SOLUTIONS FOR HW2 - don't' distribute!

(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 κ (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 ρ is the chain density and β 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

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

where

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

(a) A *normal mode* is a periodic collective motion where all particles move at the same frequency. A *phonon* is a quantum of vibration.

[I do not like the definition "a quantum of vibrational energy". The vibration does carry energy, but it carries momentum as well, so why specify energy only?]

Each classical normal mode of vibration corresponds to a quantum mode of vibration which can be excited multiple times. A single mode may be occupied by a single phonon, or it may be occupied with multiple phonons corresponding to a larger amplitude oscillation. The fact that the same state may be multiply occupied by phonons means that phonons must be bosons.

(b) The equation of motion for the n^{th} particle along the chain is given by

$$m\ddot{x}_n = \kappa(x_{n+1} - x_n) + \kappa(x_{n-1} - x_n) = \kappa(x_{n+1} + x_{n-1} - 2x_n)$$

note that na is the equilibrium position of the n^{th} particle. Using the ansatz

$$x_n = Ae^{i\omega t - ikna}$$

we obtain

$$\begin{aligned} -\omega^2 m e^{i\omega t - ikna} &= \kappa e^{i\omega t}(e^{ik(n+1)a} + e^{ik(n-1)a} - 2e^{ikn}) \\ \omega^2 m = &= 2\kappa(\cos(ka) - 1) \end{aligned}$$

or

$$\omega = \sqrt{(2\kappa/m)(\cos(ka) - 1)} = 2\sqrt{\kappa/m}\,|\sin(ka/2)|$$

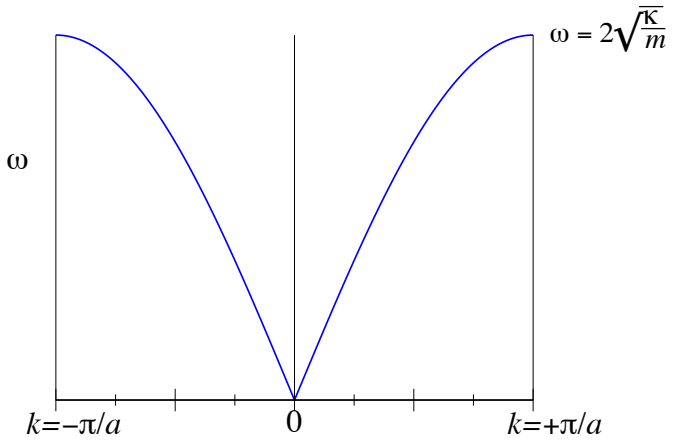


Fig. 9.1 Dispersion relation for vibrations of the one-dimensional monatomic harmonic chain. The dispersion is periodic in $k \to k + 2\pi/a$.

(c)

$$e^{-i(k+2\pi/a)na} = e^{-i(k+2\pi/a)na} = e^{-ikna}$$

If you assume periodic boundary conditions, then $k = 2\pi m/L$ but k is identified with $k + 2\pi/a$ so that there are therefore exactly $N = L/a$ different normal modes.

(d)

$$v_{phase} = \omega(k)/k = 2\sqrt{\kappa/m}\,|\sin(ka/2)|/k$$

and

$$v_{group} = d\omega(k)/dk = \sqrt{\kappa/m}\,a\cos(|k|a/2) = (a/2)\omega_0\sqrt{1-\omega^2/\omega_0^2}$$

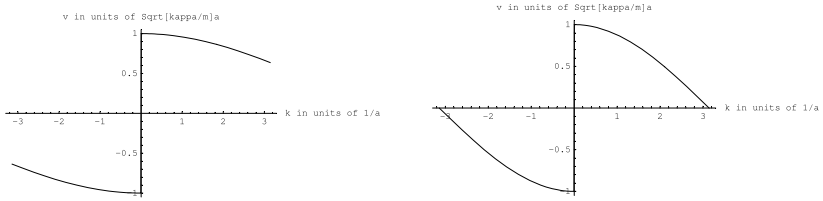


Fig. 9.2 The monatomic harmonic chain. Right: Phase velocity. Left: Group velocity. Note velocities are signed quantities, to the left of the origin, the velocity should have negative sign.

