ECE-656: Fall 2011

Lecture 13: Phonon Transport

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heat flux and thermal conductivity

1) Electrons can carry heat, and we have seen how to evaluate the electronic thermal conductivity.

$$J_x^q = \pi\sigma\mathcal{E}_x - \kappa_0\, dT_L/dx \qquad \kappa_0 = \int \frac{(E-E_F)^2}{q^2T_L}\sigma'(E)\,dE$$

$$J_x^q = \pi J_x - \kappa_e\, dT_L/dx \qquad \kappa_e = \kappa_0 - \pi S\sigma$$

2) In metals, electrons carry most of the heat.

3) But in semiconductors and insulators, most of the heat is carried by lattice vibrations (***phonons***).

this lecture…

$$J_x^q = \pi J_x - \kappa_e \, dT_L / dx$$

$$J_x^Q = -\kappa_L \, dT_L / dx$$

is a brief introduction to phonon transport. We also discuss the differences between electron and phonon transport (i.e. why does the electrical conductivity vary over **>20** orders of magnitude while the thermal conductivity only varies only over **~3** orders of magnitude?)

for more information

To hear a longer lecture on this topic, see:
http://nanohub.org/resources/11869

Also, see Chapter 9 in:
Near-equilibrium Transport: Fundamentals and Applications, World Scientific, to be published, 2012.

The techniques used to produce the plots in this lecture are described in:

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.

outline

1) Introduction
2) Electrons and Phonons
3) General model for heat conduction
4) Thermal conductivity
5) Debye model
6) Scattering
7) Discussion
8) Summary

electron dispersion

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

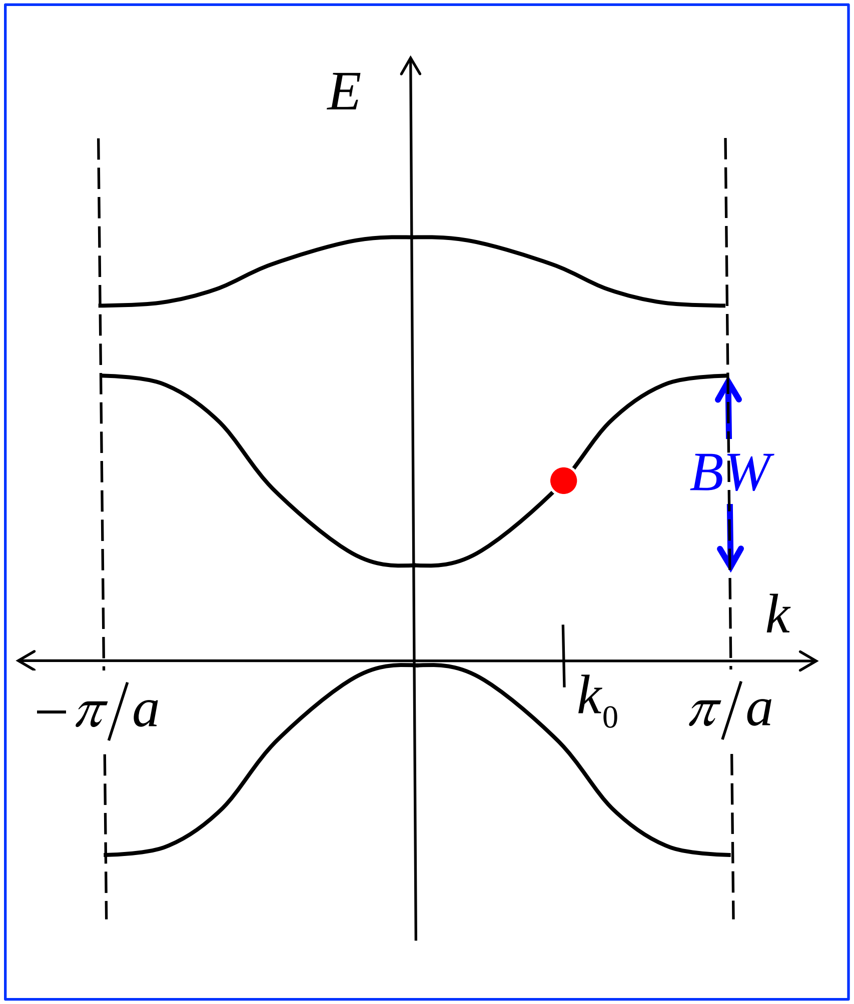
Electron waves are described by a "dispersion:" $E\left(\vec{k}\right) = \hbar\omega\left(\vec{k}\right)$

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:

$$\vec{\upsilon}_g\left(\vec{k}\right) = \nabla_k E\left(\vec{k}\right)/\hbar$$



phonon dispersion

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

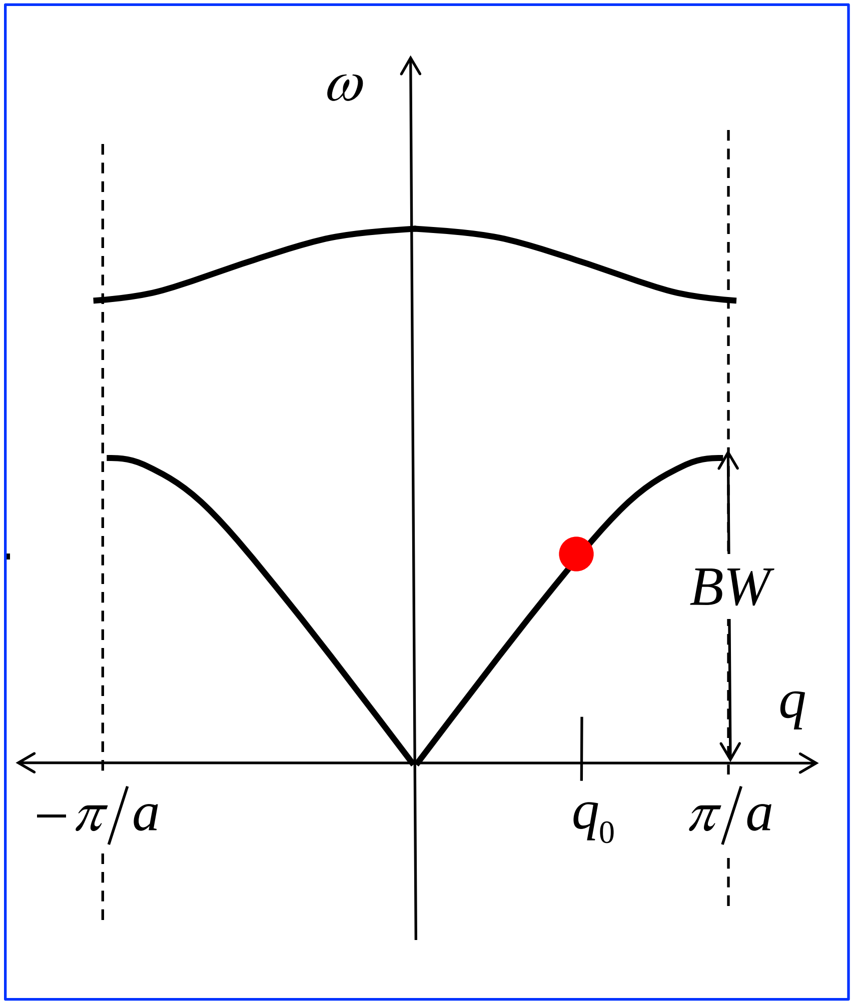
Lattice vibrations are described by a "dispersion:" $\omega(\vec{q}) = E(\vec{q})/\hbar$

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

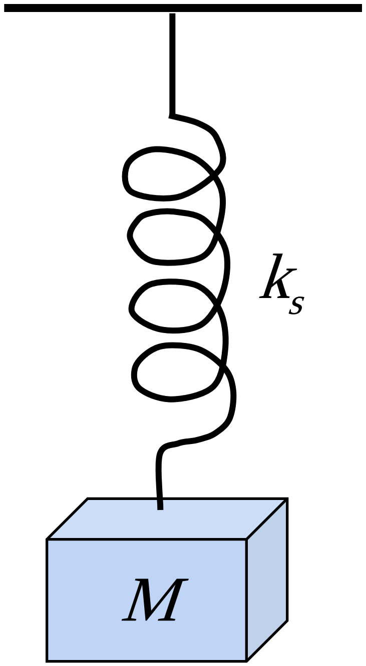
Particles described by a "wavepacket."

