HW 7 ECE 65600 by Peide Ye

Due on November 12 Tuesday Lecture Time

1) The probability that an electron state is occupied is given by the Fermi function. The probability that a phonon is occupied is given by the Bose-Einstein distribution, which is:

   a) $n_0 = \frac{1}{e^{\frac{\hbar\omega}{k_B T}}+1}$

   b) $n_0 = \frac{1}{e^{\frac{\hbar\omega}{k_B T}}-1}$

   c) $n_0 = \frac{1}{e^{\frac{(\hbar\omega - E_F)}{k_B T}}+1}$

   d) $n_0 = \frac{1}{e^{\frac{(\hbar\omega - E_F)}{k_B T}}-1}$

   e) $n_0 = \frac{1}{e^{\frac{(\hbar\omega - E_F)}{k_B T}}-2}$

Answer: b)

The Bose-Einstein distribution formula for particles that do not obey the Pauli exclusion principle (like phonons) is given by:

$$n_0 = \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$

This formula differs from the Fermi-Dirac distribution (which applies to electrons) because phonons are bosons, not fermions, so they can occupy the same energy state. The factor $e^{\hbar\omega/k_B T} - 1$ in the denominator reflects the Bose-Einstein statistics, where $\hbar\omega$ is the phonon energy, k_B is the Boltzmann constant, and T is the temperature.

2) What is a plot of $\hbar\omega(\vec{q})$ *vs.* $\vec{q}$ for lattice vibrations called?

   a) The Einstein approximation.
   b) The Debye approximation.
   c) The gray approximation.
   d) The phonon dispersion.
   e) The Brillouin zone.

Answer: d)

The phonon dispersion relation $\hbar\omega(\vec{q})$ describes how the frequency (or energy) of phonons varies with their wavevector $\vec{q}$. This relation gives an idea into the vibrational properties of the lattice and how phonons propagate through it.

3) How can we obtain the phonon group velocity from a plot of $\hbar\omega(\vec{q})$ *vs.* $\vec{q}$?

   a) The group velocity is $\vec{v}_g(\vec{q}_0) = \omega(\vec{q})/d\vec{q}|_{\vec{q}=\vec{q}_0}$.
   b) The group velocity is $\vec{v}_g(\vec{q}_0) = d\omega(\vec{q})/d\vec{q}|_{\vec{q}=\vec{q}_0}$.
   c) The group velocity is $\vec{v}_g(\vec{q}_0) = \omega(\vec{q}_0)\vec{q}_0$.

d) The group velocity is $v_g(\vec{q}_0) = \vec{c}$.
e) The group velocity is $v_g(\vec{q}_0) = \vec{v}_s$.

Answer: b)

The phonon group velocity, which represents the speed at which energy or information is transported by phonons, is the derivative of the phonon frequency $\omega(\vec{q})$ with respect to the wavevector $\vec{q}$. This derivative $\vec{v}_g(\vec{q}_0) = d\omega(\vec{q})/d\vec{q}$ at a specific $q = q_0$ (Different values of q correspond to different vibrational modes in the lattice) gives the group velocity, indicating how fast phonons propagate energy at that specific wavevector.

4) What is the biggest difference between the electron dispersion and the phonon dispersion of a material?

a) The size in q-space of the Brillouin zone for phonons is smaller than the Brillouin zone for electrons.
b) The size in q-space of the Brillouin zone for phonons is larger than the Brillouin zone for electrons.
c) The bandwidth in energy of the phonon dispersion is much less than the bandwidth of the electron dispersion.
d) The bandwidth in energy of the phonon dispersion is much greater than the bandwidth of the electron dispersion.
e) For a given material, the two dispersions are identical.

Answer: c)

Phonon dispersion has a relatively limited energy bandwidth because it depends on lattice vibrations, which have lower energy scales than electronic excitations. In contrast, electron dispersion spans a much broader energy range because of the higher energy levels associated with electronic states in solids. This difference reflects the distinct nature of phonons versus electrons.

5) Comparing the electrical conductivity to the lattice thermal conductivity, which of the following statements is true?

a) The electrical conductivity can be positive or negative, but the lattice thermal conductivity is always positive.
b) The lattice thermal conductivity varies over <u>many</u> orders of magnitude.
c) The electrical conductivity varies over <u>many</u> orders of magnitude.
d) The two are related by Wiedemann-Franz Law.
e) The two are related by the Lorenz number.

