

Phonon Transport: A Landauer Approach

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Outline

- 1) **Quick review**
- 2) General model
- 3) Ballistic phonon transport
- 4) Diffusive phonon transport
- 5) Discussion
- 6) Questions?

Electrons and phonons

electrons

$$E(\vec{k})$$

$$\vec{v}_e(\vec{k}) = \frac{1}{\hbar} \vec{\nabla}_k E(\vec{k})$$

$$f_0(E) = \frac{1}{e^{(E-E_F)/k_B T_e} + 1}$$

phonons

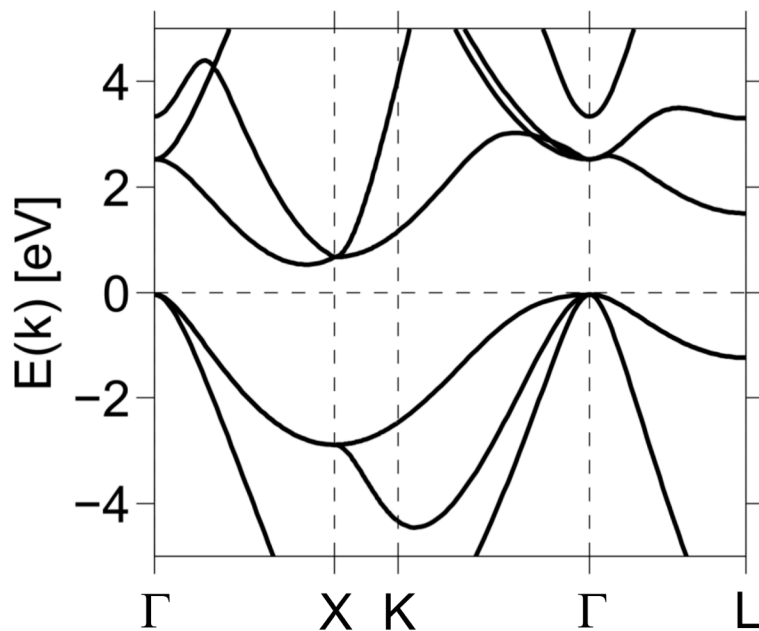
$$\omega(\vec{q}) \quad \{E(\vec{q}) = \hbar\omega(\vec{q})\}$$

$$\vec{v}_p(\vec{q}) = \vec{\nabla}_q \omega(\vec{q})$$

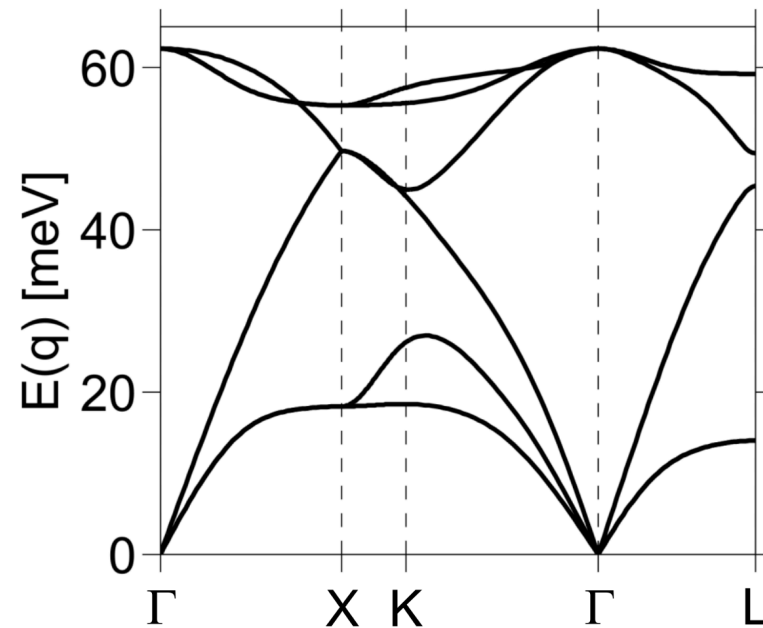
$$n_0(\hbar\omega) = \frac{1}{e^{\hbar\omega/k_B T_L} - 1}$$

Electrons and phonon dispersion

electrons in Si



phonons in Si



note the different energy scales!

(DFT calculations by Dr. J. Maassen, Dalhousie)

Heat flow by lattice vibrations (phonons)

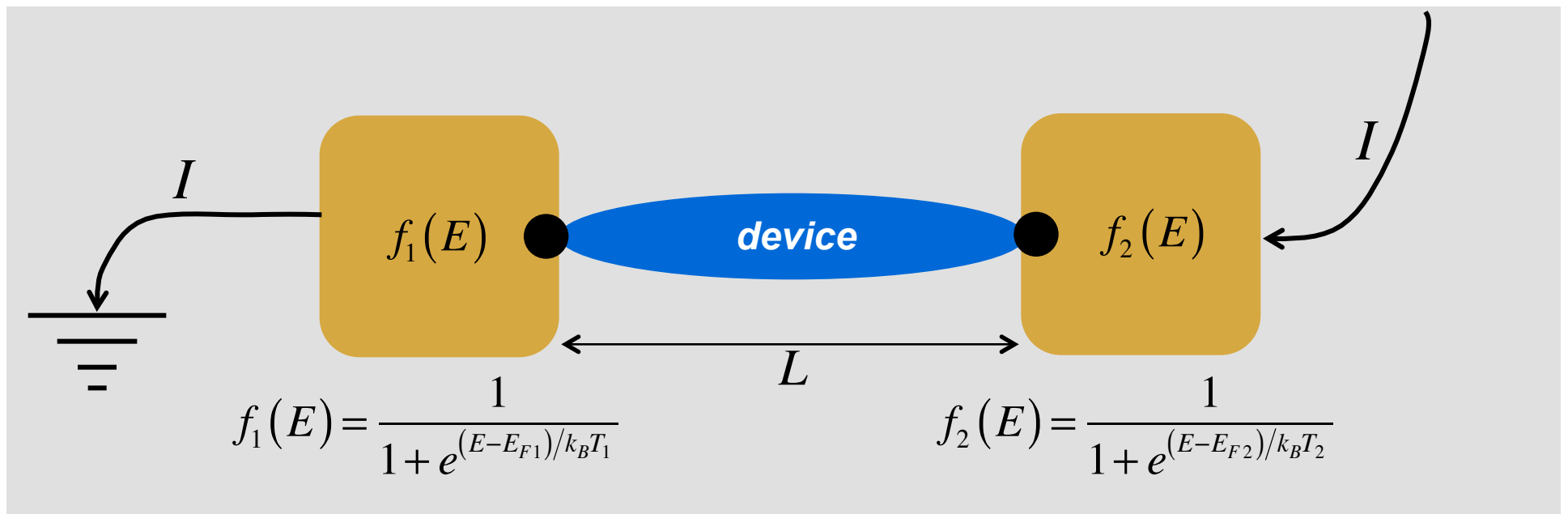
$$J_Q = -\kappa_L \frac{dT_L}{dx} \quad (\text{Watts / m}^2)$$

$$\kappa_L = \frac{1}{3} \Lambda_{ph} v_{ph} C_V \quad (\text{Watts/m-K})$$

$$E_L = \int_0^{\infty} (\hbar\omega) D_{ph}(\hbar\omega) n_0(\hbar\omega) d(\hbar\omega) \quad C_V = \left. \frac{\partial E_L}{\partial T} \right|_V$$

Review: electron transport (3D)