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

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



mass and spring



$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

$$U = \frac{1}{2} k_s \left(x - x_0\right)^2$$

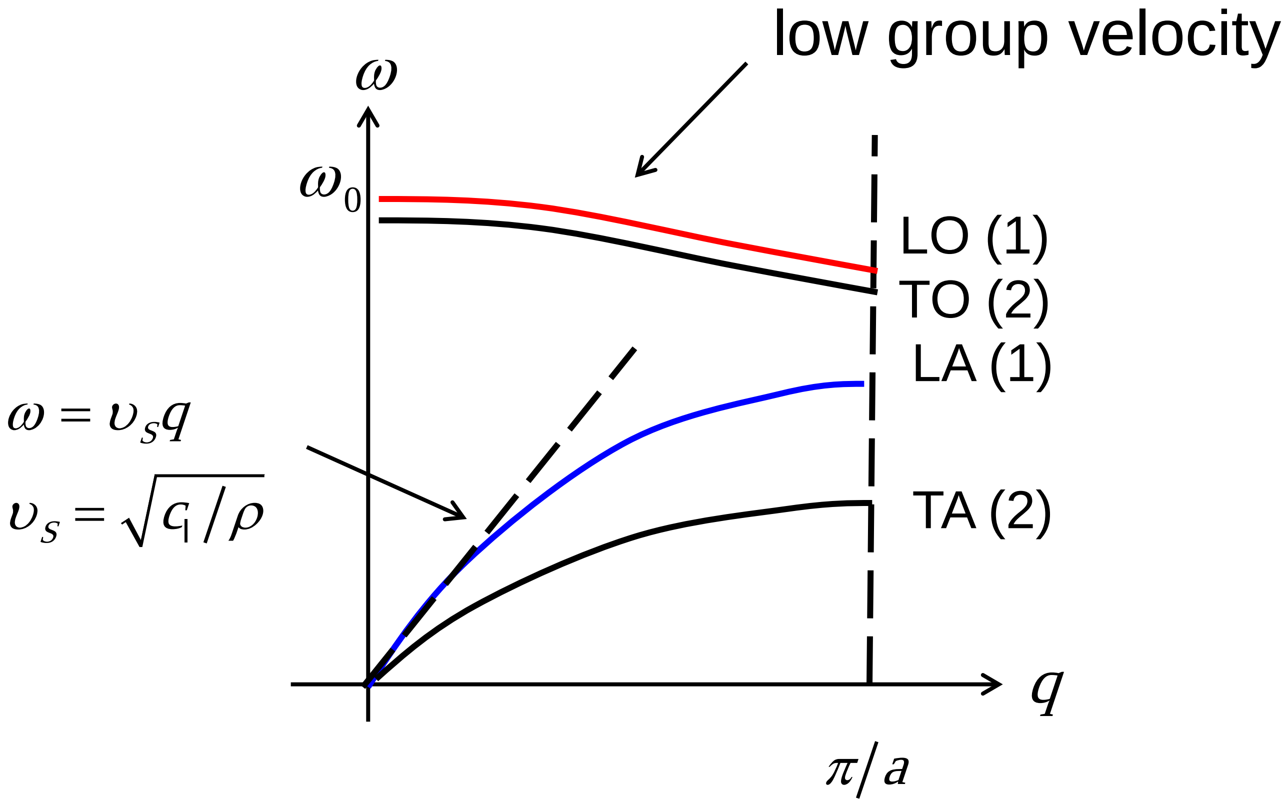
$$F = -\frac{dU}{dx} = -k_s\left(x - x_0\right)$$

$$M\frac{d^2x}{dt^2} = -k_s\left(x - x_0\right)$$

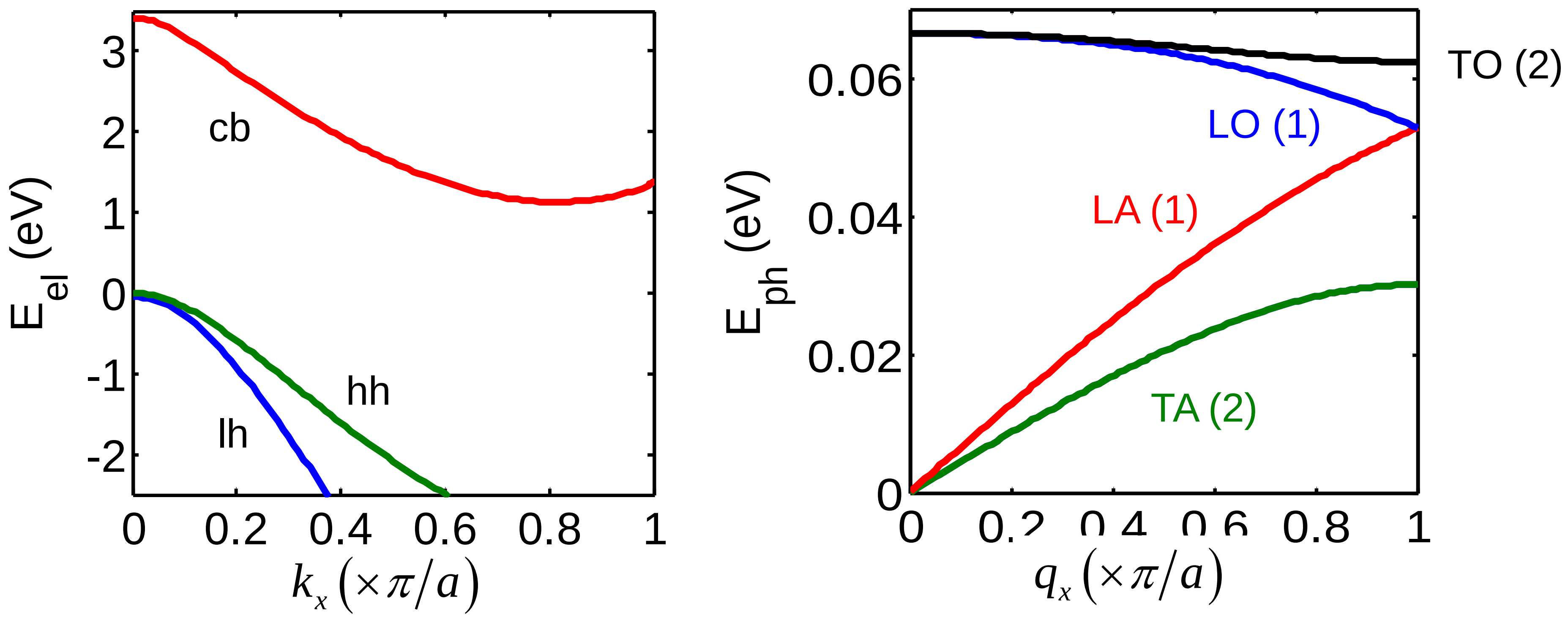
$$x(t) - x_0 = Ae^{i\omega t}$$

$$\omega = \sqrt{k_s/M}$$

general features of phonon dispersion



real dispersion



note the different energy scales!

electrons in Si (along [100]) phonons in Si (along [100])

