

## Physics 489 Problem Set 4 Due Monday, Oct. 3

(1) Specific heat in the Debye model for 2D square lattice, 2 degenerate modes:

(a) Find the density of modes vs.  $\omega$  for the case that the speed of sound is  $c$  and the lattice is a simple square lattice, one atom per cell, with lattice constant  $a$ .

(b) Calculate the cutoff frequency,  $\omega_D$ .

(c) Following the procedure for specific heat calculation, write down the integral expression for the average energy, and by change of variables change the integral to dimensionless units.

(d) Evaluate the integral for the low temperature regime, and then take the derivative to find the specific heat for this temperature range. In this case we are looking for the leading term; you will have to find the integral in a table or perhaps in Mathematica. What is the temperature exponent for the specific heat in this case?

(e) Evaluate the integral in the limit of the high temperature regime, and again take the derivative to get  $C_V$  for high temperatures. Compare to the expectation for a classical harmonic lattice.

(2) Group velocity in 2D rectangular lattice: Consider the transverse waves in a 2-D lattice which were determined in the last homework set, problem 4.

(a) Find the group velocity, as a 2D vector, as a general function of  $k$  for this case.

(b) Find the points in the first Brillouin zone where the group velocity magnitude is zero.

(c) Show that the component of the velocity in the direction perpendicular to the zone boundary is zero, at all points on the boundary.

(d) Find the speed of sound for small wavevectors, and show that it is not isotropic. Find specifically the sound velocity for waves traveling in the x direction and in the y direction.

(e) Find the phonon density of modes for this case, limited to the case of small wavevectors where the trig functions can be Taylor expanded to lowest order.

(3) Thermal conductivity of germanium: See fig. 5.19 in your text showing a plot. At 200 K, normal Ge has  $k \sim 1$  W/(cm.K). The decrease with increasing  $T$  is due mostly to Umklapp scattering as noted in class.

(a) Ge has a lattice constant of  $5.7 \text{ \AA}$  (conventional cubic cell, for Ge in the diamond structure). From this determine the molar density of Ge, moles/cm<sup>3</sup>.

(b) Assume that at 200 K the phonon contribution to the specific heat for Ge has already reached the classical limit, and determine the specific heat per cm<sup>3</sup>. [Alternatively, you can make a slightly better estimate from the plot earlier in chapter 5, where you can see that  $C$  is still  $\sim 10\%$  below the classical limit at this temperature.]

(c) Ge has TA and LA phonon velocities of about 5000 and 3500 m/s, however the optical branches have considerably smaller velocities. Assume for a rough approximation a mean phonon velocity of 2000 m/s, and then based on your above results determine the phonon Umklapp mean free path at 200 K. Compare this to the period of the highest-frequency lattice vibration mode for Ge (see the slide I showed in class; vertical units are  $10^{12}$  Hz).

(4) Average square displacement of an atom in a harmonic crystal:

(a) Consult appendix C regarding the formalism for quantized harmonic crystals, and note that equation (32) in the appendix gives a relationship for the displacement of a given atom in terms of the phonon raising and lowering operators, which are defined in equations (28) and (29).

Suppose that a crystal is in a specific vibrational state, with wavefunction corresponding to a specific set of quantum numbers  $\{n_{ks}\}$ . For the case of a basis of 1, this set of quantum numbers is a set of  $N$  integers, and as we have seen each integer specifies the number of phonons present in each of the vibrational modes. We want the expectation value of the squared displacement of a given atom, in other words  $\langle \{n_{ks}\} | q^2 | \{n_{ks}\} \rangle$ . The square in the middle can be rewritten as products of raising and lowering operators using (32), however since the wavefunctions on the right and left are the same, we can have nonzero result only for a product of terms that raise and lower the same phonon mode, in either order. Thus, using the relations (23-26) for these operators applied to the vibrational states, find an expression for  $\langle \{n_{ks}\} | q^2 | \{n_{ks}\} \rangle$  as a sum over  $k$ ; the sum will contain the numbers of phonons,  $n_{ks}$  along with the atom mass and phonon frequencies.

(b) For  $T=0$  we have the zero-point motion limit; all phonon occupation numbers will be zero but there is still a nonzero expectation value. Find the expectation value in this case.

(c) I hope you obtained an expression in (b) that is proportional to a sum of  $(1/\omega)$  over all modes. This can be evaluated in the Debye approximation using the density of modes. To do this you need to turn the sum over  $k$  into an integral over  $\omega$ , and use the density of modes  $D(\omega)$  given by (22) in chapter 5. This is easier if you use (23) to eliminate the sound velocity  $v$  in (22) and write  $D(\omega)$  in terms of  $\omega_D$ . Do this, and finally express the  $T=0$  expectation value  $\langle q^2 \rangle$  in terms of  $\omega_D$  as well as  $\hbar$  and  $M$ .