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

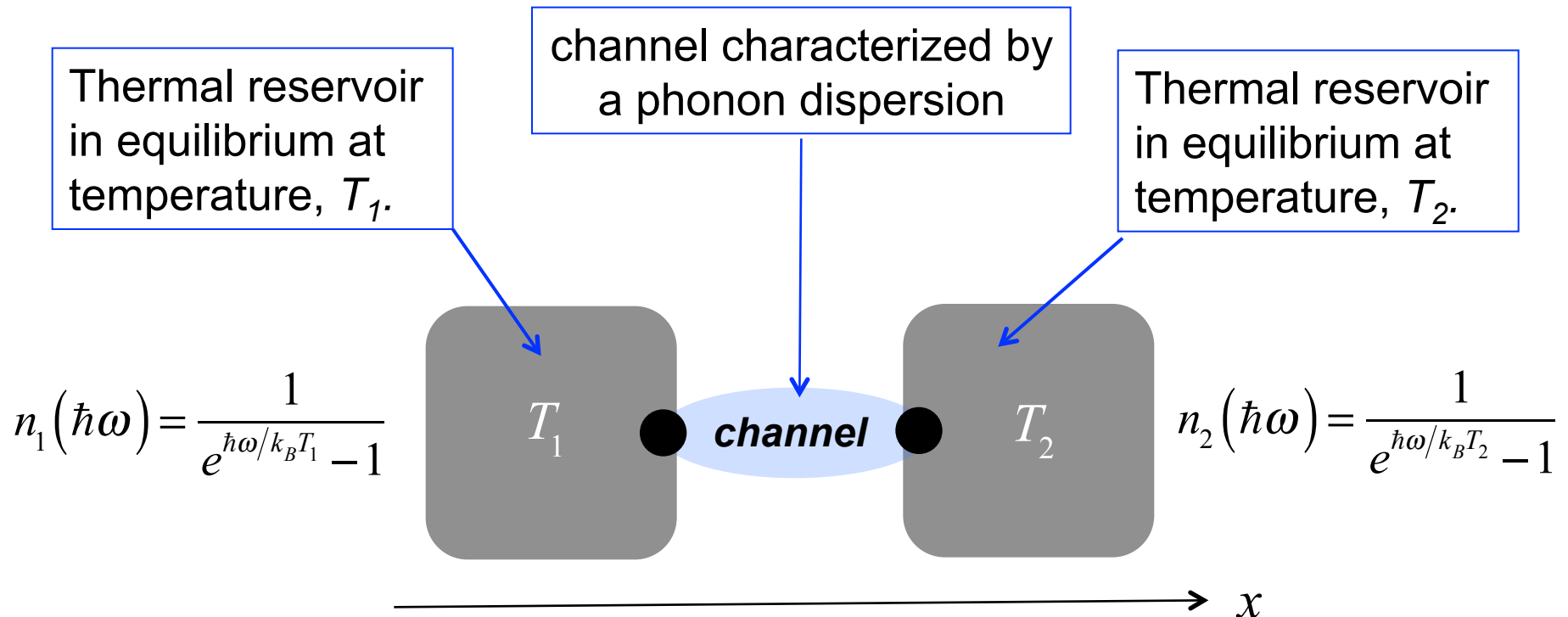


$$M_{el}(E) = A \frac{h}{4} \langle v_x^+ \rangle D_{3D}(E) \quad \mathcal{T}_{el}(E) = \frac{\lambda(E)}{\lambda(E) + L}$$

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Landauer approach to phonon transport



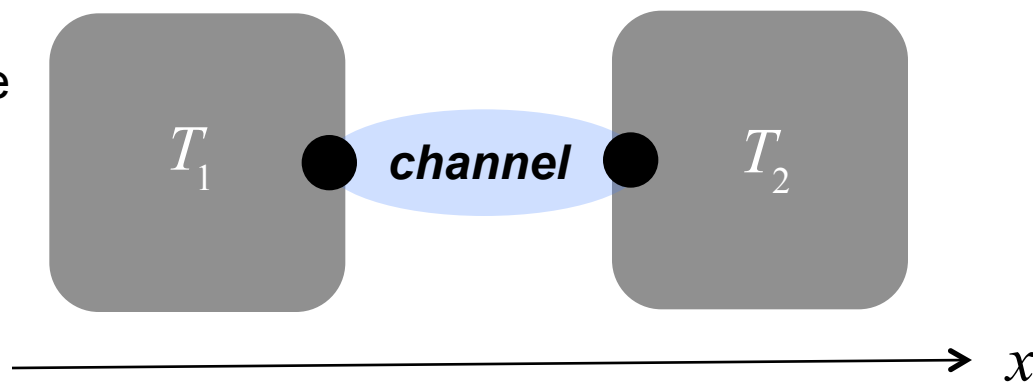
$$I = \frac{2q}{h} \int \mathcal{T}_{el}(E) M_{el}(E) (f_1 - f_2) dE \Rightarrow I_Q = ?$$

Heat flux

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

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

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



Near-equilibrium heat flux

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

$$n_2 \approx n_1 + \frac{\partial n_1}{\partial T_L} \Delta T_L \quad \Delta T_L = T_2 - T_1 \quad (n_1 - n_2) \approx -\frac{\partial n_1}{\partial T_L} \Delta T_L \approx -\frac{\partial n_0}{\partial T_L} \Delta T_L$$

$$\frac{\partial n_0}{\partial T_L} = \frac{\partial}{\partial T_L} \left\{ \frac{1}{e^{\hbar\omega/k_B T_L} - 1} \right\}$$

$$\frac{\partial n_0}{\partial T_L} = \frac{\hbar\omega}{T_L} \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right)$$

$$(n_1 - n_2) \approx -\frac{\hbar\omega}{T_L} \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right) \Delta T_L$$

$$I_Q = -K_L \Delta T_L$$

Lattice thermal conductance (i)

$$I_Q = \frac{1}{h} \int (\hbar\omega) \mathcal{T}_{ph}(\hbar\omega) M_{ph}(\hbar\omega) (n_1 - n_2) d(\hbar\omega) \quad (n_1 - n_2) \approx -\frac{\hbar\omega}{T_L} \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right) \Delta T_L$$

$$I_Q = -K_L \Delta T_L$$

$$K_L = \frac{(k_B T_L)^2}{h T_L} \int \mathcal{T}_{ph}(\hbar\omega) M_{ph}(\hbar\omega) \left\{ \left(\frac{\hbar\omega}{k_B T_L} \right)^2 \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right) \right\} d(\hbar\omega)$$

Lattice thermal conductance (ii)

$$I_Q = -K_L \Delta T_L$$

$$K_L = \frac{k_B^2 T_L}{h} \int \mathcal{T}_{ph}(\hbar\omega) M_{ph}(\hbar\omega) \left\{ \left(\frac{\hbar\omega}{k_B T_L} \right)^2 \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right) \right\} d(\hbar\omega)$$

Recall the electrical conductance:

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

“window function”:

$$W_{el}(E) = (-\partial f_0 / \partial E) \int_{-\infty}^{+\infty} (-\partial f_0 / \partial E) dE = 1$$

Lattice thermal conductance (iii)

$$Q = -K_L \Delta T_L \quad K_L = \frac{k_B^2 T_L}{h} \int \mathcal{T}_{ph}(\hbar\omega) M_{ph}(\hbar\omega) \left\{ \left(\frac{\hbar\omega}{k_B T_L} \right)^2 \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right) \right\} d(\hbar\omega)$$

