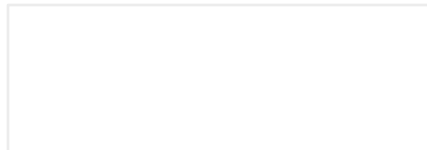


# ECE-656: Fall 2009

## Lecture 11: Discussion

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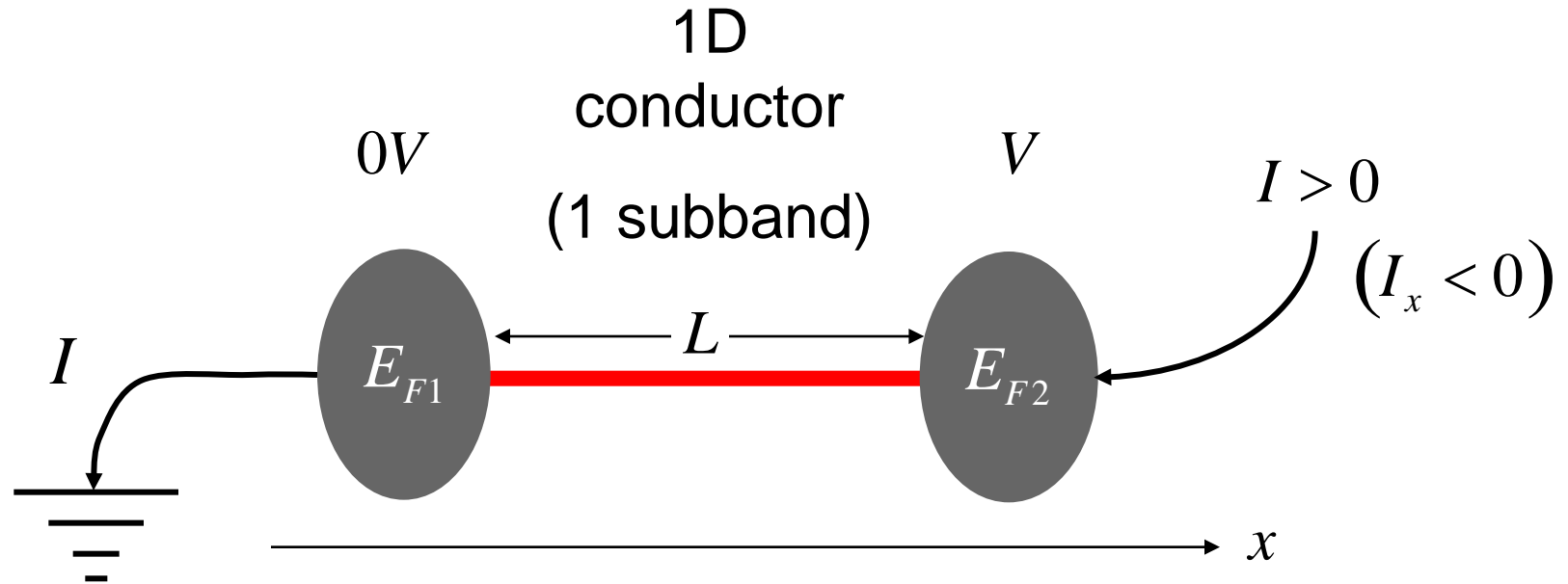


# outline

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- 1) P-type conductors and thermoelectrics
- 2) ZT figure of merit
- 3) Maximizing the “power factor”
- 4) TE parameters for non-degenerate semiconductor

# Lecture 5: 1D conductor



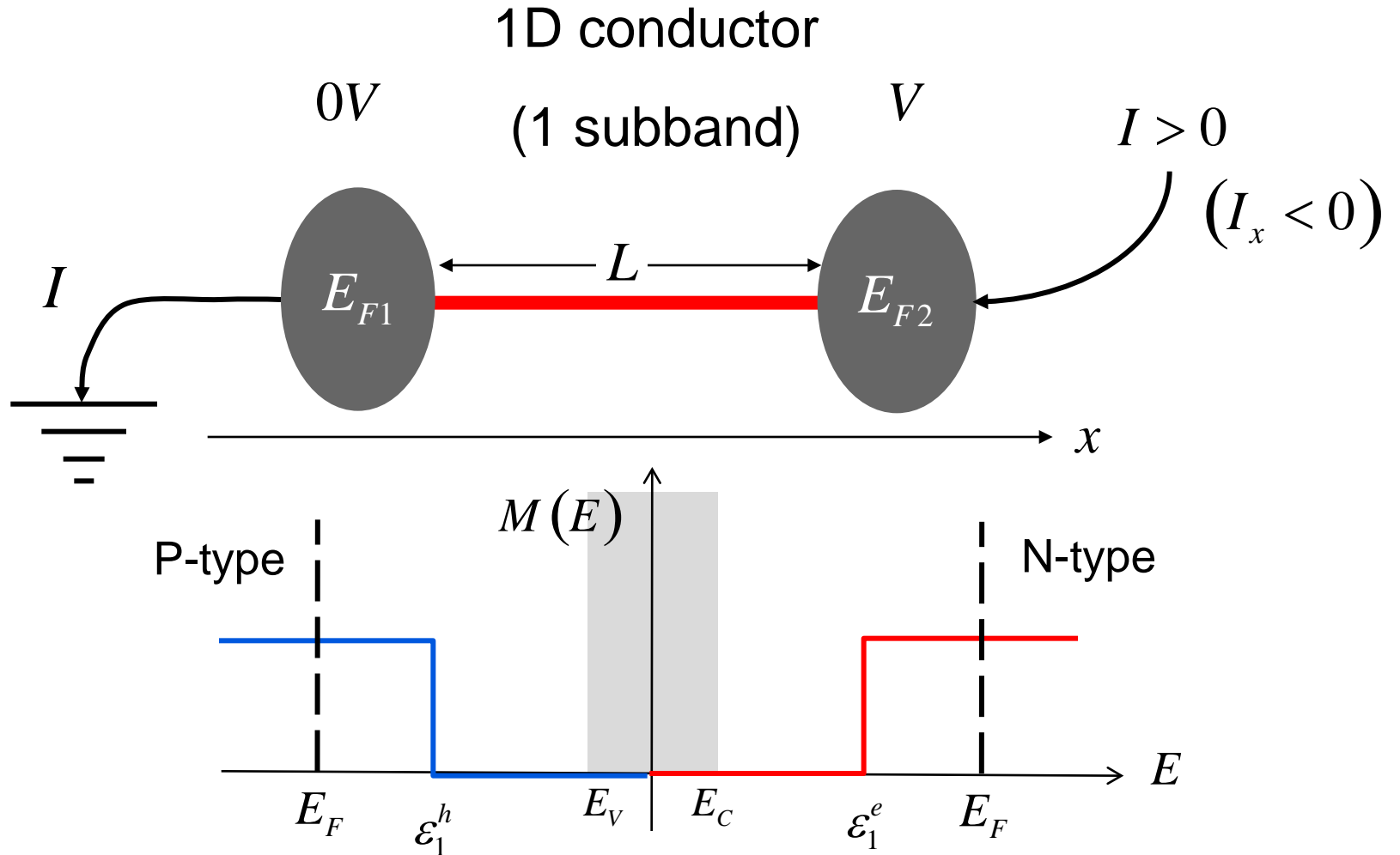
$$G = \frac{2q^2}{h} \int_{-\infty}^{+\infty} T(E) M(E) \left( -\frac{\partial f_0}{\partial E} \right) dE$$

