

ECE-656: Fall 2009

Lecture 8: Thermoelectric Effects

Professor Mark Lundstrom
Electrical and Computer Engineering
Purdue University, West Lafayette, IN USA

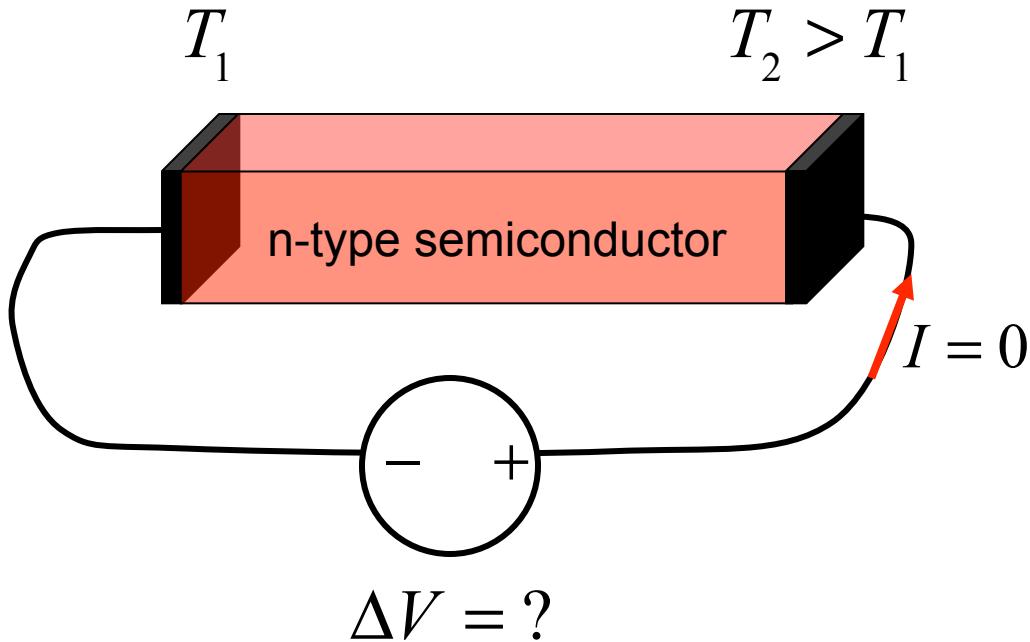
acknowledgement

The author would like to thank Ms. Raseong Kim and Mr. Changwook Jeong for their many contributions to this lecture.

outline

- 1) Introduction**
- 2) One energy level formulation
- 3) Distribution of energy levels
- 4) Discussion
- 5) Summary

Seebeck effect



$$\Delta V \propto \Delta T$$

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

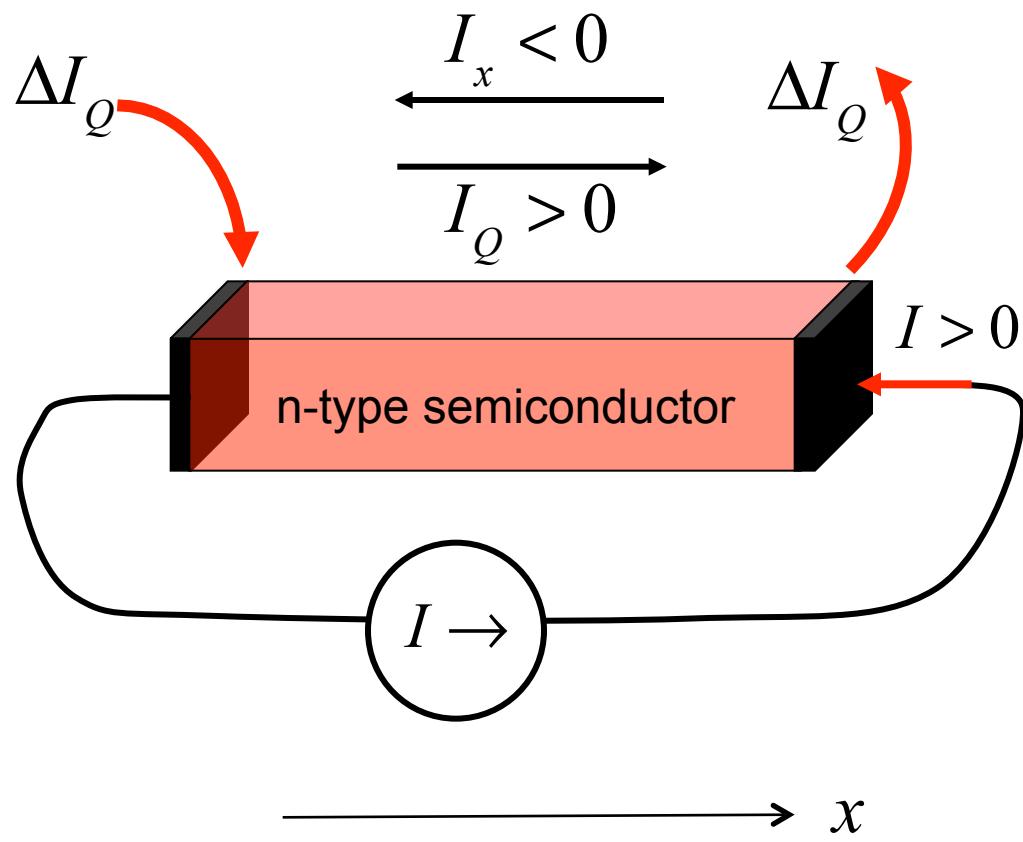
S is the “Seebeck coefficient” in V/K

$S < 0$ for n-type conduction

S is also called the thermopower, α

The Seebeck effect was discovered in 1821 by Thomas Seebeck. It also occurs between the junction of two dissimilar metals at different temperatures. It is the basis for temperature measurement with thermocouples and for thermoelectric power generation.

Peltier effect



$$I_Q \propto I$$

$$I_Q = -\pi I$$

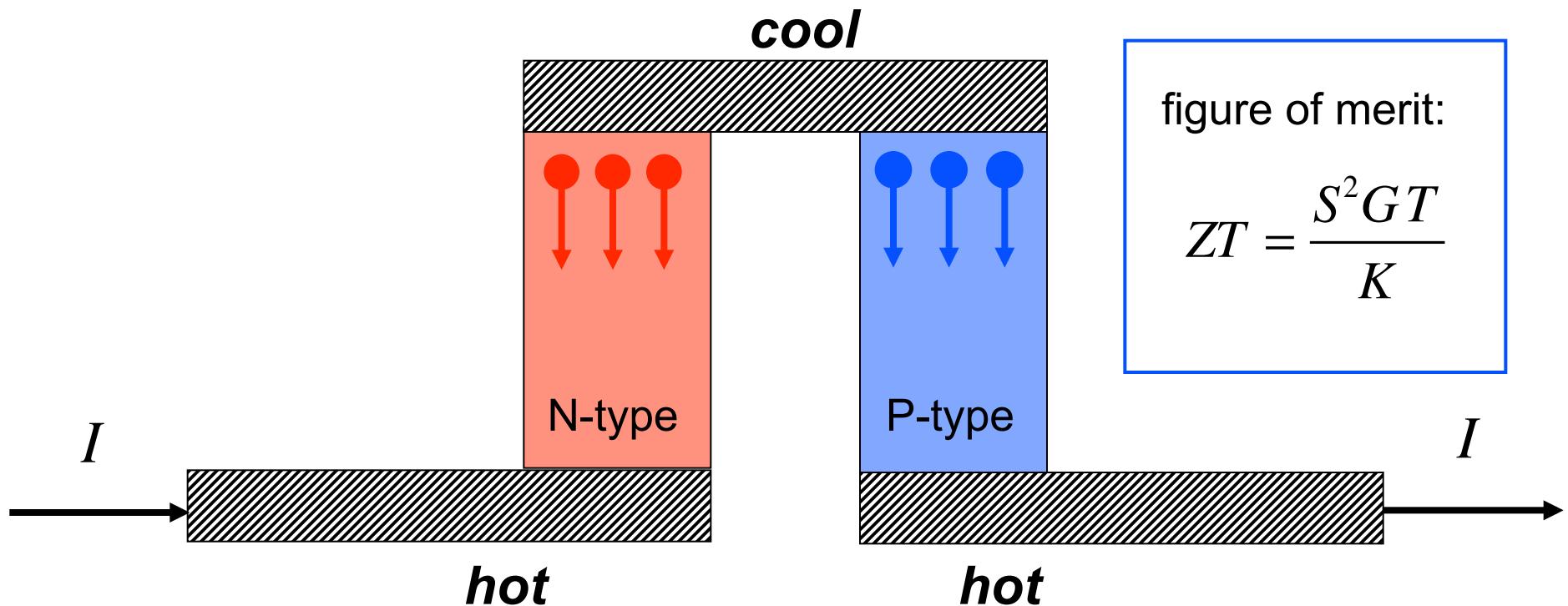
π is the Peltier coefficient in W/A

There is a close connection between the Peltier coefficient and the Seebeck coefficient.

$$\pi = TS \quad \text{“Kelvin relation”}$$

The Peltier effect was discovered in 1834 by Jean-Charles Peltier and explained in 1838 by Lenz. It finds use in thermoelectric cooling.

thermoelectric devices



- 1) refrigeration and electronic cooling
- 2) power generation from waste heat
(also thermionic devices)

materials characterization

“Thermoelectric and Magneto-thermoelectric Transport Measurements of Graphene,” Y.M. Zuev, W. Chang, and P. Kim, *Phys. Rev. Lett.*, **102**, 096807, 2009.

