

## HW 2 - PHONONS, DUE WED 17th, 5pm

Solve these problems from Simon's The Oxford Solid State Basics

### (9.2) Normal Modes of a One-Dimensional Monatomic Chain

(a)‡ Explain what is meant by “normal mode” and by “phonon”.

▷ Explain briefly why phonons obey Bose statistics.

(b)‡ Derive the dispersion relation for the longitudinal oscillations of a one-dimensional mass-and-spring crystal with  $N$  identical atoms of mass  $m$ , lattice spacing  $a$ , and spring constant  $\kappa$  (motion of the masses is restricted to be in one dimension).

(c)‡ Show that the mode with wavevector  $k$  has the same pattern of mass displacements as the mode with wavevector  $k + 2\pi/a$ . Hence show that the dispersion relation is periodic in reciprocal space ( $k$ -space).

▷ How many *different* normal modes are there.

(d)‡ Derive the phase and group velocities and sketch them as a function of  $k$ .

▷ What is the sound velocity?

▷ Show that the sound velocity is also given by  $v_s =$

$1/\sqrt{\beta\rho}$  where  $\rho$  is the chain density and  $\beta$  is the compressibility.

(e) Find the expression for  $g(\omega)$ , the density of states of modes per angular frequency.

▷ Sketch  $g(\omega)$ .

(f) Write an expression for the heat capacity of this one-dimensional chain. You will inevitably have an integral that you cannot do analytically.

(g)\* However, you can expand exponentials for high temperature to obtain a high-temperature approximation. It should be obvious that the high-temperature limit should give heat capacity  $C/N = k_B$  (the law of Dulong–Petit in one dimension). By expanding to next non-trivial order, show that

$$C/N = k_B(1 - A/T^2 + \dots)$$

where

$$A = \frac{\hbar^2 \kappa}{6mk_B^2}.$$

### (9.3) More Vibrations

Consider a one-dimensional spring and mass model of a crystal. Generalize this model to include springs not only between neighbors but also between second nearest neighbors. Let the spring constant between neighbors be

called  $\kappa_1$  and the spring constant between second neighbors be called  $\kappa_2$ . Let the mass of each atom be  $m$ .

(a) Calculate the dispersion curve  $\omega(k)$  for this model.

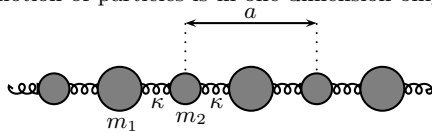
(b) Determine the sound wave velocity. Show the group velocity vanishes at the Brillouin zone boundary.

### (10.1) Normal modes of a One-Dimensional Diatomic Chain

(a) What is the difference between an acoustic mode and an optical mode.

▷ Describe how particles move in each case.

(b) Derive the dispersion relation for the longitudinal oscillations of a one-dimensional diatomic mass-and-spring crystal where the unit cell is of length  $a$  and each unit cell contains one atom of mass  $m_1$  and one atom of mass  $m_2$  connected together by springs with spring constant  $\kappa$ , as shown in the figure (all springs are the same, and motion of particles is in one dimension only).



(c) Determine the frequencies of the acoustic and optical modes at  $k = 0$  as well as at the Brillouin zone boundary.

▷ Describe the motion of the masses in each case (see margin note 4 of this chapter!).

▷ Determine the sound velocity and show that the group velocity is zero at the zone boundary.

▷ Show that the sound velocity is also given by  $v_s = \sqrt{\beta^{-1}/\rho}$  where  $\rho$  is the chain density and  $\beta$  is the compressibility.

(d) Sketch the dispersion in both reduced and extended zone scheme.

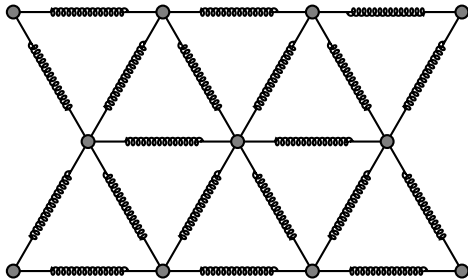
▷ If there are  $N$  unit cells, how many different normal modes are there?

▷ How many *branches* of excitations are there? I.e., in reduced zone scheme, how many modes are there there at each  $k$ ?

(e) What happens when  $m_1 = m_2$  ?

If you feel strong and theory inclined, Instead of solving 9.3 problems you can try instead this problem.

(9.8) Phonons in 2d\*



Consider a mass and spring model of a two-dimensional triangular lattice as shown in the figure (assume the lattice is extended infinitely in all directions). Assume that identical masses  $m$  are attached to each of their six neighbors by equal springs of equal length and spring constant  $\kappa$ . Calculate the dispersion curve  $\omega(\mathbf{k})$ . The two-dimensional structure is more difficult to handle than the one-dimensional examples given in this chapter. In Chapters 12 and 13 we study crystals in two and three dimensions, and it might be useful to read those chapters first and then return to try this exercise again.