$$T(E) \approx \frac{\lambda_0}{L} \quad (\text{diffusive})$$

Does this apply to an n- or p-type conductor?

**Answer: both**

# modes



case i): n-type,  $T = 0\text{K}$

$$G_{1D} = \frac{2q^2}{h} \int_{\varepsilon_1}^{+\infty} T(E) \left( -\frac{\partial f_0}{\partial E} \right) dE$$

$$G_{1D} = \frac{2q^2}{h} \frac{\lambda(E_F)}{L}$$

$$G = n_L q \mu_n \frac{1}{L}$$

$$\mu_n = \frac{q \tau(E_F)}{m_n^*}$$

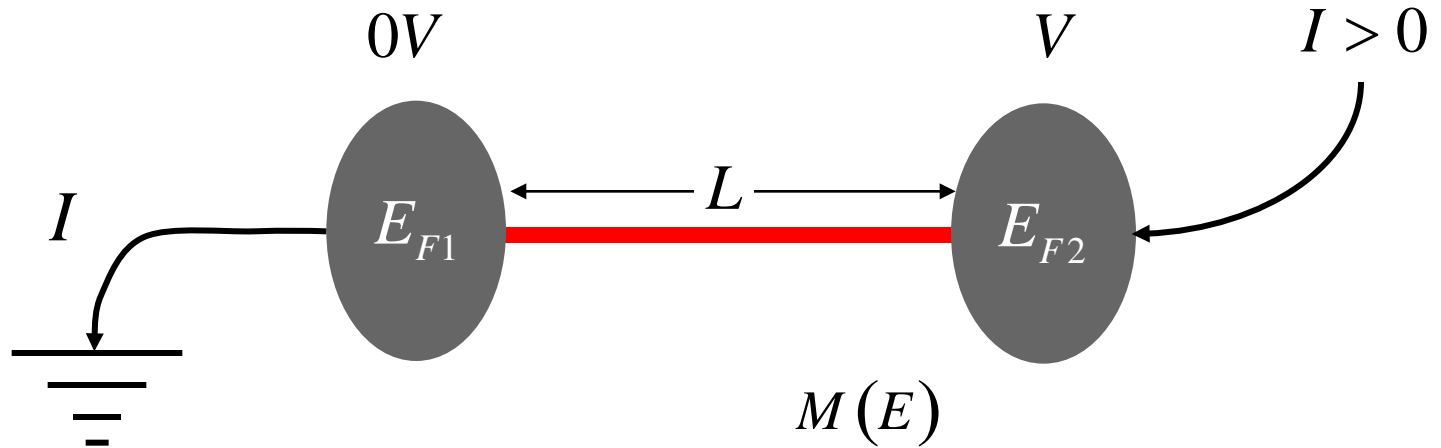
$$N = \frac{2k_F}{2\pi/L} \times 2$$

$$n_L = \frac{2k_F}{\pi} = \frac{2\sqrt{2m_n^*(E_F - \varepsilon_1)}}{\pi\hbar}$$