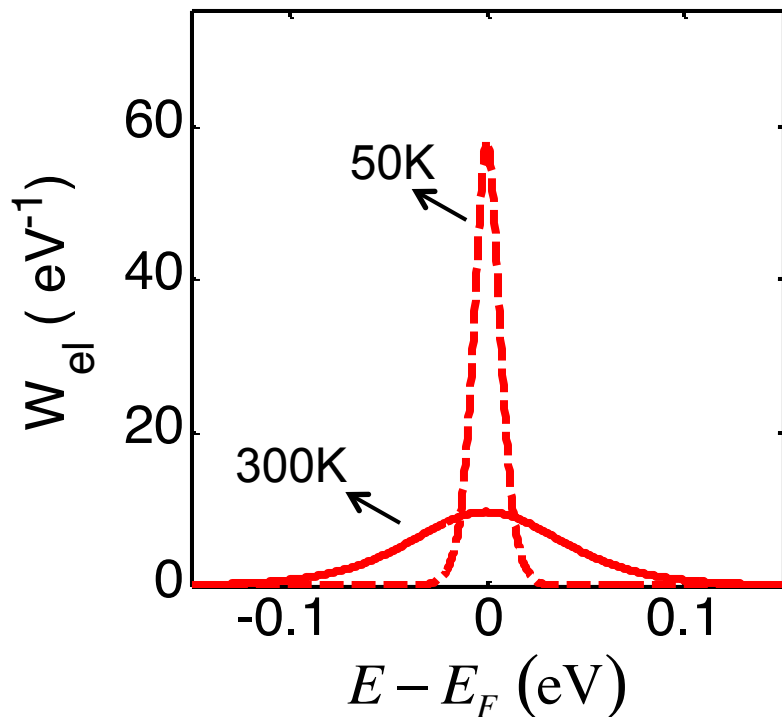
$$\int_0^{+\infty} \left(\frac{\hbar\omega}{k_B T_L} \right)^2 \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right) d(\hbar\omega) = \frac{\pi^2}{3}$$

$$K_L = \frac{\pi^2 k_B^2 T_L}{3h} \int \mathcal{T}_{ph}(\hbar\omega) M_{ph}(\hbar\omega) \left\{ \frac{3}{\pi^2} \left(\frac{\hbar\omega}{k_B T_L} \right)^2 \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right) \right\} d(\hbar\omega)$$

$$W_{ph}(\hbar\omega)$$

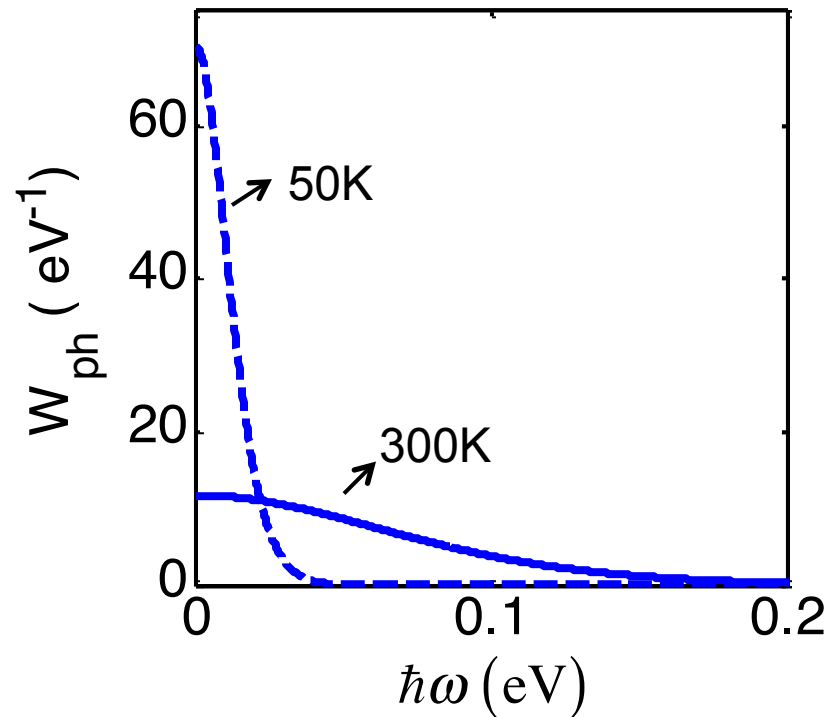
Window functions: electrons vs. phonons

Electrons



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

Phonons



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

Recap: Heat conduction

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

2) Thermal conductance:

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

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

4) Window function for phonons:

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

Compare to: Electrical conduction

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

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Ballistic phonon transport

$$I_Q = -K_L \Delta T_L = \frac{\Delta T_L}{R_L} \quad K_L = \frac{\pi^2 k_B^2 T_L}{3h} \int \mathcal{T}_{ph}(\hbar\omega) M_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega)$$

Ballistic phonon transport: $\mathcal{T}_{ph}(\hbar\omega) = 1$

$$K_L = \frac{\pi^2 k_B^2 T_L}{3h} \int M_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega)$$

Finite thermal conductance even for ballistic phonon transport.

Analogous to quantum contact resistance for electrons
“Kapitza resistance”

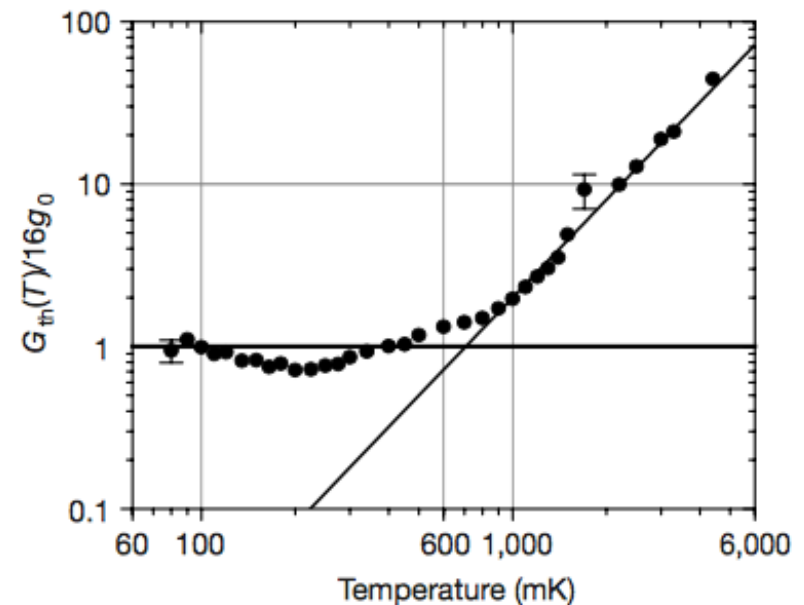
Quantized thermal transport

Measurement of the quantum of thermal conductance

K. Schwab*, E. A. Henriksen*, J. M. Worlock*† & M. L. Roukes*

* Condensed Matter Physics 114-36, California Institute of Technology, Pasadena, California 91125, USA

The physics of mesoscopic electronic systems has been explored for more than 15 years. Mesoscopic phenomena in transport processes occur when the wavelength or the coherence length of the carriers becomes comparable to, or larger than, the sample dimensions. One striking result in this domain is the quantization of electrical conduction, observed in a quasi-one-dimensional constriction formed between reservoirs of two-dimensional electron gas^{1,2}. The conductance of this system is determined by the number of participating quantum states or 'channels' within the