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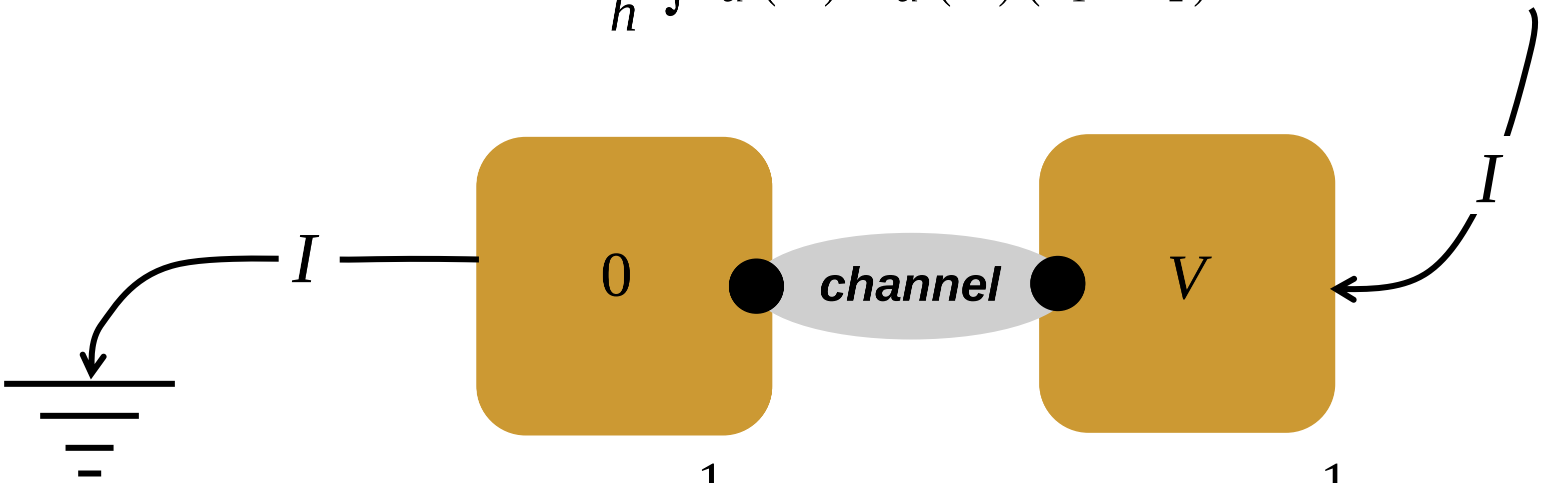
general model for **electronic** conduction

From Lecture 4:

$$I = \frac{2q}{h}\int T_{el}(E) M_{el}(E)\left(f_1 - f_2\right) dE$$



$$f_1(E) = \frac{1}{e^{(E-E_{F1})/k_B T_L} + 1} \qquad f_2(E) = \frac{1}{e^{(E-E_{F1}+qV)/k_B T_L} + 1}$$

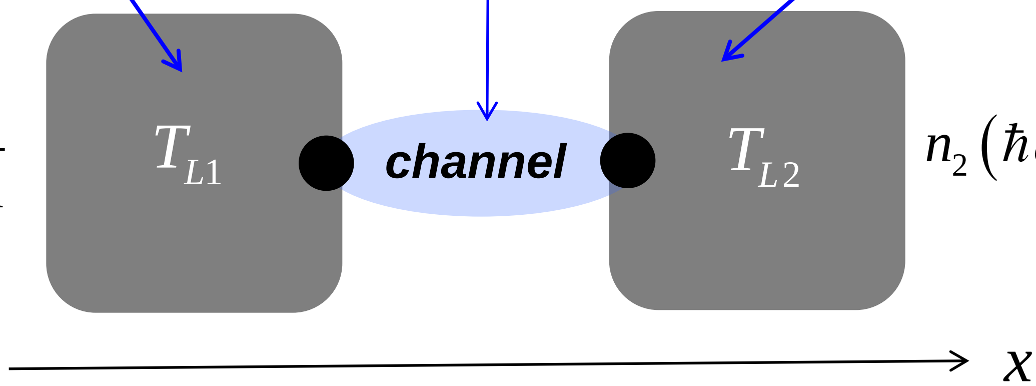
for **phonon** conduction

Thermal reservoir in equilibrium at temperature, T_{L1}.

channel characterized by a phonon dispersion

Thermal reservoir in equilibrium at temperature, T_{L2}.

$$n_1(\hbar\omega) = \frac{1}{e^{\hbar\omega/k_B T_{L1}} - 1}$$



$$n_2(\hbar\omega) = \frac{1}{e^{\hbar\omega/k_B T_{L2}} - 1}$$

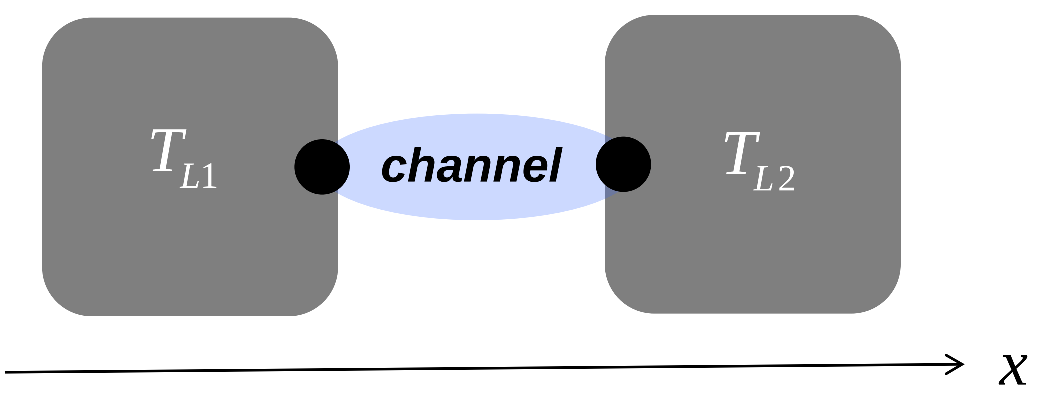
$$I = \frac{2q}{h}\int T_{el}(E) M_{el}(E)\left(f_1 - f_2\right) dE \quad \Rightarrow \quad Q = ?$$

heat flux

$$I = \frac{2q}{h}\int T_{el}\left(E\right)M_{el}\left(E\right)\left(f_1 - f_2\right)dE$$

$$Q = \frac{1}{h}\int \left(\hbar\omega\right)T_{ph}\left(\hbar\omega\right)M_{ph}\left(\hbar\omega\right)\left(n_1 - n_2\right)d\left(\hbar\omega\right)$$

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



near-equilibrium heat flux

$$Q = \frac{1}{h}\int (\hbar\omega) T_{ph}(\hbar\omega) M_{ph}(\hbar\omega)(n_1 - n_2)\, d(\hbar\omega)$$

$$n_2 \approx n_1 + \frac{\partial n_1}{\partial T_L}\Delta T_L \qquad (n_1 - n_2) \approx -\frac{\partial n_1}{\partial T_L}\Delta T_L \approx -\frac{\partial n_0}{\partial T_L}\Delta T_L$$

$$\frac{\partial n_0}{\partial T_L} = \frac{\partial}{\partial T_L}\left\{\frac{1}{e^{\hbar\omega/k_B T_L} - 1}\right\} = \left(\frac{\hbar\omega}{k_B T_L^2}\right)\frac{e^{\hbar\omega/k_B T_L}}{\left(e^{\hbar\omega/k_B T_L} - 1\right)^2}$$

$$\frac{\partial n_0}{\partial(\hbar\omega)} = \frac{\partial}{\partial(\hbar\omega)}\left\{\frac{1}{e^{\hbar\omega/k_B T_L} - 1}\right\} = \left(-\frac{1}{k_B T_L}\right)\frac{e^{\hbar\omega/k_B T_L}}{\left(e^{\hbar\omega/k_B T_L} - 1\right)^2}$$

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

$$\boxed{Q = -K_L \Delta T_L}$$

lattice thermal conductance

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

Recall the electrical conductance:

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

"window function":

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

$$Q = -K_L \Delta T_L \qquad K_L = \frac{k_B^2 T_L}{h} \int T_{ph}(\hbar\omega) M_{ph}(\hbar\omega) \boxed{\left\{ \left(\frac{\hbar\omega}{k_B T_L} \right)^2 \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right) \right\}} d(\hbar\omega)$$

$$\int_0^{+\infty} \left(\frac{\hbar\omega}{k_B T_L} \right)^2 \left(-\frac{\partial n_0}{\partial(\hbar\omega)} \right) d(\hbar\omega) = \int_0^{+\infty} \left\{ \frac{\left(\hbar\omega/k_B T_L\right)^2 e^{\hbar\omega/k_B T_L}}{\left(e^{\hbar\omega/k_B T_L} - 1\right)^2} \right\} d\left(\frac{\hbar\omega}{k_B T_L} \right) = \int_0^{+\infty} \left\{ \frac{x^2 e^x}{\left(e^x - 1\right)^2} \right\} dx = \frac{\pi^2}{3}$$