where $\omega_0 = 2\sqrt{\kappa/m}$. Note that the phase velocity is not periodic in the Brillouin zone! One can understand this if you think carefully about aliasing of waves. The phase velocity is the velocity at which the peaks of waves move. However, the waves are only defined at the position of the masses along the chain. We write $\cos(kna)$ for the positions of the masses at some time, but this only defines the value of the wave for integer n. For integer n, we have k is the same as $k + 2\pi/a$. However, the "peak" of this function may be between the integer values of n. However, when we make n non-integer, then k is no longer the same as $k + 2\pi/n$.

For sketches see figure 9.2

The sound velocity is the velocity at small k. This is

$$v = a\sqrt{\kappa/m}$$

. The density of the chain is $\rho = m/a$ and the compressibility is $\beta = -(1/L)dL/dF = 1/(\kappa a)$. Thus we obtain $v^{-2} = \rho\beta$

(e) Note first that

$$(\omega(k)/2)^2 + (v_{group}(k)/a)^2 = \kappa/m \tag{9.1}$$

Density of states is uniform in k. If there are N sites in the system, there are N modes total. The density of states in k is therefore $dN/dk = Na/(2\pi) = L/(2\pi)$ where L is the length of the system.

Thus we have

$$\begin{aligned} g(\omega) &= dN/d\omega = (dN/dk)(dk/d\omega) = \frac{Na}{2\pi v_{group}} \\ &= \frac{N}{2\pi\sqrt{\kappa/m}\cos(|k|a/2)} \\ &= \frac{2N}{2\pi\sqrt{(\kappa/m) - (\omega(k)/2)^2}} \end{aligned} \tag{9.2}$$

where we have used Eq. 9.1.

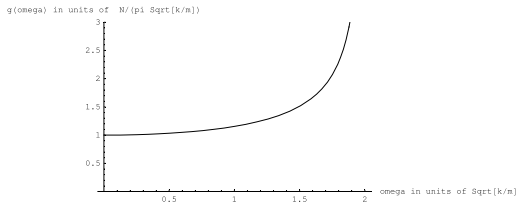


Fig. 9.3 The one dimensional harmonic chain. Density of states $g(\omega)$. Note that the DOS diverges at $\omega = 2\sqrt{k/m}$ where the group velocity goes to zero.

The additional factor of 2 that appears up top is to account for the fact that for each value of $\omega > 0$ there are actually two values of k with that ω. (Note if you integrate over frequency you correctly get back N degrees of freedom).

(f) The energy stored in the chain is given by

$$U = \int d\omega g(\omega)\hbar\omega(n_B(\omega) + 1/2)$$

so the heat capacity is $C = \partial U/\partial T$. Note that we can drop the $+1/2$ since it has no derivative.

(g) To recover the law of Dulong-Petit, one takes the high temperature limit of $n_B(\omega) = k_B T/\hbar\omega$ so th at we have

$$C = \frac{\partial}{\partial T}\int d\omega g(\omega)(k_B T) = k_B \int d\omega g(\omega) = k_B N$$

To go further, we use the high temperature expansion (expanding $1/(e^x - 1)$ for small x)

$$n_B(\omega) + 1/2 = \frac{k_B T}{\hbar\omega} + \frac{1}{12}\frac{\hbar\omega}{k_B T} + \ldots$$

So that we now have

$$C = \frac{\partial U}{\partial T} = k_B N - \frac{1}{T^2}\int d\omega \hbar\omega g(\omega)\left[\frac{1}{12}\frac{\hbar\omega}{k_B}\right]$$

So that the coefficient A defined in the problem has the values

$$A = \frac{\hbar^2}{12 N k_B^2}\int d\omega \omega^2 g(\omega)$$

Inserting our expression for $g(\omega)$ we obtain

$$A = \frac{\hbar^2}{12\pi k_B^2}\int_0^{\omega_{max}} d\omega \frac{\omega^2}{\sqrt{(\kappa/m) - (\omega/2)^2}}$$

Defining $x = (\omega/2)\sqrt{m/\kappa}$ we obtain

$$A = \frac{\hbar^2}{12\pi k_B^2}\frac{8\kappa}{m}\int_0^1 dx \frac{x^2}{\sqrt{1 - x^2}}$$

The integral is evaluated to give $\pi/4$ (make the substitution $x = \sin\theta$). Thus we obtain

$$A = \frac{\hbar^2}{6 k_B^2}\frac{\kappa}{m}$$

as required.

