Note on chapter Two

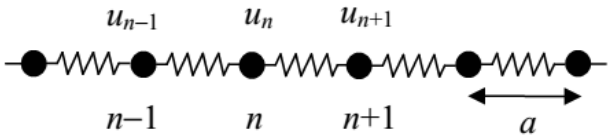
Lattice Vibration

When the lattice is at equilibrium each atom is positioned exactly at its lattice site. Now suppose that an atom displaced from its equilibrium site by a small amount. Due to force acting on this atom, it will tend to return to its equilibrium position. This results in lattice vibrations. Due to interactions between atoms, various atoms move simultaneously, so we have to consider the motion of the entire lattice.

1- One-dimensional lattice

For simplicity we consider, first, a one-dimensional crystal lattice and assume that the forces between the atoms in this lattice are proportional to relative displacements from the equilibrium positions.

Fig.1



This is known as the *harmonic approximation*, which holds well provided that the displacements are small. One might think about the atoms in the lattice as interconnected by elastic springs. Therefore, the force exerted on n-the atom in the lattice is given by

where M is the mass of the atom. Note that we neglected here by the interaction of the n-th atom with all but its nearest neighbors. A similar equation should be written for each atom in the lattice, resulting in N coupled differential equations, which should be solved simultaneously (N is the total number of atoms in the lattice). In addition the boundary conditions applied to the end atom in the lattice should be taken into account. Now let us attempt a solution of the form

(i) *Reducing to the first Brillouin zone*. The frequency (5.6) and the displacement of the atoms (5.3) do not change when we change q by $q+2\pi/a$. This means that these solutions are physically identical. This allows us to set the range of independent values of q within the first Brillouin zone, i.e.

$$-\frac{\pi}{a} \le q \le \frac{\pi}{a}.$$

Within this range of q the ω versus q is shown in Fig.2.

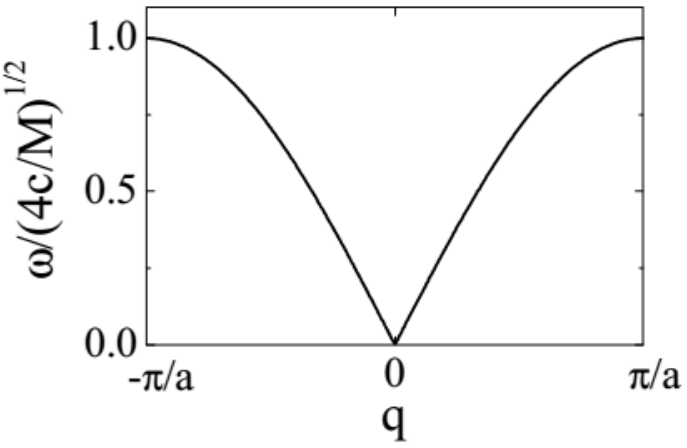


Fig.2

The maximum frequency is $4C / M$. The frequency is symmetric with respect to the sign change in q, i.e. $\omega(q)= \omega(-q)$. This is not surprising because a mode with positive q corresponds to the wave traveling in the lattice from the left to the right and a mode with a negative q corresponds to the wave traveling from the right tot the left. Since these two directions are equivalent in the lattice the frequency does not change with the sign change in q.

At the boundaries of the Brillouin zone $q=\pm\pi/a$ the solution represents a standing wave

$un = A(-1)n\ e-i\omega t$: atoms oscillate in the opposite phases depending on whether n is even or odd. The wave moves neither right nor left.

(ii) *Phase and group velocity*. The phase velocity is defined by

$$v_p = \frac{\omega}{q}$$

and the

(iii) group velocity by

$$v_g = \frac{d\omega}{dq}.$$

The physical distinction between the two velocities is that v_p is the velocity of the propagation of the plane wave, whereas the v_g is the velocity of the propagation of the wave packet. The latter is the velocity for the propagation of energy in the medium. For the particular dispersion relation ( ) the group velocity is given by

As is seen from Eq.( ) the group velocity is zero at the edge of the zone where $q=\pm\pi/a$. Here the wave is standing and therefore the transmission velocity for the energy is zero.

(iii) *Long wavelength limit*. The long wavelength limit implies that $\lambda >> a$. In this limit $qa << 1$. We can then expand the sine in Eq.(5.6) and obtain for the positive frequencies:

We see that the frequency of vibration is proportional to the wavevector. This is equivalent to the statement that velocity is independent of frequency. In this case

This is the velocity of sound for one dimensional lattice which is consistent with the expression we obtained earlier for elastic waves.

2 - Diatomic 1D lattice

Now we consider a one-dimensional lattice with two non-equivalent atoms in a unit cell. It appears that the diatomic lattice exhibit important features different from the monoatomic case. Fig.3 shows a diatomic lattice with the unit cell composed of two atoms of masses M and m with the distance between two neighboring atoms a.

We can treat the motion of this lattice in a similar fashion as for monoatomic lattice. However, in this case because we have two different kinds of atoms, we should write two equations of motion:

In analogy with the monoatomic lattice we are looking for the solution in the form of traveling mode fo r the two atoms:

The lower curve is called the *acoustic branch*, while the upper curve is called the *optical branch*. The optical branch begins at q=0 and ω=0. Then with increasing q the frequency increases in a linear fa shion. This is why this branch is called

acoustic: it corresponds to elastic waves or sound. Eventually this curve saturates at the edge of the Brillouin zone. On the other hand, the optical branch has a nonzero frequency at zero q

and it does not change much with q.

The distinction between the acoustic and optical branches of lattice vibrations can be seen most clearly by comparing them at q=0 (infinite wavelength). As follows from Eq.( ), for the acoustic branch ω=0 and .So in this limit the two atoms in the cell have the same amplitude and the phase. Therefore, the molecule oscillates as a rigid body, as shown in Fig.5 for the acoustic mode.