$$\lambda(E_F) = 2v(E_F)\tau(E_F)$$

$$v(E_F) = \sqrt{\frac{2(E_F - \varepsilon_1)}{m_n^*}}$$

# case i): result

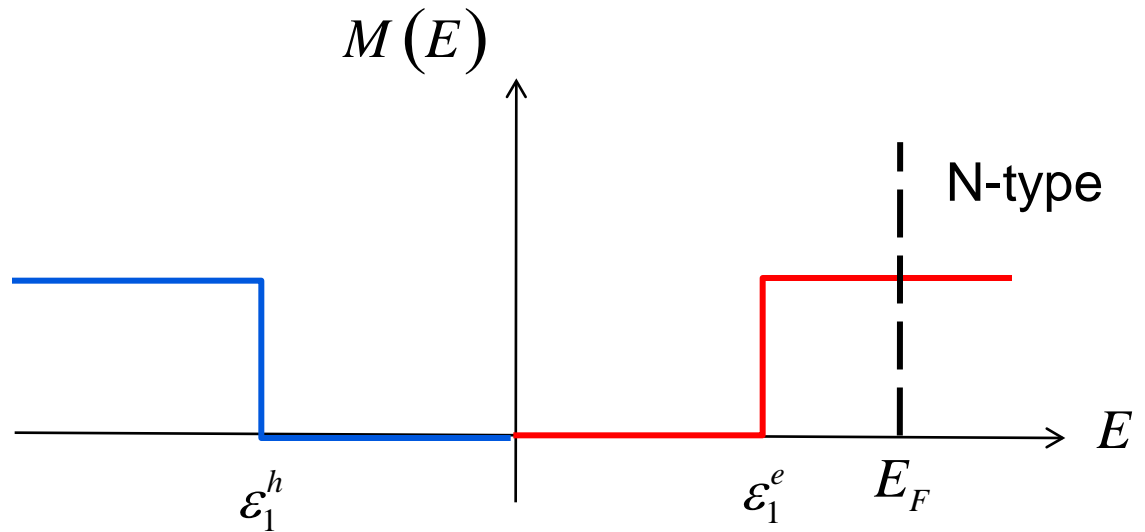


$$G_{1D} = \frac{2q^2}{h} \lambda(E_F) / L$$

$$G = n_L q \mu_n / L$$

$$\mu_n = q \tau(E_F) / m_n^*$$

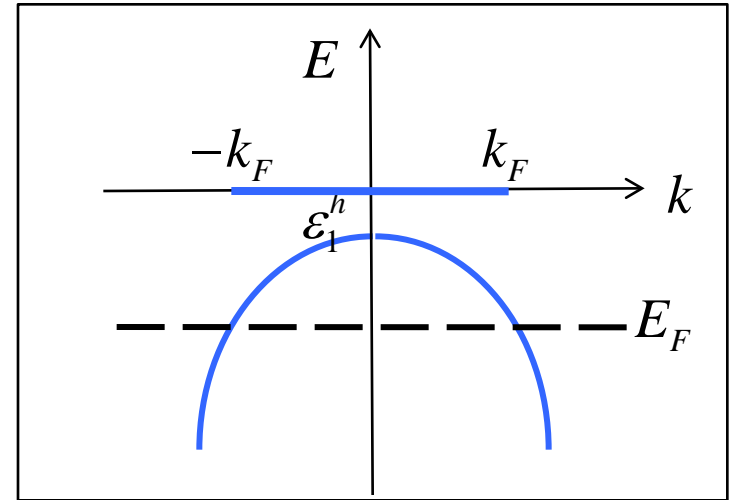
$$V > 0 \Rightarrow I > 0$$



case ii): p-type,  $T = 0\text{K}$

$$G_{1D} = \frac{2q^2}{h} \int_{-\infty}^{\varepsilon_1^h} T(E) \left( -\frac{\partial f_0}{\partial E} \right) dE$$

$$G_{1D} = \frac{2q^2}{h} \frac{\lambda(E_F)}{L}$$



$$P = \frac{2k_F}{2\pi/L} \times 2$$

$$\frac{p_L}{\square} = \frac{2k_F}{\pi} = \frac{2\sqrt{2m^*(\varepsilon_1^h - E_F)}}{\pi\hbar}$$