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

heat conduction

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

2) Thermal conductance: $K_L = \dfrac{\pi^2 k_B^2 T_L}{3h} \int T_{ph}\left(\hbar\omega\right) M_{ph}\left(\hbar\omega\right) W_{ph}\left(\hbar\omega\right) d\left(\hbar\omega\right)$

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

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

electrical conduction

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

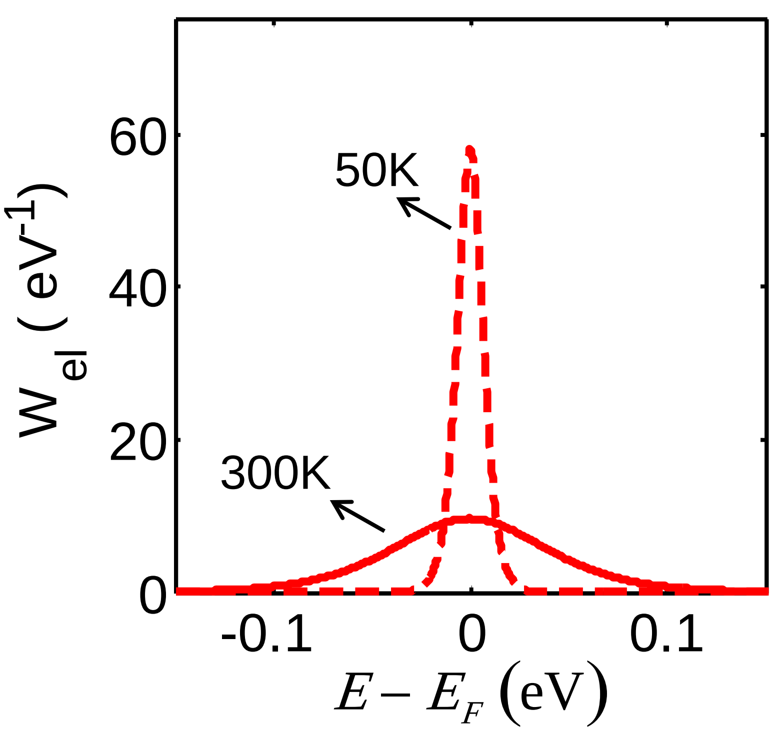
2) Electrical conductance: $G = \dfrac{2q^2}{h}\int T_{el}(E) M_{el}(E) W_{el}\, dE$

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

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

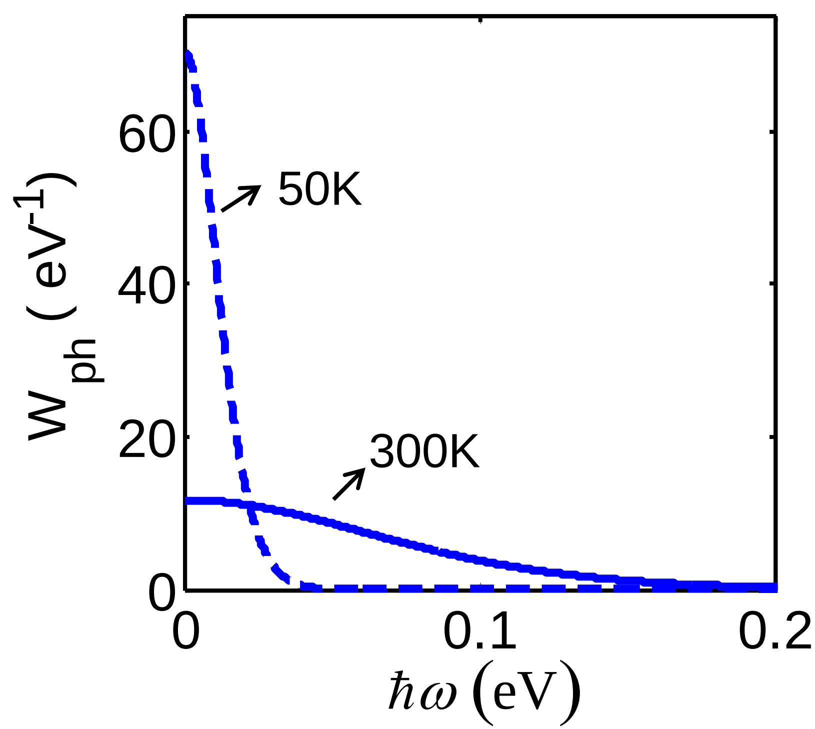
window functions: electrons vs. phonons

Electrons



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

Phonons



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

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diffusive heat transport (3D)

$$Q = -K_L \Delta T_L \qquad \text{(Watts)}$$

$$K_L = \frac{\pi^2 k_B^2 T_L}{3h} \int T_{ph}(\hbar\omega) M_{ph}(\hbar\omega) W_{ph}(\hbar\omega)\, d(\hbar\omega) \qquad \text{(Watts/K)}$$

$$T_{ph}(\hbar\omega) = \frac{\lambda_{ph}(\hbar\omega)}{\lambda_{ph}(\hbar\omega) + L} \to \frac{\lambda_{ph}(\hbar\omega)}{L} \qquad \text{(diffusive phonon transport)}$$

$$M_{ph}(\hbar\omega) \propto A \qquad \text{(large, 3D sample)}$$

$$Q = -\left(K_L \frac{L}{A}\right) A \frac{\Delta T_L}{L} \qquad J_x^Q = \frac{Q}{A} = -\kappa_L \frac{dT_L}{dx} \qquad \kappa_L = K_L\left(\frac{L}{A}\right) \quad \text{(W/m-K)}$$

diffusive heat transport (3D)

$$J_x^Q = -\kappa_L \frac{dT_L}{dx}$$ (Watts / m²)

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

$$J_x = \sigma \frac{d(F_n/q)}{dx}$$ (Amperes / m²)

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

diffusive heat transport (3D)

$$J_x^Q = -\kappa_L \frac{dT_L}{dx}$$ (Watts / m²)

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

$$J = \sigma \frac{d(F_n/q)}{dx}$$ (Amperes / m²)

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

relation to specific heat

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

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

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.