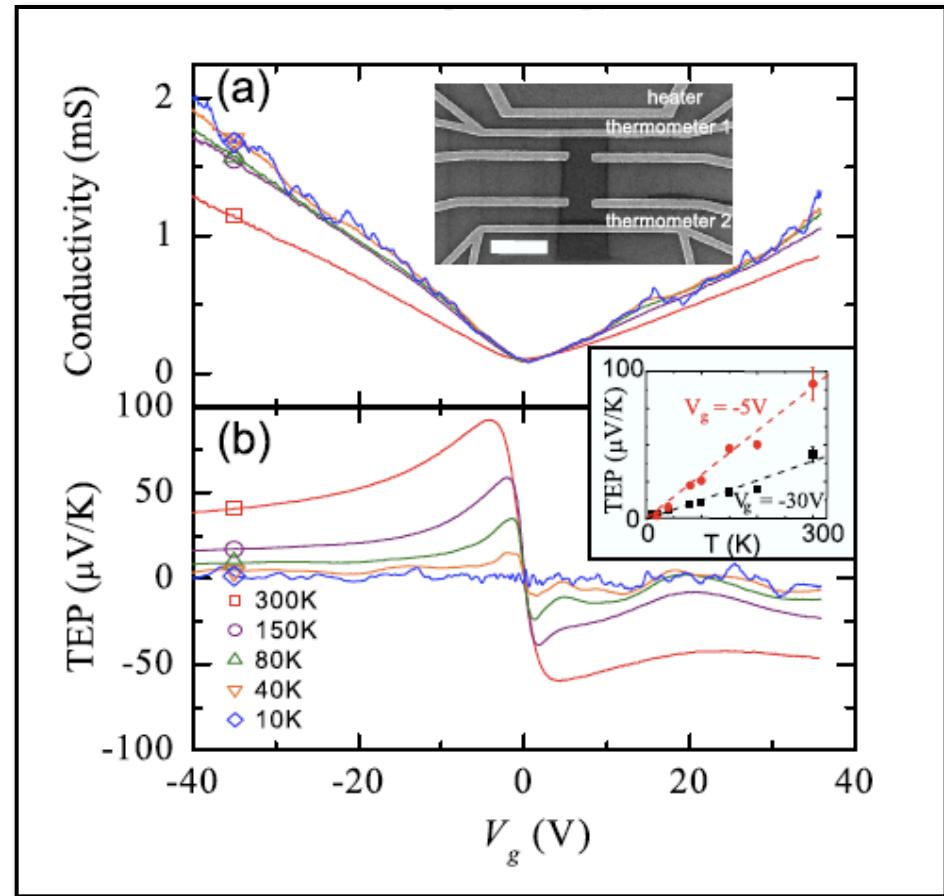


FIG. 1 (a) Conductivity and (b) TEP of a graphene sample as a function of V_g for $T_L = 300\text{ K}$ (square), 150 K (circle), 80 K (up triangle), 40 K (down triangle), and 10 K (diamond).

Upper inset: SEM image of a typical device, the scale bar is 2 microns.

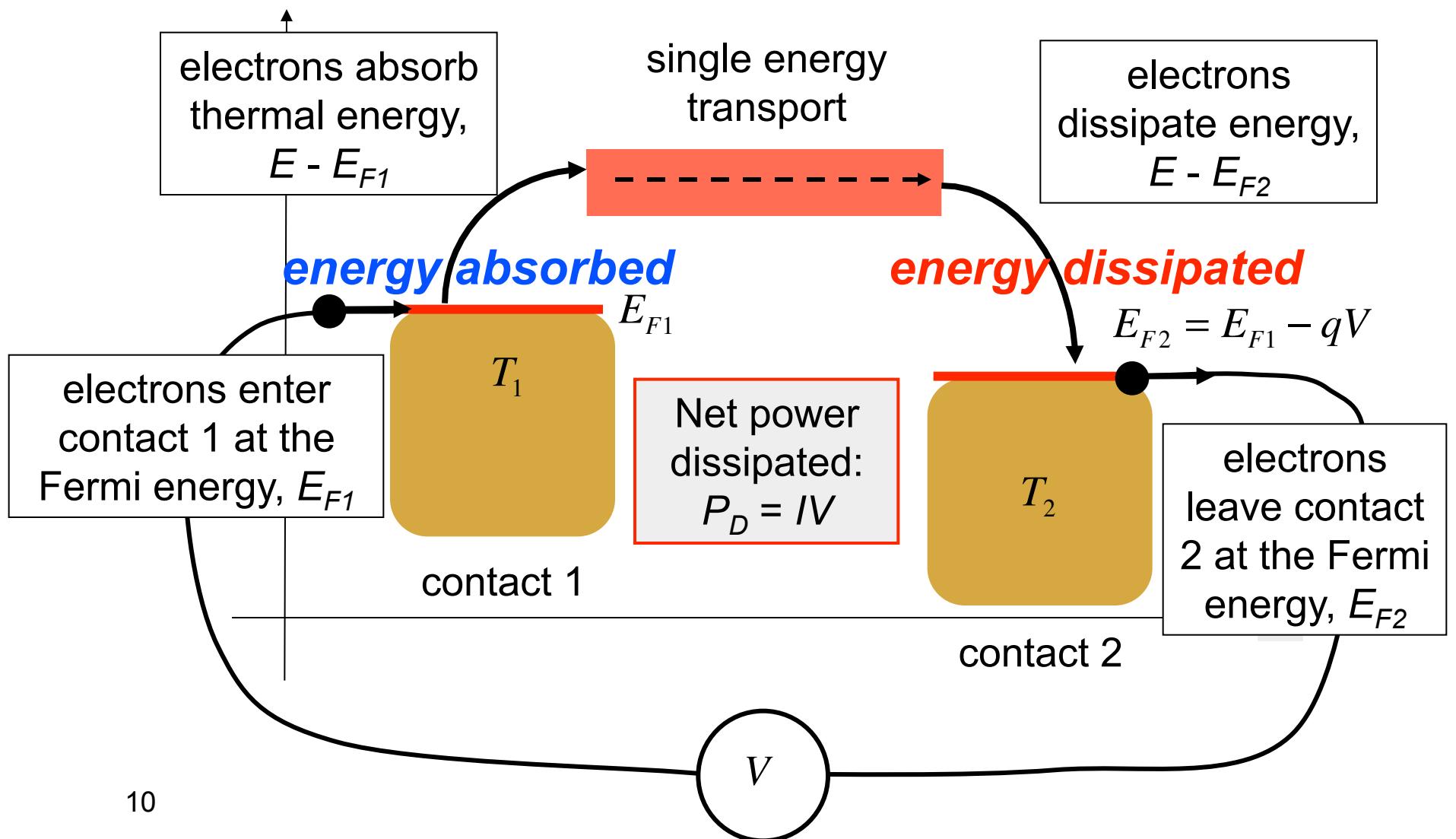
questions

- 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?

