

# Homework #2

ME 433: Nanoscale Energy Transport and Conversion  
University of Rochester  
Fall 2019

**Assigned:** Tuesday 9/24/19

**Due:** Thursday 10/3/19 (beginning of class)

## Topics:

- Photon heat capacity
- Group vs. phase velocity
- Density of states
- Heat capacity of bulk silicon

## 1. Heat capacity of photons in an oven

In class, we showed that the internal energy of photons on a per volume basis is  $u_{\text{photon}} = \frac{\pi^2 k_B^4 T^4}{15 \hbar^3 c^3} \left[ \frac{J}{m^3} \right]$ .

- Find an expression for the volumetric photon heat capacity  $C_{\text{photon}}$  [J/m<sup>3</sup>-K]
- Consider photons in an oven at a temperature  $T = 500$  K. Given that the heat capacity of air molecules in the oven is  $C_{\text{air}} = 517$  J/(m<sup>3</sup>-K), for most engineering applications is it important to consider  $C_{\text{photon}}$  when calculating the total heat capacity  $C_{\text{total}} = C_{\text{air}} + C_{\text{photon}}$ ?

## 2. Group vs. phase velocity

For photons, the linear dispersion relation  $\omega = ck$  means that the “phase velocity”  $v_{\text{phase}} = \frac{\omega}{k}$  and the “group velocity”  $v_g = \frac{\partial \omega}{\partial k}$  are identical:  $v_{\text{phase}} = v_g = c$ . However, in general,  $v_{\text{phase}} \neq v_g$ , as we noticed when we derived the non-linear Born-von Karman dispersion in our study of phonons, for example. This problem will help us understand why we use the group velocity, not the phase velocity, in our calculations of material properties.

- Consider an imaginary energy carrier with a dispersion relation  $\omega = \gamma k^2$ , where  $\gamma$  is a constant with units of m<sup>2</sup>/s. Provide analytical expressions for  $v_{\text{phase}}$  and  $v_g$ .
- Now consider two standing waves with fields  $E_1 = \cos(\omega_1 t - k_1 x)$  and  $E_2 = \cos(\omega_2 t - k_2 x)$  (here, we don’t necessarily mean an electric field; instead, we are using the term “field” generically, and could be referring to an electric field, a displacement field, etc.) We will add these two waves together to form a *wavepacket* with a field  $E = E_1 + E_2$ .

Consider a specific case where  $\gamma = 0.3$  m<sup>2</sup>/s,  $k_1 = 5.0$  m, and  $k_2 = 5.4$  m. At time  $t = 0$  s, plot  $E (= E_1 + E_2)$  as a function of  $x$  for  $x$  between -15 to 15 m.

- Now plot  $E(x)$  for three additional times,  $t = 1$  s,  $t = 2$  s, and  $t = 3$  s. By looking at each plot, estimate  $x_c$ , the location of the center of the wavepacket at time  $t$ . For example, at  $t = 0$  s,  $x_c = 0$  m. Since you are estimating  $x_c$  by eye, do not worry about being perfectly accurate.
- Plot  $x_c$  as a function of  $t$  using the values of  $x_c$  at times  $t = 0, 1, 2$ , and  $3$  s that you found in (c). On the same plot, also plot  $x_{c,\text{phase}} = v_{\text{phase}} t$  and  $x_{c,g} = v_g t$ . Evaluate both the group and phase velocities using an average wavevector  $k_{\text{avg}} = \frac{1}{2}(k_1 + k_2)$ .
- Based on your plot from (d), does the group velocity or the phase velocity do a better job at describing the wavepacket’s movement?

### 3. Density of states

Consider a special type of energy carrier with four identical polarizations and a power law dispersion relation  $\omega = bk^6$ , where  $b$  is a constant. The allowed frequencies go from 0 to  $\infty$ .

Find the density of states  $D(\omega)$ . **Hint:** Just as we found for photons and phonons, the allowed wavevector components are  $k_x = \frac{2\pi N_x}{L}$ ,  $k_y = \frac{2\pi N_y}{L}$ , and  $k_z = \frac{2\pi N_z}{L}$  where  $N_x$ ,  $N_y$ , and  $N_z$  are integers, and the size of the sample is  $L \times L \times L$ . Therefore, you can begin by constructing  $D(k)$  for a *single* polarization exactly as we did in class for photons and phonons.

### 4. Heat capacity of bulk silicon

Because silicon has a diamond crystal structure, it has 2 atoms per primitive unit cell, and therefore has both acoustic and optical phonon modes.

- a) Construct a Debye model for the acoustic phonon modes. You may use an identical effective velocity of  $v_{eff} = 6,000 \frac{m}{s}$  for all three polarizations. Given that  $\eta_{PUC} = 2.5 \times 10^{28}$ , find the Debye wavevector  $k_D$  (and then the Debye frequency  $\omega_D$  and the Debye temperature  $\theta_D$ ) to determine the upper bound of your integral.

Write down an expression for  $C_{acoustic} \left[ \frac{J}{m^3 K} \right]$  based on the information given above. You will not actually evaluate the integral yet, since doing so will require numerical integration.

- b) Construct an Einstein model for the optical phonon modes. Use  $\omega_E = 2\pi \cdot 14 THz \approx 8.8 \times 10^{13} rad/s$ . Write down an expression for  $C_{optical} \left[ \frac{J}{m^3 K} \right]$ .
- c) Plot  $C_{total} = C_{acoustic} + C_{optical}$  as a function of temperature for  $T$  between 0 K and 1000 K. You will need to do a simple numerical integral to calculate  $C_{acoustic}$ .
- d) To compare your results for the volumetric heat capacity of silicon with other materials, look at the *Ashby chart* below, which shows thermal conductivity (here called  $\lambda$ , but what we usually call  $k$ ) as a function of thermal diffusivity ( $a = \frac{k}{\rho c} = \frac{k}{C_v}$ ) for a variety of materials near room temperature. Therefore, a line on this plot is a line of constant volumetric heat capacity. Remarkably, we note that the many materials represented on this plot essentially all fall along a straight line: in other words, nearly all fully dense materials have the same volumetric heat capacity with a factor of  $\sim 3$ .

Does this result surprise you? How can you explain this result?