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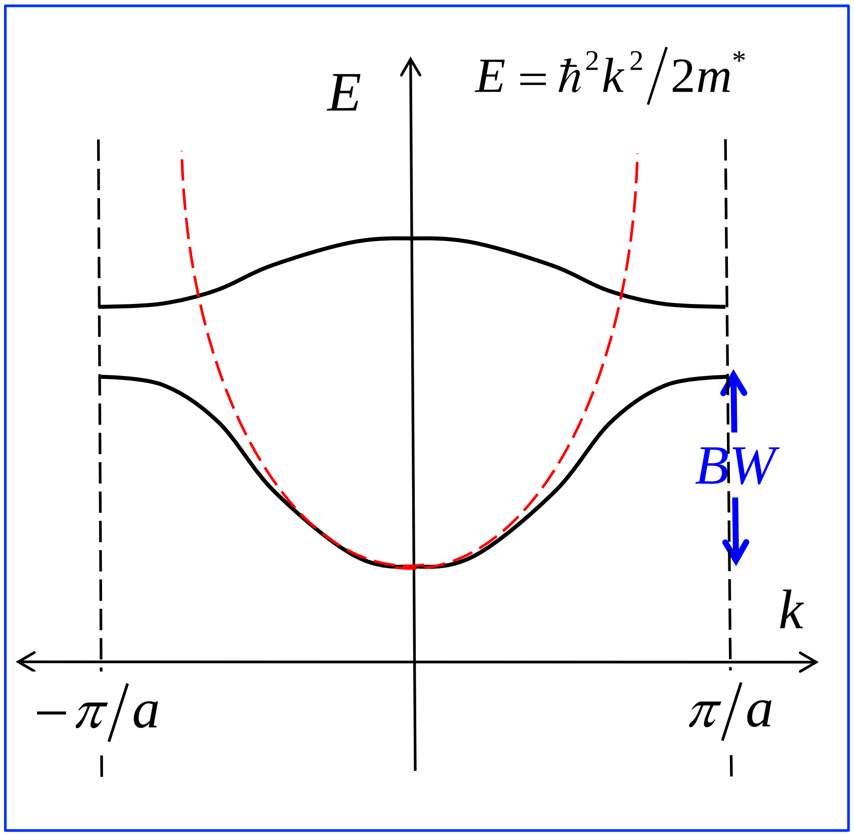
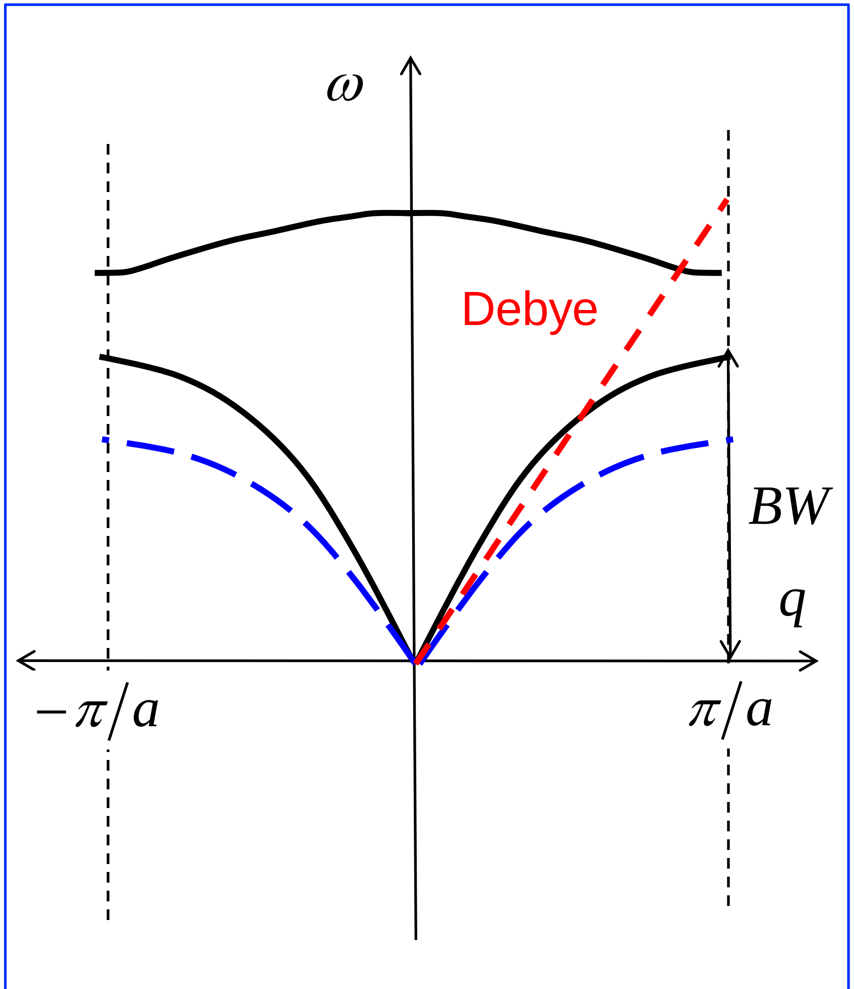
effective mass model for electrons



As long as the BW >> $k_B T_L$, the effective mass model generally works ok.

This is the typical case for electronic dispersions. Only states near the bottom of the conduction band or top of the valence band matter, and these regions can be described by an eff mass model.

Debye model for acoustic phonons



Linear dispersion model

$$\omega = \upsilon_D q$$

$$D_{ph}(\hbar\omega) = \frac{3(\hbar\omega)^2 \Omega}{2\pi^2(\hbar\upsilon_D)^3} \quad (\text{no./J})$$

$$M_{ph}(\hbar\omega) = \frac{3(\hbar\omega)^2 A}{2\pi\hbar\upsilon_D^2} \quad (\text{no./J})$$

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

Debye model: cutoff frequency / wavevector

For phonons, BW ~ $k_B T_L$ (recall slide 10)

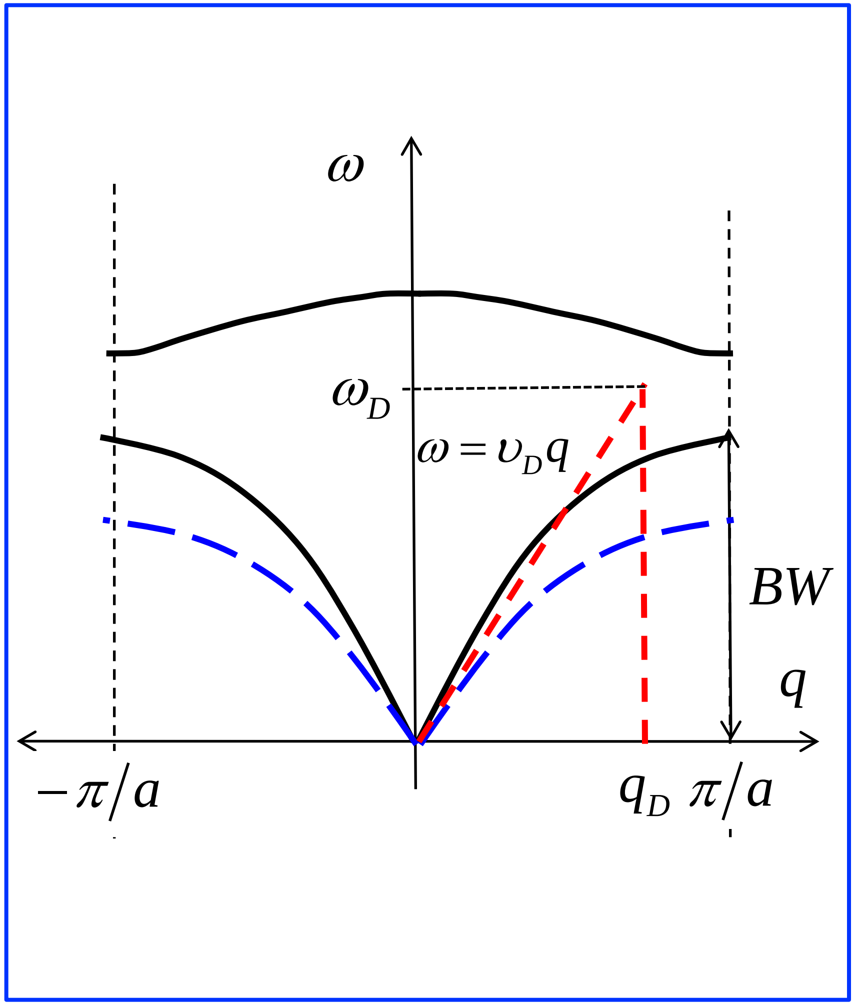
No. of states in a band = N.

$$\int_0^{\omega_D} D_{ph}(\hbar\omega)\,d(\hbar\omega) = \int_0^{\hbar\omega_D} \frac{3(\hbar\omega)^2}{2\pi^3(\hbar\upsilon_D)^3}\,d(\hbar\omega) = 3\frac{N}{\Omega}$$

$$\hbar\omega_D = \hbar\upsilon_D\left(\frac{6\pi^2 N}{\Omega}\right)^{1/3} \equiv k_B T_D$$

$$q_D = \frac{\omega_D}{\upsilon_D} = \left(\frac{6\pi^2 N}{\Omega}\right)^{1/3}$$

