NanoEnergy

ECE 597/697 Special Topics: Energy Transport and Conversion at the Nanoscale
http://blogs.umass.edu/eceng597en-zlatana/

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Meeting time and place: MWF 12:20 in Elab 306

*Office Hours*: Tue 10:30am, Fri after class, or by appt
Schedule for the rest of the semester

– HW3 Due Friday Oct. 31st
– HW4 Due Friday Nov. 7th (no Quiz!)
– Last day to turn in homework for credit Nov. 7th
– Midterm Exam distributed Monday Nov. 10th in class (no lecture)
– Midterm due Wed. Nov 12th beginning of class
– Final Project proposal and team members due Friday Nov. 14th (1 page statement of problem, methods, outcomes)
– Reading Assignment Reports Due Monday Nov. 17th (electronic submission preferred).
– Final Project presentations at final exam time Dec. 8th
– Final Reports due Dec. 8th (electronic submission, will accept until Friday Dec. 12th)
Recap so far

• So far we have discussed energy storage (expressed as heat capacity) of a single isolated structure
• First we calculated the energy per state/mode $E(k)$ or $\hbar \omega(k)$
• Next we calculated how many states/modes have that particular energy—the density of states
• We then derived the probability/number of carriers (electrons, phonons, photons) per state—the distribution function
• Then we just multiplied the three together and integrated over the energy variable—energy density $U(T)$
• Finally we looked at how much the energy density changes if we change temperature—heat capacity $C(T) = dU/dT$
### Recap so far

<table>
<thead>
<tr>
<th>Property</th>
<th>Electrons</th>
<th>Phonons</th>
<th>Photons</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Energy</strong></td>
<td>( E(k) = \frac{\hbar^2 k^2}{2m^*} )</td>
<td>( E(k) = \hbar \omega(k) = \hbar c_s</td>
<td>k</td>
</tr>
<tr>
<td><strong>Density of States</strong></td>
<td>( D(E) = \frac{1}{4\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \sqrt{E - E_0} )</td>
<td>( D(\omega) = \frac{N(\omega)}{V d\omega} = \frac{\omega^2}{2\pi^2 c_s^3} )</td>
<td>( D(\omega) = \frac{\omega^2}{\pi^2 c_s^3} )</td>
</tr>
<tr>
<td><strong>Type/Statistics</strong></td>
<td>Fermions: Fermi Dirac</td>
<td>Bosons: Bose-Einstein</td>
<td>Bosons: Bose-Einstein</td>
</tr>
<tr>
<td><strong>Distribution Function</strong></td>
<td>( f_{FD}(E,T) = \frac{1}{\exp \left( \frac{E - E_F}{k_B T} \right) + 1} )</td>
<td>( f_{BE}(E,T) = \frac{1}{\exp \left( \frac{\hbar \omega}{k_B T} \right) - 1} )</td>
<td>( f_{BE}(E,T) = \frac{1}{\exp \left( \frac{\hbar \omega}{k_B T} \right) - 1} )</td>
</tr>
<tr>
<td><strong>Heat Capacity, Low T</strong></td>
<td>( C_V(T) = \frac{\pi^2}{2} n_e k_B \frac{T}{T_F} )</td>
<td>( C_V(T) = k_B \frac{12\pi^4}{15} \left( \frac{N}{V} \right) \left( \frac{T}{T_D} \right)^3 )</td>
<td>( C_V(T) = k_B \frac{N}{V} )</td>
</tr>
<tr>
<td><strong>High T</strong></td>
<td></td>
<td>Black-body radiation</td>
<td></td>
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<tr>
<td></td>
<td></td>
<td>( e_b(T) = \frac{\pi^2 k_B^4}{60\hbar^3 c^2} T^4 = \sigma T^4 )</td>
<td></td>
</tr>
</tbody>
</table>
Moving energy around

- Let us now consider a system where two isolated solids are connected by a nanostructure.
- The two solids are assumed to be "reservoirs".
- They maintain a constant temperature $T_1$ and $T_2$ and constant density $E_{F1}$ and $E_{F2}$.
Moving energy around, cont.

- Both “reservoirs” are emitting carriers into the nanostructure.
- We want to compute the rate of energy transfer from each reservoir into the nanostructure – the energy/heat flux $Q_{1,2}$.
- Let’s first consider reservoir 1 on the left; only particles going left to right (positive “x” direction, $k_x$ and $v_x > 0$) contribute.
- The rate at which any given state transfers energy is

$$Q_1(k) = \frac{E(k)v_x(k)}{L}$$

- To get the total we simply multiply by the distribution and sum over states going right:

$$Q_1 = \sum_{k_x > 0} Q_1(k) = \frac{1}{L} \sum_{k_x > 0} f(E, T)E(k)v_x(k)$$
Moving energy around, cont.