(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 κ_1 and the spring constant between second neighbors be called κ_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.

(a) Use the same approach

$$\begin{aligned} m\ddot{x}_n &= \kappa_1(x_{n+1}-x_n)+\kappa_1(x_{n-1}-x_n)+\kappa_2(x_{n+2}-x_n)+\kappa_1(x_{n-2}-x_n) \\ &= \kappa_1(x_{n+1}+x_{n-1}-2x_n)+\kappa_2(x_{n+2}+x_{n-2}-2x_n) \end{aligned}$$

Using the same ansatz

$$x_n = Ae^{i\omega t-ikna}$$

we obtain

$$-m\omega^2 = 2\kappa_1(\cos(ka)-1)+2\kappa_2(\cos(2ka)-1) \qquad (9.3)$$

so

$$\omega = \sqrt{\frac{2\kappa_1}{m}(\cos(ka)-1)+\frac{2\kappa_2}{m}(\cos(2ka)-1)}$$

(b) To obtain the sound velocity, expand for small k to obtain

$$\omega = \sqrt{\frac{2\kappa_1}{m}\frac{(ka)^2}{2}+\frac{2\kappa_2}{m}\frac{(2ka)^2}{2}} = \left(a\sqrt{\frac{\kappa_1+4\kappa_2}{m}}\right)k$$

Thus the sound velocity is

$$v_s = a\sqrt{\frac{\kappa_1+4\kappa_2}{m}}$$

The easiest way to examine $\partial\omega/\partial k$ at the zone boundary is to differentiate Eq. 9.3 to given

$$m\omega\partial\omega/\partial k = -2a\kappa_1\sin(ka)-4a\kappa_2\sin(2ka)$$

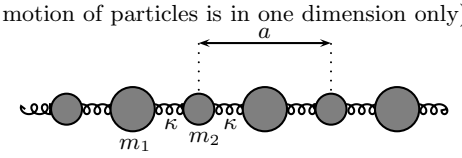
At the zone boundary $k=\pi/2$ both terms on the right hand side are zero, hence we have zero group velocity.

(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 κ, 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 ρ is the chain density and β is the compressibility.

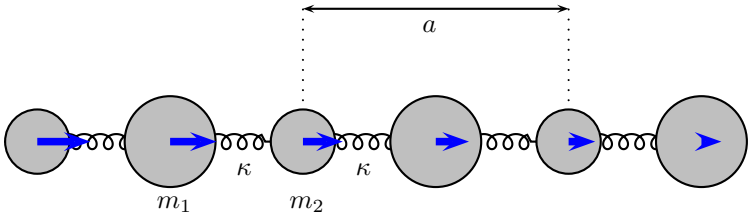
(d) Sketch the dispersion in both reduced and extended zone scheme.

▷ 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?

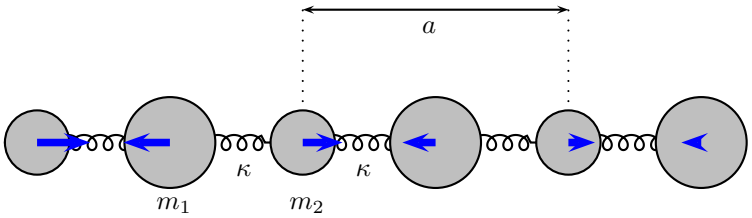
(e) What happens when $m_1 = m_2$?