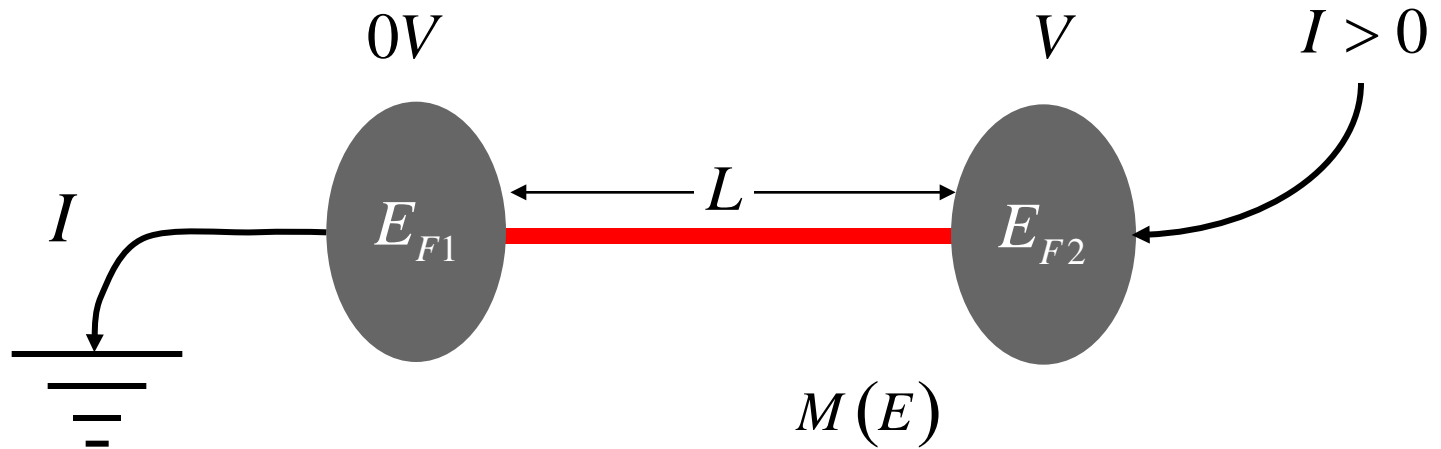
$$\lambda(E_F) = 2v(E_F)\tau(E_F)$$

$$v(E_F) = \sqrt{2(\varepsilon_1^h - E_F)/m^*} \quad 7$$

$$G = p_L q \mu_p \frac{1}{L}$$

$$\mu_p = \frac{q\tau(E_F)}{m_p^*}$$

# case ii): result

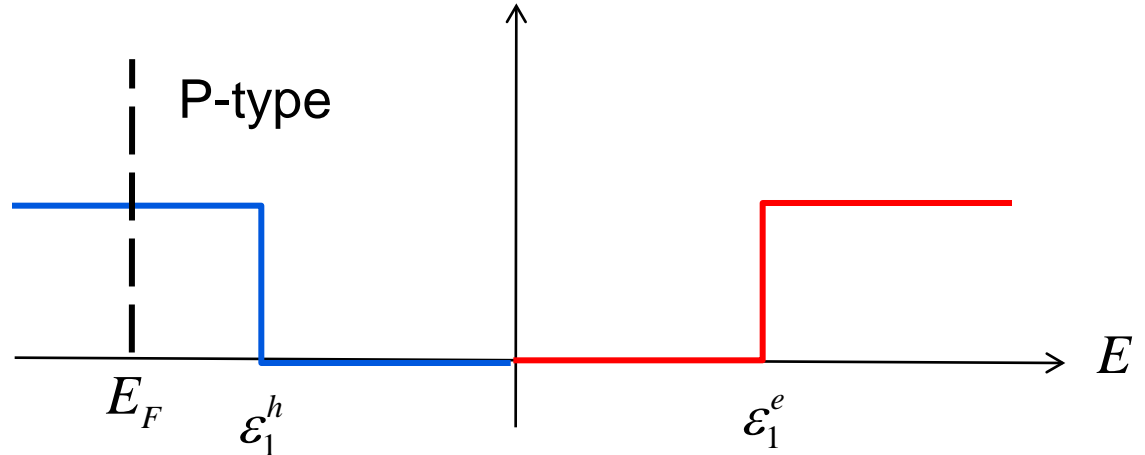


$$G_{1D} = \frac{2q^2}{h} \lambda(E_F)/L$$

$$G = p_L q \mu_n / L$$

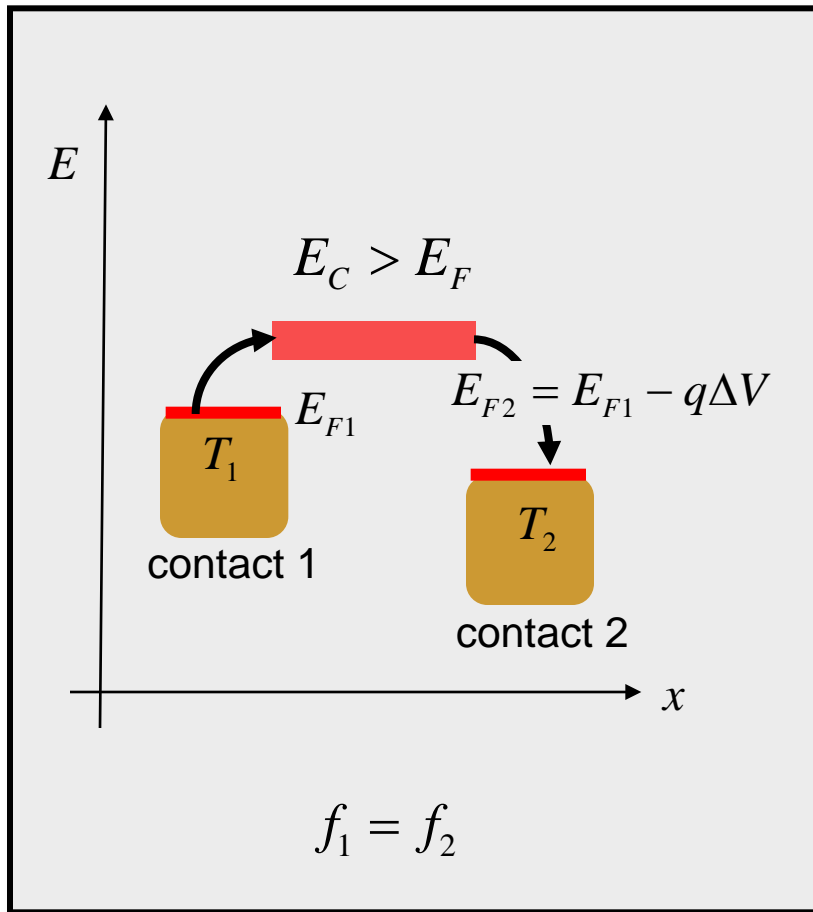