K. Schwab, E. A. Henriksen, J. M. Worlock, and M. L. Roukes, *Nature*, **404**, 974, 2000.

$$g_0 = \frac{\pi^2 k_B^2 T_L}{3h}$$

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Diffusive heat transport (3D)

$$I_Q = -K_L \Delta T_L \quad (\text{Watts})$$

$$K_L = \frac{\pi^2 k_B^2 T_L}{3h} \int \mathcal{T}_{ph}(\hbar\omega) M_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega) \quad (\text{Watts/K})$$

$$\mathcal{T}_{ph}(\hbar\omega) = \frac{\lambda_{ph}(\hbar\omega)}{\lambda_{ph}(\hbar\omega) + L} \rightarrow \frac{\lambda_{ph}(\hbar\omega)}{L} \quad (\text{diffusive phonon transport})$$

$$K_L = \frac{\pi^2 k_B^2 T_L}{3h} \int \frac{\lambda_{ph}(\hbar\omega)}{L} M_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega)$$

Conductance and conductivity

$$I_Q = -K_L \Delta T_L \quad (\text{Watts})$$

$$J_Q = -\kappa_L \frac{dT_L}{dx} \quad (\text{Watts/m}^2)$$

$$K_L = \kappa_L \frac{A}{L} \quad (\text{Watts/K})$$

$$\kappa_L = K_L \frac{L}{A} \quad (\text{Watts/m-K})$$

Conductance and conductivity

$$I_Q = -K_L \Delta T_L \quad (\text{Watts})$$

$$J_Q = -\kappa_L \frac{dT_L}{dx} \quad (\text{Watts/m}^2)$$

$$\kappa_L = K_L \frac{L}{A}$$

$$K_L = \frac{\pi^2 k_B^2 T_L}{3h} \int \frac{\lambda_{ph}(\hbar\omega)}{L} M_{ph}(\hbar\omega) W_{ph}(\hbar\omega) d(\hbar\omega)$$

$$\kappa_L = \frac{\pi^2 k_B^2 T_L}{3h} \int \lambda_{ph}(\hbar\omega) \left(M_{ph}(\hbar\omega) / A \right) W_{ph}(\hbar\omega) d(\hbar\omega) \quad \checkmark$$

Diffusive heat transport (3D)

$$J_Q = -\kappa_L \frac{dT_L}{dx} \quad (\text{Watts / m}^2)$$

$$\kappa_L = \frac{\pi^2 k_B^2 T_L}{3h} \int \lambda_{ph}(\hbar\omega) \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega) d(\hbar\omega) \quad (\text{Watts/m-K})$$

$$J_n = \sigma \frac{d(F_n/q)}{dx} \quad (\text{Amperes / m}^2)$$

$$\sigma = \frac{2q^2}{h} \int \lambda_{el}(E) \frac{M_{el}(E)}{A} W_{el}(E) dE \quad (1/\text{Ohm-m})$$

Diffusive heat transport (3D)

$$J_Q = -\kappa_L \frac{dT_L}{dx} \quad (\text{Watts / m}^2)$$

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

$$J_n = \sigma \frac{d(F_n/q)}{dx} \quad (\text{Amperes / m}^2)$$

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

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 - Debye model
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 - MFP distribution
- 5) Summary

Connection to traditional approach

Recall that for electrons, we related our Landauer approach to the mobility, because mobility is a traditional quantity that is widely used.

$$\sigma = \frac{2q^2}{h} \langle M_{el}/A \rangle \langle \langle \lambda_{el} \rangle \rangle \leftrightarrow n_0 q \mu_n$$

Connection to traditional approach

The traditional expression for the lattice thermal conductivity is:

$$\kappa_L = \frac{1}{3} \Lambda_{ph} v_{ph} C_V \quad (\text{Watts/m-K})$$

Where C_V is the specific heat at constant volume.

$$E_L = \int_0^{\infty} (\hbar\omega) D_{ph}(\hbar\omega) n_0(\hbar\omega) d(\hbar\omega) \quad C_V = \left. \frac{\partial E_L}{\partial T} \right|_V$$

Specific heat is related to DOS.

Connection to traditional approach

$$\kappa_L = \frac{\pi^2 k_B^2 T}{3h} \langle M_{ph}/A \rangle \langle \langle \lambda_{ph} \rangle \rangle \leftrightarrow \frac{1}{3} \Lambda_{ph} v_{ph} C_V \quad (\text{Watts/m-K})$$

$$\lambda_{ph}(\hbar\omega) = \frac{4}{3} v_{ph}(\hbar\omega) \tau_m(\hbar\omega) = \frac{4}{3} \Lambda(\hbar\omega)$$

$$M_{ph}/A = \frac{h}{2} \langle v_{ph}^+ \rangle D_{ph}(\hbar\omega) \quad \langle v_{ph}^+ \rangle = \frac{v_{ph}^+}{2}$$

See Lundstrom and Jeong, NET, Exercise 9.1, p. 180.

Outline

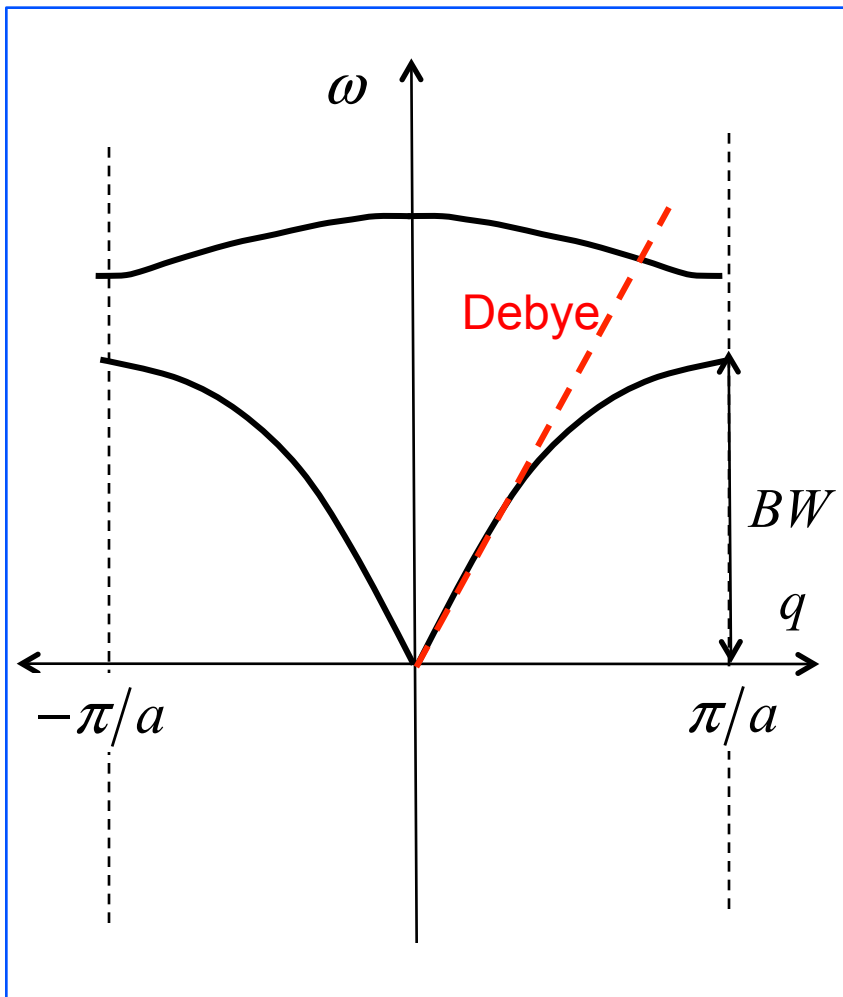
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Debye model for acoustic phonons



