ECE 656: Fundamentals of Carrier Transport Fall 2013

Week 9 Summary:

Transmission and Phonon Transport

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10/19/13

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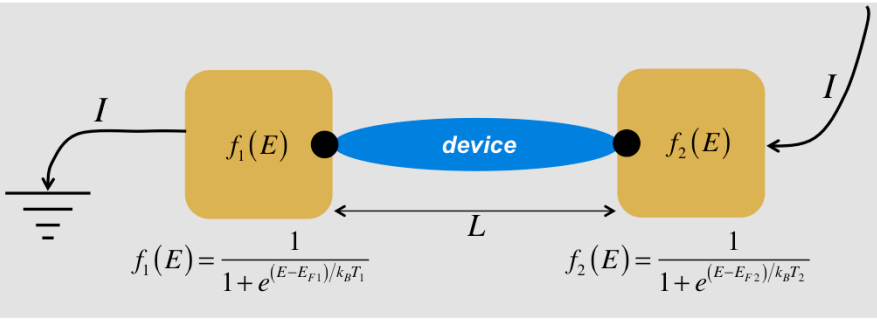
nano to macro device

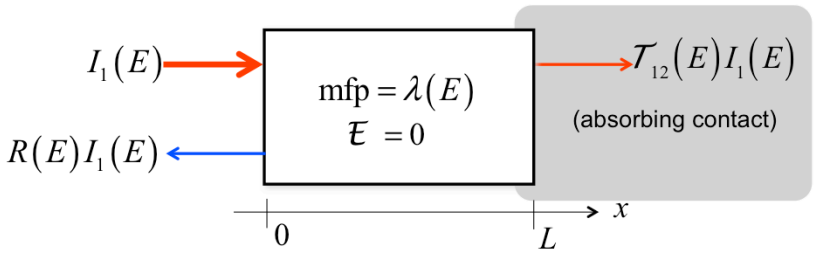
$$I = \frac{2q}{h}\int \mathcal{T}(E)M(E)(f_1 - f_2)\,dE$$



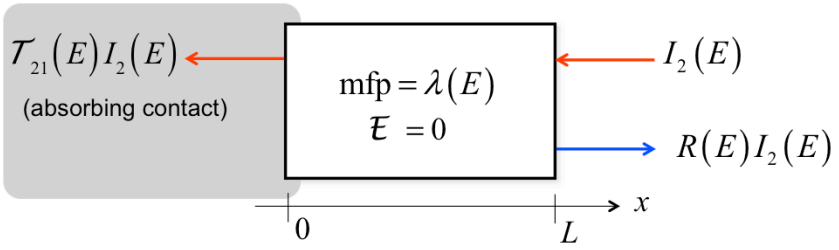
$$M_{3D}(E)A = A\frac{h}{4}\langle v_x^+ \rangle D_{3D}(E)$$

$$\mathcal{T}(E) = \frac{\lambda(E)}{\lambda(E)+L}$$

transmission across a field-free slab



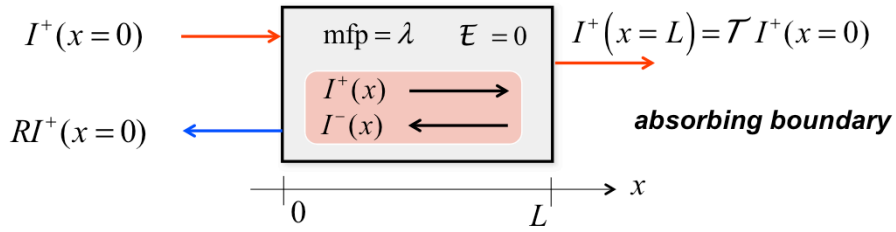
transmission across a field-free slab



In general, there *could* be injection from both the left and the right contacts.