$$\mu_n = q \tau(E_F) / m_p^*$$

$$V > 0 \Rightarrow I > 0$$





# Seebeck coefficient: n-type

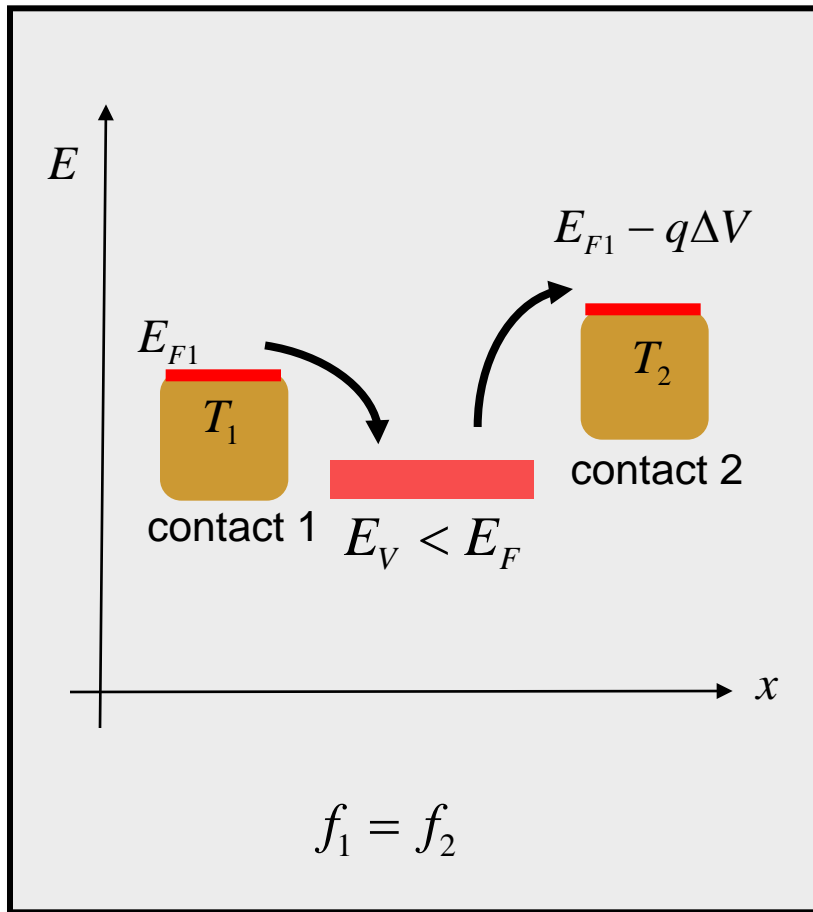


$$\Delta V = -S(E)\Delta T > 0$$

$$S(E) < 0$$

$$S(E) \approx \left( -\frac{k_B}{q} \right) \frac{(E_C - E_F)}{k_B T_L}$$

# Seebeck coefficient: p-type



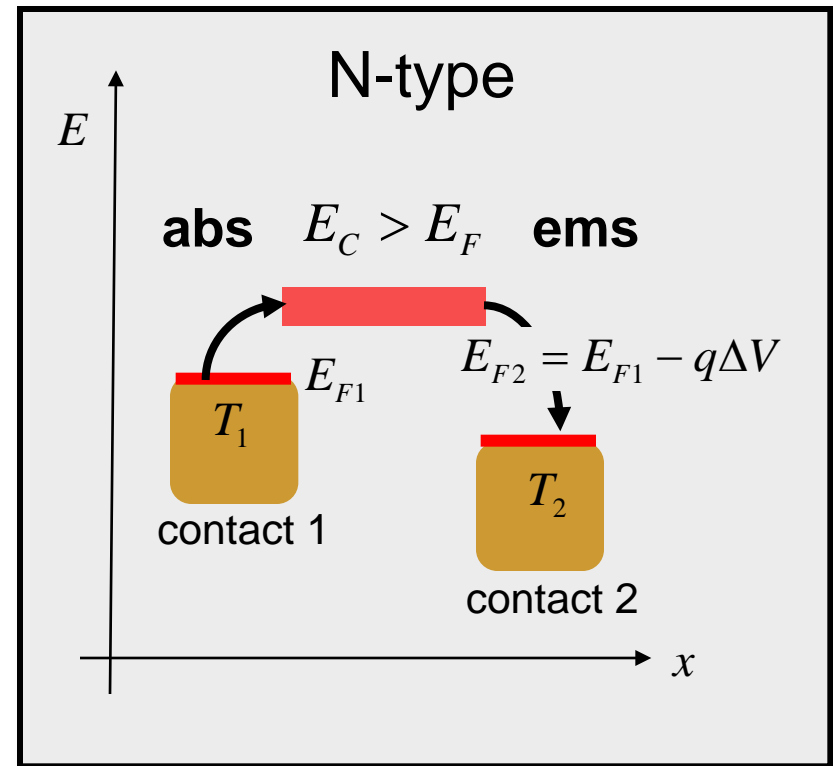
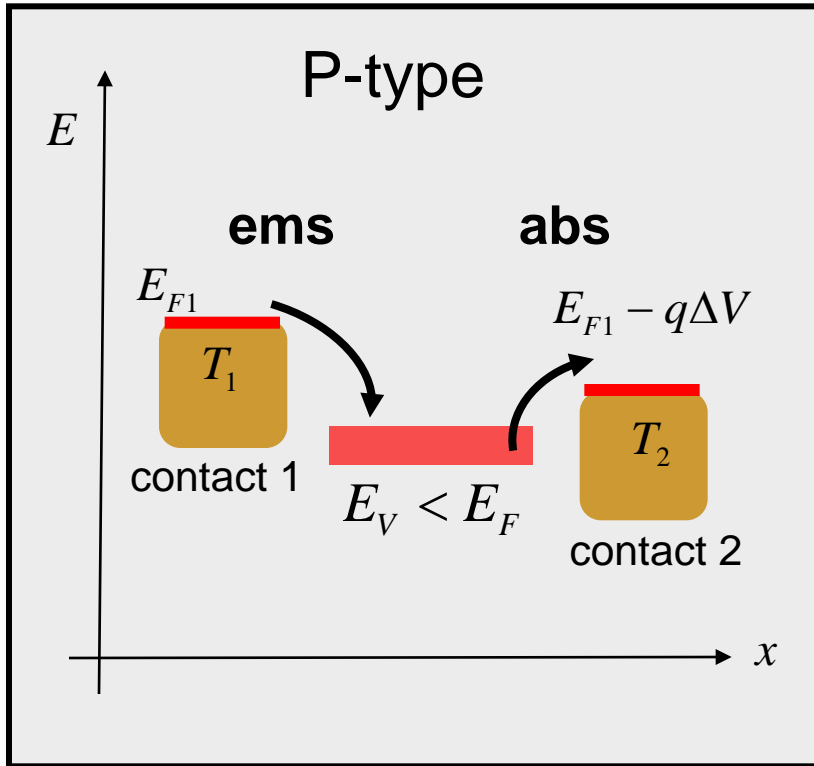
$$\Delta V = -S(E)\Delta T < 0$$

