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Near-equilibrium Transport: Fundamentals and Applications

Lecture 9: 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.

\[ J^q_x = \pi \sigma E_x - \kappa_0 \frac{dT_L}{dx} \]

\[ \kappa_0 = \int \frac{(E - E_F)^2}{q^2 T_L} \sigma'(E) dE \]

\[ J^q_x = \pi J_x - \kappa_e \frac{dT_L}{dx} \]

\[ \kappa_e = \kappa_0 - \pi S \sigma \]

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).

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This lecture 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?)
9.1 Introduction
9.2 Electrons and Phonons
9.3 General model for heat conduction
9.4 Thermal conductivity
9.5 Debye model
9.6 Scattering
9.7 Discussion
9.8 Summary
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:

\[
\vec{v}_g(\vec{k}) = \nabla_k E(\vec{k})/\hbar
\]
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:

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

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

\[ U = \frac{1}{2} k_s (x - x_0)^2 \]

\[ F = -\frac{dU}{dx} = -k_s (x - x_0) \]

\[ M \frac{d^2 x}{dt^2} = -k_s (x - x_0) \]

\[ x(t) - x_0 = A e^{i\omega t} \]

\[ \omega = \sqrt{\frac{k_s}{M}} \]
general features of phonon dispersion

LO and TO degenerate at $q = 0$ for non-polar semiconductors

$\omega = \nu_s q$
$\nu_s = \sqrt{c_1 / \rho}$

LO (1)  TO (2)  LA (1)  TA (2)

low group velocity

LO and LA degenerate at zone boundary for non-polar semiconductors
real dispersion

- note the different energy scales!

- electrons in Si (along [100])

- phonons in Si (along [100])
wavelengths: electrons vs. phonons

\[ \langle \lambda_B^{el} \rangle = \frac{\hbar}{\sqrt{3m^*k_B T_L}} \approx 60\,\text{Å} \]

\[ \langle \lambda_B^{ph} \rangle = \frac{4\pi\hbar \nu_S}{3k_B T_L} \approx 5\,\text{Å} \]

\( (m^* = m_0, T_L = 300\,\text{K}) \)

\( (\nu_S \approx 5000\,\text{m/s}) \)

(see appendix for derivation)

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general model for **electronic** conduction

From Lecture 2:

\[ I = \frac{2q}{h} \int T_{el}(E)M_{el}(E)(f_1 - f_2) \, dE \]

\[ f_1(E) = \frac{1}{e^{(E-E_{F1})/k_BT_L} + 1} \]

\[ f_2(E) = \frac{1}{e^{(E-E_{F1}+qV)/k_BT_L} + 1} \]
for phonon conduction

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

channel characterized by a dispersion

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

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

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

\[ I = \frac{2q}{h} \int T_{el}(E)M_{el}(E)(f_1 - f_2) dE \quad \Rightarrow \quad Q = ? \]
heat flux

\[ I = \frac{2q}{\hbar} \int T_{el}(E)M_{el}(E)(f_1 - f_2) \, dE \]

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

Assume **ideal contacts**, so that the transmission describes the transmission of the channel.
near-equilibrium heat flux

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

\[ n_2 \approx n_1 + \frac{\partial n_1}{\partial T_L} \Delta T_L \]

\[ (n_1 - n_2) \approx - \frac{\partial n_1}{\partial T_L} \Delta T_L \approx - \frac{\partial n_0}{\partial T_L} \Delta T_L \]

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

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

\[ \frac{\partial n_0}{\partial T_L} = \frac{\hat{\hbar} \omega}{T_L} \left( - \frac{\partial n_0}{\partial (\hat{\hbar} \omega)} \right) \]

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

\[ Q = -K_L \Delta T_L \]
Recall the electrical conductance:

\[ Q = -K_L \Delta T_L \]

\[ K_L = \frac{k_B^2 T_L}{\hbar} \int T_{ph}(\hbar \omega) M_{ph}(\hbar \omega) \left\{ \left( \frac{\hbar \omega}{k_B T_L} \right) \left( -\frac{\partial n_0}{\partial (\hbar \omega)} \right) \right\} d(\hbar \omega) \]