The following figure depicts a long wavelength acoustic wave: All atoms in the unit cell move in-phase with a slow spatial modulation. Acoustic waves $\omega \sim k$ for small k.



acoustic

The following depicts a long wavelength optical wave: The two different types of atoms move out of phase, with a slow spatial modulation. (In general a long wavelength optical mode is any long wavelength mode where not all atoms in the unit cell are moving in phase). Note that the amplitude of motion of the different atoms in the cells is generally not the same. Optical modes have ω nonzero as $k \to 0$.



optical

(b) Let x_n be the position of the n^{th} particle of mass m_1 and y_n be the position of the n^{th} particle of mass m_2. We can assume that the equilibrium position of x_n is given by na and the equilibrium position of y_n is given by $na + d$.

We write the equations of motion for the *deviations* from these equilibrium positions δx_n and δy_n.

$$\begin{aligned} m_1\ddot{\delta x}_n &= -\kappa(\delta x_n - \delta y_{n-1}) - \kappa(\delta x_n - \delta y_n) \\ m_2\ddot{\delta y}_n &= -\kappa(\delta y_n - \delta x_n) - \kappa(\delta y_n - \delta x_{n+1}) \end{aligned}$$

Writing the ansätze

$$\begin{aligned} \delta x_n &= A_x e^{ikan - i\omega t} \\ \delta y_n &= A_y e^{ikan - i\omega t} \end{aligned}$$

we obtain the equations

$$\begin{aligned} -m_1\omega^2 A_x e^{ikna} &= -2\kappa A_x e^{ikna} + \kappa A_y(e^{ikna} + e^{ik(n-1)a}) \\ -m_2\omega^2 A_y e^{ikna} &= -2\kappa A_y e^{ikna} + \kappa A_x(e^{ikna} + e^{ik(n+1)a}) \end{aligned}$$

or

$$\omega^2 A_x = 2(\kappa/m_1)A_x - (\kappa/m_1)(1 + e^{-ika})A_y \qquad (10.1)$$

$$\omega^2 A_y = 2(\kappa/m_2)A_y - (\kappa/m_2)(1 + e^{ika})A_x \qquad (10.2)$$

which is an eigenvalue problem from ω^2. Thus we need to find the roots of the determinant

$$\begin{vmatrix} 2(\kappa/m_1) - \omega^2 & -(\kappa/m_1)(1 + e^{-ika}) \\ -(\kappa/m_2)(1 + e^{ika}) & 2(\kappa/m_2) - \omega^2 \end{vmatrix}$$

which gives the equation

$$\begin{aligned} 0 &= \omega^4 - \omega^2\left(2\kappa(1/m_1 + 1/m_2)\right) + \frac{\kappa^2}{m_1 m_2}\left(4 - (1 + e^{ika})(1 + e^{-ika})\right) \\ 0 &= \omega^4 - \omega^2\left(\frac{2(m_1 + m_2)\kappa}{m_1 m_2}\right) + \frac{\kappa^2}{m_1 m_2}\left(2 - 2\cos(ka)\right)) \end{aligned}$$

with the solution (skipping a few steps)

$$\begin{aligned} \omega^2 &= \frac{\kappa}{m_1 m_2}\left(m_1 + m_2 \pm \sqrt{m_1^2 + m_2^2 + 2m_1 m_2\cos(ka)}\right) \\ &= \frac{\kappa}{m_1 m_2}\left(m_1 + m_2 \pm \sqrt{(m_1 + m_2)^2 - 4m_1 m_2\sin^2(ka/2)}\right) \end{aligned}$$

(c) At $k = 0$, $\cos(ka) = 1$, the acoustic mode has zero energy, whereas the optical mode has energy

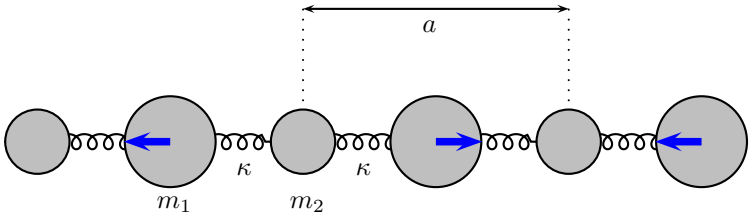
$$\omega = \sqrt{\frac{2\kappa(m_1 + m_2)}{m_1 m_2}}$$

At the zone boundary $\cos(ka) = -1$, so the two modes have energy

$$\omega = \sqrt{\frac{2\kappa m_1}{m_1 m_2}} \quad \text{and} \quad \sqrt{\frac{2\kappa m_2}{m_1 m_2}}$$

the greater of which is the optical mode, the lesser being the acoustic mode.