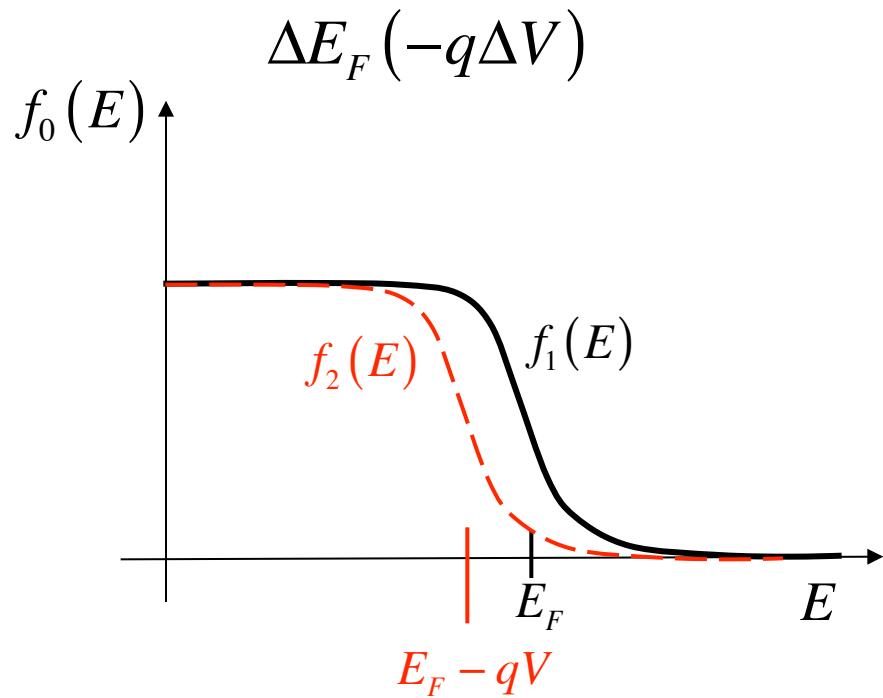
outline

- 1) Introduction
- 2) **One level energy formulation**
- 3) Distribution of energy levels
- 4) Discussion
- 5) Summary

one energy model



when $\Delta T = 0$, the driving force is: ΔE_F



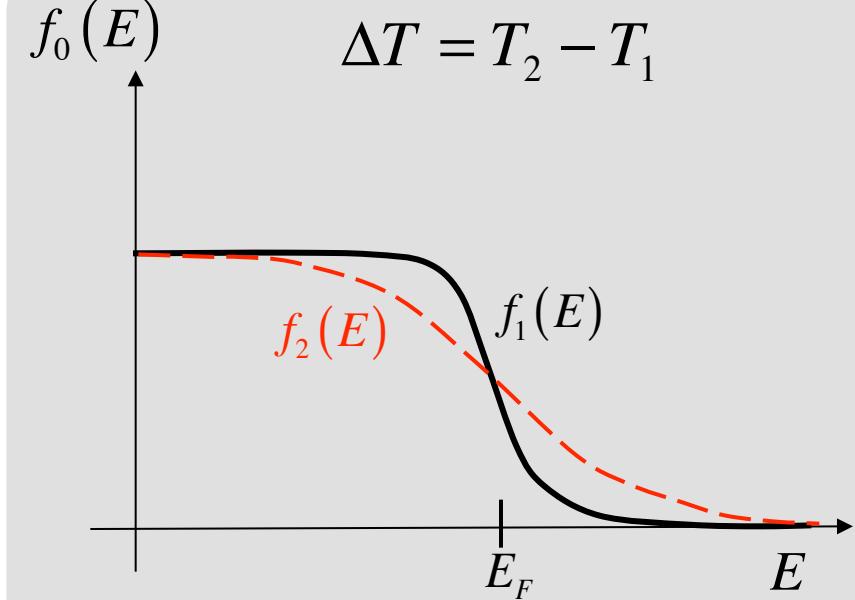
$$(f_1 - f_2) \approx \left(-\frac{\partial f_0}{\partial E} \right) q \Delta V$$

driving force: differences in temperature

$$\begin{aligned}(f_1 - f_2) &\approx f_1 - \left(f_1 + \frac{\partial f_1}{\partial T} \Delta T \right) \\ &= -\frac{\partial f_1}{\partial T} \Delta T\end{aligned}$$

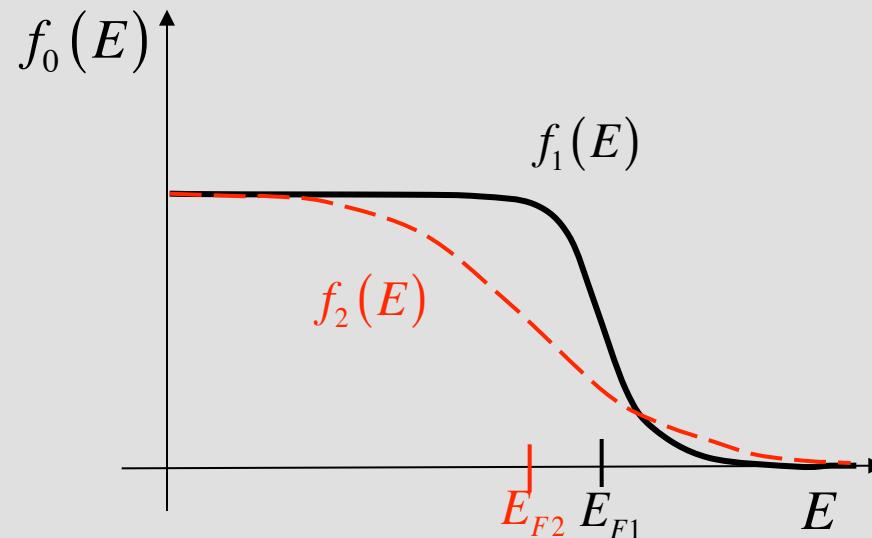
$$\frac{\partial f_1}{\partial T} = -\frac{(E - E_F)}{T} \left(\frac{\partial f_0}{\partial E} \right)$$

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



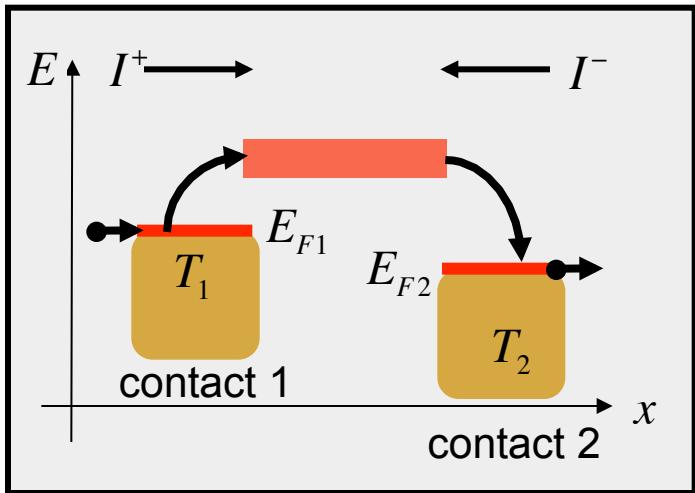
$$(f_1 - f_2) \approx -\left(-\frac{\partial f_0}{\partial E}\right) \frac{(E - E_F)}{T} \Delta T$$

driving force: differences in both E_F and T



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

one energy model: result



$$I(E_0) = \frac{2q}{h} T(E_0) M(E_0) (f_1 - f_2)$$

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

$$I(E_0) = G(E_0) \Delta V - [SG(E_0)] \Delta T$$

$$G(E_0) = \frac{2q^2}{h} T(E_0) M(E_0) \left(-\frac{\partial f_0}{\partial E} \right)$$

$$[SG(E_0)] = \frac{2q}{h} T(E_0) M(E_0) \left(-\frac{\partial f_0}{\partial E} \right) \left(\frac{E - E_F}{T} \right)$$

two forms of the result

$$I(E_0) = G(E_0)\Delta V - [SG(E_0)]\Delta T$$

$$G(E_0) = \frac{2q^2}{h} T(E_0) M(E_0) \left(-\frac{\partial f_0}{\partial E} \right)$$

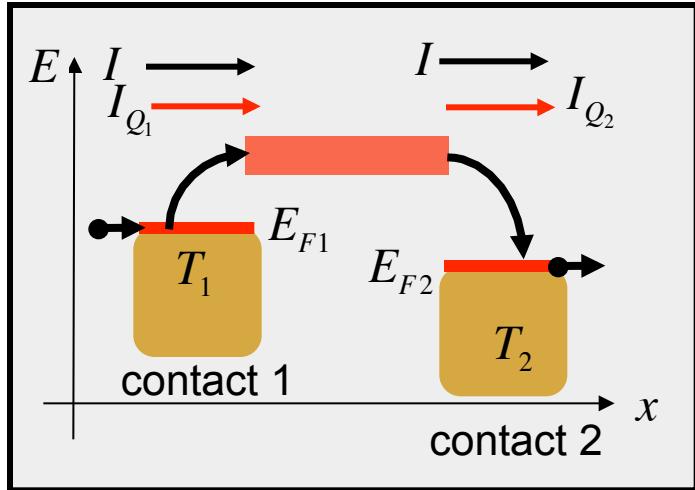
$$[SG(E_0)] = \frac{2q}{h} T(E_0) M(E_0) \left(-\frac{\partial f_0}{\partial E} \right) \left(\frac{E_0 - E_F}{T} \right)$$

$$\Delta V = R(E_0) I(E_0) - S(E_0) \Delta T$$

$$R(E_0) = 1/G(E_0)$$

$$S(E_0) = -[SG(E_0)]/G(E_0) \quad S(E_0) = \left(-\frac{k_B}{q} \right) \frac{(E_0 - E_F)}{k_B T}$$

but there is more to the story....