Answer: c)

Electrical conductivity can vary significantly across materials, from insulators with negligible conductivity (low as 10^{-12} S/m) to metals with very high conductivity (low as 10^6-10^8 S/m). This wide range reflects the diversity of electronic structures and bonding types in different materials. In contrast, lattice thermal conductivity typically varies over a smaller range because it is governed by phonon transport, which is less affected by electronic band structure than electrical conductivity.

6) For electrons, the band structure is a plot of energy, $E(\vec{k})$, vs. wavevector, $\vec{k}$. For phonons, the dispersion is a plot of phonon energy, $\hbar\omega(\vec{q})$, vs. phonon wavevector, $\vec{q}$.

For electrons, we <u>often</u> approximate the band structure with simple, parabolic bands,

$$E(\vec{k}) = \frac{\hbar^2 k^2}{2m^*}$$

For phonons, we can sometimes approximate the phonon dispersion with the Debye approximation,

$$\hbar\omega = \hbar v_D q$$

where v_D is the Debye velocity (an average of the longitudinal and transverse acoustic velocities.)

6a) Compute the density of states, $D_{ph}(\hbar\omega)$, for phonons in the Debye model.

$$\frac{1}{\Omega} N_q dq = \frac{1}{8\pi^3} \times 3(4\pi q^2) dq = D_{ph}(\hbar\omega) d(\hbar\omega) \quad (1)$$

In this case, there is no factor of 2 for spin, unlike in electron-related calculations where spin degeneracy typically introduces a factor of 2. However, we do include a factor of 3 here to account for the three possible polarization modes of acoustic phonons: one longitudinal mode and two transverse modes.

$$\hbar\omega = \hbar v_D q \quad (2)$$

Given by the question, this is the linear dispersion relation for acoustic phonons in the Debye model, where v_D is the Debye velocity. By solving q in terms of $\hbar\omega$, we can rewrite q^2 as following.

$$q^2 = (\frac{\hbar\omega}{\hbar v_D})^2 \quad (3)$$

This relation is derived by differentiating the dispersion relation.

$$dq = \frac{d(\hbar\omega)}{\hbar v_D} \quad (4)$$

By substituting q^2 and dq from equations (3) and (4), we can express $D_{ph}(\hbar\omega)$ as a function of $\hbar\omega$.

$$D_{ph}(\hbar\omega) d(\hbar\omega) = \frac{3}{2\pi^2} q^2 dq = \frac{3}{2\pi^2} (\frac{\hbar\omega}{\hbar v_D})^2 \frac{d(\hbar\omega)}{\hbar v_D} \quad (5)$$

$$D_{ph}(\hbar\omega) = \frac{3(\hbar\omega)^2}{2\pi^2 (\hbar v_D)^3} \quad [\mathrm{J^{-1}\text{-}m^{-3}}] \quad (6)$$

6b) Compute the distribution of channels, $M_{ph}(\hbar\omega)$, for phonons in the Debye model.

$$M_{ph}(\hbar\omega) = \frac{h}{2} \langle v_z^+ \rangle D_{ph}(\hbar\omega) \quad (7)$$

To compute the distribution of channels $M_{ph}(\hbar\omega)$ for phonons, we start with the definition above. In the Debye model, the phonon velocity $v(\hbar\omega)$ is approximated as a constant v_D, the Debye velocity.

$$v(\hbar\omega) = v_D \quad (8)$$

When averaging over all angles in three dimensions, the average component of velocity along one direction (e.g., z-axis) is $v_D/2$.

$$\langle v_z^+ \rangle = \frac{v_D}{2} \tag{9}$$

We substitute $D_{ph}(\hbar\omega)$ and $\langle v_z^+ \rangle$ in Eq. (7) by Eq. (6) and Eq. (9).

$$M_{ph}(\hbar\omega) = \frac{h}{2}\langle v_z^+ \rangle D_{ph}(\hbar\omega) = \frac{h}{2}\frac{v_D}{2}\frac{3(\hbar\omega)^2}{2\pi^2(\hbar v_D)^3} = \frac{\hbar v_D}{2}\frac{3(\hbar\omega)^2}{2\pi(\hbar v_D)^3} \tag{10}$$

$$\boxed{M_{ph}(\hbar\omega) = \frac{3(\hbar\omega)^2}{4\pi(\hbar v_D)^2}} \tag{11}$$