ECE215A/Materials206A Winter 2008
Prof. Brown/ECE Dept/UCSB

Homework 4

1. *Monatomic linear lattice*. Consider a longitudinal wave $u_s = u\cos(\omega t - sKa)$ which propagates in a monatomic linear lattice of atoms of mass M, spacing a, and nearest-neighbor interaction C.
   (a) Show that the total energy of the wave is given by
   $$E = \tfrac{1}{2} M \sum_s (du_s/dt)^2 + \tfrac{1}{2} C \sum_s (u_s - u_{s+1})^2,$$
   where s runs over all atoms.

   (b) By substitution of u_s, in this expression, show that the time-average total energy per atom is
   $$\tfrac{1}{4} M\omega^2 u^2 + \tfrac{1}{2} C(1-\cos Ka)u^2 = \tfrac{1}{2} M\omega^2 u^2,$$
   where in the last step we have used the longitudinal-wave dispersion relation.

2. *Diatomic chain.* Consider the normal modes of linear chain in which the force constants between nearest-neighbor atoms are alternately C and 10C. Let the masses be equal, and let the nearest-neighbor separation be $a/2$. Find ω(k) at $k = 0$ and k = π/a.

3. Show that for long wavelengths the lattice-wave equation of motion reduces to the continuum elastic wave equation
   $$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2},$$
   where v is the velocity of sound.

4. Consider a two-dimensional lattice of area A containing N atoms and having two types of acoustical phonons. Using the Debye model (v = velocity of sound) , find expressions for:

(a) The two-dim energy for acoustical phonons excluding the "zero-point" term (Clues: D(ω) dω = (dN(K)/dK)(dK/dω) dω

(b) energy and heat capacity at low temperatures (Clue: let $\hbar\omega / kT \to \infty$; $\int_0^\infty \frac{x^2 dx}{e^x - 1} = 2.40$)

(c) energy and heat capacity at high temperatures (Clue: $\frac{1}{e^x - 1} \to \frac{1}{x}$

5. Use the results of Problem 4 to analyze a quasi-two dimensional crystal in which phonons propagate in parallel planes but not along the direction perpendicular to the planes. Evaluate the case of graphite in which each plane of phonon propagation is a hexagonal lattice with nearest-neighbor separation a = 3.0 Ang, and the separation between parallel planes is 2.4a. Assume the velocity of sound for both in-plane acoustical phonons is 5000 m/s and that the volume of the sample is 1 cm^3. Find:

(a) the phonon energy and heat capacity of the sample at 77-K using the low-temperature approximation.
(b) the phonon energy and heat capacity of the sample in the high-temperature limit.

6. A 3-dim solid sample has a crystal structure consisting of a Bravais lattice with four atoms per primitive cell (one primary plus three satellites).

(a) What is the number of acoustical lattice waves ? What is the number of optical lattice waves ? Of all the optical waves, how many are longitudinal and how many are transverse ?

(b) Use the Debye model for acoustic phonons to find expressions for the energy and specific heat capacity at low temperatures in terms of N_C, ω_D, T, and fundamental constants [clue: $\int_0^\infty \frac{x^3 dx}{e^x - 1} = \frac{\pi^4}{15}$].

(c) Evaluate the Debye frequency and Debye temperature assuming an average velocity of sound (for all three acoustical waves) of 5000 m/s, and a cubic crystal having a primitive cell of volume 30 Ang^3.

(d) Estimate the specific heat capacity in MKSA units at 77 K.

(e) Evaluate the classical (Dulong-Petit) specific heat capacity for the same sample as in (c).