Optical and Acoustic Phonons

When we are first introduced to lattice vibrations in solid state physics we study the simplest solids which possess one atom per unit cell. Our first mathematical model is that of a one-dimensional chain of atoms connected by springs. (More correctly, we say that we follow the motion of a single atom in a plane and characterise the coherent vibration of all atoms in the plane by observing the displacement of that particular atom.)

We choose the equilibrium separation of the atoms to be d, the mass to me m and label each atom's displacement from its equilibrium position by u_s, where s is an integer index identifying the plane. With a Hook's law restoring force (per atom) given by,

$$F_s = -C\,(u_s - u_{s+1}) - C\,(u_s - u_{s-1})\ ,$$

the equation of motion for displacments of atoms in the s-plane, $u_s(t)$, is

$$m\frac{d^2\,u_s}{dt^2} = -C\,(2u_s - u_{s+1} - u_{s-1})\ . \tag{1}$$

With periodic boundary condition, the solutions to this set of differential equations are sinusoidal, i.e. plane waves,

$$u_s(t) = Ae^{iksd - i\omega t}\,,$$

with amplitude A. The wave vector, k, is related to the vibration frequency by

$$\omega(k) = 2\sqrt{\frac{C}{m}}\left|\sin\left(\frac{kd}{2}\right)\right|\ .$$

When dealing with solids with more than a one-atom basis, we usually start by considering an idealized solid with two atoms per unit cell and a phonon propagating in a direction such that sucessive planes of atoms are all of one type. The resulting one-dimensional model is used to illustrate optical and acoustic phonons, i.e. the existence of two vibrational modes for each wave vector.

With atoms of mass m_1 and m_2 that experience displacments from equilibrium u_s and v_2 respectively the equations of motions for the two types of atoms becomes,

$$\begin{aligned} m_1\frac{d^2\,u_s}{dt^2} &= -C\,(2u_s - v_s - v_{s-1})\ , \\ m_2\frac{d^2\,v_s}{dt^2} &= -C\,(2v_s - u_{s+1} - u_s)\ . \end{aligned} \tag{2}$$

A plane wave for each atom type,

$$u_s(t) = Ae^{iksd - i\omega t}\,, \tag{3}$$

$$v_s(t) = Be^{iksd - i\omega t}\,, \tag{4}$$

is a solution. When these are substituted into Eq. 2, the determinant to obtain the eigenvalues produces a 4-th order equation,

$$m_1 m_2 \omega^4 - 2C(m_1 + m_2)\omega^2 + 2C^2(1 - \cos kd) = 0$$

which has two roots for ω^2,

$$\omega^2 = \frac{2C(m_1+m_2) \pm \sqrt{4c^2(m_1+m_2)^2 - 8m_1m_2C^2(1-\cos kd)}}{2m_1m_2}\,.$$

At zero wave vector, this reduces to

$$\omega^2(k=0) = \left[\begin{array}{cc} 2C\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\left(1-\frac{k^2d^2}{4}\right) & \text{optic} \\ \\ 0+\frac{C}{2(m_1+m_2)}k^2d^2 & \text{acoustic} \end{array}\right]$$