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”:

\[ W_{el}(E) = \left( -\frac{\partial f_0}{\partial E} \right) \int_{-\infty}^{+\infty} \left( -\frac{\partial f_0}{\partial E} \right) dE = 1 \]
lattice window function

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

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

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

\[ W_{ph} (\hbar \omega) \]
heat conduction

1) Fourier’s Law of heat conduction: \[ Q = -K_L \Delta T_L \]

2) Thermal conductance: \[ K_L = \frac{\pi^2 k_B^2 T_L}{3h} \int T_{ph} (\hbar \omega) M_{ph} (\hbar \omega) W_{ph} (\hbar \omega) d(\hbar \omega) \]

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

4) Window function for phonons: \[ W_{ph} (\hbar \omega) = \left\{ \frac{3}{\pi^2} \left( \frac{\hbar \omega}{k_B T_L} \right)^2 \left( -\frac{\partial n_0}{\partial (\hbar \omega)} \right) \right\} \]
electrical conduction

1) Electrical current: \[ I = G \Delta V \]

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

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

4) Window function for electrons: \[ W_{el}(E) = \left( -\frac{\partial f_0}{\partial E} \right) \]
window functions: electrons vs. phonons

Electrons

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

Phonons

\[ W_{ph}(\hbar \omega) = \left\{ \frac{3}{\pi^2} \left( \frac{\hbar \omega}{k_B T_L} \right)^2 \left( -\frac{\partial n_0}{\partial (\hbar \omega)} \right) \right\} \]
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diffusive heat transport (3D)

\[ Q = -K_L \Delta T_L \]  (Watts)

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

\[ T_{ph}(\hbar\omega) = \frac{\lambda_{ph}(\hbar\omega)}{\lambda_{ph}(\hbar\omega) + L} \rightarrow \frac{\lambda_{ph}(\hbar\omega)}{L} \]  (diffusive phonon transport)

\[ M_{ph}(\hbar\omega) \propto A \]  (large, 3D sample)

\[ Q = -\left( K_L \frac{L}{A} \right) A \frac{\Delta T_L}{L} \]

\[ J^Q_x = \frac{Q}{A} = -\kappa_L \frac{dT_L}{dx} \]

\[ \kappa_L = K_L \left( \frac{L}{A} \right) \]  (W/m-K)
diffusive heat transport (3D)

\[ J^Q_x = -\kappa_L \frac{dT_L}{dx} \quad \text{(Watts / m}^2\text{)} \]

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

\[ J_x = \sigma \frac{d(F_n/q)}{dx} \quad \text{(Amperes / m}^2\text{)} \]

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

\[
\kappa_{L\ell} = \frac{\pi^2 k_B^2 T_L}{3h} \left[ \int \lambda_{ph}(\hbar\omega) \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega) d(\hbar\omega) \right] \quad \text{(Watts/m-K)}
\]

\[
\kappa_{L\ell} = \frac{\pi^2 k_B^2 T_L}{3h} \left[ \int \lambda_{ph}(\hbar\omega) \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega) d(\hbar\omega) \right] \frac{\left[ \int M_{ph}(\hbar\omega) d(\hbar\omega) \right]}{A}
\]

\[
\kappa_{L\ell} = \frac{\pi^2 k_B^2 T_L}{3h} \left[ \langle M_{ph} / A \rangle \langle \lambda_{ph} \rangle \right]
\]

\[
\langle M_{ph} / A \rangle = \int \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega) d(\hbar\omega)
\]

\[
\langle \lambda_{ph} \rangle = \int \frac{\lambda_{ph}(\hbar\omega)}{A} \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega) d(\hbar\omega)
\]

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diffusive heat transport (3D)

\[ J_x^Q = -\kappa_L \frac{dT_L}{dx} \quad \text{(Watts / m}^2\text{)} \]

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

\[ J = \sigma \frac{d(F_n/q)}{dx} \quad \text{(Amperes / m}^2\text{)} \]

\[ \sigma = \frac{2q^2}{h} \left\langle \frac{M_{el}}{A} \left\langle \lambda_{el} \right\rangle \right\rangle \quad \text{(1/Ohm-m)} \]
diffusive heat transport (3D)

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

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

To evaluate the lattice thermal conductivity, we must specify:
1) the mean-free-path for phonon scattering
2) the number of channels per unit area for phonon conduction.