For elastic scattering: $\mathcal{T}_{12}(E) = \mathcal{T}_{21}(E) = \mathcal{T}(E)$

transmission and mfp



$$\frac{dI^+(x)}{dx}=-\frac{I^+(x)}{\lambda}+\frac{I^-(x)}{\lambda}$$

$I=I^+(x)-I^-(x)$ (constant)

$$\mathcal{T}(E)=\frac{\lambda(E)}{\lambda(E)+L} \qquad \mathcal{T}(E)+R(E)=1$$

$\mathcal{T}\to 0 \quad L>>\lambda$

$\mathcal{T}\to 1 \quad L<<\lambda$

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mean-free-path

$$\lambda(E) \equiv 2\frac{\langle v_x^2 \tau_m \rangle}{\langle |v_x| \rangle}$$

This is an average over angle at a specific energy, *E*.

$$\lambda(E) = 2v(E)\tau_m(E) \quad \text{1D}$$

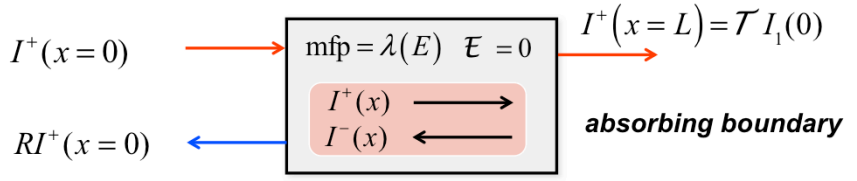
$$\lambda(E) = \frac{\pi}{2}v(E)\tau_m(E) \quad \text{2D}$$

$$\lambda(E) = \frac{4}{3}v(E)\tau_m(E) \quad \text{3D}$$

ECE-656 Lecture 17. http://nanohub.org/resources/7281.

Changwook Jeong, et al. "On Landauer vs. Boltzmann and Full Band vs. Effective Mass Evaluation of Thermoelectric Trans-port Coefficients," *J. Appl. Phys.*, **107**, 023707, 2010.

Fick's law of diffusion

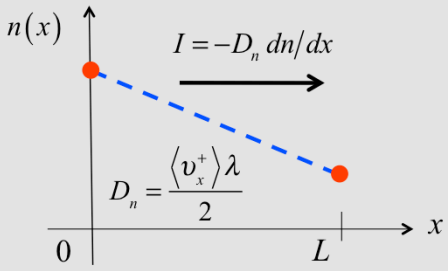


$$I = \frac{\langle v_x^+ \rangle}{2} \frac{\mathcal{T} L}{1-T} \times \left[\frac{n(0) - n(L)}{L} \right]$$

$$I = -D_n \frac{dn}{dx} \qquad D_n = \frac{\langle v_x^+ \rangle}{2} \frac{\mathcal{T} L}{1-\mathcal{T}}$$

$$\mathcal{T} = \frac{\lambda}{\lambda + L}$$

Fick's Law



estimating mfp from measurements

$$\mu_n \rightarrow D_n \rightarrow \frac{\left\langle \upsilon_x^+ \right\rangle \left\langle \left\langle \lambda \right\rangle \right\rangle}{2} \rightarrow \left\langle \left\langle \lambda \right\rangle \right\rangle$$

electrons and phonons

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electrons

Electrons in a solid behave as both particles (quasi-particles) and as waves.

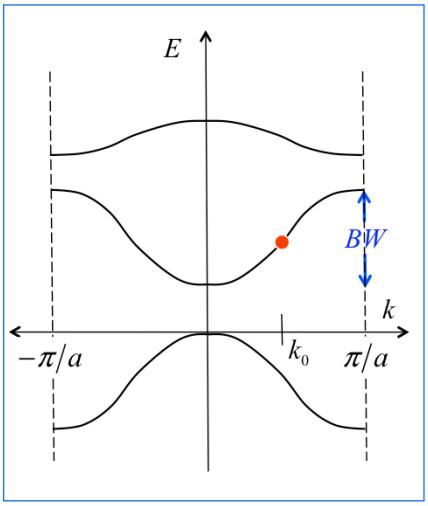
Electron waves are described by a "dispersion:" $E(\vec{k}) = \hbar\omega(\vec{k})$

Because the crystal is periodic, the dispersion is periodic in *k* (Brillouin zone).

Particles described by a "wavepacket."

The "group velocity" of a wavepacket is determined by the dispersion:

$$\vec{v}_g(\vec{k}) = \nabla_k E(\vec{k})/\hbar$$



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phonons

Lattice vibrations behave both as particles (quasi-particles) and as waves.