Debye model: cutoff frequency / wavevector



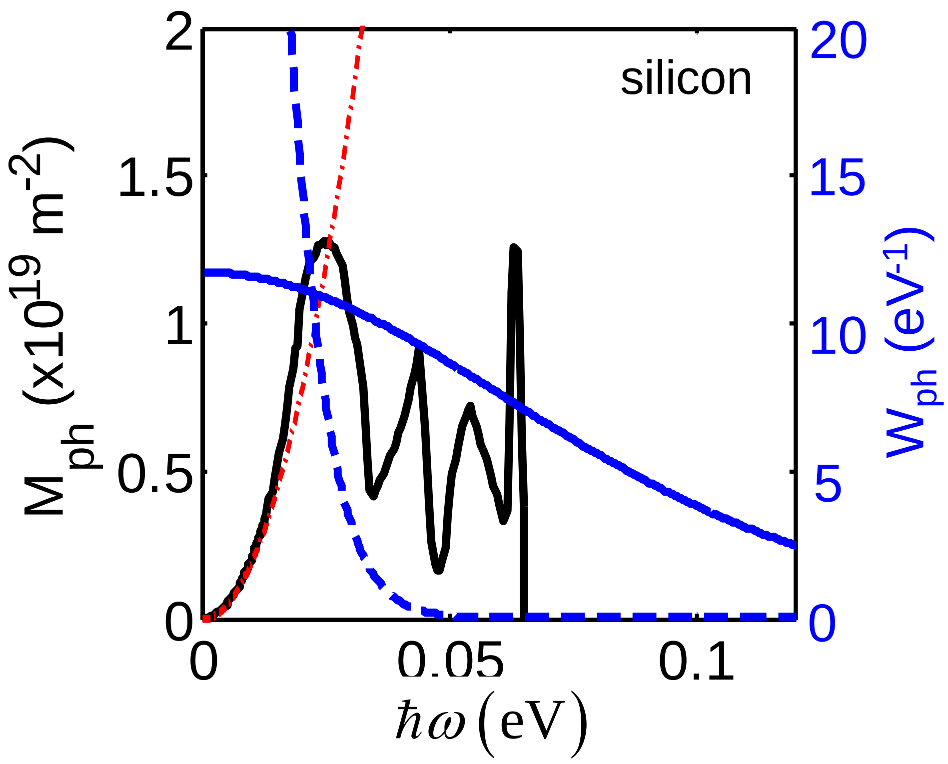
$$\hbar\omega_D = \hbar\upsilon_D\left(\frac{6\pi^2 N}{\Omega}\right)^{1/3}$$

$$q_D = \frac{\omega_D}{\upsilon_D} = \left(\frac{6\pi^2 N}{\Omega}\right)^{1/3}$$

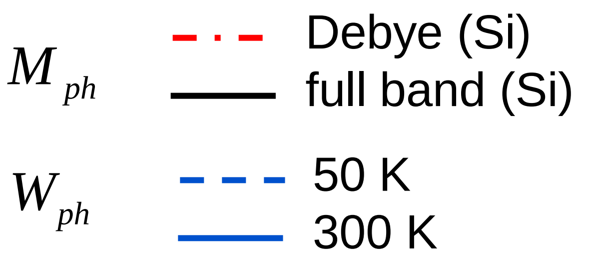
$$k_B T_D \equiv \hbar\omega_D$$

Debye model valid when $T_L << T_D$ (generally means T_L << 300K)

limitation of Debye model



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

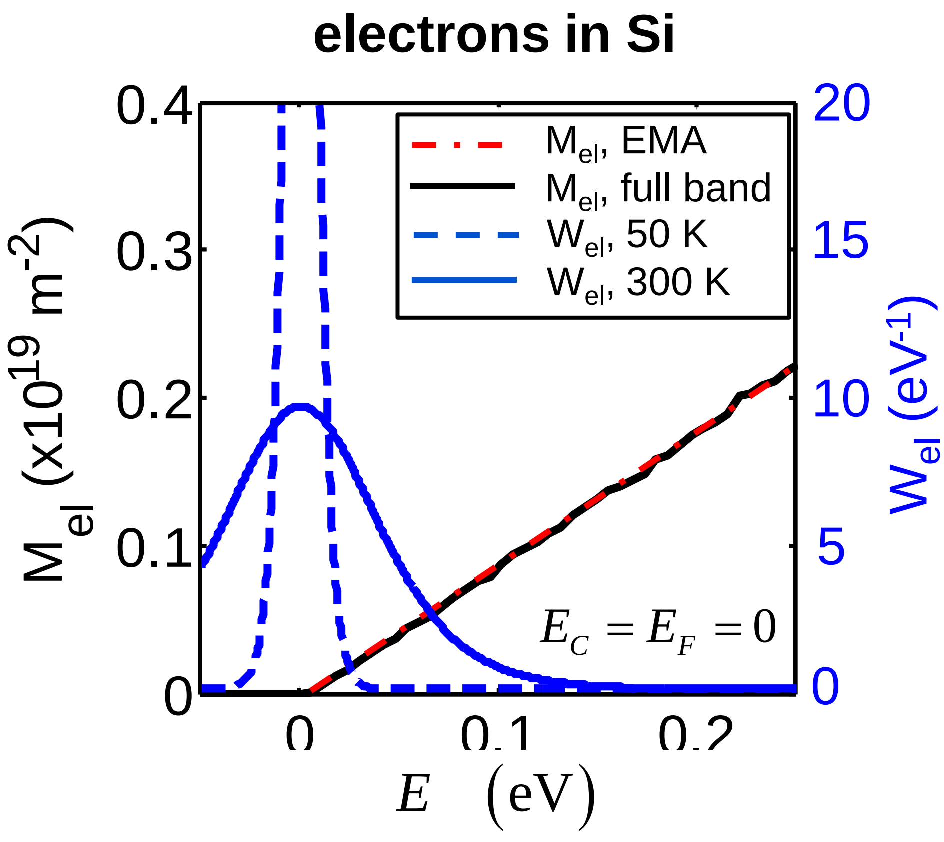


Window function spans the entire BZ at room temp.

Debye model works well at very temperatures below 50 K.

effective mass model for electrons

Parabolic dispersion assumption for electrons works well at room temperature.



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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. (Lecture 12)

Phonons scatter from:

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

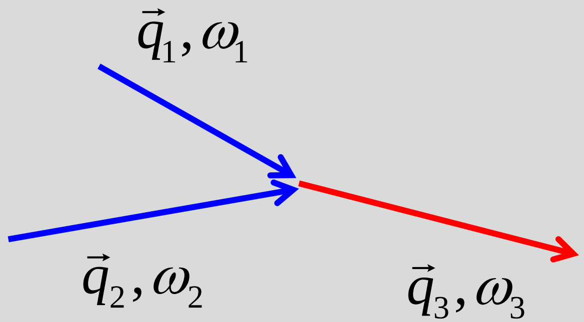
2) other phonons

3) surfaces and boundaries

4) electrons ("phonon drag")

Scattering rates are computed from Fermi's Golden Rule.

phonon-phonon scattering



i) momentum conservation:

$$\hbar\vec{q}_3 = \hbar\vec{q}_1 + \hbar\vec{q}_2$$

ii) energy conservation:

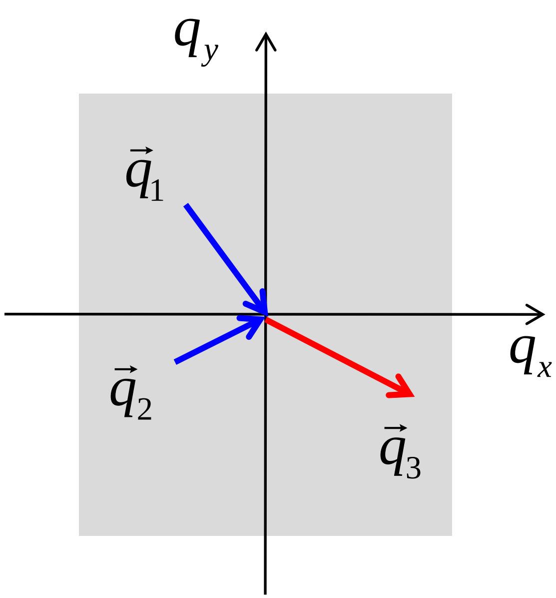
$$\hbar\omega_3 = \hbar\omega_1 + \hbar\omega_2$$

little effect on thermal conductivity!

