Coefficients,” *J. Appl. Phys*., **107**, 023707, 2010.

inverting the equations (ii)

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

$$I_Q = -T_L S_T \Delta V - K_0 \Delta T$$

$$\Delta V = RI - S\Delta T \qquad S = \frac{S_T}{G}$$

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

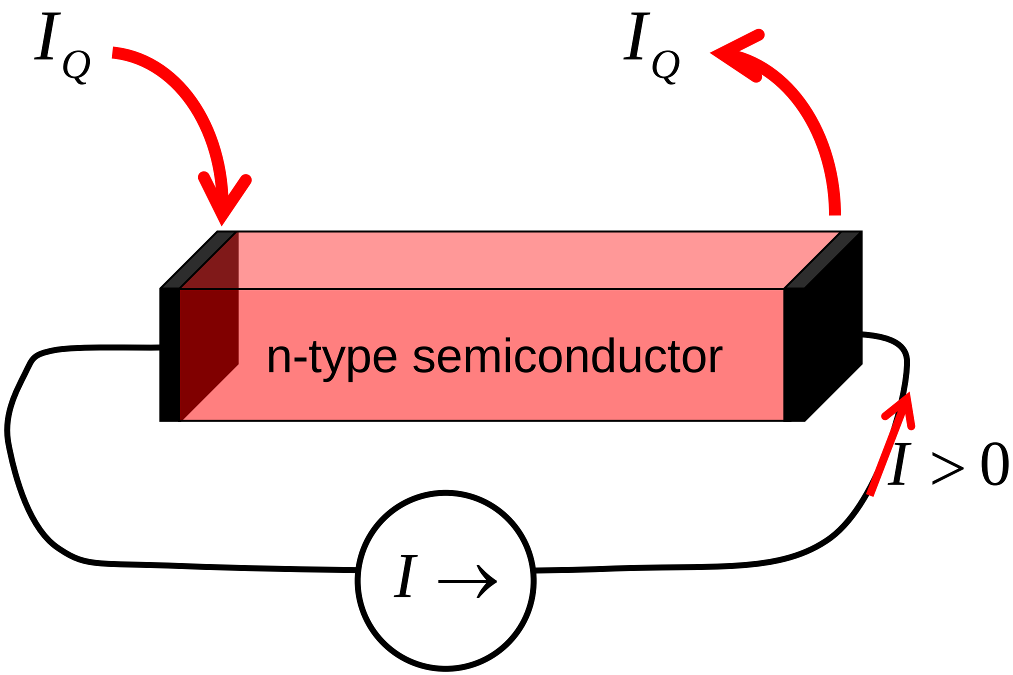
$$\pi = T_L S$$ (Peltier coefficient)

(Kelvin relation)

$$K_e = K_0 - \pi S G$$

(open-circuit thermal conductance)

Peltier coefficient



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

$$\pi = T_L S$$

$\pi < 0$ for *n*-type
$\pi > 0$ for *p*-type

summary

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

$$I_Q = -T_L S_T \Delta V - K_0 \Delta T$$

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

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

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

$$S_T = -\int \frac{(E-E_F)}{qT_L} G'(E)\,dE$$

$$K_0 = \int \frac{(E-E_F)^2}{q^2 T_L} G'(E)\,dE$$

$$S = \frac{S_T}{G}$$

$$K_e = K_0 - \pi S G$$

for bulk 3D semiconductors

$$J_x = \sigma \mathcal{E}_x - s_T \, dT_L/dx$$

$$J_x^q = T_L S_T \mathcal{E}_x - \kappa_0 \, dT_L/dx$$

$$\mathcal{E}_x = \rho J_x + S \frac{dT_L}{dx}$$

$$J_x^q = \pi J_x - \kappa_e \frac{dT}{dx}$$

(diffusive transport)

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

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

$$s_T = -\int \frac{(E - E_F)}{qT_L} \sigma'(E)\, dE$$

$$\kappa_0 = \int \frac{(E - E_F)^2}{q^2 T_L} \sigma'(E)\, dE$$

$$S = S_T/\sigma \qquad \pi = T_L S$$

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

transport parameters

$$S = -\frac{1}{qT_L}\frac{\int (E - E_F)\sigma'(E)\,dE}{\int \sigma'(E)\,dE} = \frac{1}{qT_L}\langle (E - E_F)\rangle = -\frac{(E_J - E_F)}{qT_L}$$