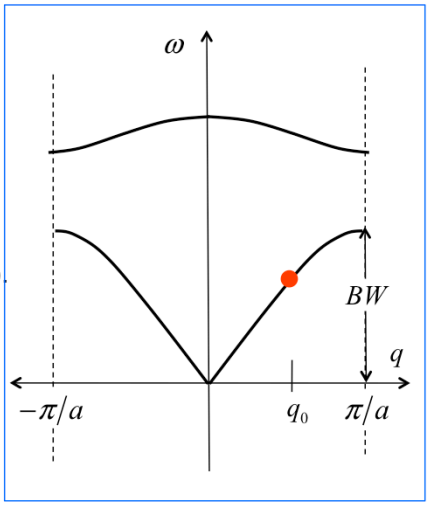
Lattice vibrations are described by a "dispersion:" $\omega(\vec{q}) = E(\vec{q})/\hbar$

Because the crystal is periodic, the dispersion is periodic in *k* (Brillouin zone).

Particles described by a "wavepacket."

The "group velocity" of a wavepacket is determined by the dispersion:

$$\vec{v}_g(\vec{q}) = \nabla_q \omega(\vec{q})$$



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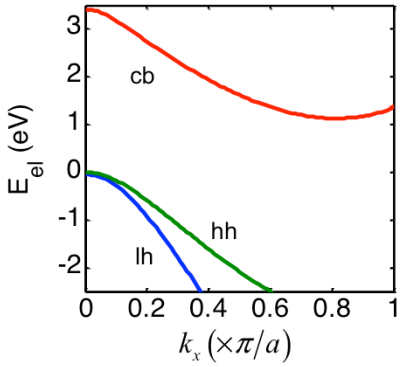
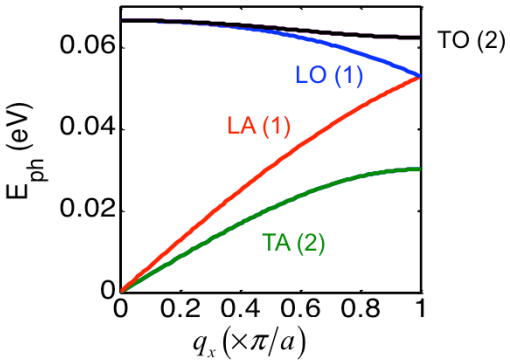
electron vs. phonon dispersion



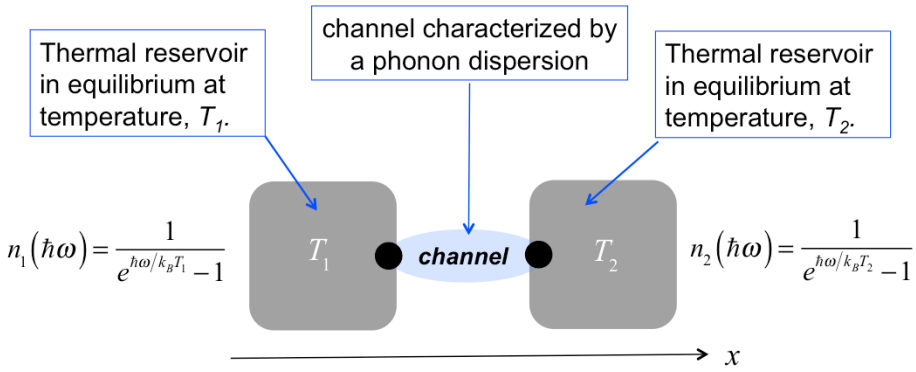


note the different energy scales!

electrons in Si (along [100])

phonons in Si (along [100])

Landauer approach to phonon transport



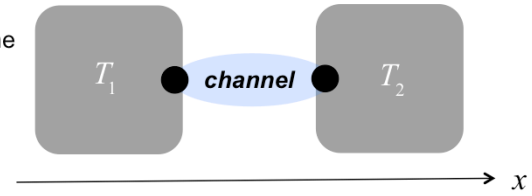
$$I = \frac{2q}{h}\int \mathcal{T}_{el}(E) M_{el}(E)(f_1 - f_2)\,dE \quad \Rightarrow \quad q = ?$$

heat flux

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

$$q = \frac{1}{h}\int (\hbar\omega)\mathcal{T}_{ph}(\hbar\omega) M_{ph}(\hbar\omega)(n_1 - n_2)\,d(\hbar\omega)$$

Assume **ideal contacts**, so that the transmission describes the transmission of the channel.



thermal conductance

1) Fourier's Law of heat conduction: $q = -K_L \Delta T_L$

2) Thermal conductance: $K_L = \frac{\pi^2 k_B^2 T}{3h} \int \mathcal{T}_{ph}(\hbar\omega) M_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega)$