Before we do that……the lattice thermal conductivity is often related to the lattice specific heat. Let’s see how that works.
The total energy (per unit volume) of the lattice vibrations is:

\[ E_L = \int_0^{\infty} (\hbar\omega) D_{ph}(\hbar\omega) n_0(\hbar\omega) d(\hbar\omega) \]

where \( D_{ph} \) is the phonon density of states per unit volume.

The **specific heat** is the change in energy per degree change in \( T_L \):

\[ C_V = \frac{\partial E_L}{\partial T_L} = \frac{\partial}{\partial T_L} \int_0^{\infty} (\hbar\omega) D_{ph}(\hbar\omega) n_0(\hbar\omega) d(\hbar\omega) \]

\[ C_V \approx \int_0^{\infty} (\hbar\omega) D_{ph}(\hbar\omega) \left( \frac{\partial n_0(\hbar\omega)}{\partial T_L} \right) d(\hbar\omega) \]
specific heat (ii)

\[ C_V \approx \int_0^\infty (\hbar \omega) D_{ph}(\hbar \omega) \left( \frac{\partial n_0(\hbar \omega)}{\partial T_L} \right) d(\hbar \omega) \quad \text{Recall:} \quad \frac{\partial n_0}{\partial T_L} = \frac{\hbar \omega}{T_L} \left( - \frac{\partial n_0}{\partial (\hbar \omega)} \right) \]

\[ C_V \approx k_B^2 T_L \int_0^\infty D_{ph}(\hbar \omega) \left( \frac{\hbar \omega}{k_B T_L} \right)^2 \left( - \frac{\partial n_0}{\partial (\hbar \omega)} \right) d(\hbar \omega) \]

\[ C_V \approx \frac{\pi^2 k_B^2 T_L}{3} \int_0^\infty D_{ph}(\hbar \omega) W_{ph}(\hbar \omega) d(\hbar \omega) \]

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specific heat and thermal conductivity

\[
C_V = \frac{\pi^2 k_B^2 T_L}{3} \int_0^\infty D_{ph}(\hbar \omega) W_{ph}(\hbar \omega) \, d(\hbar \omega)
\]

\[
\kappa_{L\ell} = \frac{\pi^2 k_B^2 T_L}{3h} \int \lambda_{ph}(\hbar \omega) \frac{M_{ph}(\hbar \omega)}{A} W_{ph}(\hbar \omega) \, d(\hbar \omega)
\]

one can show…. (see appendix)

\[
\kappa_{L\ell} = \frac{1}{3} \left\langle \left\langle \Lambda_{ph} \right\rangle \right\rangle \left\langle \nu_{ph} \right\rangle C_V
\]
Specific heat and thermal conductivity

\[ \kappa_{L\ell} = \frac{\pi^2 k_B^2 T_L}{3h} \int \lambda_{ph}(\hbar\omega) \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega) d(\hbar\omega) \]

\[ \kappa_{L\ell} = \frac{1}{3} \left\langle \left\langle \Lambda_{ph} \right\rangle \right\rangle \left\langle \nu_{ph} \right\rangle C_V \]

\[ \left\langle \left\langle \Lambda_{ph} \right\rangle \right\rangle = \left\{ \frac{\int \Lambda_{ph} \nu_{ph} D_{ph} W_{ph} d(\hbar\omega)}{\int_0^\infty \nu_{ph} D_{ph} W_{ph} d(\hbar\omega)} \right\} \]

\[ \langle \nu_{ph} \rangle = \frac{1}{3} \left\{ \frac{\int_0^\infty \nu_{ph} D_{ph} W_{ph} d(\hbar\omega)}{\int_0^\infty D_{ph} W_{ph} d(\hbar\omega)} \right\} \]

