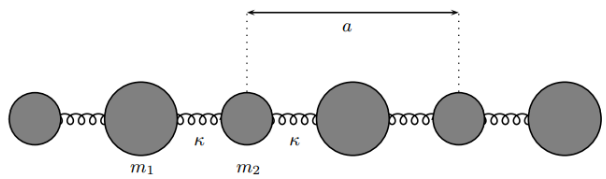
Problem 1

Simon - Solid State Basics - Problem 10.1: Normal Modes of a One-Dimensonal Diatomic Chain

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

- Describe how the 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 frequences of the acoustic and optical modes at $k = 0$ as well as the Brillouin zone boundary.

- Describe the motion of the masses in each case. (Margin note 4 in Chapter 10 of Simon's Solid State Basics)
- 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 $v_s = \sqrt{\frac{1}{\beta\rho}}$, where β is the compressibility.

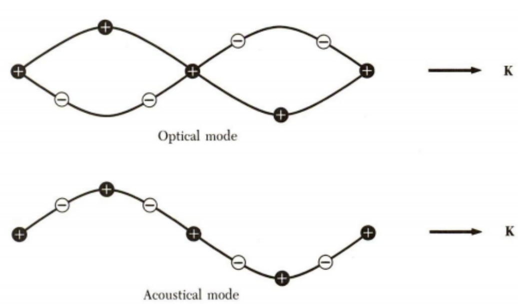
(d) Sketch the dispersion in both reduced and extended zone scheme.

- If there are N unit cells, how many different normal modes are there?
- How many *branches* of excitations are there? In other words, in the reduced zone scheme, how many modes are there at each k?

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

Solution

(a) Optical phonon modes occur when each neighboring atom within the lattice is out of phase with the atom considered. Acoustic phonon modes occur when all of the atoms within the lattice are in phase (on the same wave). The image below provides a description of how these two phonon modes appear in real space. The optical modes are typically excited by energies within the visible region of light ($\sim$ 1-3 eV), which is a much larger energy than that required for acoustic phonon modes.



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(b) Starting with versions of equations 10.1 and 10.2 from Simon's Solid State Basics adapted for different masses and same spring cosntants:

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

Which gives us the equations of motion as:

$$m_1 \delta\ddot{x}_n = \kappa(\delta y_n + \delta y_{n-1} - 2\delta x_n)$$
$$m_2 \delta\ddot{y}_n = \kappa(\delta x_{n+1} + \delta x_n - 2\delta y_n)$$

We then assume this can be viewed as a wave:

$$\delta x_n = A_x e^{i(qna-\omega t)}$$
$$\delta y_n = A_y e^{i(qna-\omega t)}$$

Therefore we have :

$$m_1\omega^2 A_x e^{i(qna-\omega t)} = \kappa(A_y e^{i(qna-\omega t)} - A_x e^{i(qna-\omega t)}) + \kappa(A_y e^{i(q(n-1)a-\omega t)} - A_x e^{i(qna-\omega t)})$$
$$m_2\omega^2 A_y e^{i(qna-\omega t)} = \kappa(A_x e^{i(q(n+1)a-\omega t)} - A_y e^{i(qna-\omega t)}) + \kappa(A_x e^{i(qna-\omega t)} - A_y e^{i(qna-\omega t)})$$

$$\Rightarrow m_1\omega^2 A_x = \kappa(A_y - A_x + A_y e^{ika} - A_x)$$
$$m_2\omega^2 A_y = \kappa(A_x e^{-ika} - A_y + A_x - A_y)$$

$$\Rightarrow m_1\omega^2 A_x = \kappa(A_y(1+e^{ika}) - 2A_x)$$
$$m_2\omega^2 A_y = \kappa(A_x(1+e^{ika}) - 2A_y)$$

$$\Rightarrow m_1\omega^2 \begin{vmatrix} A_x \\ A_y \end{vmatrix} = \begin{vmatrix} -2\kappa & \kappa(1+e^{ika}) \\ \kappa(1+e^{ika}) & -2\kappa \end{vmatrix} \begin{vmatrix} A_x \\ A_y \end{vmatrix}$$

Now take the determinant:

$$0 = \begin{vmatrix} -2\kappa & \kappa(1+e^{ika}) \\ \kappa(1+e^{ika}) & -2\kappa \end{vmatrix} \begin{vmatrix} A_x \\ A_y \end{vmatrix}$$