S is proportional to the average energy above the Fermi level at which current flows.

$$\pi = T_L S$$

Kelvin relation

$$\kappa_0 = \int \frac{(E - E_F)^2}{q^2 T_L}\sigma'(E)\,dE = \frac{\int \frac{(E - E_F)^2}{q^2 T_L}\sigma'(E)\,dE}{\int \sigma'(E)\,dE}\sigma = \left\langle \frac{(E - E_F)^2}{q^2 T_L} \right\rangle \sigma$$

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

Wiedemann-Franz “Law”

$$\frac{\kappa_0}{\sigma} = \left(\frac{k_B}{q}\right)^2 \left\langle \left(\frac{E - E_F}{k_B T_L}\right)^2 \right\rangle T_L = L' T_L$$

“Wiedeman Franz Law”

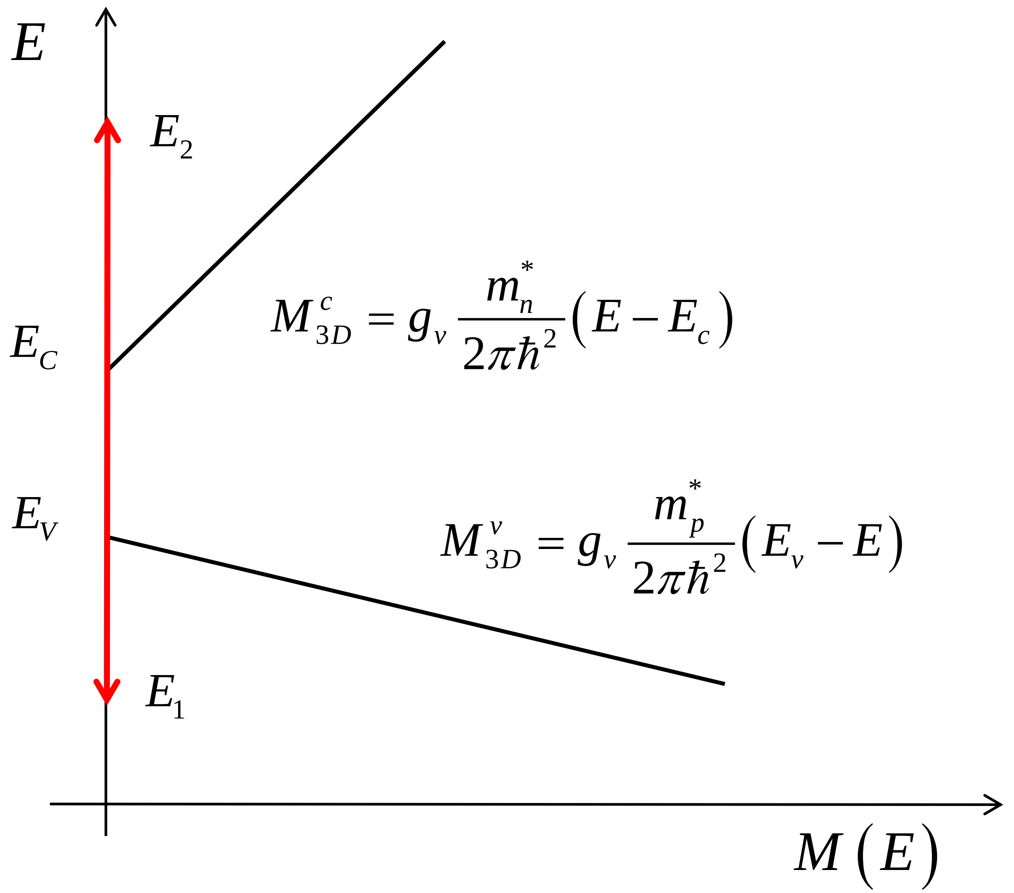
$$\frac{\kappa_e}{\sigma} = \left(\frac{k_B}{q}\right)^2 \left\{ \left\langle \left(\frac{E - E_F}{k_B T_L}\right)^2 \right\rangle - \left\langle \left(\frac{E - E_F}{k_B T_L}\right) \right\rangle^2 \right\} T_L = L T_L$$