\( \lambda_{ph}(\hbar\omega) = \frac{4}{3} \Lambda_{ph}(\hbar\omega) \)

\( \Lambda_{ph}(\hbar\omega) \equiv \nu(\hbar\omega) \tau(\hbar\omega) \)

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Why did we do this?

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

But, we now have a precise definition of the mfp and average phonon velocity.
\[ \kappa_{L\ell} = \frac{1}{3} \left\langle \Lambda_{ph} \right\rangle \left\langle \nu_{ph} \right\rangle C_V \]


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As long as the \( BW \gg k_B T_L \), 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 effective mass model.
Debye model for acoustic phonons

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

**Linear dispersion model**

$$\omega = \nu_D q$$

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

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

Most textbooks derive the phonon DOS in frequency space, not energy space as we have.

\[
D_{ph}(\omega) = \frac{3\omega^2}{2\pi^2\nu_D^3} \quad \text{(no./Hz)}
\]

\[
D_{ph} (\hbar\omega) = \frac{3(\hbar\omega)^2}{2\pi^2(\hbar\nu_D)^3} \quad \text{(no./J)}
\]

\[
D_{ph}(\omega) = \frac{D_{ph} (\hbar\omega)}{\hbar}
\]
Debye model: cutoff frequency / wavevector

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

No. of states in a band $= N$.

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

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

$$q_D = \frac{\omega_D}{\nu_D} = \left( \frac{6\pi^2 N}{\Omega} \right)^{1/3}$$
Debye model: cutoff frequency / wavevector

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

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

\[ k_B T_D = \hbar \omega_D \]

Debye model valid when \( T_L << T_D \) (generally means \( T_L << 300K \))
Debye model: thermal conductivity

\[ \kappa_L = \frac{\pi^2 k_B^2 T_L}{3h} \int_{0}^{\omega_D} \lambda_{ph}(\hbar \omega) \frac{M_{ph}(\hbar \omega)}{A} W_{ph}(\hbar \omega) d(\hbar \omega) \]

\[ \omega_D = v_D \left( \frac{6\pi^2 N}{\Omega} \right)^{1/3} \quad M_{ph}(\omega) = \frac{3h\omega^2}{8\pi^2 v_D^2} \quad W_{ph}(\hbar \omega) = \left\{ \frac{3}{\pi^2} \left( \frac{\hbar \omega}{k_B T_L} \right)^2 \left( -\frac{\partial n_0}{\partial (\hbar \omega)} \right) \right\} \]

See:

limitation of Debye model

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

\( M_{ph} \)  \hspace{1cm} \text{Debye (Si)}
\( W_{ph} \)  \hspace{1cm} \text{full band (Si)}

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.

**electrons in Si**

![Graph showing effective mass and density of states for electrons in Si.](image)

- $M_{el}$, EMA
- $M_{el}$, full band
- $W_{el}$, 50 K
- $W_{el}$, 300 K

$E_C = E_F = 0$
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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 6)

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.
To compute the phonon dispersion, we expand the bonding energy in a Taylor series expansion. To first order, the potential energy is harmonic:

\[ U = \frac{1}{2} k (x - x_0)^2 \]

To this order, the normal modes are independent, there is no scattering. Higher order terms, give an anharmonic potential and scattering electrons from one mode to another.

\[ \hbar q_3 = \hbar q_1 + \hbar q_2 \]

\[ \hbar \omega_3 = \hbar \omega_1 + \hbar \omega_2 \]

\textit{little effect on thermal conductivity!}
N and U processes

Normal (N) process (momentum conserved)
Little effect on $\kappa_L$.

Umklapp (U) process (momentum not conserved)
Lowers $\kappa_L$.