To find the motions corresponding to these modes we need to plug our frequencies back into Eqs. 10.1 and 10.2 to find the relation between A_x and A_y. For the acoustic mode at $k = 0$ we obtain $A_x = A_y$ which means the two masses move in phae with the same amplitude. For the optical mode at $k = 0$ we have $A_x = -(m_2/m_1)A_y$ meaning that the two different masses move in opposite directions with the heavier mass moving with lower amplitude. At the zone boundary the two modes correspond to one of the masses staying still and the other mass moving. For example, for the lower frequency mode, the higher mass particles move and the lower mass particle stays fixed. Since we are at the zone boundary, every other higher mass particle moves in the opposite direction (thus compressing symmetrically around the fixed particle. An example of a zone boundary mode is shown in the following figure



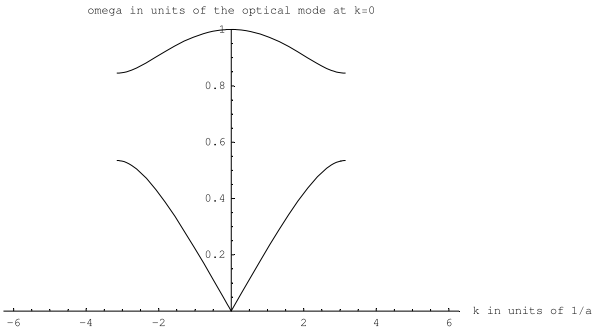
zone boundary

To find the sound velocity, expand the cos around $k = 0$, one obtains the acoustic mode velocity $\omega = vk$ with

$$v = a\sqrt{\frac{\kappa}{2(m_1 + m_2)}}$$

We check that $v^{-2} = \rho\beta$. The density of the chain is $\rho = (m_1 + m_2)/a$, the compressibility of two springs in series is $\kappa/2$ so the compressibility of the chain is $\beta = -(1/L)dL/dF = 2/(\kappa a)$.

Near the zone boundary, since the group velocity is $d\omega/dk$ and since $d\omega/d\cos(ka)$ is nonsingular, the group velocity must be zero by using the chain rule since $d\cos(ka)/dk = a\sin(ka) = 0$ at the zone boundary $(k = \pi/a)$.



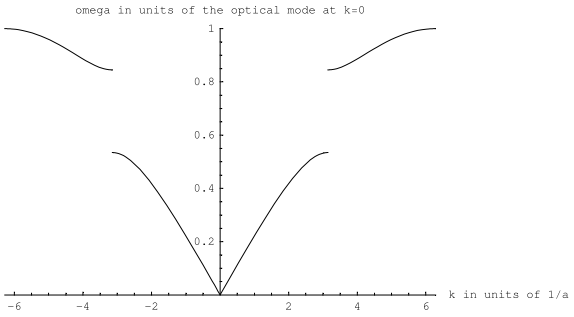


Fig. 10.1 Diatomic Chain. Top Reduced Zone Scheme. Bottom Extended Zone Scheme. Both pictures use $m_1/m_2 = .4$.

If there are N unit cells, therefore $2N$ atoms, there are 2N modes. There are 2 modes per k in the reduced zone scheme, therefore two branches.

(e) When $m_1 = m_2$ the unit cell is now of size $a/2$ so the Brillouin zone is doubled in size. In this limit, the gap at the Brillouin zone boundary vanishes and the two branches become the single branch of the monatomic chain (this is most easily described in extended zone scheme).