Linear dispersion model

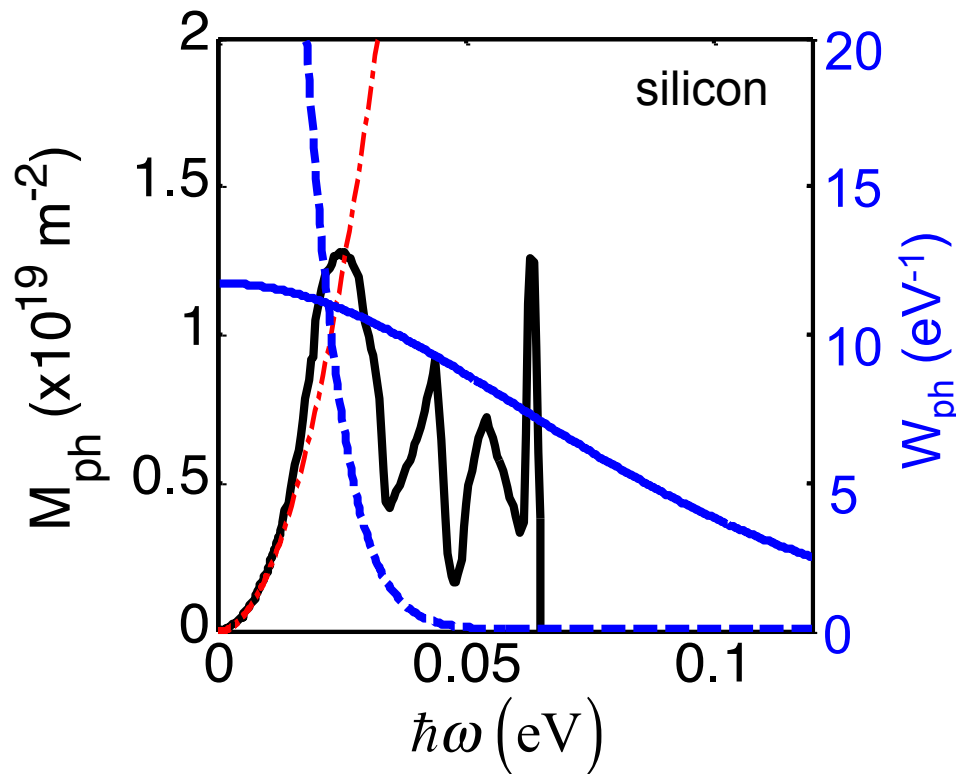
$$\omega = v_D q$$

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

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

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

Debye model in practice



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

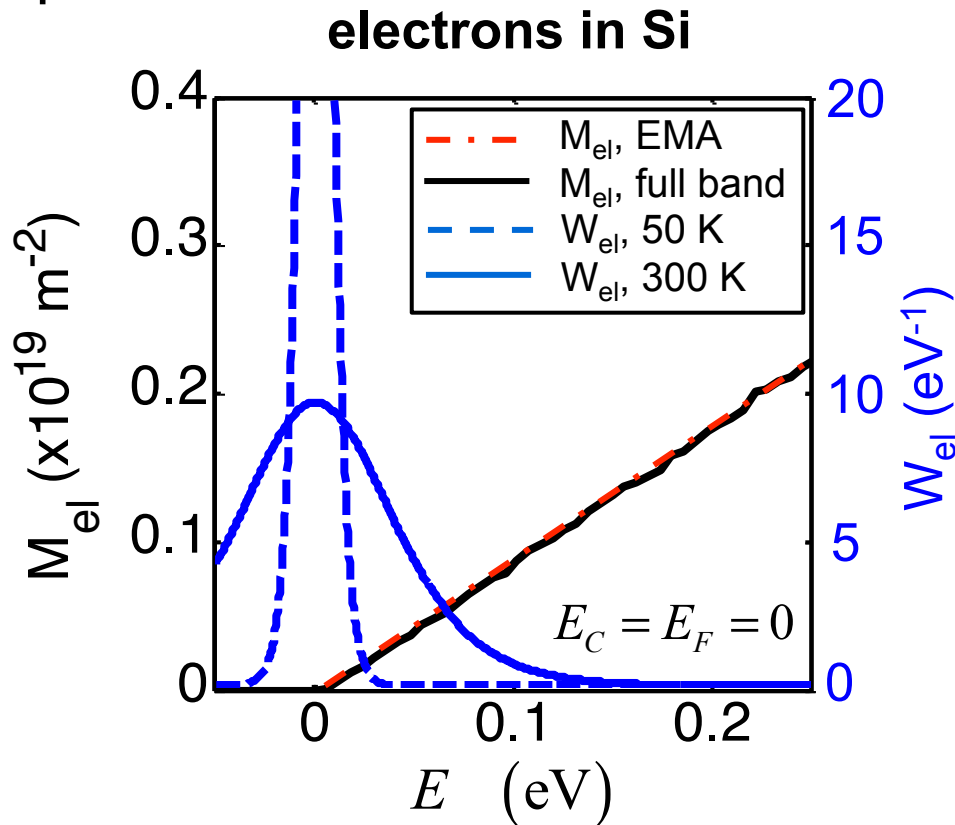
- M_{ph} - · - Debye (Si)
 — full band (Si)
- W_{ph} - - - 50 K
 — 300 K

Window function spans the entire BZ at room temp.

Debye model works well at very temperatures below 50 K.

Compare to: Effective mass model for electrons

Parabolic dispersion assumption for electrons works well at room temperature.



Outline

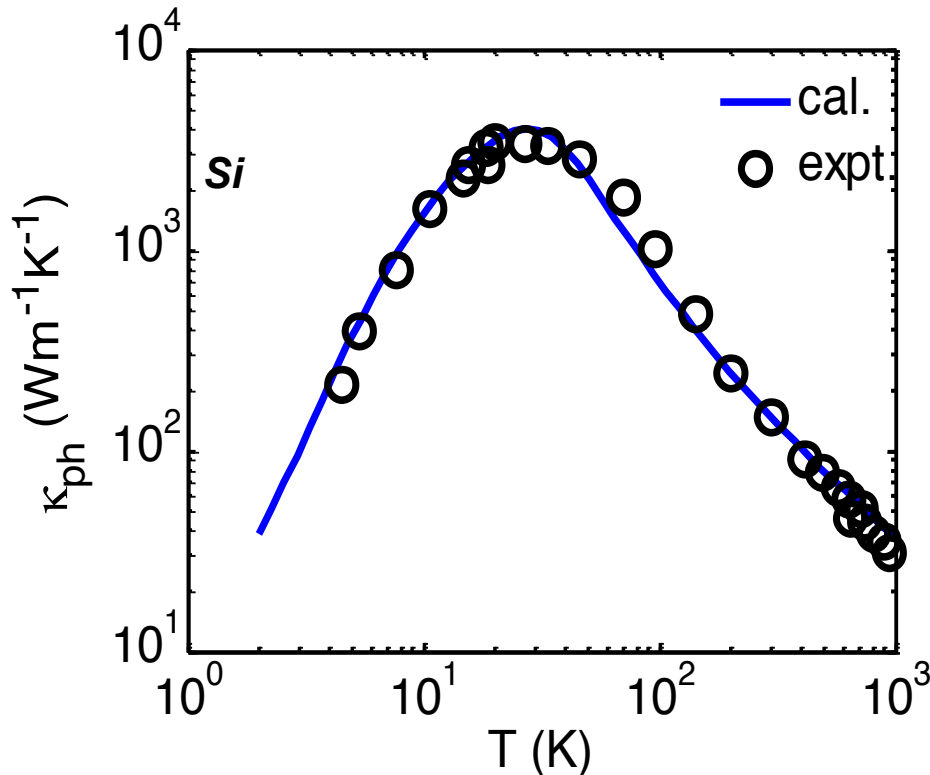
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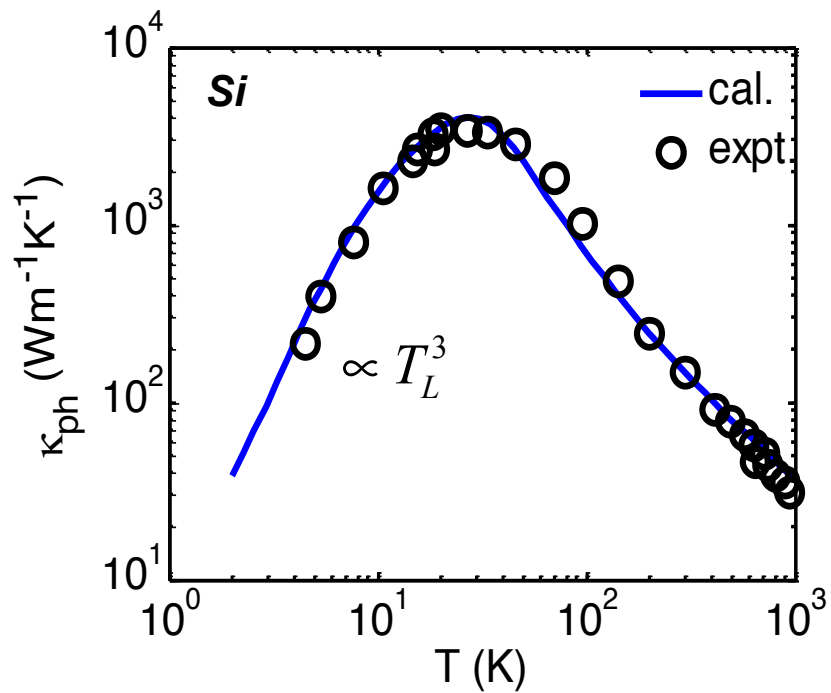
i) measured vs. calculated $\kappa_L(T_L)$ for silicon