- Note that we have not yet specified the type of carrier—they could be electrons, phonons, or even photons.
- Also note that we have neglected to consider the possibility that a carrier never makes it to the other end.
- To account for this possibility, we need to multiply by a probability of transmission $0 < \tau(k) < 1$

\[
Q_1 = \sum_{k_x > 0} Q_1(k) = \frac{1}{L} \sum_{k_x > 0} f(E, T_1) E(k) v_x(k) \tau(k) \]

- The energy flux from the other reservoir will look the same, except with $T_2$ and only left-moving carriers instead.

\[
Q_2 = \sum_{k_x < 0} Q_2(k) = \frac{1}{L} \sum_{k_x < 0} f(E, T_2) E(k) v_x(-k) \tau(-k) \]
Moving energy around, cont.

- The net energy flux is just the difference between the two terms

\[ Q_{tot} = Q_1 - Q_2 = \frac{1}{L} \left[ \sum_{k_x > 0} f(E, T_1)E(\vec{k})v_x(\vec{k})\tau(\vec{k}) - \sum_{k_x < 0} f(E, T_2)E(\vec{k})v_x(\vec{k})\tau(\vec{k}) \right] \]

- If \( T_1 = T_2 = T \), we have equilibrium and the net flux must be zero

\[ Q_{tot} = \frac{1}{L} \left[ \sum_{k_x > 0} f(E, T)E(\vec{k})v_x(\vec{k})\tau(\vec{k}) - \sum_{k_x < 0} f(E, T)E(\vec{k})v_x(\vec{k})\tau(\vec{k}) \right] = 0 \]

- Consequently the two summations (left-going and right-going) have to be exactly the same; otherwise we would have a flux

- Now let’s apply a temperature gradient \( \Delta T \) so that the temperature on the left is \( T + \Delta T \) and the right is \( T \).
Moving energy around, cont.

- The net energy flux is no longer zero

\[ Q_{\text{tot}} = \frac{1}{L} \left[ \sum_{k_x > 0} f(E, T + \Delta T) E(\vec{k}) v_x(\vec{k}) \tau(\vec{k}) - \sum_{k_x < 0} f(E, T) E(\vec{k}) v_x(\vec{k}) \tau(\vec{k}) \right] \]

- We can group the terms since the summations are the same

\[ Q_{\text{tot}} = \frac{1}{L} \sum_{k_x > 0} \left[ f(E, T + \Delta T) - f(E, T) \right] E(\vec{k}) v_x(\vec{k}) \tau(\vec{k}) \]

- In the limit of small gradient, we can expand the distribution function into a Taylor series and take the first two terms

\[ f(E, T + \Delta T) = f(E, T) + \Delta T \frac{\partial f(E, T)}{\partial T} \]

- Plugging into the above, we can write the conductance as

\[ K(T) = \frac{Q_{\text{tot}}}{\Delta T} = \frac{1}{L} \sum_{k_x > 0} \left[ f(E, T) + \Delta T \frac{\partial f(E, T)}{\partial T} - f(E, T) \right] E(\vec{k}) v_x(\vec{k}) \tau(\vec{k}) \]
Quantum Conductance

- We simplify the expression by cancelling the $\Delta T$ terms

\[
K(T) = \frac{1}{L} \sum_{k_x>0} \frac{\partial f(E,T)}{\partial T} E(\vec{k}) v_x(\vec{k}) \tau(\vec{k}) = \frac{1}{L} \sum_{k_x>0} C(\vec{k},T) v_x(\vec{k}) \tau(\vec{k})
\]

- For phonons and photons, we would replace $E$ with $\hbar \omega$ and use the Bose-Einstein distribution function

- For electrons, we would use the Fermi-Dirac distribution

- However, electrons carry both charge and energy—so far we’ve derived the energy/heat conductance

- The charge conductance would look the same except we replace the $E(k)$ with “$e$”, the electron charge to get

\[
Q_1 = \sum_{k_x>0} Q_1(k) = e \frac{L}{L} \sum_{k_x>0} f(E - E_{F1}, T_1) v_x(\vec{k}) \tau(\vec{k})
\]
Quantum Conductance

- Likewise, for the current going from right to left, we have

$$Q_2 = \sum_{k_x>0} Q_2(k) = \frac{e}{L} \sum_{k_x>0} f(E - E_{F2}, T_2) v_x \left( \vec{k} \right) \tau \left( \vec{k} \right)$$