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

$$I(E_0) = \frac{2q}{h} T(E_0) M(E_0) (f_1 - f_2)$$

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

$$I_{Q_1}(E_0) = \frac{2(E_0 - E_{F1})}{h} T(E_0) M(E_0) (f_1 - f_2)$$

$$I_{Q_2}(E_0) = \frac{2(E_0 - E_{F2})}{h} T(E_0) M(E_0) (f_1 - f_2)$$

near-equilibrium heat current

$$I_{Q_1} \approx I_{Q_2} = I_Q(E_0) = \frac{2(E_0 - E_F)}{h} T(E_0) M(E_0)(f_1 - f_2) \quad f_1 \approx f_2 \approx f_0$$

$$(f_1 - f_2) \approx C_1(E_0) q \Delta V + C_2(E_0) \Delta T$$

$$I_Q(E_0) = \frac{2}{h} T(E_0) M(E_0) \left(-\frac{\partial f_0}{\partial E} \right) \left\{ (E_0 - E_F) q \Delta V - \frac{(E_0 - E_F)^2}{T} \Delta T \right\}$$

$$I_Q(E_0) = T [SG(E_0)] \Delta V - K_0(E_0) \Delta T$$

$$[K_0(E_0)] = \frac{2}{h} \frac{(E_0 - E_F)^2}{T} T(E_0) M(E_0) \left(-\frac{\partial f_0}{\partial E} \right)$$

one level summary

$$I(E_0) = G(E_0)\Delta V - [SG(E_0)]\Delta T_L$$

$$I_Q(E_0) = T[SG(E_0)]\Delta V - K_0(E_0)\Delta T$$

$$\Delta V = R(E_0)I(E_0) - S(E_0)\Delta T$$

$$I_Q(E_0) = -\pi(E_0)I(E_0) - K_e(E_0)\Delta T$$

But is there a more **physical** way to understand these coefficients?

$$G(E_0) = \frac{2q^2}{h}T(E_0)M(E_0)\left(-\frac{\partial f_0}{\partial E}\right)$$

$$[SG(E_0)] = \frac{(E_0 - E_F)}{qT}G(E_0)$$

$$[K_0(E_0)] = \left(\frac{E_0 - E_F}{q}\right)^2 \frac{1}{T}G(E_0)$$

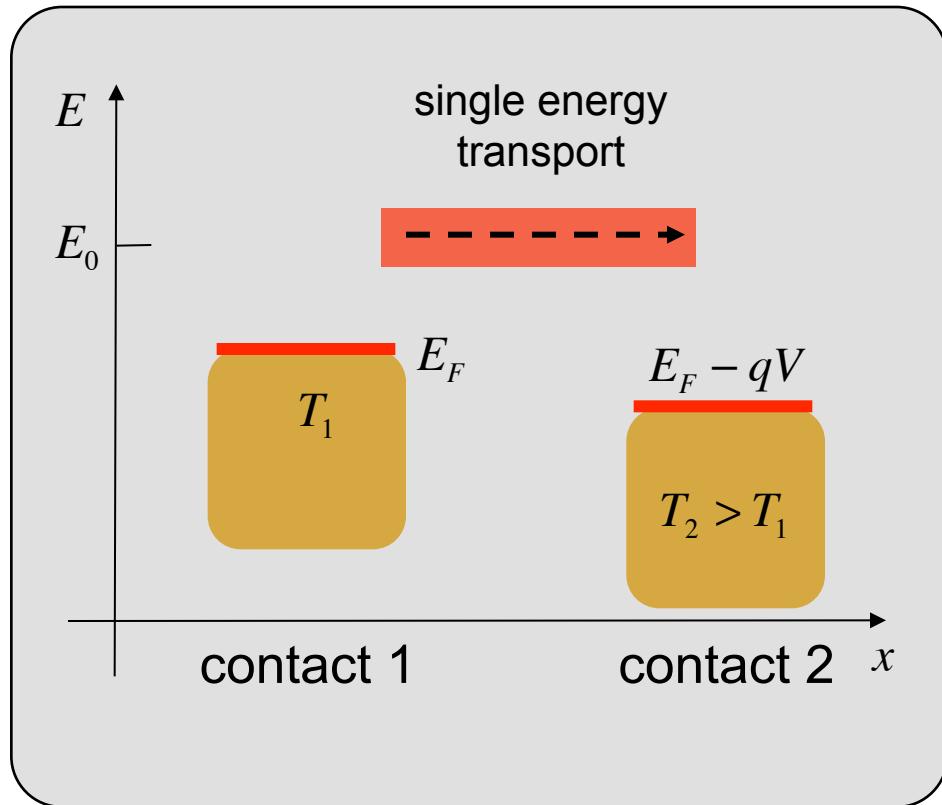
$$R(E_0) = \frac{1}{G(E_0)}$$

$$S(E_0) = \left(-\frac{k_B}{q}\right) \frac{(E_0 - E_F)}{k_B T}$$

$$\pi(E_0) = T S(E_0)$$

$$K_e(E_0) = K_0(E_0) - T S(E_0)^2 G(E_0)$$

Seebeck coefficient



$$S \equiv \frac{V_{OC}}{\Delta T}$$

$$f_1(E_0) = f_0(E_0)$$

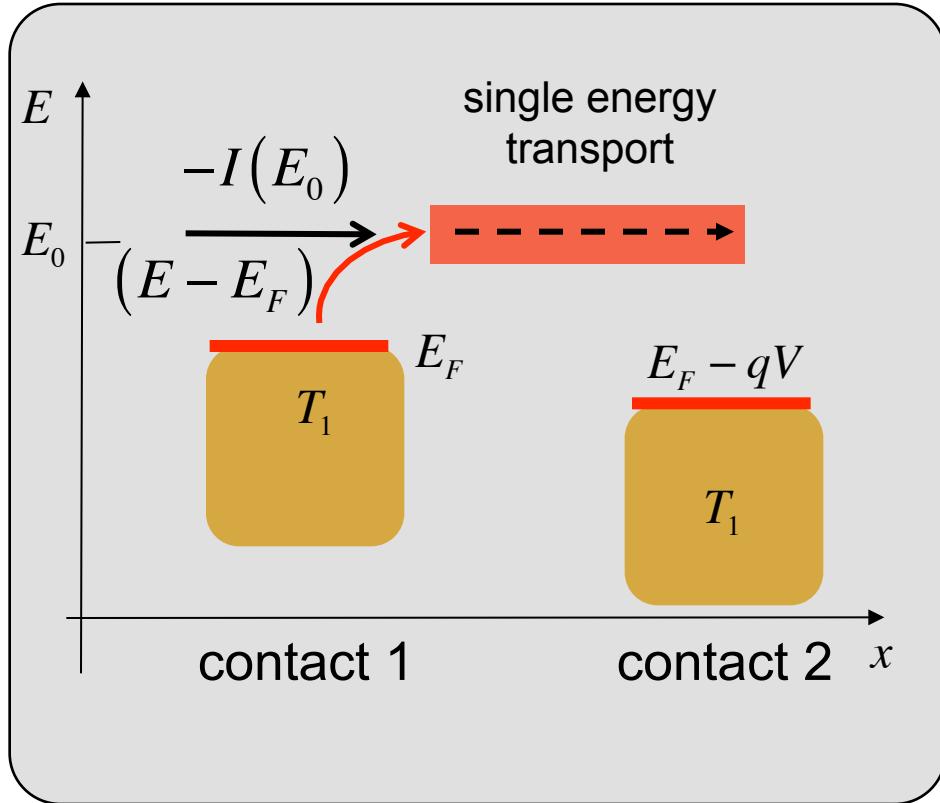
$$\frac{1}{1 + e^{(E_0 - E_F)/k_B T_1}} = \frac{1}{1 + e^{(E_0 - E_F + qV_{OC})/k_B T_2}}$$

