Homework # 14

Exercise 1 - 1D monoatomic chain

Let us consider a linear chain of atoms, with one atom per unit cell, of mass M connected to the nearest neighbors by springs with force constant K. During the lectures we saw that in such a system there is a single dispersion curve (called acoustic branch) given by:

$$\omega(k) = 2\sqrt{\frac{K}{M}}\left|\sin\left(\frac{ka}{2}\right)\right|, \tag{1}$$

where k is the wave vector confined to the first Brillouin zone ($-\frac{\pi}{a} \leq k < \frac{\pi}{a}$) and a is the distance between nearest neighbors.

1. Calculate the group velocity $v_g(k) = \frac{d\omega(k)}{dk}$ and show that it is zero at the border of the Brillouin zone.

Sound propagates in solids as long-wavelength compression/dilation waves that are nothing but longitudinal acoustic phonons. In our system the speed of sound is therefore given by $|v_g(k=0)| := \lim_{k\to 0} |v_g(k)|$.

2. Write the expression for the speed of sound of the one-dimensional chain.
3. Show that in the long-wavelength limit ($k \to 0$) the group velocity is equal to the phase velocity $|v_p| = \frac{\omega(k)}{|k|}$.

Exercise 2 - 1D diatomic chain

Let us consider a linear chain of atoms, with two atoms per unit cell of mass M_1 and M_2 connected to nearest neighbors by springs with force constant K.

1. Write the classical equations of motions for the two atoms in the unit cell.

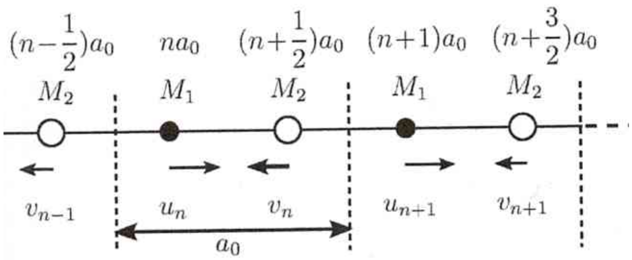

Figure 1: Longitudinal displacements in a 1D diatomic chain (adapted from *Solid State Physics* by Grosso and Pastori Parravicini.)

2. By imposing the ansatzs:

$$u_n(t) = A_1 e^{i(kna_0 - \omega t)} \tag{2}$$

$$v_n(t) = A_2 e^{i(k(n+1/2)a_0 - \omega t)}, \tag{3}$$

compute the phonon dispersion.

3. How many acoustic and optical phonon branches are present?

4. If $M_1 = M_2$, how does the phonon spectrum change qualitatively?
   At the Brillouin zone border, is there still an energy gap between acoustic and optical phonons?
   How do you recover the case discussed in Exercise 1?

Exercise 3 – The Debye model

Peter Debye was a physicist and physical chemist, who got the Nobel prize in Chemistry in 1936. His first major scientific contribution was the application of the concept of dipole moment to the charge distribution in asymmetric molecules in 1912, developing equations relating dipole moments to temperature and dielectric constant. In 1923, he worked with his assistant Erich Hückel (Hückel model), and developed an improvement of Svante Arrhenius' theory of electrical conductivity in electrolyte solutions.

In the Debye model, the phonon dispersion is assumed to be linear, $\omega = v_s\, q$ (v_s being the sound velocity), for all wave vectors $\mathbf{q}$. In addition, the Brillouin zone is replaced by a sphere of radius q_D. Several physical quantities can be expressed in term of the the Debye frequency $\omega_D = v_s\, q_D$.

1. Considering a monoatomic crystal (one atom per unit cell), determine the value of q_D as a function of the number density $n = N/V$ by imposing that the total number of q-points allowed in the sphere is equal to the number N of atoms in the crystal of volume V.

2. Compute an expression for ω_D as a function of the density ρ.

Sodium atoms have a mass of 23 amu, the sodium density is $\rho = 0.97\,\mathrm{g/cm^3}$. The mean velocity of sound (low frequencies) is $v_s = 3200\,\mathrm{m/s}$. Approximating the sodium structure with a simple cubic crystal:

3. Compute the Debye frequency ω_D for sodium.

4. At high temperatures the average displacement of atoms is given by:

$$\bar{u} = \sqrt{\langle u^2 \rangle} = \sqrt{\frac{9 k_B T}{M \omega_D^2}}\,. \qquad (4)$$

   According to Lindemann's criterion, a crystal melts when this average displacement is equal to 10% of the lattice constant. Evaluate the corresponding melting temperature of sodium.
   (*Hint: Remember that the density is an intensive quantity.*)