$$S(E) > 0$$

$$S(E) \approx \left( -\frac{k_B}{q} \right) \frac{(E_V - E_F)}{k_B T_L}$$

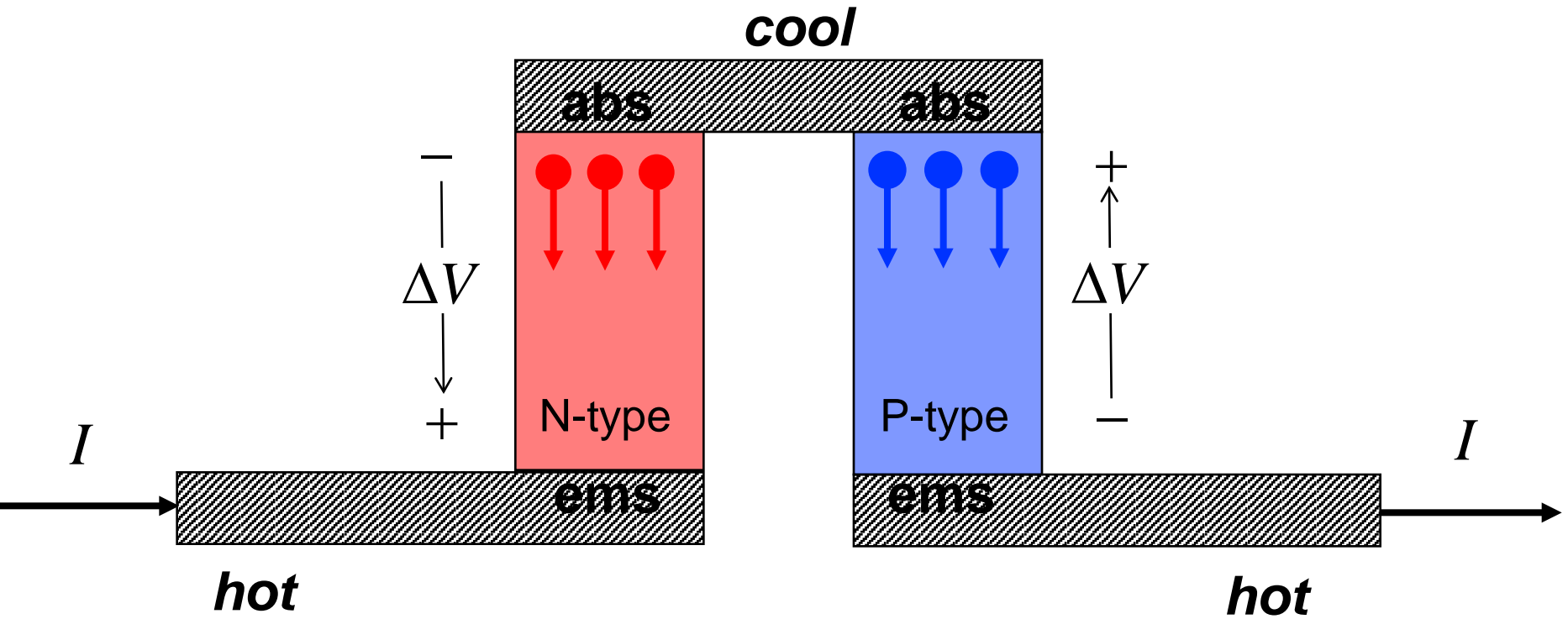
$$S(E) \approx \left( +\frac{k_B}{q} \right) \frac{(E_F - E_V)}{k_B T_L}$$

# Peltier coefficient: p-type

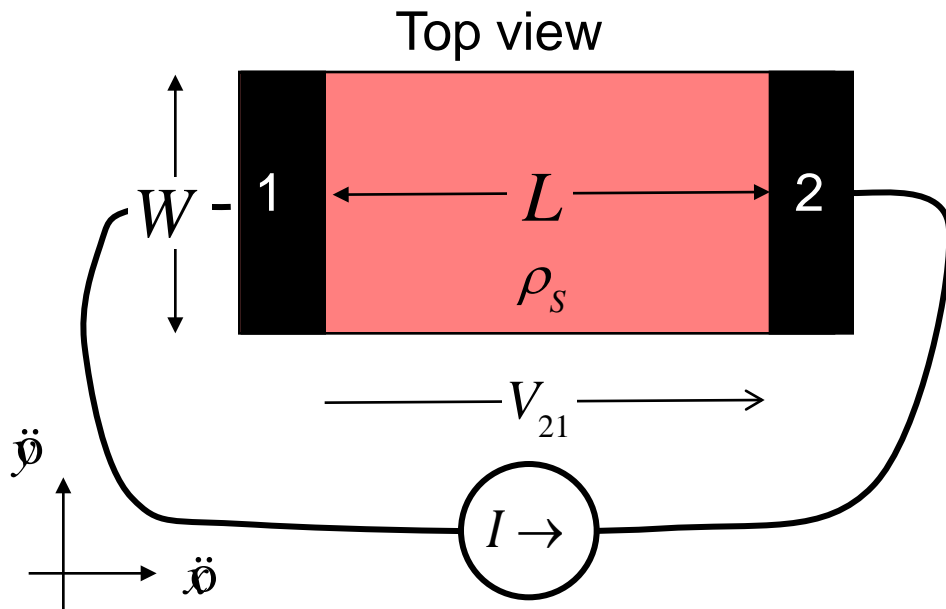


For the same sign voltage at contact 2, the contacts that absorb and emit heat are interchanged.

