

Solutions of homework # 14

Exercise 1 - 1D monoatomic chain

1. The group velocity represents the velocity of energy propagation in the medium and it can be interpreted as the transmission velocity of a wave packet. For a linear chain of atoms, the group velocity is given by:

$$v_g(k) = \frac{d\omega(k)}{dk} = a\sqrt{\frac{K}{M}} \cos\left(\frac{1}{2}ka\right) \operatorname{sgn}\left(\sin\frac{ka}{2}\right) = a\sqrt{\frac{K}{M}} \cos\left(\frac{1}{2}ka\right) \operatorname{sgn}(k), \quad (1)$$

where $\operatorname{sgn}(x)$ is the sign function and we have used the fact that $\sin\frac{ka}{2}$ has the same sign of k inside the first Brillouin zone. At the border of the Brillouin zone we find

$$v_g(k = \pm\frac{\pi}{a}) = a\sqrt{\frac{K}{M}} \cos\left(\pm\frac{\pi}{2}\right) = 0. \quad (2)$$

This is in agreement with the fact that the mode at the border of the Brillouin zone corresponds to a standing wave and, as a consequence, there is no net energy propagation inside the chain.

2. The speed of sound inside the linear chain is given by

$$|v_g(k=0)| = a\sqrt{\frac{K}{M}}. \quad (3)$$

3. Because in the long-wavelength limit $\sin\left(\frac{1}{2}ka\right) \simeq \frac{1}{2}ka$, we can write the dispersion relation as:

$$\omega(k) \simeq 2\sqrt{\frac{K}{M}} \frac{1}{2}|k|a = a\sqrt{\frac{K}{M}}|k| \quad (4)$$

The phase velocity for $k \rightarrow 0$ is $|v_p(k \rightarrow 0)| = \lim_{k \rightarrow 0} \omega(k)/|k| = a\sqrt{\frac{K}{M}}$, and is equal to the group velocity $|v_g(k=0)|$.

Exercise 2 - 1D diatomic chain

1. We denote by u_n and v_n the displacements of the atoms of mass M_1 and M_2 , respectively and we assume that the atoms of mass M_1 occupy the sublattice positions $R_n^{(1)} = na_0$ and those of mass M_2 occupy the positions $R_n^{(2)} = (n + 1/2)a_0$, as reported in Fig. 1.

If we consider the interactions with the nearest neighbors only, the classical equations of motion for the two types of particles read:

$$\begin{cases} M_1 \ddot{u}_n = -K(u_n - v_{n-1}) - K(u_n - v_n) \\ M_2 \ddot{v}_n = -K(v_n - u_n) - K(v_n - u_{n+1}) \end{cases} \implies \begin{cases} M_1 \ddot{u}_n = -K(2u_n - v_{n-1} - v_n) \\ M_2 \ddot{v}_n = -K(2v_n - u_n - u_{n+1}) \end{cases} \quad (5)$$

2. The system above represents a set of two coupled differential equations that can be readily solved looking for traveling waves (i.e. solutions periodic both in space and time):

$$u_n(t) = A_1 e^{i(kna_0 - \omega t)}, \quad (6)$$

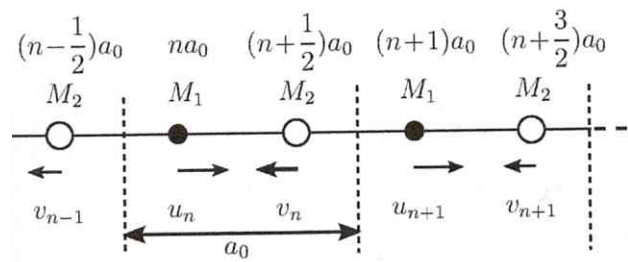


Figure 1: Longitudinal displacements in a 1D diatomic chain (adapted from *Solid State Physics* by Grosso and Pastori Parravicini.)

$$v_n(t) = A_2 e^{i(k(n+1/2)a_0 - \omega t)} . \quad (7)$$

By inserting (6)-(7) in (5), we obtain

$$\begin{cases} (M_1\omega^2 - 2K)A_1 + 2K \cos(ka_0/2)A_2 = 0 \\ 2K \cos(ka_0/2)A_1 + (M_2\omega^2 - 2K)A_2 = 0 \end{cases} \quad (8)$$