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

\[
n_0 = \frac{1}{e^{\hbar\omega/k_B T_L} - 1}
\]

\[
e^{\hbar\omega/k_B T_L} \approx 1 - \hbar\omega/k_B T_L
\]

\[
n_0 \approx \frac{k_B T_L}{\hbar\omega}
\]

\[
\frac{1}{\tau_U} \propto n_0 \propto T_L
\]
scattering summary

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

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

\[\lambda_{ph}(\hbar\omega) \propto \nu_{ph}(\hbar\omega) \tau_{ph}(\hbar\omega)\]

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

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

3) Umklapp scattering: \(1/\tau_U(\hbar\omega) \propto T_L\) \(\begin{cases} 1/\tau_U(\hbar\omega) \propto e^{-T_D/b_T}T_L^3\omega^2 \end{cases}\)
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   i) Temperature dependent $\kappa_L$
   ii) Electrons vs. phonons
   iii) Quantized heat flow
9.8 Summary
i) measured vs. calculated $\kappa_L(T_L)$ for silicon

\[ \kappa_L = \frac{\pi^2 k_B^2 T_L}{3h} \left\langle M_{ph} \right\rangle \times \left\langle \lambda_{ph} \right\rangle \]

\[ \kappa_{L\ell} = \frac{1}{3} C_V \left\langle \nu_{ph} \right\rangle \left\langle \Lambda_{ph} \right\rangle \]

population of modes vs. $T_L$

\[ \left\langle \frac{M_{ph}}{A} \right\rangle \]

\[ \propto T_L^3 \]

more modes

\[ \left\langle \frac{M_{ph}}{A} \right\rangle \equiv \int \frac{M_{ph}(\hbar\omega)}{A} W_{ph}(\hbar\omega) d(\hbar\omega) \]
mean-free-path vs. $T_L$

\begin{equation}
\kappa_{ph}(T) \propto T_L^3
\end{equation}

\begin{align*}
\left\langle \lambda_{ph} \right\rangle & \text{ Limited by boundaries} \\
\text{defect scattering important} & \\
\text{dominated by phonons (U-processes)} & \\
\frac{1}{\lambda_{ph}(\hbar \omega)} & = \frac{1}{\lambda_D(\hbar \omega)} + \frac{1}{\lambda_B(\hbar \omega)} + \frac{1}{\lambda_U(\hbar \omega)}
\end{align*}

Lundstrom and Jeong 2011
temperature-dependent thermal conductivity

\[ \kappa_{ph} (\text{Wm}^{-1}\text{K}^{-1}) \]

population of modes and boundary scattering

phonon scattering by U-processes

\[ \kappa_L = \frac{\pi^2 k_B^2 T_L}{3h} \left\langle M_{ph} \right\rangle \times \left\langle \left\langle \lambda_{ph} \right\rangle \right\rangle \]

Lundstrom and Jeong 2011
ii) electron vs. phonon conductivities

The expressions look similar:

\[ \kappa_{L\ell} = \frac{\pi^2 k_B^2 T_L}{3h} \langle M_{ph}/A \rangle \langle \lambda_{ph} \rangle \]
\[ \sigma = \frac{2q^2}{\hbar} \langle M_{el}/A \rangle \langle \lambda_{el} \rangle \]

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.
quantized heat flow

Both the charge and heat currents are quantized.

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

\[ \approx \frac{\pi^2 k_B^2 T_L}{3h} T_{ph}(0) M_{ph}(0) \text{ at low temp} \]

Nanostructure at low temperatures can have nearly ballistic phonon transport with a small number of modes occupied. See the paper by Schwab, et al. for experimental confirmation of quantized heat flow.

9.1 Introduction
9.2 Electrons and Phonons
9.3 General model for heat conduction
9.4 Thermal conductivity
9.5 Debye model
9.6 Scattering
9.7 Discussion
9.8 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.
for more about heat transport


quantized thermal transport

for more about this lecture

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