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**

\[ E(\vec{k}) \]

\[ \tilde{v}_e(\vec{k}) = \frac{1}{\hbar} \tilde{k} E(\vec{k}) \]

\[ f_0(E) = \frac{1}{e^{(E-E_F)/k_BT_e} + 1} \]

**Phonons**

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

\[ \tilde{v}_p(\vec{q}) = \tilde{\nu}_q \omega(\vec{q}) \]

\[ n_0(\hbar \omega) = \frac{1}{e^{\hbar \omega/k_BT_L} - 1} \]
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\(^2\))} \]

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

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

\[ C_V = \left. \frac{\partial E_L}{\partial T} \right|_V \]
Review: electron transport (3D)

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

\[ f_1(E) = \frac{1}{1 + e^{(E - E_{F1})/k_B T_1}} \]

\[ f_2(E) = \frac{1}{1 + e^{(E - E_{F2})/k_B T_2}} \]

\[ M_{el}(E) = A \frac{h}{4} \left\langle v_x^+ \right\rangle D_{3D}(E) \]

\[ \mathcal{T}_{el}(E) = \frac{\lambda(E)}{\lambda(E) + L} \]
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Landauer approach to phonon transport

Thermal reservoir in equilibrium at temperature, $T_1$.

$n_1(\hbar \omega) = \frac{1}{e^{\hbar \omega/k_B T_1} - 1}$

channel characterized by a phonon dispersion

Thermal reservoir in equilibrium at temperature, $T_2$.

$n_2(\hbar \omega) = \frac{1}{e^{\hbar \omega/k_B T_2} - 1}$

channel

$x$

$I = \frac{2q}{h} \int T_{el}(E) M_{el}(E)(f_1 - f_2) dE \Rightarrow I_Q =$?
Heat flux

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

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

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

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

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

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

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

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

\[ I_Q = -K_L \Delta T_L \]
Lattice thermal conductance (i)

\[ I_Q = \frac{1}{h} \int (\hbar \omega) T_{ph}(\hbar \omega) M_{ph}(\hbar \omega)(n_1 - n_2) d(\hbar \omega) \quad (n_1 - n_2) \approx -\frac{\hbar \omega}{T_L} \left( -\frac{\partial n_0}{\partial (\hbar \omega)} \right) \Delta T_L \]

\[ I_Q = -K_L \Delta T_L \]

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

\[ Q = -K_L \Delta T_L \]

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

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

\[ K_L = \frac{\pi^2 k_B^2 T_L}{3h} \int \mathcal{T}_{ph} (\hbar \omega) M_{ph} (\hbar \omega) \left\{ \frac{3}{\pi^2} \left( \frac{\hbar \omega}{k_B T_L} \right)^2 \left( \frac{\partial n_0}{\partial (\hbar \omega)} \right) \right\} d(\hbar \omega) \]
Window functions: electrons vs. phonons

Electrons

\[ W_{el}(E) = \left( -\frac{\partial f_0}{\partial E} \right) \]

Phonons

\[ W_{ph}(\hbar \omega) = \left\{ \frac{3}{\pi^2} \left( \frac{\hbar \omega}{k_B T_L} \right)^2 \left( -\frac{\partial n_0}{\partial (\hbar \omega)} \right) \right\} \]
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: \( W_{el}(E) = (-\frac{\partial f_0}{\partial E}) \)
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Ballistic phonon transport

\[ I_Q = -K_L \Delta T_L = \frac{\Delta T_L}{R_L} \]

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

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


\[ g_0 = \frac{\pi^2 k_B^2 T}{3h} \]
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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

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

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

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

\[ \kappa_L = K_L \frac{L}{A} \quad \text{(Watts/m-K)} \]
Conductance and conductivity

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

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

\[ \kappa_L = K_L \frac{L}{A} \]

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

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

Lundstrom ECE-656 F17
Diffusive heat transport (3D)

\[ J_Q = -\kappa_L \frac{dT_L}{dx} \] (Watts / m\(^2\))

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

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

\[ \sigma = \frac{2q^2}{h} \int \lambda_{el}(E) \frac{M_{el}(E)}{A} W_{el}(E) dE \] (1/Ohm-m)
Diffusive heat transport (3D)

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

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

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

\[ \sigma = \frac{2q^2}{h} \langle M_{el}/A \rangle \langle \langle \lambda_{el} \rangle \rangle \quad \text{(1/Ohm-m)} \]
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   - connection to traditional approach
   - Debye model
   - thermal conductivity vs. temperature
   - MFP distribution