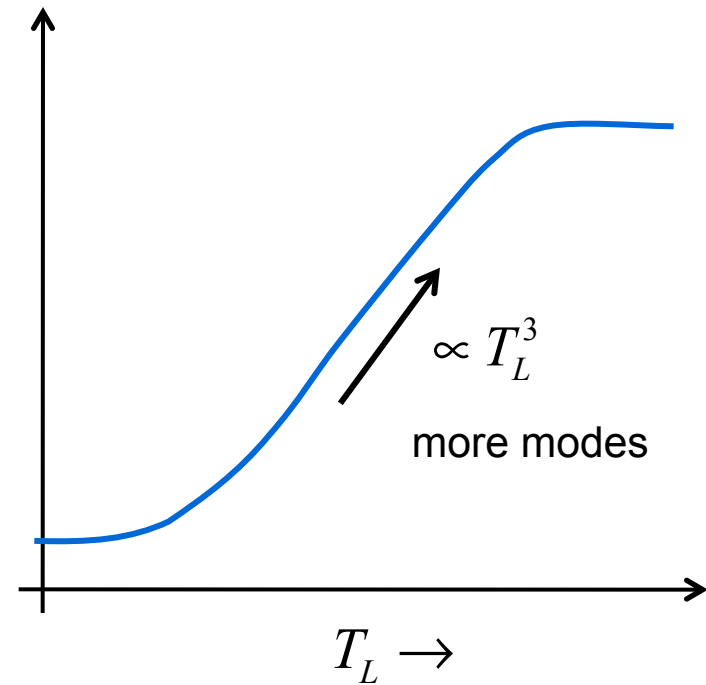
$$\kappa_L = \frac{\pi^2 k_B^2 T_L}{3h} \langle M_{ph} \rangle \times \langle \langle \lambda_{ph} \rangle \rangle$$

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 modes vs. T_L

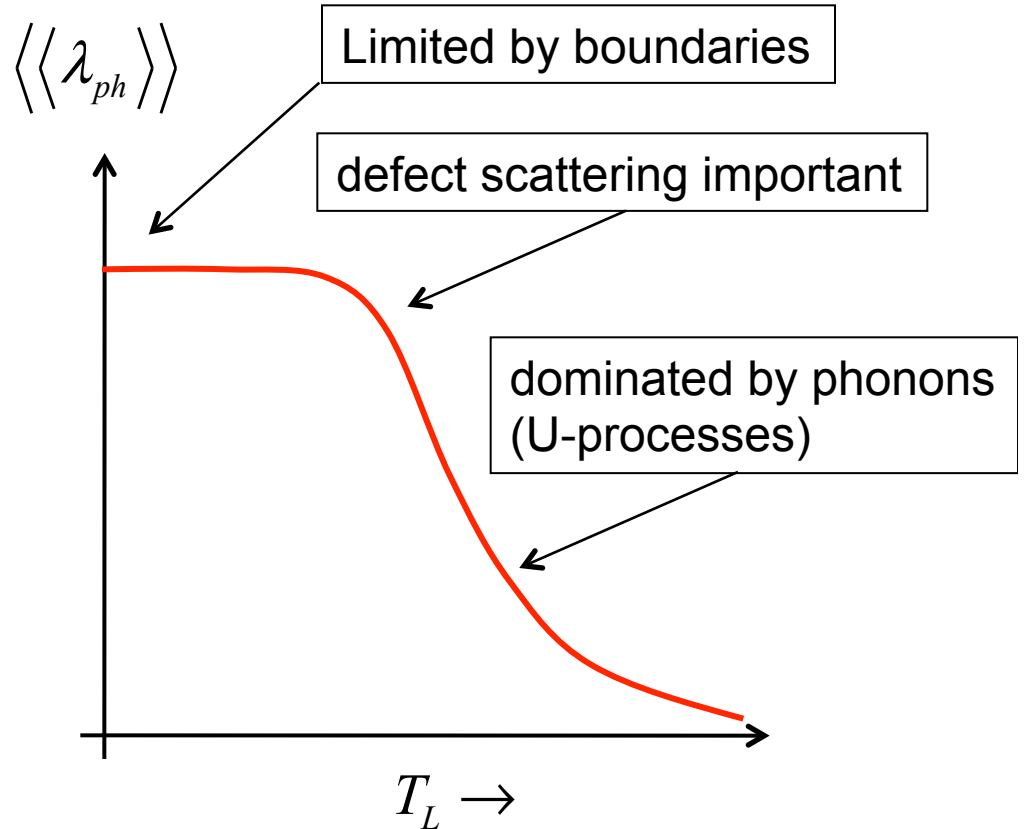
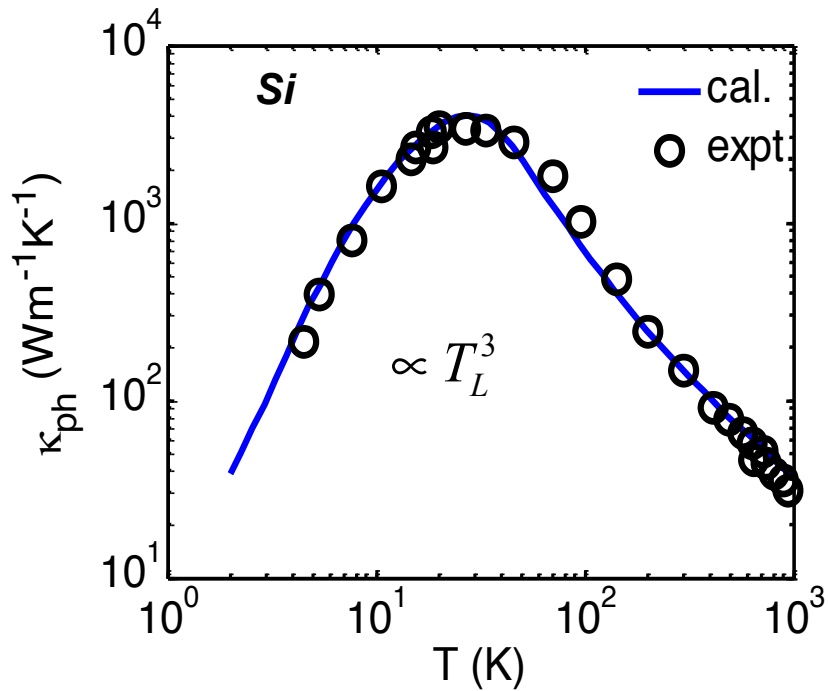