3) Quantum of heat conduction: $\frac{\pi^2 k_B^2 T}{3h}$

4) Window function for phonons: $W_{ph}(\hbar\omega) = \left\{ \frac{3}{\pi^2} \left(\frac{\hbar\omega}{k_B T} \right)^2 \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right) \right\}$

electrical conductance

1) Electrical current: $I = G\Delta V$

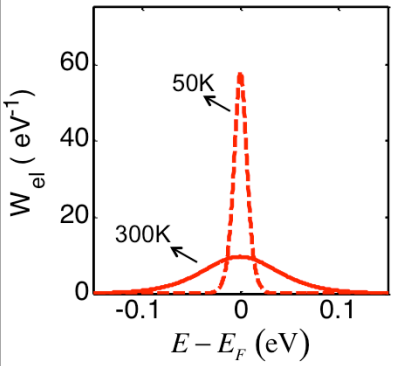
2) Electrical conductance: $G = \frac{2q^2}{h}\int \mathcal{T}_{el}(E) M_{el}(E) W_{el}\, dE$

3) Quantum of electrical conduction: $\frac{2q^2}{h}$

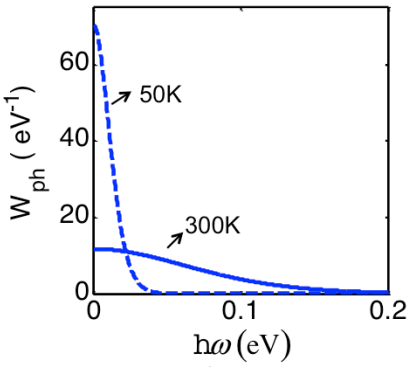
4) Window function for electrons: $W_{el}(E) = \left(-\partial f_0 / \partial E\right)$

window functions

Electrons



Phonons



$$W_{el}(E) = (-\partial f_0 / \partial E)$$

$$W_{ph}(\hbar\omega) = \left\{ \frac{3}{\pi^2} \left(\frac{\hbar\omega}{k_B T} \right)^2 \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right) \right\}$$

diffusive transport

$$q_x = -\kappa_L \frac{dT}{dx} \qquad \text{(Watts / m}^2\text{)}$$

$$\kappa_L = \frac{\pi^2 k_B^2 T}{3h} \left\langle M_{ph}/A \right\rangle \left\langle\left\langle \lambda_{ph} \right\rangle\right\rangle \qquad \text{(Watts/m-K)}$$

$$J_x = \sigma \frac{d\left(F_n/q\right)}{dx} \qquad \text{(Amperes / m}^2\text{)}$$

$$\sigma = \frac{2q^2}{h} \left\langle M_{el}/A \right\rangle \left\langle\left\langle \lambda_{el} \right\rangle\right\rangle \qquad \text{(1/Ohm-m)}$$

relation to specific heat

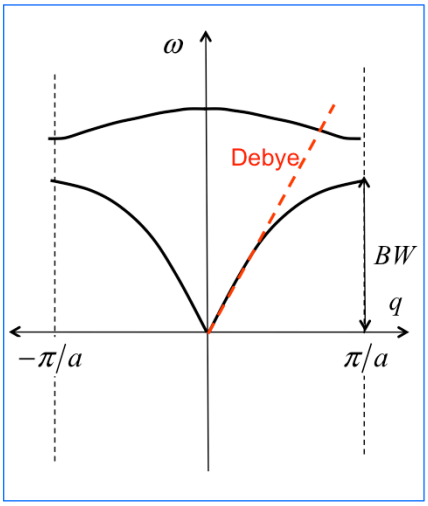
$$\kappa_L = \frac{\pi^2 k_B^2 T}{3h} \int \lambda_{ph}(\hbar\omega) \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega)\, d(\hbar\omega)$$

$$\kappa_L = \frac{1}{3} \langle\langle \Lambda_{ph} \rangle\rangle \langle v_{ph} \rangle C_V \qquad \lambda_{ph}(\hbar\omega) = (4/3)\Lambda_{ph}(\hbar\omega)$$

This expression can be simply derived from kinetic theory and is widely-used.

But the Landauer approach gives us a precise definition of the mfp and average phonon velocity.