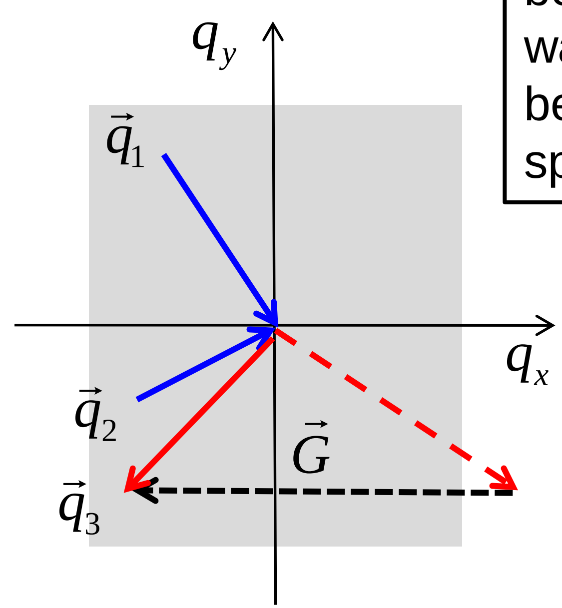
N and U processes

Need population of large q states for U-scattering. Need high T_L 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.

scattering summary

$$\frac{1}{\tau_{ph}(\hbar\omega)} = \frac{1}{\tau_D(\hbar\omega)} + \frac{1}{\tau_B(\hbar\omega)} + \frac{1}{\tau_U(\hbar\omega)}$$

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

$$\lambda_{ph}(\hbar\omega) \propto \upsilon_{ph}(\hbar\omega)\tau_{ph}(\hbar\omega)$$

1) point defects and impurities: $1/\tau_D(\hbar\omega) \propto \omega^4$ "Raleigh scattering"

2) boundaries and surfaces: $1/\tau_B(\hbar\omega) \propto \upsilon_{ph}(\hbar\omega)/t$

3) Umklapp scattering: $1/\tau_U(\hbar\omega) \propto T_L$

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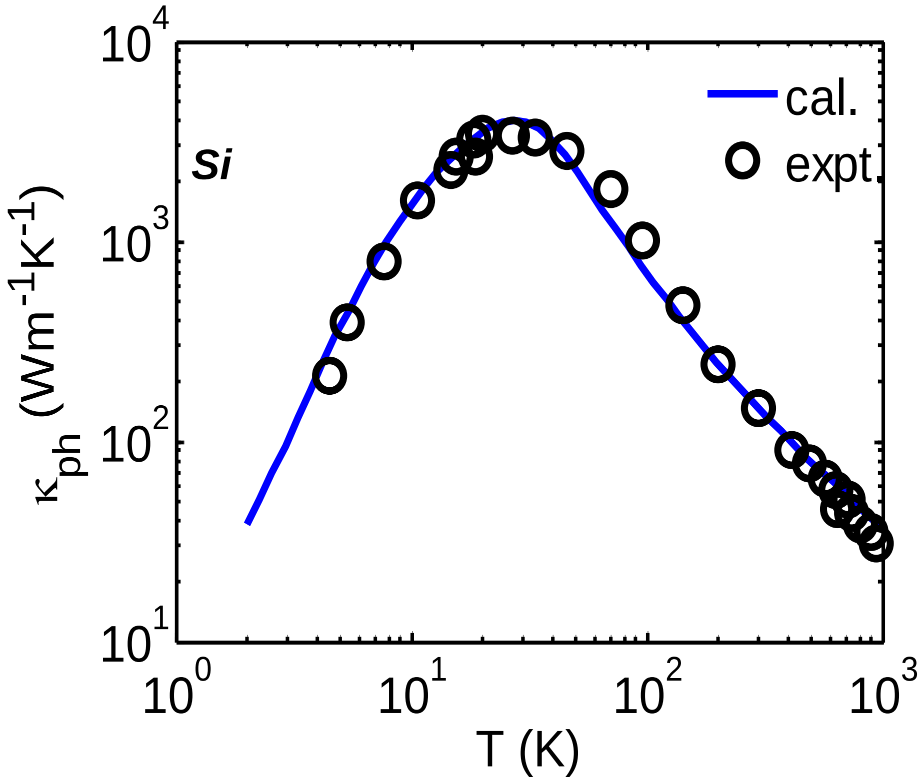
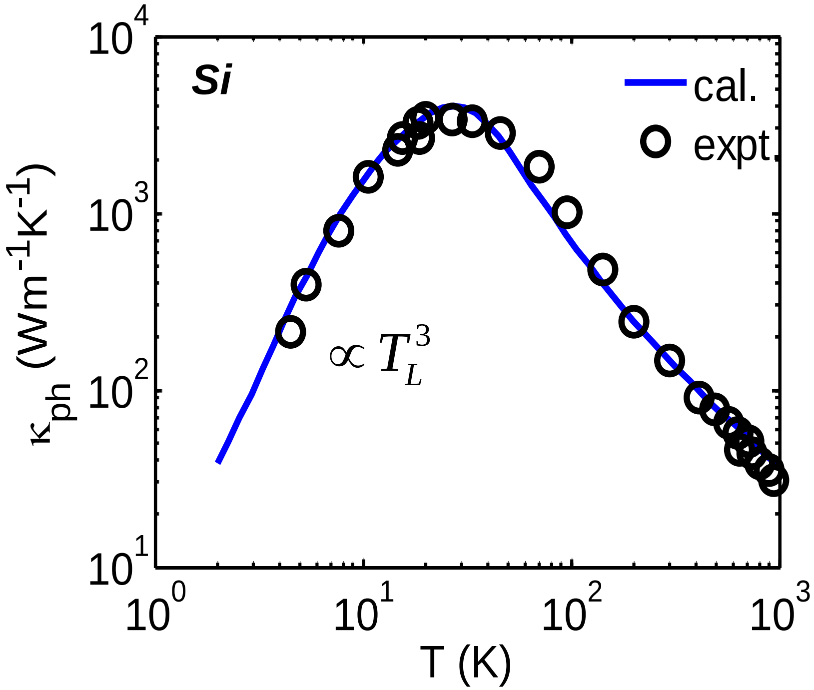
i) measured vs. calculated $\kappa_L(T_L)$ for silicon

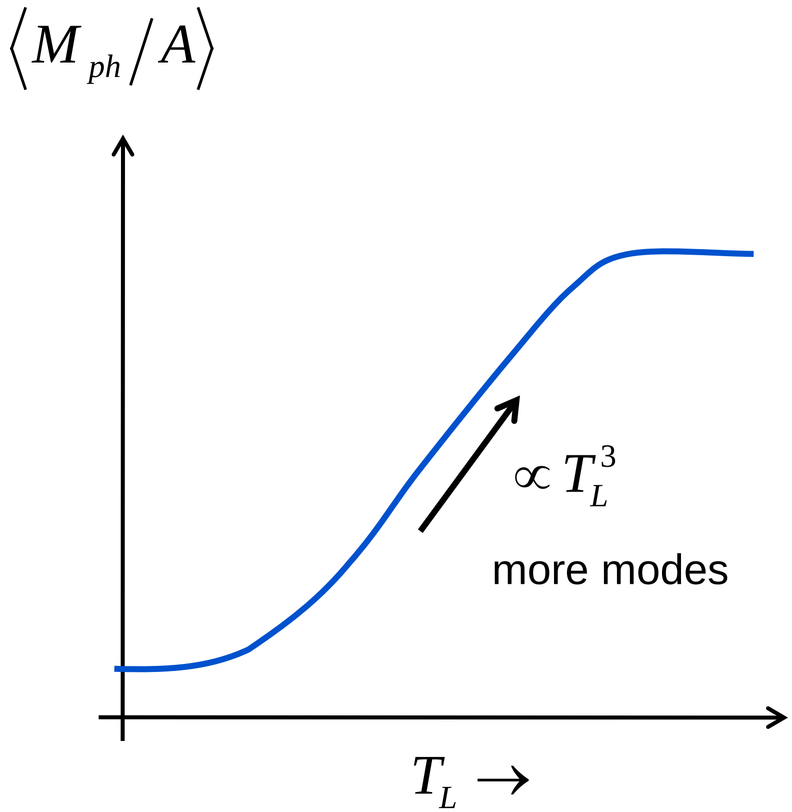


$$\kappa_L = \frac{\pi^2 k_B^2 T_L}{3h} \langle M_{ph} \rangle \times \langle\langle \lambda_{ph} \rangle\rangle$$

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.