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

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

\[ E_L = \int_0^\infty (\hbar \omega) D_{ph}(\hbar \omega) n_0(\hbar \omega) d(\hbar \omega) \quad C_V = \frac{\partial E_L}{\partial T} \bigg|_V \]

Specific heat is related to DOS.
Connection to traditional approach

\[ \kappa_L = \frac{\pi^2 k_B^2 T}{3h} \left\langle M_{ph} / A \right\rangle \left\langle \left( \lambda_{ph} \right) \right\rangle \leftrightarrow \frac{1}{3} \Lambda_{ph} v_{ph} C_V \]  

(Watts/m-K)

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

\[ M_{ph} / A = \frac{h}{2} \left\langle \nu_{ph}^+ \right\rangle D_{ph}(\hbar \omega) \quad \left\langle \nu_{ph}^+ \right\rangle = \frac{v_{ph}^+}{2} \]

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Debye model for acoustic phonons

Linear dispersion model

\[ \omega = \nu_D q \]

\[ D_{ph}(\hbar\omega) = \frac{3(\hbar\omega)^2 \Omega}{2\pi^2 (\hbar\nu_D)^3} \quad (\text{J}-\text{m}^3)^{-1} \]

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

If acoustic phonons near \( q = 0 \) mostly contribute to heat transport, the Debye model works well.
Debye model in practice

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

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.

Electrons in Si

\[ E_C = E_F = 0 \]

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

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

Population of modes vs. $T_L$

\[ \left< \frac{M_{ph}}{A} \right> \]

\[ \kappa_{ph} \propto T_L^3 \]

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

more modes


Mean-free-path vs. $T_L$

\[ \left\langle \lambda_{ph} \right\rangle \]

Limited by boundaries

Defect scattering important

dominated by phonons (U-processes)

\[ \frac{1}{\lambda_{ph}(\hbar\omega)} = \frac{1}{\lambda_D(\hbar\omega)} + \frac{1}{\lambda_B(\hbar\omega)} + \frac{1}{\lambda_U(\hbar\omega)} \]
Temperature-dependent thermal conductivity

\[ \kappa_{ph} = \frac{\pi^2 k_B^2 T}{3hf} \left\langle M_{ph} \right\rangle \times \left\langle \lambda_{ph} \right\rangle \]

population of modes and boundary scattering

defects

phonon scattering by U-processes

Si
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MFP and thermal conductivity

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

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

\[ \kappa_L = \int \kappa_\lambda d\lambda_{ph} \]

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

“MFP distribution”
MFP and thermal conductivity


\[
\text{Cumm } \kappa_L \left( \lambda_1 \right) = \left( \int_0^{\lambda_1} \kappa \lambda \, d\lambda \right) / \kappa_L^{\text{bulk}}
\]
MFP spectra – phonons vs. electrons

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

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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:

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

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 \( \gg k_B T_L \) which for phonons, BW \( \sim k_B T_L \). Most of the modes are occupied for phonons but only a few for electrons.
The lattice thermal conductivity of Bi$_2$Te$_3$ is much lower than that of Si.

<table>
<thead>
<tr>
<th>Material</th>
<th>Lattice Thermal Conductivity</th>
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<tbody>
<tr>
<td>Bi$_2$Te$_3$</td>
<td>$\kappa_L \approx 1$ W/m-K</td>
</tr>
<tr>
<td>Silicon</td>
<td>$\kappa_L \approx 150$ W/m-K</td>
</tr>
</tbody>
</table>

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

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

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

<table>
<thead>
<tr>
<th>Material</th>
<th>( \kappa_L ) (W/m·K)</th>
<th>( \left&lt; \lambda_{ph} \right&gt; ) (nm)</th>
<th>( \left&lt; M_{ph} \right&gt; ) (m(^{-2}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bi(_2)Te(_3)</td>
<td>( \approx 1 )</td>
<td>( \approx 11 )</td>
<td>( \approx 3.2 \times 10^{17} )</td>
</tr>
<tr>
<td>Silicon</td>
<td>( \approx 150 )</td>
<td>( \approx 140 )</td>
<td>( \approx 3.3 \times 10^{18} )</td>
</tr>
</tbody>
</table>

(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 information about Landauer Approach


Questions?

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

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

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

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

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

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