Debye model for acoustic phonons



Linear dispersion model

$$\omega = \upsilon_D q$$

$$D_{ph}(\hbar\omega) = \frac{3(\hbar\omega)^2 \Omega}{2\pi^2 (\hbar\upsilon_D)^3} \quad \left(\text{J-m}^3\right)^{-1}$$

$$M_{ph}(\hbar\omega) = \frac{3(\hbar\omega)^2 A}{2\pi\hbar\upsilon_D^2} \quad \left(\text{m}^2\right)^{-1}$$

If acoustic phonons near q =0 mostly contribute to heat transport, the Debye model works well.

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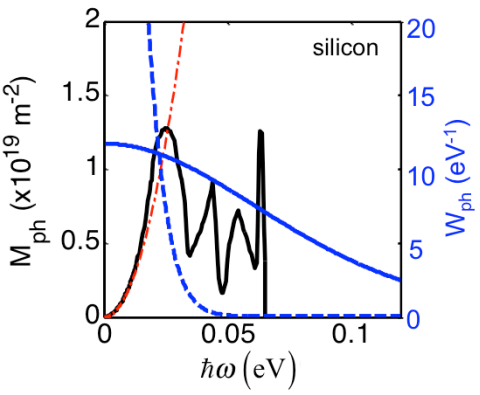
Debye model in practice



$$\kappa_L = \frac{\pi^2 k_B^2 T}{3h} \int \lambda_{ph} \frac{M_{ph}}{A} W_{ph}\, d(\hbar\omega)$$

M_{ph} Debye (Si)
full band (Si)

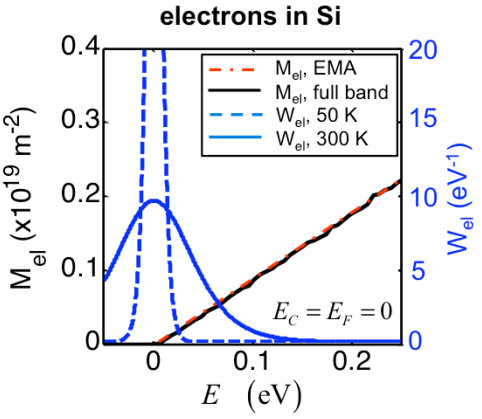
W_{ph} 50 K
300 K

Window function spans the entire BZ at room temp.

Debye model works well at very temperatures below 50 K.

effective mass model in practice

Parabolic dispersion assumption for electrons works well at room temperature.



phonon scattering

Electrons scatter from:

1) defects
   -e.g. charged impurities, neutral impurities, dislocations, etc.

2) phonons

3) surfaces and boundaries

4) other electrons

Scattering rates are computed from Fermi's Golden Rule.

Phonons scatter from:

1) defects
   -e.g. impurities, dislocations, isotopes, etc.

2) other phonons

3) surfaces and boundaries

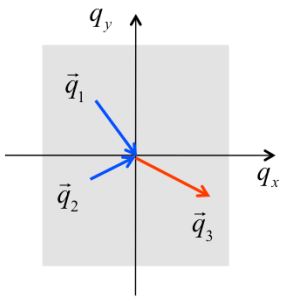
4) electrons ("phonon drag")

Scattering rates are computed from Fermi's Golden Rule.

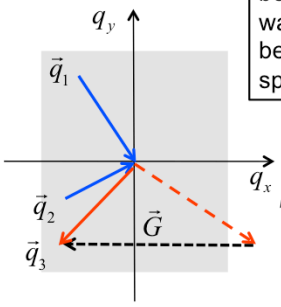
N and U processes

Need population of large q states for U-scattering. Need high T so that window function is broad and large q states are populated.

High q implies short wavelength. Unphysical because wavelength would be less than lattice spacing.

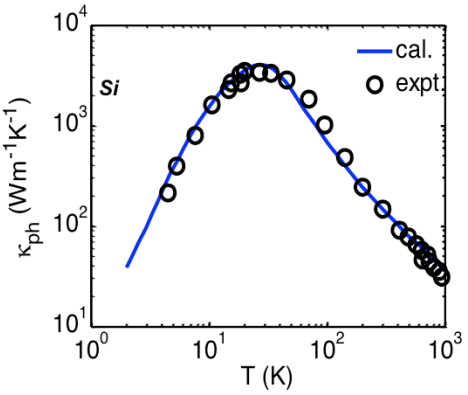


Normal (N) process
(momentum conserved)
Little effect on κ_L.



Umklapp (U) process
(momentum not conserved)
Lowers κ_L.