$$\langle M_{ph} / A \rangle$$



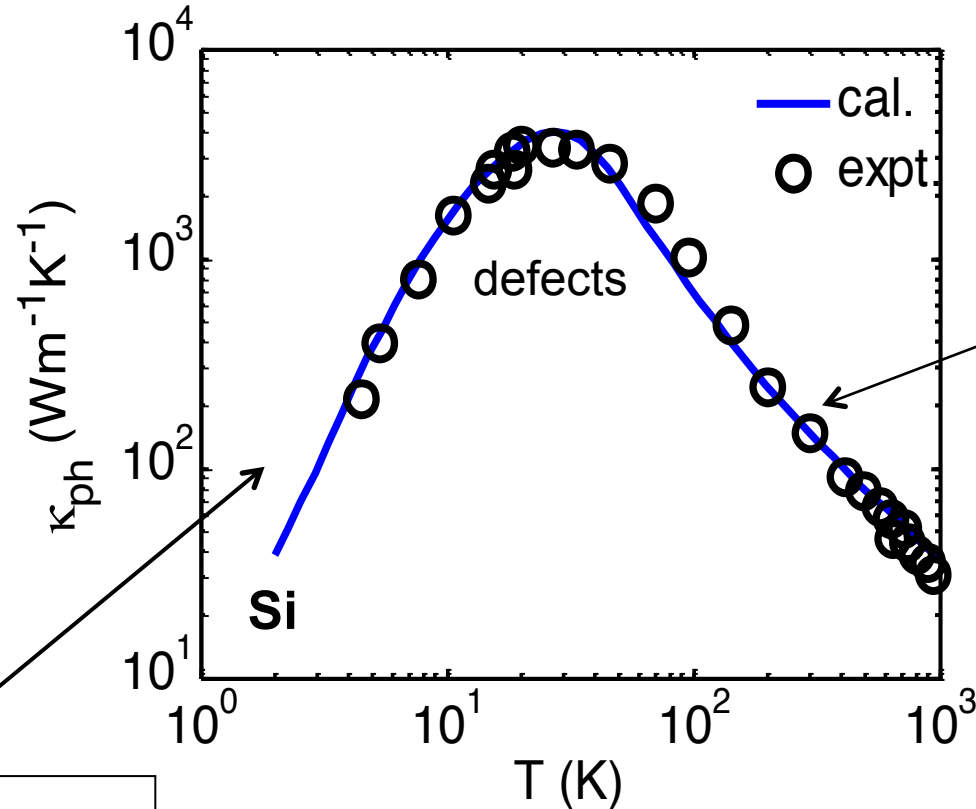
$$\langle M_{ph} / A \rangle \equiv \int \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega) d(\hbar\omega)$$

Mean-free-path vs. T_L



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

Temperature-dependent thermal conductivity



population of modes and boundary scattering

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

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MFP and thermal conductivity

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

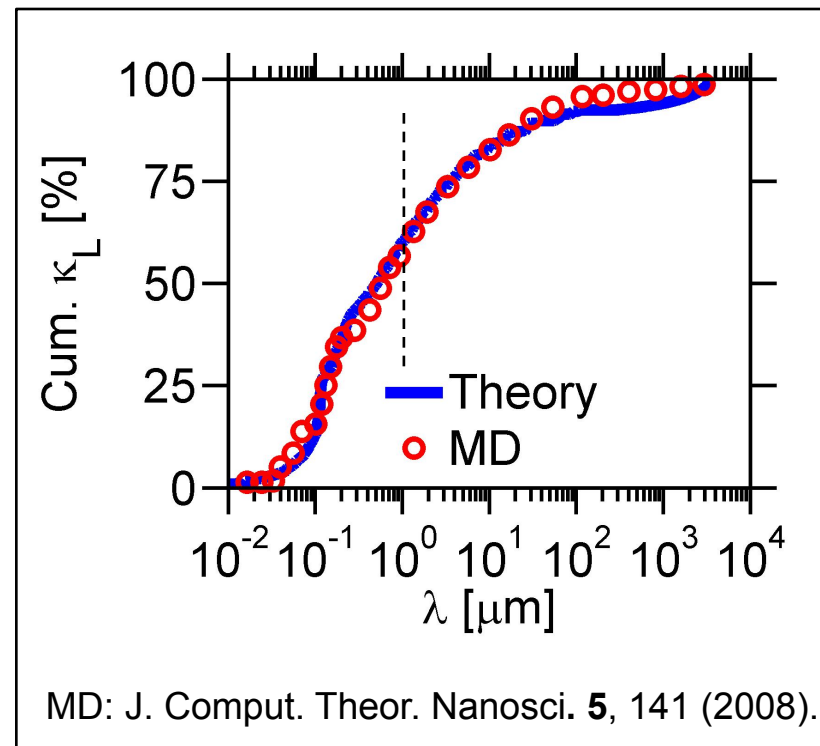
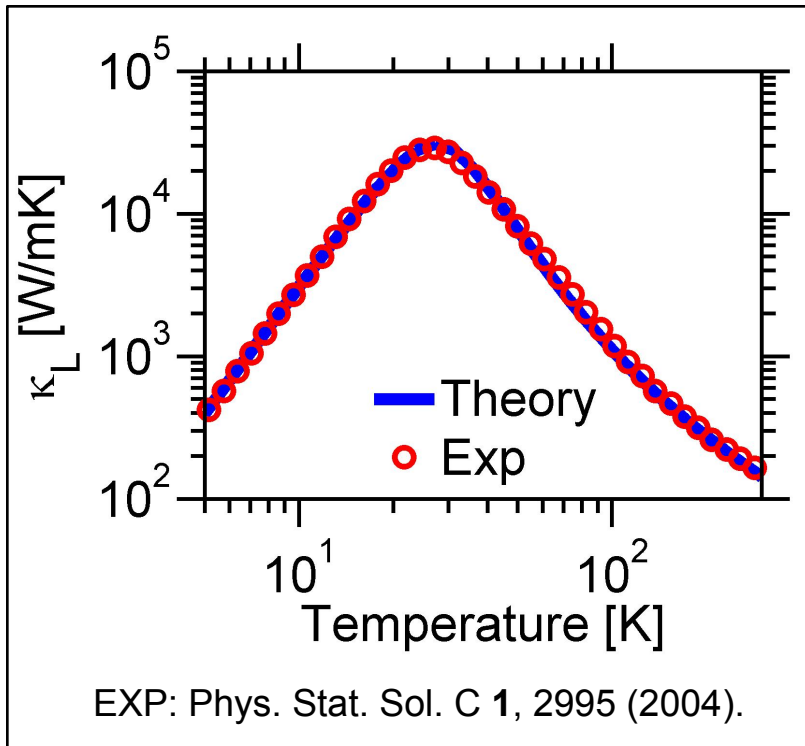
$$\kappa_L = \frac{\pi^2 k_B^2 T}{3h} \int \left[\lambda_{ph}(\hbar\omega) \left(M_{ph}(\hbar\omega) / A \right) W_{ph}(\hbar\omega) \frac{d(\hbar\omega)}{d\lambda_{ph}} \right] d\lambda_{ph}$$

$$\kappa_L = \int \kappa_\lambda d\lambda_{ph}$$

$$\kappa_\lambda(\lambda_{ph}) = \frac{\pi^2 k_B^2 T}{3h} \lambda_{ph}(\hbar\omega) \left(M_{ph}(\hbar\omega) / A \right) W_{ph}(\hbar\omega) \frac{d(\hbar\omega)}{d\lambda_{ph}}$$

