Phonons

Untill now we have assumed a lattice with fixed cores. But even at zero temperature the lattice vibrates, due to the zero-point motion of the cores.

Let us consider a monoatomic chain. The equilibrium spacing between the atoms is a and their mass is M.

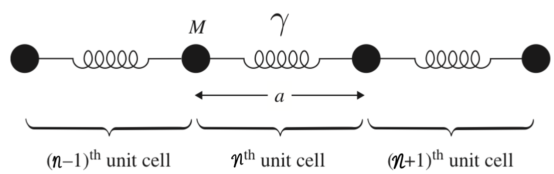
The position of the n^{th} atom is x_n and at equilibrium $x_n^{eq} = na$, where $n \in \mathbb{Z}$.

As soon as we allow for the motion of the atoms x_n will deviate from its equilibrium positin, so we define

$$\delta x_n = x_n - x_n^{eq}$$

This consideration means that the masses meve in 1D only.

If a solid is at low enough energies we can consider the potential holding the atoms together to be a quadratic one (this is to say that we Tylor expanded arround a minimum). So we have a harmonic chain. Within these considerations the total potential energy of the chain is



$$V_{tot} = \sum_i V(x_{i+1} - x_i) = \sum_i \frac{\gamma}{2}(x_{i+1} - x_i - a)^2 \quad (\gamma \text{ is the spring constant}).$$

$$V_{tot} = \sum_i \frac{\gamma}{2}(\delta x_{i+1} - \delta x_i)^2,$$

then the force on the n^{th} mass of the chain is

$$F_n = -\frac{\partial V_{tot}}{\partial x_n} = \gamma(\delta x_{n+1} - \delta x_n) + \gamma(\delta x_{n-1} - \delta x_n).$$

Thus we have the Newton's equation of motion

$$M \delta \ddot{x}_n = K(\delta x_{n+1} + \delta x_{n-1} - 2\delta x_n)$$

The Key idea to solve this equation is to use the plane-wave ansatz, where

$$\delta x_n = A e^{i\omega t - iq x_n^{eq}} = A e^{i\omega t - iqna},$$

A is the amplitude of oscillations, q and ω are the wavector and the frequency of the proposed wave.

Substituting the ansatz in the equations of motion, we get

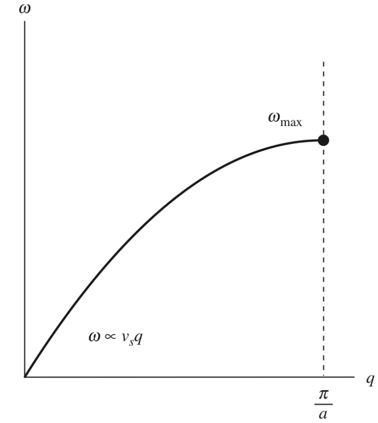
$$-m\omega^2 e^{i\omega t - iqna} = \gamma A e^{i\omega t}\left[e^{-iqa(n+1)} + e^{-iqa(n-1)} - 2e^{-iqan}\right]$$

$$m\omega^2 = 2\gamma\left[1 - \cos(qa)\right] = 4\gamma \sin^2(qa/2).$$

Then we obtain $\omega = 2\sqrt{\frac{\gamma}{M}}\left|\sin\left(\frac{qa}{2}\right)\right|$ and this is the phonon dispersion relation

Notice tha ω_{max} happens at the B.Z. boundary, and therfore $\omega_{max} = 2\sqrt{\frac{\gamma}{M}}$.

The saturation of the dispersion curve results from the discreteness of the atomic arrangment in a solid, where q is only has a meaning in the B.Z.



Acoustic phonon band structure for a monatomic chain of atoms.

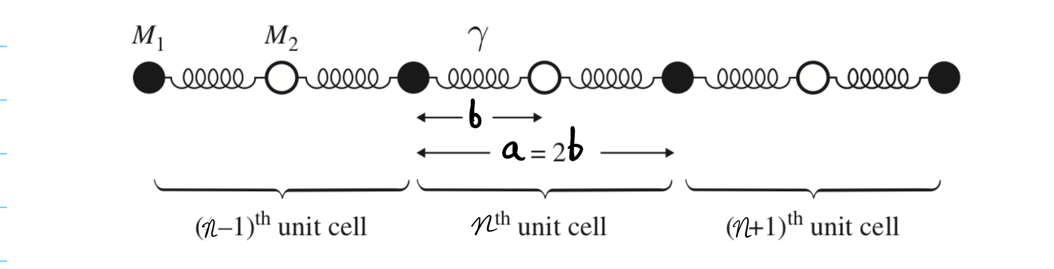
If we examine

$$\lim_{q\to 0} w^2 = \frac{2\gamma}{M}\frac{1}{2}(qa)^2 \qquad \text{(The long wavelength limit)}$$

$$w(q\to 0) = \sqrt{\frac{\gamma}{M}}\, aq = v_s q \text{ , where}$$

$v_s = \sqrt{\frac{\gamma}{M}}\, a$ represents the velocity of sound. Hence the name Acoustic phonons.