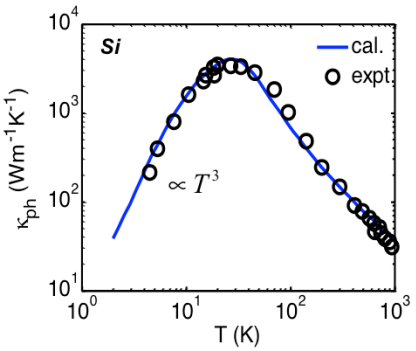
phonon conductivity vs. *T*



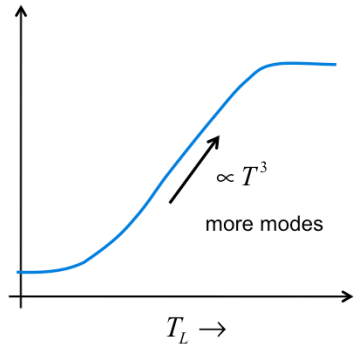
$$\kappa_L = \frac{\pi^2 k_B^2 T}{3h} \langle M_{ph} \rangle \times \langle\langle \lambda_{ph} \rangle\rangle$$

C. Jeong, S. Datta, M. Lundstrom, "Full Dispersion vs. Debye Model Evaluation of Lattice Thermal Conductivity with a Landauer approach," *J. Appl. Phys*. **109,** 073718-8, 2011.

population of phonon modes

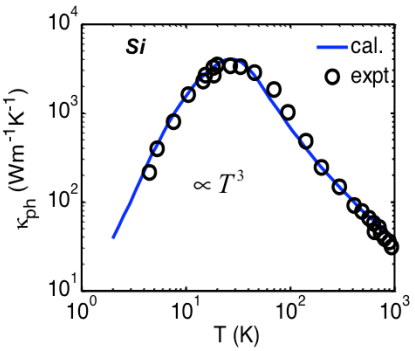


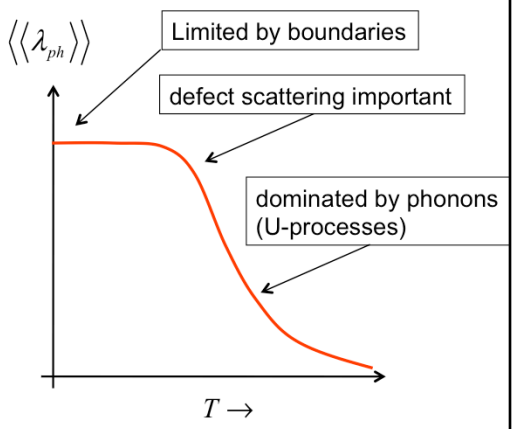
$\langle M_{ph}/A \rangle$



$$\langle M_{ph}/A \rangle \equiv \int \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega)\, d(\hbar\omega)$$

mfp vs. T





$$\frac{1}{\lambda_{ph}(\hbar\omega)} = \frac{1}{\lambda_D(\hbar\omega)} + \frac{1}{\lambda_B(\hbar\omega)} + \frac{1}{\lambda_U(\hbar\omega)}$$

electrons vs. phonons

The expressions look similar:

$$\kappa_L = \frac{\pi^2 k_B^2 T}{3h}\left\langle M_{ph}/A\right\rangle\left\langle\left\langle \lambda_{ph}\right\rangle\right\rangle \qquad \sigma = \frac{2q^2}{h}\left\langle M_{el}/A\right\rangle\left\langle\left\langle \lambda_{el}\right\rangle\right\rangle$$

In practice, the mfps often have similar values. **The difference is in <*M*>.**

For electrons, the location E_F can vary <*M*> over many orders of magnitude.

But even when $E_F = E_C$, <*M*> is much smaller for electrons than for phonons because for electrons, the BW >> k_BT which for phonons, BW ~ k_BT. Most of the modes are occupied for phonons but only a few for electrons.

summary

1) Our model for electrical conduction can readily be extended to describe phonon transport. The mathematical formulations are very similar.

2) Just as for electrons, phonon transport is quantized.

3) The difference BW's of the electron and phonon dispersions has important consequences. For electrons, a simple dispersion (effective mass) often gives good results, but for phonons, the simple dispersion (Debye model) is not very good.

4) There is no Fermi level for phonons, so the lattice thermal conductivity cannot be varied across many orders of magnitude like the electrical conductivity.