Wiedeman Franz Law

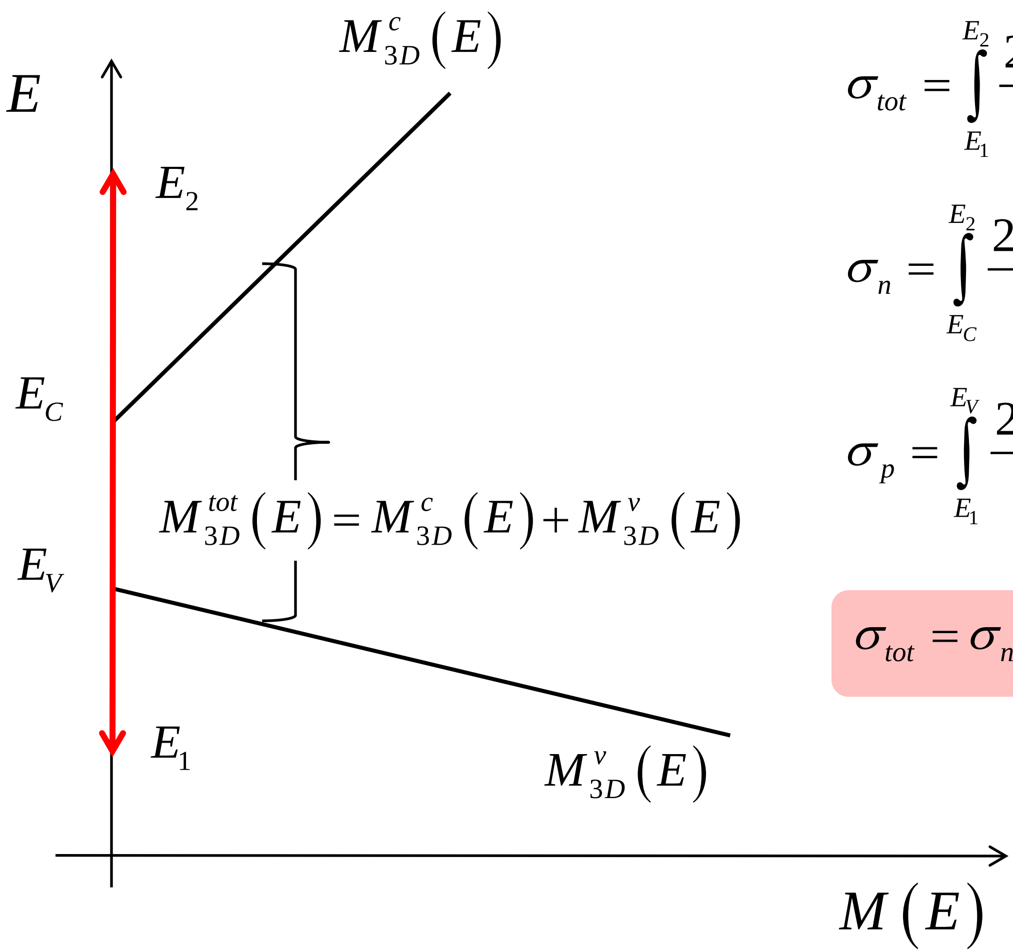
For parabolic bands and degenerate conditions: $\frac{\kappa_e}{\sigma} = \left(\frac{k_B}{q}\right)^2 \frac{\pi^2}{3} T_L$

For parabolic bands and non-degenerate conditions: $\frac{\kappa_e}{\sigma} = \left(\frac{k_B}{q}\right)^2 2 T_L$

what about the valence band?