$$\frac{(E_0 - E_F)}{k_B T_1} = \frac{(E_0 - E_F + qV_{OC})}{k_B T_2}$$

$$T_2 = T_1 + \Delta T$$

$$S = \frac{V_{OC}}{\Delta T} = -\frac{(E_0 - E_F)}{qT}$$

Peltier coefficient



$$\pi \equiv \left. \frac{I_Q}{-I} \right|_{T_1 = T_2}$$

$$\pi(E_0) = \frac{(E_0 - E_F)(I(E_0)/q)}{-I(E_0)}$$

$$\pi(E_0) = -\frac{(E_0 - E_F)}{q}$$

$$S = \frac{V_{OC}}{\Delta T} = -\frac{(E_0 - E_F)}{qT}$$

$$\pi = TS$$

coupled currents

$$\Delta V = R(E_0)I(E_0) - S(E_0)\Delta T$$

$$I_Q(E_0) = -\pi(E_0)I(E_0) - K_e(E_0)\Delta T$$

$$R(E_0) = 1/G(E_0)$$

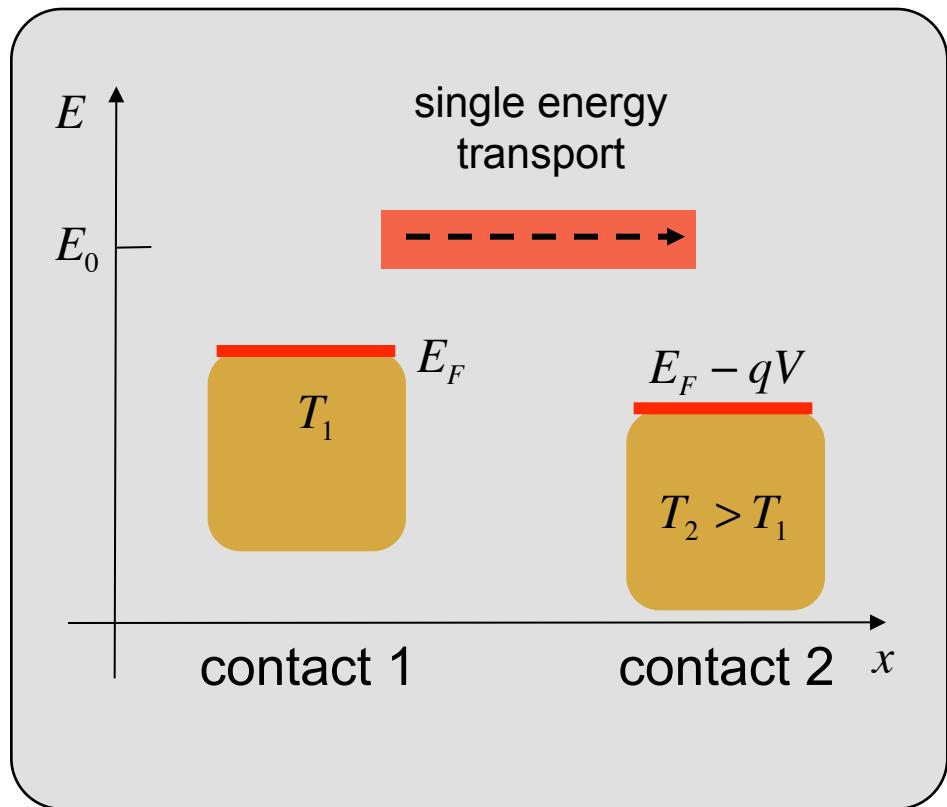
$$G(E_0) = \frac{2q^2}{h} T(E_0) M(E_0) \left(-\frac{\partial f_0}{\partial E} \right) \Big|_{E_0}$$

$$S(E_0) = -\frac{(E_0 - E_F)}{qT}$$

$$\pi(E_0) = TS(E_0)$$

$$K_e(E_0) = ?$$

thermal conductance



$$I_Q(E_0) = -\pi(E_0)I(E_0) - K_e(E_0)\Delta T$$

$$K_e(E_0) \equiv \left. \frac{-I_Q(E_0)}{\Delta T} \right|_{I(E_0)=0}$$

$$I(E_0) = 0 \Rightarrow I_Q(E_0) = 0$$

$$K_e(E_0) = 0$$

(in the single level model)

one level summary

$$\begin{aligned}
K_e(E_0) &= K_0(E_0) - T S(E_0)^2 G(E_0) \\
&= \left(\frac{E_0 - E_F}{q} \right)^2 \frac{1}{T} G(E_0) \\
&\quad - T \left\{ \left(-\frac{k_B}{q} \right) \frac{(E_0 - E_F)}{k_B T} \right\}^2 G(E_0) \\
&= 0
\end{aligned}$$

$$G(E_0) = \frac{2q^2}{h} T(E_0) M(E_0) \left(-\frac{\partial f_0}{\partial E} \right)$$

$$[SG(E_0)] = \frac{(E_0 - E_F)}{qT} G(E_0)$$

$$[K_0(E_0)] = \left(\frac{E_0 - E_F}{q} \right)^2 \frac{1}{T} G(E_0)$$

$$R(E_0) = \frac{1}{G(E_0)}$$

$$S(E_0) = \left(-\frac{k_B}{q} \right) \frac{(E_0 - E_F)}{k_B T}$$

$$\pi(E_0) = T S(E_0)$$

$$K_e(E_0) = K_0(E_0) - T S(E_0)^2 G(E_0)$$

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real materials

Real materials have a **distribution of energy channels** in the conduction and valence bands. We must add up the contributions of each of these energy channels.

linear response

$$I(E) = G(E)\Delta V - [SG(E)]\Delta T$$

$$I_Q(E) = T[SG(E)]\Delta V - K_0(E)\Delta T$$

total currents

For a **distribution of channels**, we add up the contributions of each channel.

$$I(E) = G(E)\Delta V - [SG(E)]\Delta T$$

$$I_Q(E) = T_L[SG(E)]\Delta V - K_0(E)\Delta T$$

$$I = G\Delta V - [SG]\Delta T$$

$$I_Q = T[SG]\Delta V - K_0\Delta T$$

$$I = \int_{-\infty}^{+\infty} I(E)dE = G\Delta V - [SG]\Delta T$$

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

$$\begin{aligned}[SG] &= \int_{-\infty}^{+\infty} [SG(E)]dE \\ &= \int_{-\infty}^{+\infty} \left(\frac{1}{T} \right) \frac{(E - E_F)}{q} G(E)dE\end{aligned}$$

$$K_0 = \int_{-\infty}^{+\infty} [K_0(E)]dE$$

$$= \int_{-\infty}^{+\infty} \frac{1}{T} \left(\frac{E - E_F}{q} \right)^2 G(E)dE$$

TE integrals

All TE coefficients involve similar integrals:

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

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

$$I = \int_{-\infty}^{+\infty} I(E) dE = G \Delta V - [SG] \Delta T$$

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

$$\begin{aligned} [SG] &= \int_{-\infty}^{+\infty} [SG](E) dE \\ &= \int_{-\infty}^{+\infty} \left(\frac{1}{T} \right) \frac{(E - E_F)}{q} G(E) dE \end{aligned}$$

$$\begin{aligned} K_0 &= \int_{-\infty}^{+\infty} [K_0](E) dE \\ &= \int_{-\infty}^{+\infty} \frac{1}{T} \left(\frac{E - E_F}{q} \right)^2 G(E) dE \end{aligned}$$

TE integrals (ii)

All TE coefficients involve similar integrals:

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

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

$$I = G \Delta V - [SG] \Delta T$$

$$G = \frac{2q^2}{h} I_0 \quad [SG] = \left(-\frac{k_B}{q} \right) I_1$$

$$I_Q = T [SG] \Delta V - K_0 \Delta T$$

$$K_0 = \left(\frac{k_B T}{q} \right) \left(\frac{k_B}{q} \right) I_2$$

alternative formulation

linear response

$$I = G\Delta V - [SG]\Delta T$$

$$I_Q = T[SG]\Delta V - K_e\Delta T$$

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

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

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

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

$$\pi = TS$$

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

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

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

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Seebeck coefficient of a bulk semiconductor

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

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

$$M(E) = \frac{m^*}{2\pi\hbar^2} (E - \epsilon_1) A \quad T(E) = \frac{\lambda_0}{L} \quad (\text{diffusive})$$