- Electrons have both temperature and Fermi level; when both are equal, there is no net current (equilibrium)

- Normally we think of a charge current driven by a voltage gradient: let’s add $e\Delta V$ to the Fermi level so that $E_{F1} = E_F + \Delta V$:

$$Q_{tot} = Q_1 - Q_2 = \frac{e}{L} \sum_{k_x>0} \left[ f(E - E_F - e\Delta V, T) - f(E - E_F, T) \right] v_x \left( \vec{k} \right) \tau \left( \vec{k} \right)$$

- Again after expanding $f(E - E_F - \Delta V)$, we get conductance as:

$$G = \frac{Q_{tot}}{\Delta V} = \frac{e^2}{L} \sum_{k_x>0} \left( - \frac{\partial f(E - E_F, T)}{\partial E} \right) v_x \left( \vec{k} \right) \tau \left( \vec{k} \right)$$
Quantum Thermal Conductance-phonons

• Let’s compute the thermal conductance of a 1-d conductor
• Assume, for simplicity, perfect transmission with $\tau=1$
• For phonons, we would replace $E$ with $\hbar\omega$ and use the Bose-Einstein distribution function
  \[
  K(T) = \frac{1}{L} \sum_{k_x>0} \frac{\partial f_{BE}(\hbar\omega,T)}{\partial T} \hbar \omega(k) v_x(k)
  \]
• If the spacing of $k$’s is small enough, we can replace them by a continuum—then our sum turns into an integral
  \[
  K(T) = \frac{1}{L} \left( \frac{L}{2\pi} \right)^k \int_0^{k_D} \frac{\partial f_{BE}(\hbar\omega,T)}{\partial T} \hbar \omega(k) v_x(k)
  \]
• Finally we recognize that the velocity is just a derivative of $\omega$
  \[
  K(T) = \frac{1}{2\pi} \int_0^{k_D} \frac{\partial f_{BE}(\hbar\omega,T)}{\partial T} \hbar \omega(k) \frac{d\omega}{dk} dk = \frac{1}{2\pi} \int_0^{k_D} \frac{\partial f_{BE}(\hbar\omega,T)}{\partial T} \hbar \omega d\omega
  \]
Quantum Thermal Conductance-phonons

Now we can plug in the derivative of \( f_{BE} \) wrt \( T \) and group terms

\[
K(T) = \frac{1}{2\pi} \int_0^{k_D} \frac{\hbar \omega}{k_B T^2} \frac{\exp(\hbar \omega/k_B T)}{[\exp(\hbar \omega/k_B T) - 1]^2} \hbar \omega d\omega = \frac{k_B}{2\pi} \int_0^{k_D} \left( \frac{\hbar \omega}{k_B T} \right)^2 \frac{\exp(\hbar \omega/k_B T)}{[\exp(\hbar \omega/k_B T) - 1]^2} d\omega
\]

After our standard substitution for the unitless variable “x”

\[
x = \frac{\hbar \omega}{k_B T} \quad dx = \frac{\hbar}{k_B T} d\omega \quad d\omega = \frac{k_B T}{\hbar} dx
\]

We have a familiar integral—take the upper limit to infinity

\[
K(T) = \frac{k_B}{2\pi} \left( \frac{k_B T}{\hbar} \right) \int_0^\infty \frac{x^2}{[\exp(x) - 1]^2} dx = \frac{k_B^2 T}{h} \left( \frac{\pi^2}{3} \right)
\]

The thermal conductance is a universal value per conduction channel, independent of the actual material properties
Quantum Thermal Conductance-phonons

- This universal quantum thermal conductance has been measured/observed experimentally in 2000 (predicted in 1998)
- The quantum thermal conductance $g_0=(9.456 \times 10^{-13} \text{ W/K}^2)T$ is the maximum amount of energy transported by a single "channel"
Quantum Thermal Conductance—electrons

- For comparison, let’s compute the thermal conductance of a 1-d conductor filled with electrons
- For electrons we use the Fermi-Dirac distribution function

$$K(T) = \frac{1}{L} \sum_{k_x > 0} \frac{\partial f_{FD}(E, T)}{\partial T} E(\vec{k}) v_x(\vec{k})$$

- Again we convert our sum into an integral and recognize that $v(k) = \frac{1}{\hbar} dE/dk$

$$K(T) = \frac{1}{L \left( \frac{L}{2\pi} \right)^{k_{max}}} \int_0^{k_{max}} \frac{\partial f_{FD}(\hbar \omega, T)}{\partial T} E(\vec{k}) \frac{1}{\hbar} \frac{dE}{dk} dk$$