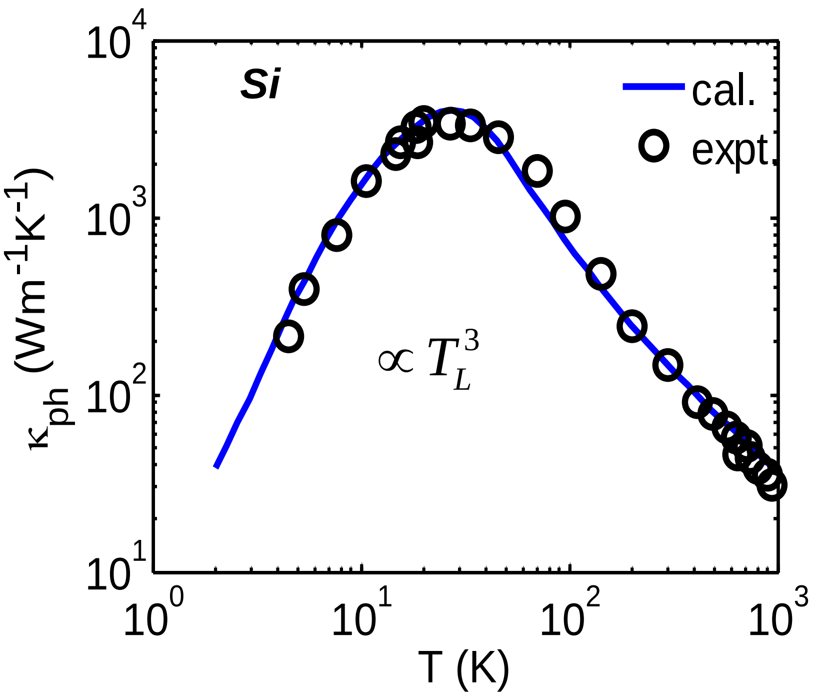
population of modes vs. T_L

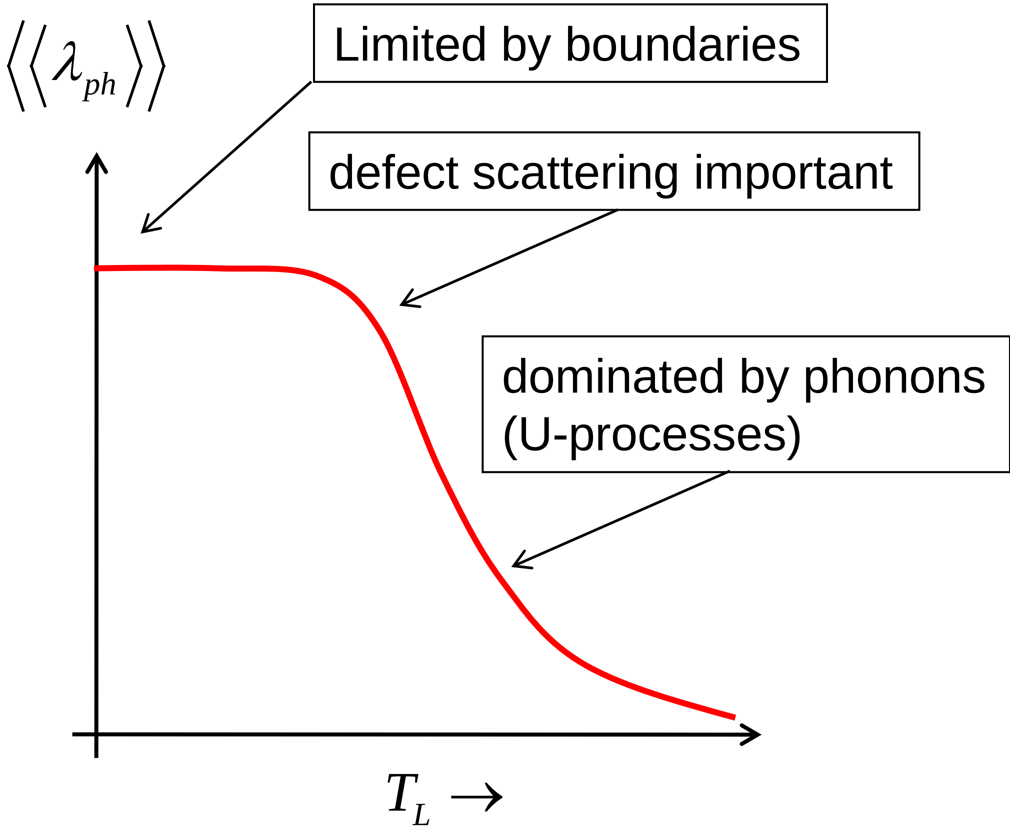




$$\langle M_{ph}/A \rangle \equiv \int \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega)\, d(\hbar\omega)$$

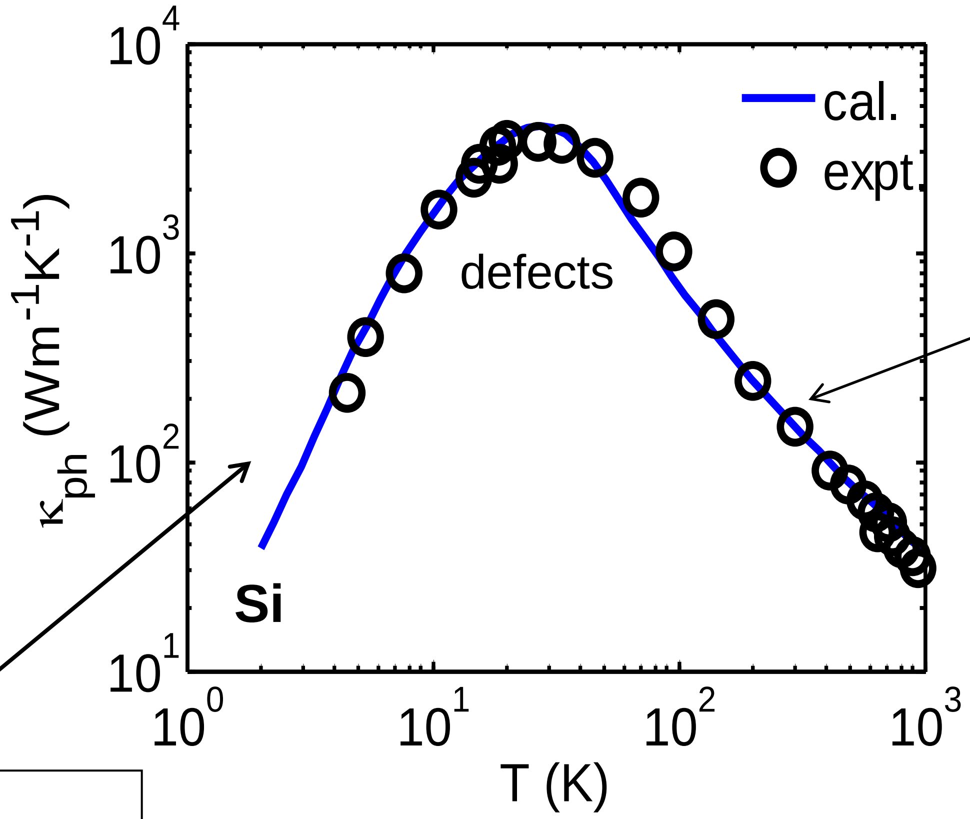
mean-free-path vs. T_L





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

temperature-dependent thermal conductivity



phonon scattering by U-processes

population of modes and boundary scattering

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

ii) electron vs. phonon conductivities

The expressions look similar:

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

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 >> $k_B T_L$ which for phonons, BW ~ $k_B T_L$. Most of the modes are occupied for phonons but only a few for electrons.

outline

1) Introduction
2) Electrons and Phonons
3) General model for heat conduction
4) Thermal conductivity
5) Debye model
6) Scattering
7) Discussion
8) Summary

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.

questions

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