Result:

$$\eta_F \equiv (E_F - E_C) / k_B T$$

non-degenerate

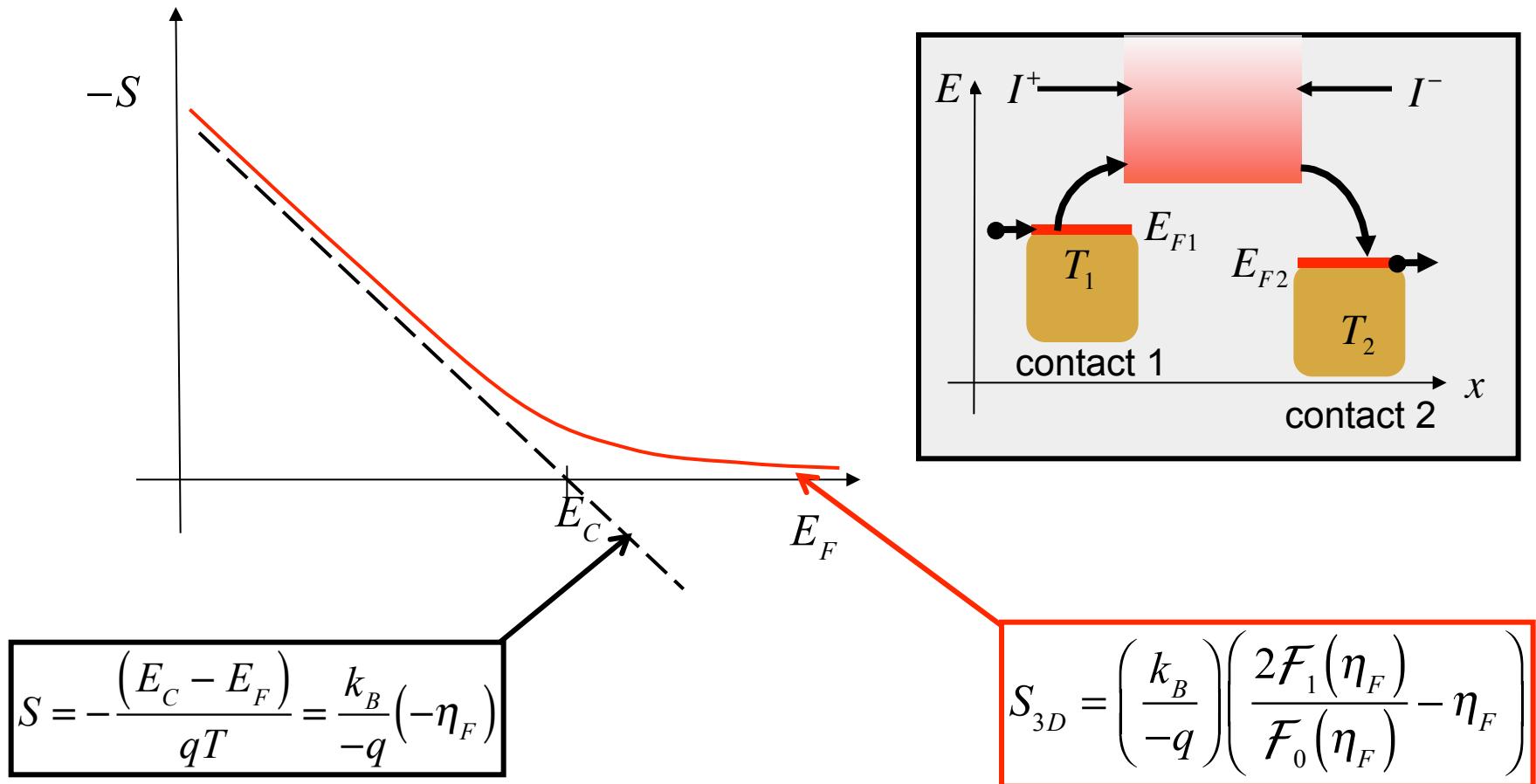
$$S_{3D} = \left(\frac{k_B}{-q} \right) \left(\frac{2\mathcal{F}_1(\eta_F)}{\mathcal{F}_0(\eta_F)} - \eta_F \right)$$

$$S_{3D} = \left(\frac{k_B}{-q} \right) \left(2 - \frac{(E_F - E_C)}{k_B T} \right)$$

Independent of scattering (if mfp is independent of energy).

Independent of m^* (for parabolic energy bands).

Seebeck coefficient of bulk semiconductors



Seebeck coefficient and scattering

$$G = \left(\frac{2q^2}{h} \right) I_0 \quad I_j = \int_{-\infty}^{+\infty} \left(\frac{E - E_F}{k_B T} \right)^j T(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right) dE$$

$$S = \left(-\frac{k_B}{q} \right) \frac{I_1}{I_0} \quad T(E) = \frac{\lambda(E)}{L} \quad \lambda(E) = \lambda_0 \left(E/k_B T \right)^s$$
$$\tau(E) = \tau_0 \left(E/k_B T \right)^r$$

$$S = -\frac{k_B}{q} \left(\frac{\left(s + \frac{D+1}{2} \right) \mathcal{F}_{s+(D-1)/2}(\eta_F) - (\eta_F)}{\mathcal{F}_{s+(D-3)/2}(\eta_F)} \right)$$

“power law scattering”

$D = 1, 2, 3$ dimensions

$$G = \frac{2q^2}{h} \mathcal{F}_{s+(D-3)/2}(\eta_F)$$

Seebeck coefficient and scattering

$$S_{3D} = -\frac{k_B}{q} \left(\frac{(s+2)\mathcal{F}_{s+1}(\eta_F)}{\mathcal{F}_s(\eta_F)} - 1 \right)$$

Common values of s :

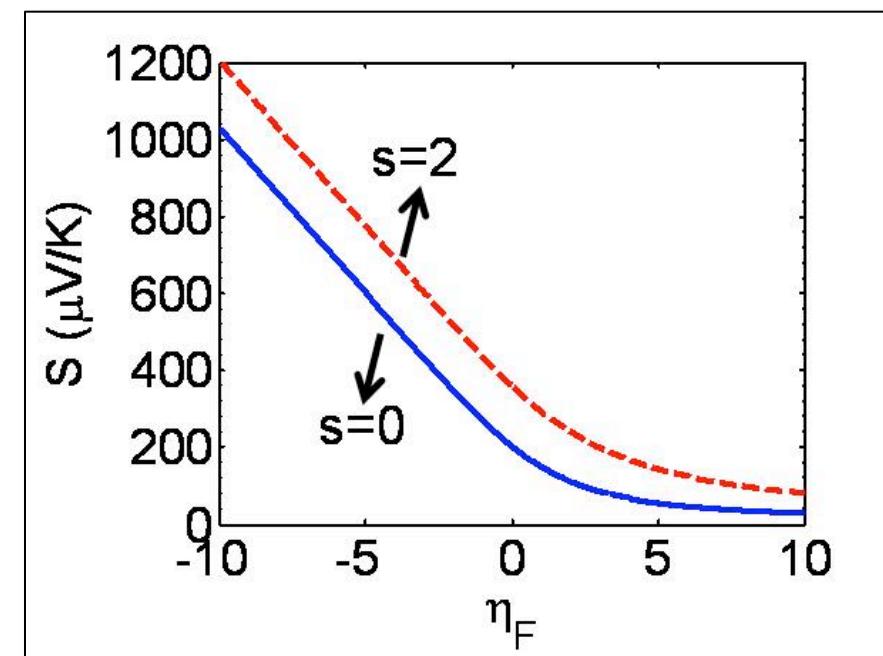
ionized impurity scattering:

$$r = 3/2 \quad s = 2$$

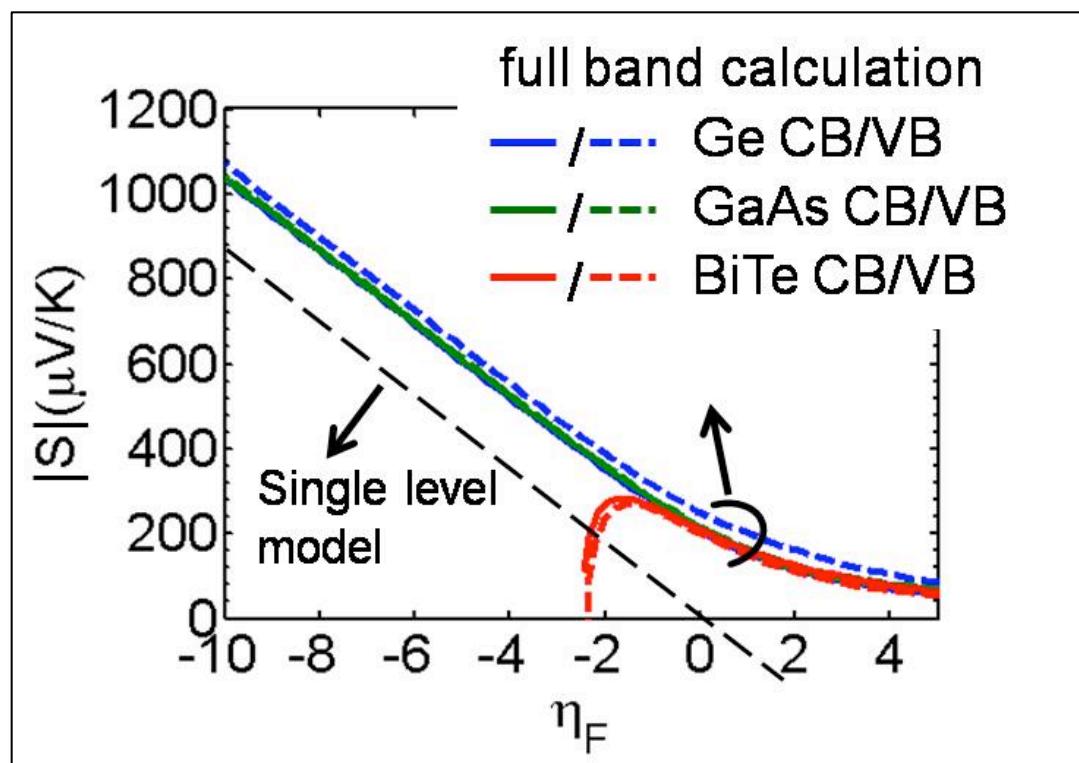
acoustic phonon scattering:

$$r = -1/2 \quad s = 0$$

$$\lambda(E) = \lambda_0 (E/k_B T)^s \quad \tau(E) = \tau_0 (E/k_B T)^r$$



“full band” Seebeck coefficient



Changwook Jeong, Purdue University 2009

thin films and nanowires

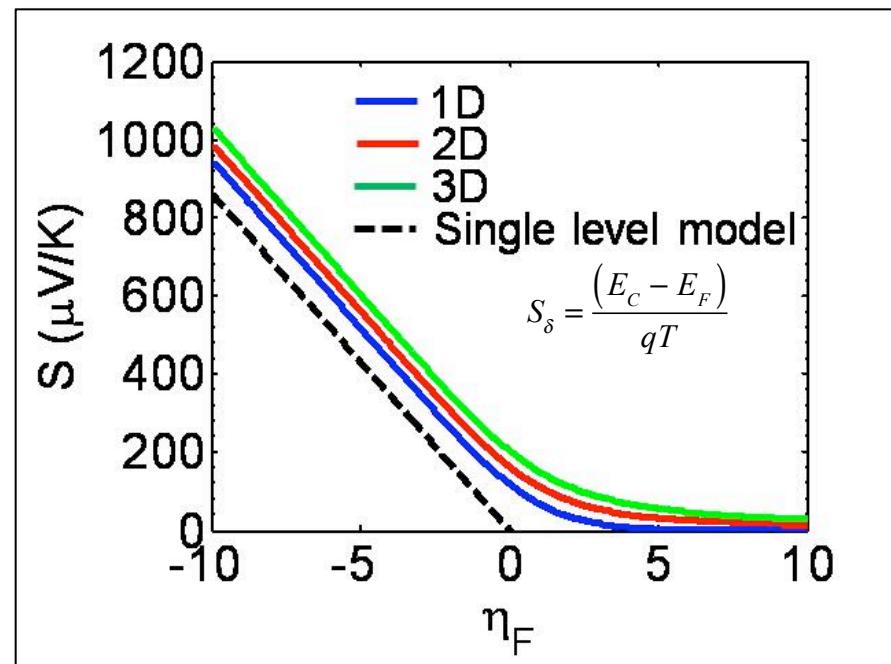
$$S_\delta = \left(\frac{k_B}{-q} \right) (-\eta_F)$$

$$S_{1D} = \left(\frac{k_B}{-q} \right) \left(\frac{\mathcal{F}_0(\eta_F)}{\mathcal{F}_{-1}(\eta_F)} - \eta_F \right)$$

$$S_{2D} = \left(\frac{k_B}{-q} \right) \left(\frac{3\mathcal{F}_{1/2}(\eta_F)}{2\mathcal{F}_{-1/2}(\eta_F)} - \eta_F \right)$$

$$S_{3D} = \left(\frac{k_B}{-q} \right) \left(\frac{2\mathcal{F}_1(\eta_F)}{\mathcal{F}_0(\eta_F)} - \eta_F \right)$$

(parabolic bands)



R. Kim, et. al, *J. Appl. Phys.*, **105**, 034506, 2009

Seebeck coefficient of graphene

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

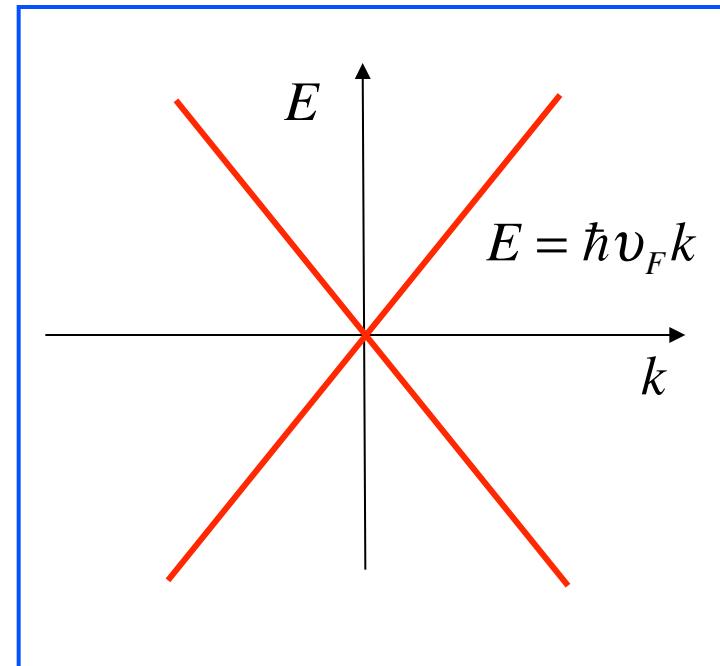
$$I_j = \int_{-\infty}^{+\infty} \left(\frac{E - E_F}{k_B T} \right)^j T(E) M(E) \left(-\frac{\partial f_0}{\partial E} \right) dE$$

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

Result:

$$S = \frac{k_B}{q} \left(-\frac{2(\mathcal{F}_1(\eta_F) - \mathcal{F}_1(-\eta_F))}{\mathcal{F}_0(\eta_F) + \mathcal{F}_0(-\eta_F)} + \eta_F \right)$$

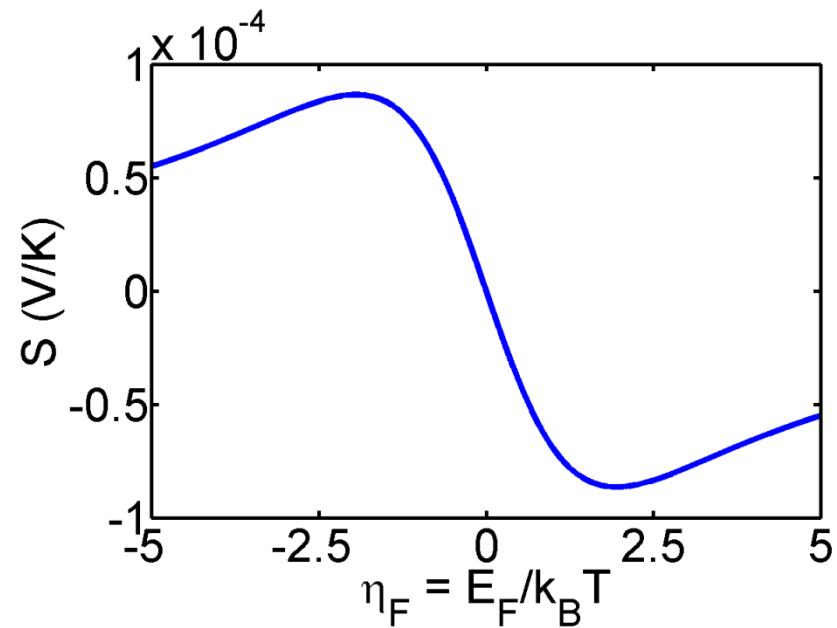
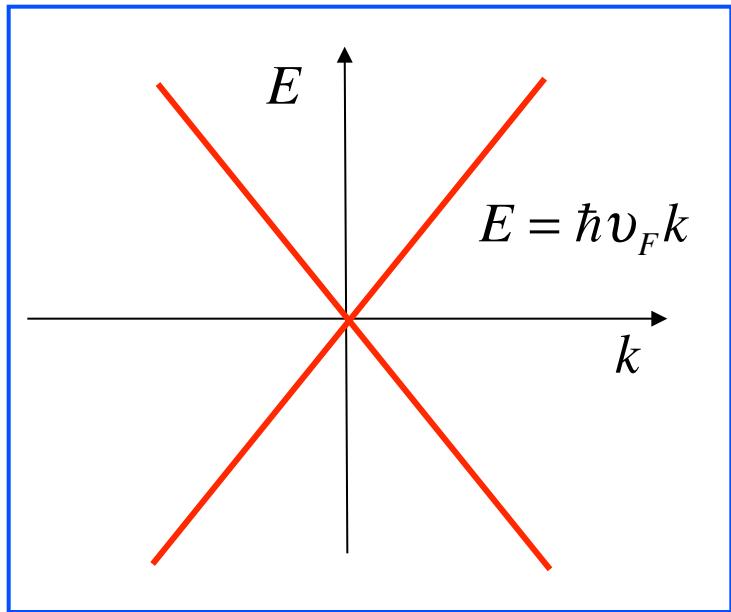
$$M_{2D}(E) = W 2E / \pi \hbar v_F \quad E > 0$$