- Group terms and plug in the derivative

$$K(T) = \frac{1}{2\pi} \int_0^{k_{max}} \frac{E - E_F}{k_B T^2} \exp \left( \frac{E - E_F}{k_B T} \right) \exp \left( \frac{E - E_F}{k_B T} \right) + 1^2 \frac{EdE}{k_B T^2}$$
Quantum Thermal Conductance—electrons

- We would like to group the terms together into \((E-E_F)/k_B T\)
- Missing a "\(-E_F\)" term—add and subtract the same value

\[
K(T) = \frac{k_B}{2\pi} \int_0^{k_{\text{max}}} \left( \frac{E-E_F}{k_B T} \right)^2 \exp \left( \frac{E-E_F}{k_B T} \right) \left[ \exp \left( \frac{E-E_F}{k_B T} \right) + 1 \right] dE + E_F \frac{1}{2\pi T} \int_0^{k_{\text{max}}} \frac{E-E_F}{k_B T} \exp \left( \frac{E-E_F}{k_B T} \right) + 1 \right] dE
\]

- Making the substitution again:
  \[x = \frac{E-E_F}{k_B T}, \quad dx = \frac{dE}{k_B T}, \quad dE = k_B T dx\]

\[
K(T) = \frac{k_B^2 T}{2\pi} \int_{-E_F/k_B T}^{(E_{\text{max}}-E_F)/k_B T} x^2 \frac{\exp(x)}{[\exp(x) + 1]^2} dx + E_F \frac{k_B}{2\pi} \int_{-E_F/k_B T}^{(E_{\text{max}}-E_F)/k_B T} x \frac{\exp(x)}{[\exp(x) + 1]^2} dx
\]

- Note the lower limit depends on \(E_F\) explicitly
- If we assume \(E_F >> k_B T\) and \(E_{\text{max}} >> K_B T\), the limits go to +/−infinity
- However, we need \(E_F > 0\)! Otherwise, our conduction channel would be empty
Quantum Thermal Conductance—electrons

• With both limits going to +/- infinity, the integrals evaluate to constants:

\[
\int_{-\infty}^{\infty} x^2 \frac{\exp(x)}{[\exp(x)+1]^2} \, dx = \frac{\pi^2}{3}
\]

\[
\int_{-\infty}^{\infty} x \frac{\exp(x)}{[\exp(x)+1]^2} \, dx = 0
\]

\[K_e(T) = \frac{\pi^2 k_B^2 T}{3h}\]

• The second term with the Fermi level does not contribute!
• We obtain the same quantum thermal conductance per “channel” for electrons as we do for phonons!
• Both conclusions hinge on \(EF>0\) (or being larger than the lowest energy level, assumed here to be zero)
• Implies that whatever states we have available for conduction, they have to be filled—otherwise we get zero conductance!
Quantum Charge Conductance

- Unlike heat/energy which can be carried by both electrons and phonons, charge is only carried by electrons.
- For electrons, we would use the Fermi-Dirac distribution.
- We derived the quantum conductance simply by replacing energy $E(k)$ with the electron charge “$e$”
- Then we applied a small potential difference and obtained:

\[
G = \frac{Q_{tot}}{\Delta V} = \frac{e^2}{L} \sum_{k_x>0} \frac{\partial f(E-E_F,T)}{\partial E} v_x(\vec{k}) \tau(\vec{k})
\]

- We want to derive the quantum conductance of a 1-dimensional conductor (single conducting channel).
- Again we convert the sum to an integral and use \( v(k) = (1/\hbar) dE/dk \)

\[
G = \frac{e^2}{L} \left( \frac{L}{2\pi} \right)^{k_{max}} \int_0^{k_{max}} \frac{\partial f_{FD}(E-E_F,T)}{\partial E} \frac{1}{\hbar} \frac{dE}{dk_x} dk_x
\]
Quantum Charge Conductance

• The derivative terms cancel so we end up with an integral over energy

\[
G = \frac{e^2}{h} \int_0^{k_{\text{max}}} \left( - \frac{\partial f_{\text{FD}}(E-E_F, T)}{\partial E} \right) dE = \frac{e^2}{h} \int_0^{k_{\text{max}}} \frac{1}{k_B T} \left[ \exp\left( \frac{E - E_F}{k_B T} \right) + 1 \right]^2 dE
\]

• After the usual substitution \( x = (E-E_F)/k_B T \), we have

\[
G = -\frac{e^2}{h} \int_{-E_F/k_B T}^{(E_{\text{max}}-E_F)/k_B T} \frac{\exp(x)}{\left[ \exp(x) + 1 \right]^2} dx
\]