# TE cooling



# maximum temperature difference

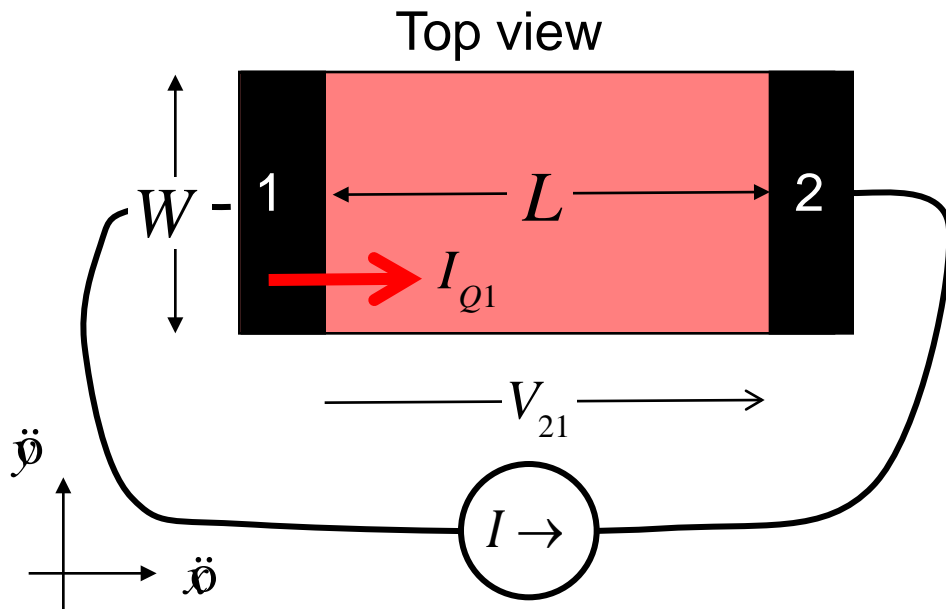


$$\Delta V = RI - S\Delta T$$

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

If we force a current through this thermoelectric device, what is the maximum temperature difference,  $\Delta T = T_2 - T_1$ , that we can produce?

# maximum temperature difference



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

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

$$I_{Q1} = -T_1 S I - K_e \Delta T - \frac{1}{2} I^2 R$$

For a fixed current, the temperature will rise until  $I_Q = 0$

$$I_{opt} = -T_1 S / R$$

$$\Delta T|_{\max} = \frac{1}{2} \frac{T_1^2 S^2 G}{K}$$

$$\Delta T = -\frac{(T_1 S I + I^2 R / 2)}{K_e}$$

$$\frac{\partial \Delta T}{\partial I} = -\frac{(T_1 S + IR)}{K_e} = 0$$

# maximum temperature difference

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$$\Delta T \Big|_{\max} = \frac{1}{2} \frac{T^2 S^2 G}{K}$$

$$\frac{\Delta T}{T} \Big|_{\max} = \frac{1}{2} \frac{S^2 G T}{K} = \frac{1}{2} ZT$$

$$ZT = \frac{S^2 G T}{K_e + K_L}$$

dimensionless figure of merit

$K_e$ : electronic heat conductance

$K_L$ : lattice heat conductance

# figure of merit

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## Power factor:

- large Seebeck coefficient
- high conductance
- depends on material parameters

$$ZT = \frac{S^2 GT}{K_e + K_L}$$

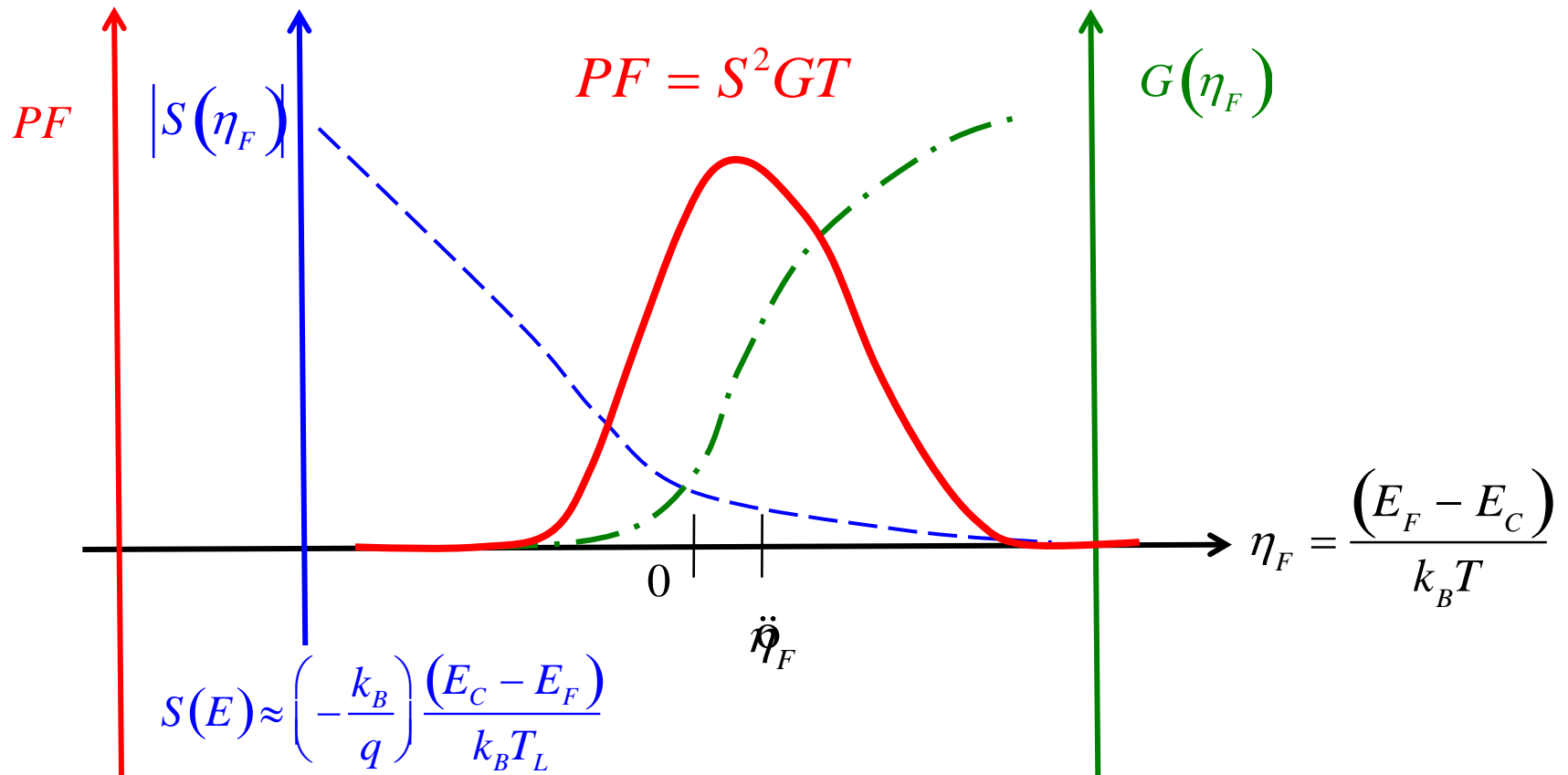
## thermal conductance:

- $K_L > K_e$
- need short mfp for phonons  
(alloys with large mass difference –  
e.g.  $\text{Bi}_2\text{Te}_3$ , SiGe)
- nanostructuring for reducing mfp
- “phonon glass - electron crystal”

G.D. Mahan and J.O. Sofo, “The Best Thermoelectric,” *Proc. Natl. Acad. Sci.*, **93**, 7436, 1996



# optimal power factor



The optimum power factor occurs when  $E_F$  is near  $E_C$ .

# TE parameters for a non-degenerate semiconductor

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

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

$$\frac{\Delta V}{L} = \frac{RA}{L} \frac{I}{A} - S \frac{\Delta T}{L}$$

$$-\mathcal{E}_x = \rho(-J_x) - S \frac{dT}{dx}$$

$$\frac{I_Q}{A} = -\pi \frac{I}{A} - \frac{K_e L}{A} \frac{\Delta T}{L}$$

$$J_Q = -\pi(-J_x) - \kappa_e \frac{dT}{dx}$$

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

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

What are the four TE parameters for a non-degenerate semiconductor?

# TE parameters for a non-degenerate semiconductor

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

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

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

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

$$G = \sigma \frac{A}{L}$$

$$K_e = \kappa_e \frac{A}{L}$$

$$T(E) = \frac{\lambda_0}{L}$$

$$G = 1/R = (2q^2/h)I_0$$

$$S = \left( -\frac{k_B}{q} \right) \frac{I_1}{I_0}$$

$$\pi = TS$$

$$K_e = \left( \frac{2k_B^2 T}{h} \right) \left[ I_2 - \frac{I_1^2}{I_0} \right]$$

$$I_j = \int_{-\infty}^{+\infty} \left( \frac{E - E_F}{k_B T_L} \right)^j T(E) M(E) \left( -\frac{\partial f_0}{\partial E} \right) dE$$

# TE parameters for a non-deg, 3D semiconductor

$$\mathcal{E}_x = \rho J_x + S \frac{dT}{dx}$$
$$J_Q = \pi J_x - \kappa_e \frac{dT}{dx}$$

$$n = 10^{15} \text{ cm}^{-3}$$

$$\mu_n = 1000 \text{ cm}^2/\text{V}\cdot\text{s}$$

$$\rho_n \approx 6 \text{ } \Omega\text{-cm}$$

$$\sigma_{3D} = nq\mu_n$$

$$n = N_C e^{\eta_F}$$

$$N_C = \frac{1}{4} \left( \frac{2m^* k_B T}{\pi \hbar^2} \right)$$

$$\eta_F = \left( \frac{E_F - E_C}{k_B T} \right)$$

$$\mu_n = \frac{v_T \lambda_0}{2} \frac{1}{(k_B T / q)}$$

# TE parameters for a non-deg, 3D semiconductor

$$\mathcal{E}_x = \rho J_x + S \frac{dT}{dx}$$
$$J_Q = \pi J_x - \kappa_e \frac{dT}{dx}$$

$$n = 10^{15} \text{ cm}^{-3}$$

$$N_C = 3.2 \times 10^{19} \text{ cm}^{-3}$$

$$k_B/q \approx 86 \text{ } \mu\text{V} / \text{K}$$

$$\eta_F \approx -10$$

$$S \approx -1 \text{ mV/K}$$

$$S_{3D} = -\frac{k_B}{q} (2 - \eta_F)$$

$$n = N_C e^{\eta_F}$$

$$S_{3D} = -\frac{k_B}{q} (2 + \ln(N_C/n))$$

$$\pi_{3D} = TS_{3D}$$

# TE parameters for a non-deg, 3D semiconductor

$$\mathcal{E}_x = \rho J_x + S \frac{dT}{dx}$$
$$J_Q = \pi J_x - \kappa_e \frac{dT}{dx}$$

for metals.....

$$\frac{\kappa_e^{3D}}{T \sigma_0} = \frac{\pi^2}{3} \left( \frac{k_B}{q} \right)^2$$

$$\kappa_e^{3D} = 2 \left( \frac{k_B}{q} \right) \left( \frac{k_B T}{q} \right) \sigma_0$$

$$\kappa_e^{3D} = 2 \left( \frac{k_B}{q} \right)^2 T \sigma_0 = L T \sigma_0$$

$L$  = "Lorenz number"

$$\frac{\kappa_e^{3D}}{T \sigma_0} = 2 \left( \frac{k_B}{q} \right)^2$$

"Wiedemann-Franz ratio"