$$M_{2D}(E) = -W 2E / \pi \hbar v_F \quad E < 0$$

S vs. Fermi level

$$S = \frac{k_B}{q} \left(-\frac{2(\mathcal{F}_1(\eta_F) - \mathcal{F}_1(-\eta_F))}{\mathcal{F}_0(\eta_F) + \mathcal{F}_0(-\eta_F)} + \eta_F \right)$$

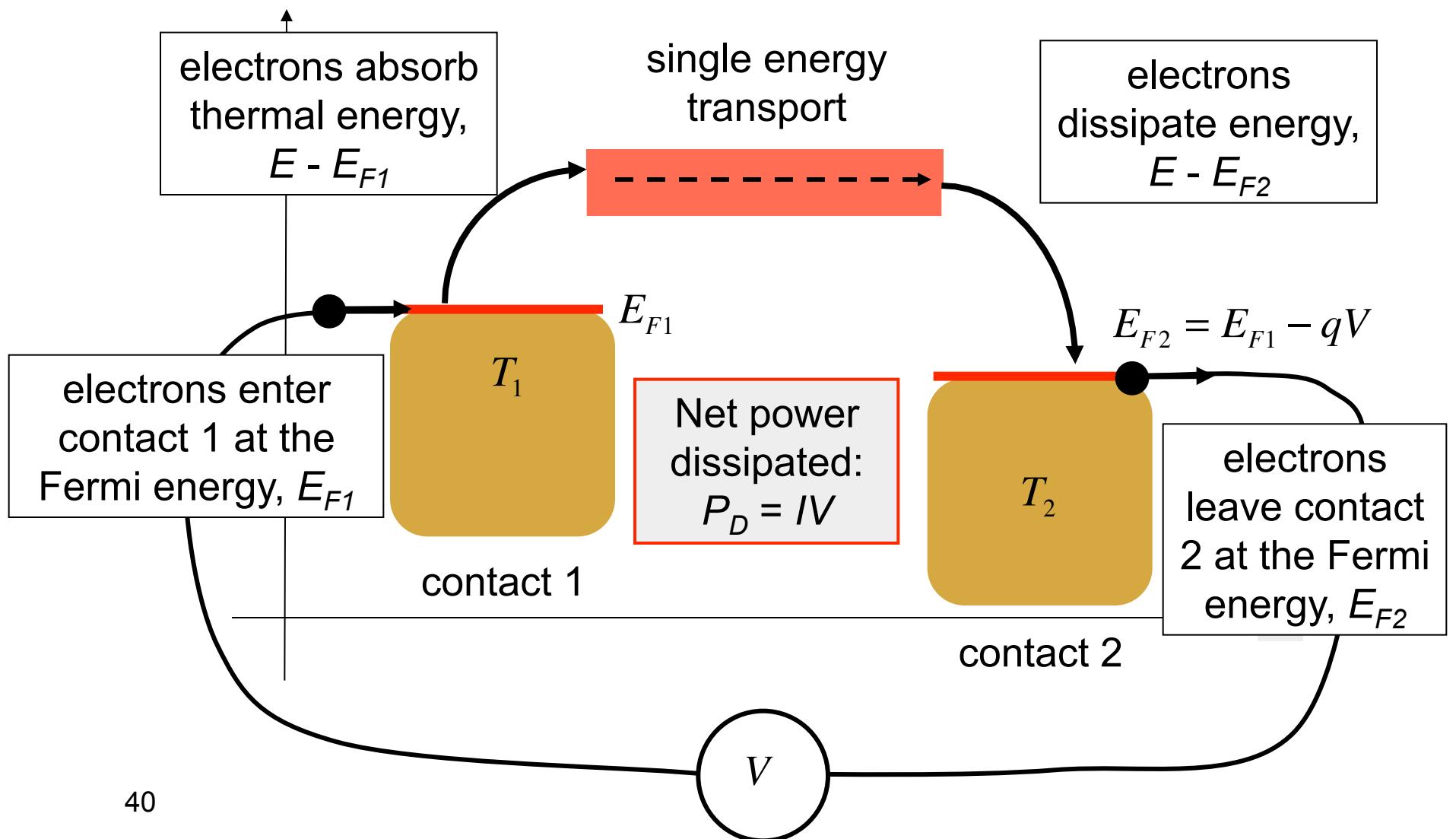


Y. M. Zuev, W. Chang, and P. Kim, "Thermoelectric and Magnetothermoelectric Transport Measurements of Graphene," *Phys. Rev. Lett.*, **109**, 096807, 2009.

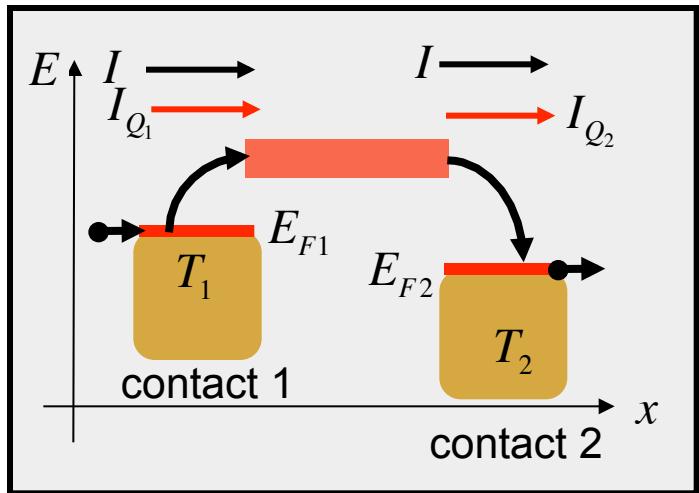
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one energy model



one-level model



$$\Delta V = R(E_0)I(E_0) - S(E_0)\Delta T$$

$$I_Q(E_0) = -\pi(E_0)I(E_0) - K_e(E_0)\Delta T$$

$$G(E_0) = \frac{2q^2}{h}T(E_0)M(E_0)\left(-\frac{\partial f_0}{\partial E}\right)$$

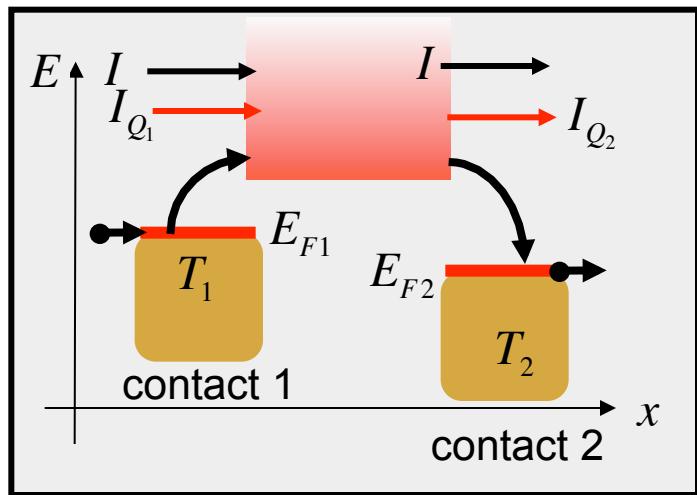
$$R(E_0) = \frac{1}{G(E_0)}$$

$$S(E_0) = \left(-\frac{k_B}{q}\right) \frac{(E_0 - E_F)}{k_B T}$$

$$\pi(E_0) = T S(E_0)$$

$$K_e(E_0) = 0$$

distribution of levels



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

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

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

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

$$\pi = TS$$

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

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

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

questions

- 1) Introduction
- 2) One energy level formulation
- 3) Distribution of energy levels
- 4) Discussion
- 5) Summary