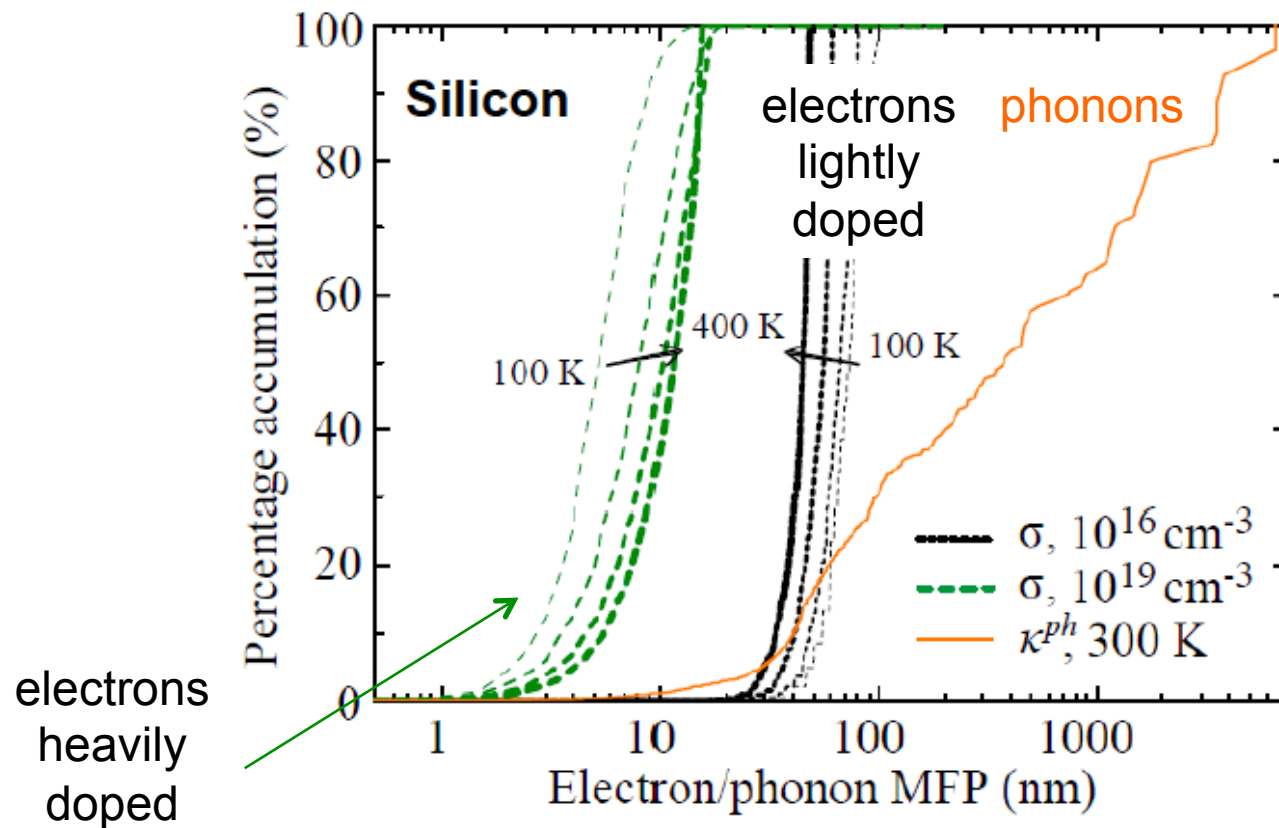
“MFP distribution”

MFP and thermal conductivity



$$\text{Cumm } \kappa_L(\lambda_1) = \left(\int_0^{\lambda_1} \kappa_\lambda d\lambda \right) / \kappa_L^{\text{bulk}}$$

MFP spectra – phonons vs. electrons



J. Zhou, B. Liao and G. Chen, "First-principles calculations of thermal, electrical, and thermoelectric transport properties of semiconductors," *Semicond. Sci. and Technol.*, **31**, 043001, 2016.

MFP spectra – phonons vs. electrons

Phonons have a broad distribution of MFPs; electrons have a much tighter distribution of MFP's.

J. Zhou, B. Liao and G. Chen, “First-principles calculations of thermal, electrical, and thermoelectric transport, properties of semiconductors,” *Semicond. Sci. and Technol.*, **31**, 043001, 2016.

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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.

Electron vs. phonon conductivities

The expressions look similar:

$$\kappa_L = \frac{\pi^2 k_B^2 T_L}{3h} \langle M_{ph}/A \rangle \langle \langle \lambda_{ph} \rangle \rangle \quad \sigma = \frac{2q^2}{h} \langle M_{el}/A \rangle \langle \langle \lambda_{el} \rangle \rangle$$

In practice, the mfps often have similar values. **The difference is in $\langle M \rangle$.**

For electrons, the location E_F can vary $\langle M \rangle$ over many orders of magnitude.

But even when $E_F = E_C$, $\langle M \rangle$ is much smaller for electrons than for phonons because for electrons, the BW $\gg k_B T_L$ which for phonons, BW $\sim k_B T_L$. Most of the modes are occupied for phonons but only a few for electrons.

A question

The lattice thermal conductivity of Bi₂Te₃ is much lower than that of Si.

Bi₂Te₃

$\kappa_L \approx 1$ W/m-K

Silicon

$\kappa_L \approx 150$ W/m-K

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

Is it the number of channels? Is it the MFP? Is it a combination of the two? What role does the sound velocity play?

A question

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

Bi₂Te₃

$$\kappa_L \approx 1 \text{ W/m-K}$$

$$\langle \langle \lambda_{ph} \rangle \rangle \approx 11 \text{ nm}$$

$$\langle M_{ph} \rangle \approx 3.2 \times 10^{17} \text{ m}^{-2}$$

Silicon

$$\kappa_L \approx 150 \text{ W/m-K}$$

$$\langle \langle \lambda_{ph} \rangle \rangle \approx 140 \text{ nm}$$

$$\langle M_{ph} \rangle \approx 3.3 \times 10^{18} \text{ m}^{-2}$$

(Calculations from Jesse Maassen, Dalhousie Univ.)

Another question to think about

Assume that the distribution of MFP's is known for a bulk material.

How does the thermal conductivity change as the sample size decreases?

For more information

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For information about Landauer Approach

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Questions?

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

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

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

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

$$\sigma = \frac{2q^2}{h} \langle M_{el}/A \rangle \langle \langle \lambda_{el} \rangle \rangle$$

$$\kappa_L = \frac{\pi^2 k_B^2 T_L}{3h} \langle M_{ph}/A \rangle \langle \langle \lambda_{ph} \rangle \rangle$$

