PHY801: Survey of Atomic and Condensed Matter Physics Michigan State University

Homework 10

10.1. Show that for a diatomic chain (two different masses M_1 and M_2 that interact with same force constant C, as given in Eq. (18) of Kittel Chapter 4), the ratio of the displacements of the two atoms u/v for the k=0 optic mode is given by

$$\frac{u}{v} = -\frac{M_2}{M_1} \; ,$$

as shown in Eq. (26) of Kittel Chapter 4.

10.2. This problem is similar to Problem 10.1., but for zone boundary modes $(k = \pi/a)$, and is based on Kittel Chapter 4, Problem #3. For the linear harmonic chain treated by Eqs. (18) to (26) in Kittel Chapter 4, find the amplitude ratios u/v for the two branches at $k_{max} = \pi/a$. Show that at this value of k the two lattices act as if they were decoupled: one lattice remains at rest while the other lattice moves.

10.3. This problem for a diatomic chain is based on Kittel Chapter 4, Problem #5. Consider the normal modes of a 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 $\omega(k)$ at k=0 and $k=\pi/a$. Sketch in the dispersion relation by eye. This problem simulates a crystal of diatomic molecules such as H_2 .

10.4. This problem on singularities in the density of vibrational states is based on Kittel Chapter 5, Problem #1.

(a) From the dispersion relation derived in Chapter 4 for a monatomic linear lattice of N atoms with nearest neighbor interactions, show that the density of vibrational states is

$$D(\omega) = \frac{2N}{\pi} \cdot \frac{1}{(\omega_m^2 - \omega^2)^{1/2}} ,$$

where ω_m is the maximum frequency. The singularity at ω_0 is called a van Hove singularity.

(b) Suppose that an optical phonon branch has the form $\omega(k) = \omega_0 - Ak^2$ near k = 0 in three dimensions. Show that $D(\omega) = (L/2\pi)^3 (2\pi/A^{3/2})(\omega_0 - \omega)^{1/2}$ for $\omega < \omega_0$ and $D(\omega) = 0$ for $\omega > \omega_0$. Here the density of vibrational states is discontinuous.

10.5. This problem on the heat capacity of a layered solid in the Debye approximation is based on Kittel Chapter 5, Problem #4.

- (a) Consider a dielectric crystal made up of layers of atoms, with rigid coupling between layers so that the motion of the atoms is restricted to the plane of the layer. Show that the phonon heat capacity in the Debye approximation in the low temperature limit is proportional to T^2 .
- (b) Suppose instead, as in many layered structures, that adjacent layers are very weakly bound to each other. What form would you expect the phonon heat capacity to approach at extremely low temperatures?