treating both bands: conductivity



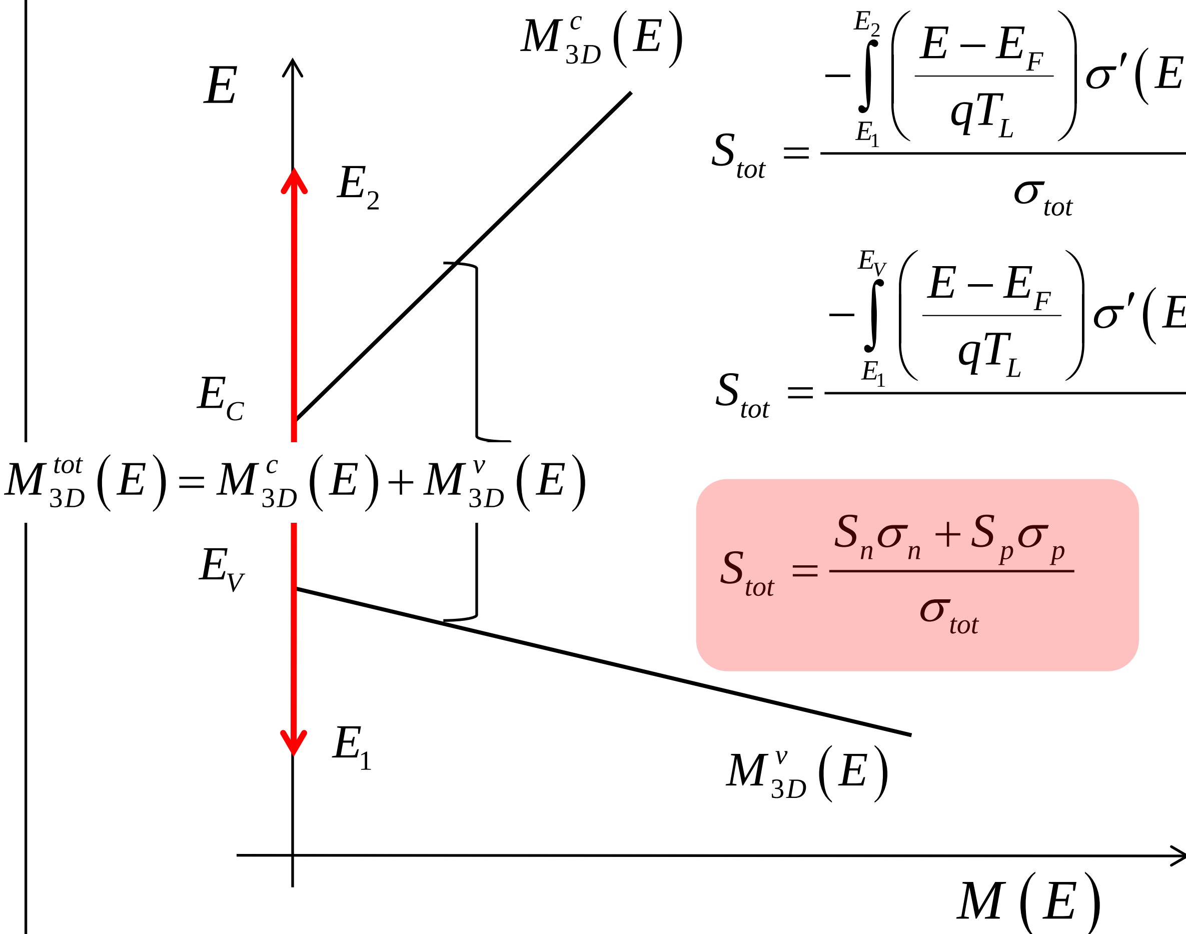
$$\sigma_{tot} = \int_{E_1}^{E_2} \frac{2q^2}{h} M_{3D}^{tot}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right) dE$$

$$\sigma_n = \int_{E_C}^{E_2} \frac{2q^2}{h} M_{3D}^{c}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right) dE$$

$$\sigma_p = \int_{E_1}^{E_V} \frac{2q^2}{h} M_{3D}^{v}(E)\lambda(E)\left(-\frac{\partial f_0}{\partial E}\right) dE$$

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

treating both bands: *S*



$$S_{tot} = \frac{-\int_{E_1}^{E_2} \left(\frac{E - E_F}{qT_L} \right) \sigma'(E)\, dE}{\sigma_{tot}}$$

