Thermal Energy at the Nanoscale

Week 4: Landauer Transport Formalism
Lecture 4.6: Wrap up

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Unidirectional Heat Flux

- The rate of heat flow leaving the hot \((T_1)\) reservoir per unit ‘area’ can be expressed as

\[
J_{Q,L\to R}(T_1) = \frac{1}{L^d} \sum_p \sum_{k;k_x>0} \nu_{gx,p}(k) \left[ E_{i,p}(k) - \mu \right] T_p(k) \left[ f_i^o(E_{i,p}(k),T_1) + c_0 \right]
\]

- Compare to internal energy

\[
U = \sum_k \sum_p E_{i,p}(k) f_i^o \left[ E_{i,p}(k), T^- \right]
\]

- Note that the \(\mu\) term accounts for ‘replacement’ carriers required to maintain thermodynamic equilibrium in the reservoir

- \(\nu_{gx,p}\) represents the x-component of velocity
2D Systems

\[ J_{Q,\text{net}} = \frac{1}{L^d} \sum_p \sum_{k; k_x > 0} v_{g,x,p} \left[ E_{i,p}(k) - \mu \right] T_p \left[ f_i^o(T_1) - f_i^o(T_2) \right] \]

\[(2D) = \sum_p \int_{-\pi/2}^{\pi/2} \int_0^\infty \frac{v_{g,p} \cos \theta [E_{i,p} - \mu]}{4\pi^2} T_p \left[ f_i^o(T_1) - f_i^o(T_2) \right] kdkd\theta \]

\[= \sum_p \int_0^\infty \frac{v_{g,p} \left[ E_{i,p}(k) - \mu \right]}{2\pi^2} T_p \left[ f_i^o(T_1) - f_i^o(T_2) \right] kdk \]

Note: \( \langle \cos \theta \rangle = \frac{\int_{-\pi/2}^{+\pi/2} \cos \theta d\theta}{\pi} = \frac{2}{\pi} \)

Note: the last equality assumes that the transmission function \( T_p(k) \) depends only on the magnitude of \( k \) and not on its direction
The Meaning of $M$

- $M$ is a dimensionless number
- Represents the number of ‘sub-bands’ that fit in the width of the device

$M$ in Frequency Space (phonons)

\[ M(\omega) = \]

\[ (1D) = \pi \left[ v_g(\omega) \right] \frac{1}{v_g(\omega) \pi} = 1 \]

\[ (2D) = W \pi \left[ \frac{2 v_g(\omega)}{\pi} \right] \frac{K(\omega)}{2 \pi v_g(\omega)} \]

\[ (3D) = A \pi \left[ \frac{v_g(\omega)}{2} \right] \frac{K(\omega)^2}{2 \pi^2 v_g(\omega)} \]
Flux to Total Heat Flow Rate

• Let $Q$ be the heat flow rate (in energy/time, e.g., Watts)

$$J_Q(1D) = Q$$

$$J_Q(2D) = Q / W$$

$$J_Q(3D) = Q / A$$
Thermal Conductance

- Assume that $T_1 - T_2 = \delta T$ is very small
- Then, $f^0(T_1) - f^0(T_2) \approx \partial f^0 / \partial T \times \delta T$
- Thermal conductance $G_Q(T)$ expressed as

$$G_Q(T) = \frac{Q(T + \delta T / 2, T - \delta T / 2)}{\delta T}$$

(phonons) = \frac{1}{2 \pi} \int_0^\infty M(\omega) \hbar \omega T(\omega) \frac{\partial f_{BE}^0}{\partial T} d\omega

(electrons) = \frac{1}{\pi \hbar} \int_0^\infty M(E)(E - \mu) T(E) \frac{\partial f_{FD}^0}{\partial T} dE
Normalized Spectral Conductance

\[ \tilde{G}_Q' = \frac{G_Q'}{C_0 k_B M T} = (\pi i \omega)^2 e^x \chi^2 \]

where

\[ C_0 = (2\pi)^{-1} \text{(phonons)} \]

\[ = (\pi \hbar)^{-1} \text{(electrons)} \]

and

\[ \chi = \frac{\hbar \omega}{k_B T} \text{(phonons)} \]

\[ = \frac{E - \mu}{k_B T} \text{(electrons)} \]
Phonon Spectral Conductance (normalized)
$\chi^\alpha \tilde{G}'_Q$ Under Debye approx, $K \sim \omega \rightarrow \alpha$ corresponds to $d-1$
An Ideal 1D Phonon Conductor

- An ideal conductor has perfect transmission ($T = 1$)
  - Called ‘ballistic’
  - 1D conductor with one phonon branch ($M = 1$)

\[
\hat{G}_{Q,ph}(T) = \frac{k_B T}{2 \pi \hbar} \int_0^\infty \hat{G}_Q'(\chi) d\chi = \frac{k_B T}{2 \pi \hbar} \int_0^\infty (f_{BE}^\infty)^2 e^\chi \chi^2 d\chi
\]

- The integrand function is
The Quantum of Thermal Conductance

- Phonons

\[ \hat{G}_{Q, ph}(T) = \frac{\pi k_B^2 T}{6\hbar} \left( = T \times 9.464 \times 10^{-13} \text{W/K}^2 \right) \]

- Electrons

\[ \hat{G}_{Q, el}(T) = \frac{\pi k_B^2 T}{3\hbar} \left( = T \times 1.893 \times 10^{-12} \text{W/K}^2 \right) \]

- Exactly 2X larger than phonon result (because of spin)