In order to have a non-trivial solution, i.e. $A_1 = A_2 = 0$, the matrix of the coefficients must be singular, that is, its determinant must be zero:

$$\begin{vmatrix} M_1\omega^2 - 2K & 2K \cos(ka_0/2) \\ 2K \cos(ka_0/2) & M_2\omega^2 - 2K \end{vmatrix} = 0 . \quad (9)$$

The solutions are:

$$\omega^2 = K \left(\frac{1}{M_1} + \frac{1}{M_2} \right) \pm K \sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2} \right)^2 - \frac{4 \sin^2(ka_0/2)}{M_1 M_2}} . \quad (10)$$

3. Such system has one acoustic (goes to 0 at the zone center) branch and one optical branch. In general, a d -dimensional system with N atoms in the primitive cell, has d acoustic branches and $d(N - 1)$ optical branches.
4. If $M_1 = M_2 = M$ the acoustic branch and the optical branch touch at the border of the Brillouin zone, hence the energy gap between the two vanishes. We can see this if we put equal masses in Eq.(10):

$$\begin{aligned} \omega^2 &= \frac{2K}{M} \pm K \sqrt{\frac{4}{M^2} - \frac{4 \sin^2(ka_0/2)}{M^2}} \\ &= \frac{2K}{M} [1 \pm \cos(ka_0/2)], \end{aligned} \quad (11)$$

and we then have:

$$\omega_1 = 2\sqrt{\frac{K}{M}} |\sin(ka_0/4)| \quad (12)$$

$$\omega_2 = 2\sqrt{\frac{K}{M}} |\cos(ka_0/4)| \quad (13)$$

which is exactly the phonon dispersion for the 1D monoatomic chain obtained in Exercise 1, simply refolded in a unit cell with lattice parameter $2a_0$. So a 1D monoatomic chain, which has only one acoustic branch (and no optical branches), can be equivalently represented

with a 1D diatomic chain of atoms with equal masses and spring constants, where the acoustic and optical branches touch at the zone border. In this case, the two branches are nothing else but the original acoustic branch refolded in a Brillouin zone which is now half of the original one.

Exercise 3 – The Debye model

1. We already know from the lectures on the density of states and on the free electron gas that the volume in reciprocal space associated with each allowed wave-vector is, in 3D, given by $(2\pi)^3/V$ where V is the volume of the system. Moreover, for a monoatomic crystal, the number of allowed wavevectors in the first Brillouin zone is equal to the number of atoms in the crystal. The volume of the first Brillouin zone then is $N(2\pi)^3/V$ and it has to be equal to $4\pi q_D^3/3$, from which we obtain:

$$q_D = \sqrt[3]{\frac{N6\pi^2}{V}} = \sqrt[3]{6\pi^2 n}. \quad (14)$$

2. The Debye frequency is given by:

$$\omega_D = v_s q_D = v_s \sqrt[3]{6\pi^2 n} = v_s \sqrt[3]{\frac{6\pi^2 \rho}{M}}, \quad (15)$$

where $\rho = nM$ and M is the atomic mass.

3. The Debye frequency for sodium is calculated as:

$$\omega_D = (3200 \text{ m/s}) \sqrt[3]{\frac{6\pi^2 \cdot 0.97 \text{ g/cm}^3}{23 \cdot 1.66 \cdot 10^{-27} \text{ g}}} = 3.67 \cdot 10^{13} \text{ s}^{-1}. \quad (16)$$

4. According to Lindemann's criterion, the melting temperature is given by

$$T_m = \frac{M\omega_D^2}{9k_B} \cdot (0.1a)^2, \quad (17)$$

where a is the lattice parameter. If we assume the sodium to have a simple cubic crystal structure, we can express the density as the ratio between the atomic mass and the volume of the primitive cell¹:

$$\rho = \frac{M}{a^3} \quad \Rightarrow \quad a = \sqrt[3]{\frac{M}{\rho}} = 3.4 \text{ \AA}. \quad (18)$$

Finally, we can calculate the melting temperature:

$$T_m = \frac{23 \cdot 1.66 \cdot 10^{-27} \cdot (3.67 \cdot 10^{13})^2}{9 \cdot 1.38 \cdot 10^{-23}} \cdot (0.1 \cdot 3.4 \cdot 10^{-10})^2 \text{ K} = 479 \text{ K}, \quad (19)$$

which is 100 K bigger than the experimental value, 370 K.

¹Here we have exploited the fact that the density is an intensive quantity.