Another useful example is the diatomic chain.



Let the position of the M_1 atoms x_n and the M_2 atoms y_n, where

$x_n^{eq} = na$ and $y_n^{eq} = na + b$ with $2b = a$, and

$\delta x_n = x_n - x_{n\,eq}$ and $\delta y_n = y_n - y_n^{eq}$.

Then the equations of motion are

$$M_1 \delta\ddot{x}_n = -\gamma(\delta x_n - \delta y_{n-1}) - \gamma(\delta x_n - \delta y_n)$$

$$M_2 \delta\ddot{y}_n = -\gamma(\delta y_n - \delta x_n) - \gamma(\delta y_n - \delta x_{n+1}).$$

Using the plane wave ansatz

$$\delta x_n = A_x e^{iqan - iwt}$$

$$\delta y_n = A_y e^{iqan - iwt}$$

after some simple math we get

$$\begin{pmatrix} 2(\gamma/M_1)-\omega^2 & -(\gamma/M_1)(1+e^{-iqa}) \\ -(\gamma/M_2)(1+e^{iqa}) & 2(\gamma/M_2)-\omega^2 \end{pmatrix}\begin{pmatrix} A_x \\ A_y \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Then the non trivial solutions are found by requiering that the determinant of the matrix above is zero.

Solving for ω from the zero determinant condition we get

$$\omega_{\pm}^2=\frac{\gamma}{M_1M_2}\left(M_1+M_2\pm\sqrt{M_1^2+M_2^2+2M_1M_2\cos(qa)}\right)$$

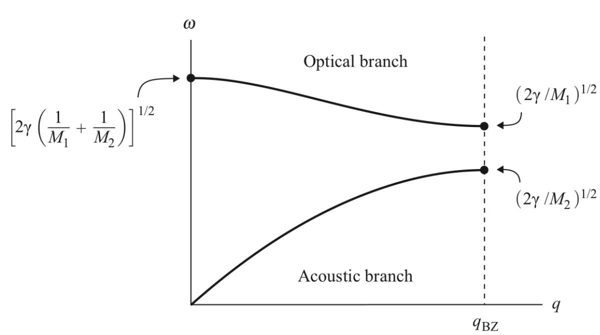
(Notice that I made few jumps in the math. Do the missing steps).

At long wavelengths ($q\to 0$)

$$\omega_+^2\to 2\gamma\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \quad \text{and} \quad \omega_-^2\to\frac{\gamma}{(M_1+M_2)}\frac{(qa)^2}{2}$$

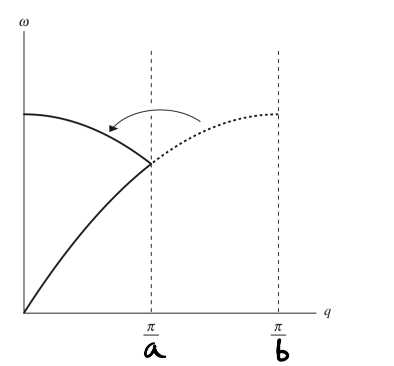
If $M_1=M_2$ $\quad \omega_-\to\sqrt{\frac{\gamma}{2M}}\left(\frac{qa}{2}\right)$ and $\omega_+\to 2\sqrt{\frac{\gamma}{M}}$. Notice that the ω_- is the same as the monoatomic chain result, and ω_+ is just the result of band folding into the 1st B.Z. (figure 2).

(1)



Lattice vibration dispersion curves for a diatomic chain of atoms with $M_2 > M_1$.

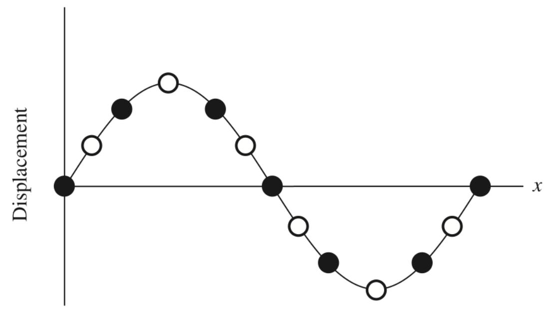
(2)



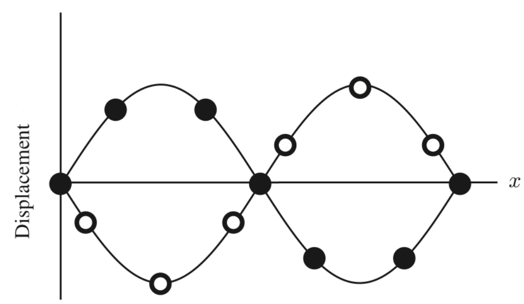
Mapping of the lattice vibration dispersion curves for a diatomic chain of equal masses from that of a r
chain.

Going back to the diatomic chain, we have a gap at the B.Z. edge, see figure (1). This gap separates the acoustic branch from the optical branch.

The two branches represent 2-distinc modes of vibration as show below



Atomic displacement versus distance *x* for an acoustic mode for a diatomic chain.



Atomic displacement versus distance *x* for an optical mode for a diatomic chain.