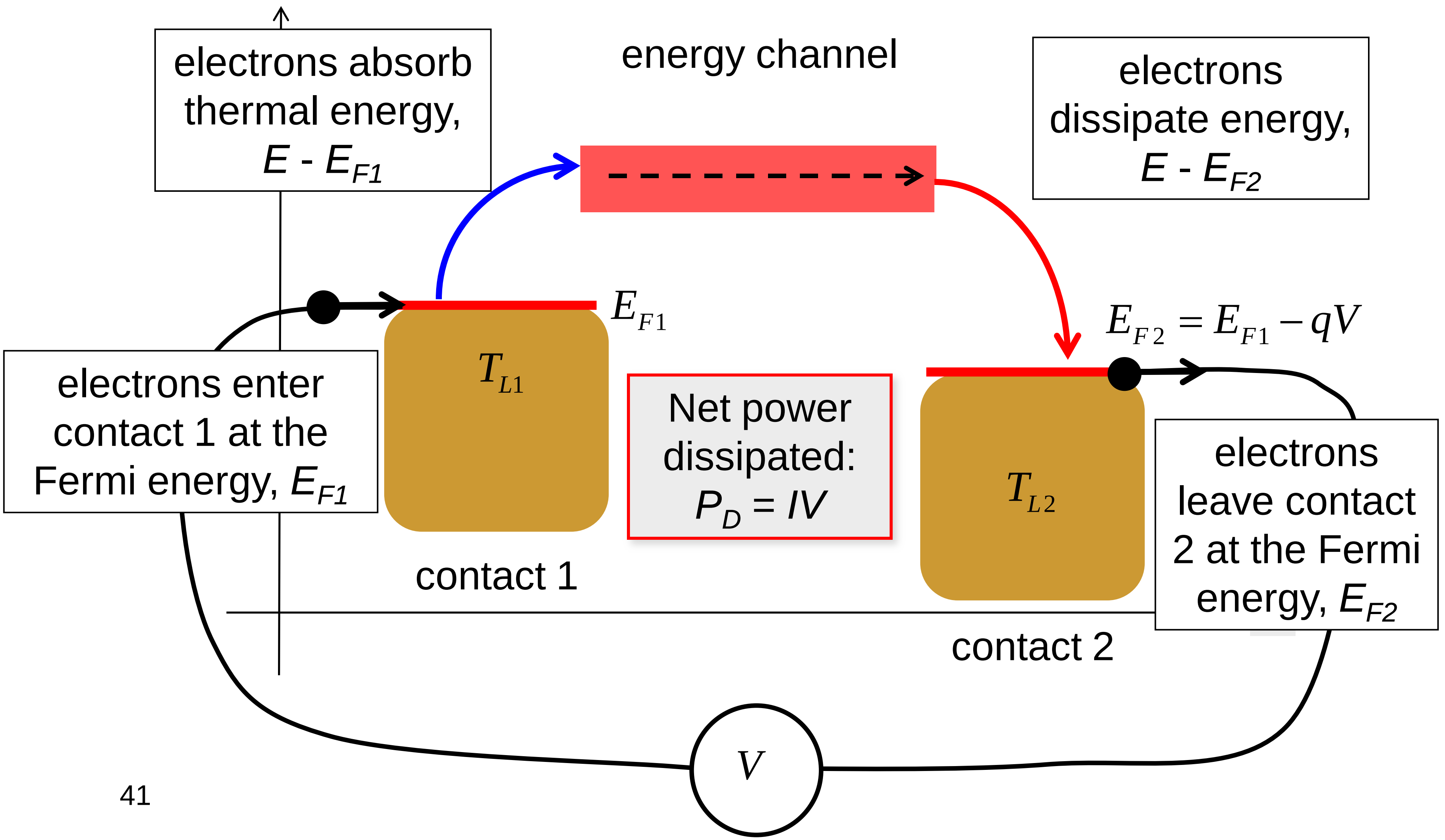
$$S_{tot} = \frac{-\int_{E_1}^{E_V} \left(\frac{E - E_F}{qT_L} \right) \sigma'(E)\, dE - \int_{E_C}^{E_2} \left(\frac{E - E_F}{qT_L} \right) \sigma'(E)\, dE}{\sigma_{tot}}$$

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

outline

1) Introduction
2) Driving forces for current
3) Charge current
4) Heat current
5) Discussion
6) **Summary**

physics of Peltier cooling



summary

1) The two “driving forces” for current flow are gradients in the electrochemical potential (quasi-Fermi level) and temperature.

2) Beginning with our general model for current flow, it is straight-forward to derive expression for the near-equilibrium charge and heat currents and for the parameters, G, S, S_T, and K_0. These expressions are valid in 1D, 2D, and 3D and from the ballistic to diffusive limits.

3) For diffusive transport, we recover the traditional expressions for the thermoelectric parameters, σ, S, π, κ_e

questions

1) Review
2) Driving forces for current flow
3) Charge current
4) Heat current
5) Discussion
6) Summary