• In the \( k_B T \ll E_F \) case, we can let the limits of integration go to \( \infty \)

\[
G_0 = -\frac{e^2}{h} \int_{-\infty}^{\infty} \frac{\exp(x)}{\left[ \exp(x) + 1 \right]^2} dx = -\frac{e^2}{h} \left[ \frac{1}{\exp(x) + 1} \right]_0^{\infty} = \frac{e^2}{h}
\]
Quantum Charge Conductance

• This value $G_0 = \frac{e^2}{h}$ is the quantum conductance—the maximum amount of conductance obtainable from a perfect 1-d conductor.
• Its inverse, the “quantum resistance” evaluates to $\sim 25k\Omega$!
• Note that electrons can have spin up and spin down so the result is typically quoted with a factor of 2 in front ($2e^2/h$).
• For such a simple answer there should be a simpler derivation!
• Let’s try the uncertainty principle: $\sigma(E)\sigma(t) \geq h$
• The usual definition of conductance is $G = I/\Delta V$ where the current is $dQ/dt$.
• For a single 1-dimensional conductor, the charge density is simply the electron charge “e” and the transit time is the variance $\sigma(t)$.
• We can write $I = e/\sigma(t)$ and $\Delta V = \sigma(E)/e$.
• Together, $G = I/\Delta V = e/\sigma(t)*e/\sigma(E) = e^2/\left[\sigma(E)\sigma(t)\right] \leq e^2/h$. 


Quantum Charge Conductance

- What do the experiments say?

Quantized Conductance of Point Contacts in a Two-Dimensional Electron Gas

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Ballistic point contacts, defined in the two-dimensional electron gas of a GaAs-AlGaAs heterostructure, have been studied in zero magnetic field. The conductance changes in quantized steps of $e^2/h$ when the width, controlled by a gate on top of the heterojunction, is varied. Up to sixteen steps are observed when the point contact is widened from 0 to 360 nm. An explanation is proposed, which assumes quantized transverse resonances in the point-contact regime.

![Graph showing point-contact conductance as a function of gate voltage](image)

**FIG. 2.** Point-contact conductance as a function of gate voltage, obtained from the data of Fig. 1 after subtraction of the lead resistance. The conductance shows plateaus at multiples of $e^2/h$. 
Quantum Thermo-electric conversion

• What happens when we apply both a temperature difference and a voltage?
• OR can we get a charge current from a temperature difference?
• Let’s try it (we actually already solved this problem!)

\[ Q_{\text{tot}} = Q_1 - Q_2 = \frac{e}{L} \sum_{k_x > 0} \left[ f(E - E_F, T + \Delta T) - f(E - E_F, T) \right] v_x(k) \tau(k) \]

• Expand into a Taylor series and keep the 2 terms:

\[ \frac{Q_{\text{tot}}}{\Delta T} = \frac{e}{L} \sum_{k_x > 0} \frac{\partial f(E - E_F, T)}{\partial T} v_x(k) \tau(k) \]

• After the sum\(\rightarrow\)integral conversion and the group velocity

\[ \frac{Q_{\text{tot}}}{\Delta T} = \frac{e}{L} \left( \frac{L}{2\pi} \right)^{k_{\text{max}}} \frac{\partial f_{\text{FD}}(E - E_F, T)}{\partial T} \frac{1}{\hbar} \frac{dE}{dk} dk \]
Quantum Thermo-electric conversion

• Now we plug in the derivative and make the substitution for $x$

\[
\frac{Q_{tot}}{\Delta T} = \frac{e^{k_{max}}}{h} \int_0^{k_{max}} \frac{\partial f_{FD}(E - E_F, T)}{\partial T} dE = \frac{e^{k_{max}}}{h} \int_0^{k_{max}} \frac{E - E_F}{k_B T^2} \left[ \exp \left( \frac{E - E_F}{k_B T} \right) - 1 \right]^2 dE
\]

\[
\frac{Q_{tot}}{\Delta T} = \frac{e^{k_{max}}}{hT} \int_0^{k_{max}} x \left[ \exp(x) - 1 \right]^2 dx \Rightarrow 0
\]

• Letting the limits of integration go to infinity tells us that we cannot obtain a thermally driven current!

• The lack of thermo-electric effect is due to the same cause as the $\leq$ sign in the derivation

• In order to couple the temperature and voltage, we need interactions/scattering between electrons and phonons

• Scattering makes the transmission imperfect $\tau<1$