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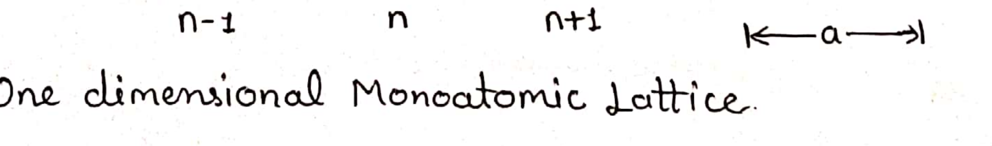
Normal modes of a one-dimensional mono-atomic lattice :->

In studying crystal structure, it is assumed that the atoms are at rest in their lattice site. Atoms, however, are not quite stationary but oscillate around their equilibrium positions as a result of thermal energy.

We shall first consider crystal vibrations in the elastic long wavelength limit, in which the crystal may be treated as a continuous medium. We shall discuss the lattice vibrations taking into account the discrete nature of the lattice.

A solid is composed of discrete atoms and this discreteness must be taken into account in the discussion of lattice vibrations. However, when the wavelength is very long, one may disregard the atomic nature and treat the solid as a continuous medium. Such vibrations are referred to as "Elastic waves".

Fig-1-



The One dimensional Monoatomic Lattice.

Figure 1 shows a one-dimensional monoatomic lattice with a lattice constant equal to "a". When the lattice is at equillibrium, each atom is positioned exactly at its lattice site.

Now, suppose that the lattice begins to vibrate, so that each atom is displaced from its site by a small amount. Because, the atoms interact with each-other, the various atoms move simultaneously, so that we must consider the motion of entire lattice.

Consider the n^{th} atom, the force exerted on it as a result of its interaction with the $(n+1)^{th}$ atom is given by

$$+\alpha(U_{n+1}-U_n) \quad \text{—— (1)}$$

where, U_n and U_{n+1} are the displacements of n^{th} and $(n+1)^{th}$ atoms, respectively and $(U_{n+1}-U_n)$ is the relative displacement of the atoms. The parameter α is known as the Interatomic force Constant.

The assumption that force is proportional to relative displacement is known as Harmonic approximation and is applicable where the displacements are small. This approximation is equivalent to the well-known Hooke's law, familiar from elementary elastic theory. It is as though the atoms were interconnected by elastic springs. The force exerted on the n^{th} atom by the $(n-1)^{th}$ atom is similarly found to be $+\alpha(U_{n-1}-U_n)$.

Applying Newton's second law to the motion of the n^{th} atom, we have therefore,

$$M\frac{d^2u_n}{dt^2} = +\alpha(U_{n+1}-U_n)+\alpha(U_{n-1}-U_n)$$

$$= -\alpha(2U_n-U_{n+1}-U_{n-1}) \quad \text{—— (2)}$$

where, M is the mass of the atom.

Note that we have neglected the interaction of the n^{th} atom with all but its nearest neighbors. Although these neglected interactions are small, as the force decreases with distance, they are not negligible, and must be taken into account in any realistic calculations. The simplified approximation will suffice, however, to illustrate the new physical concepts without involving cumbersome mathematical complexities.

To solve eqn ②, we note that the motion of the n^{th} atom is coupled to those of the $(n+1)^{th}$ and $(n-1)^{th}$ atoms. $||^{ly}$, the motion of the $(n+1)^{th}$ atom is found to be related to those of its two neighbours, and so forth.

Eqn of motion

$$U = Ae^{iqx} \quad \text{---} \quad (3)$$

for each atom in the lattice, resulting in N coupled differential eqns to be solved simultaneously, where N is the total number of the atoms. In addition, the boundary conditions applied to the end atoms of the lattice must also be taken into account.

Let us now a solution of the form

$$U_n = Ae^{i(qx_n - \omega t)}, \quad \text{---} \quad (4)$$

Where, x_n is the equillibrium position of the n^{th} atom, i.e $x_n = na$.

This equation represents a travelling wave, in which all atoms oscillate with the same frequency 'ω' and the same amplitude A. The phases of the atoms are interlocked such that the phase increases regularly from one atom to the next by an amount qa.

Note that a solution of the form (4) is possible only because of the translational symmetry of the lattice i.e the presence of equal ~~inte~~ masses at regular intervals. If, on the other hand, the masses had random values, or if they were distributed randomly along the line, then the solution would be expected to be a strongly attenuated wave. In extreme cases, a propagating solution may not even be possible at all. In the discussion of extended systems a mode of vibration such as (2), in which all elements of the system oscillate with the same frequency, is referred to as a Normal Mode. In the case of the lattice, the normal mode is a propagating wave.

If we substitute eq^n (4) into eq^n (2) and cancel the common quantities (amplitude and time factor), we find.

$$M(-\omega^2)e^{iqna} = -\alpha\left[2e^{iqna} - e^{iq(n+1)a} - e^{iq(n-1)a}\right] \quad (5)$$

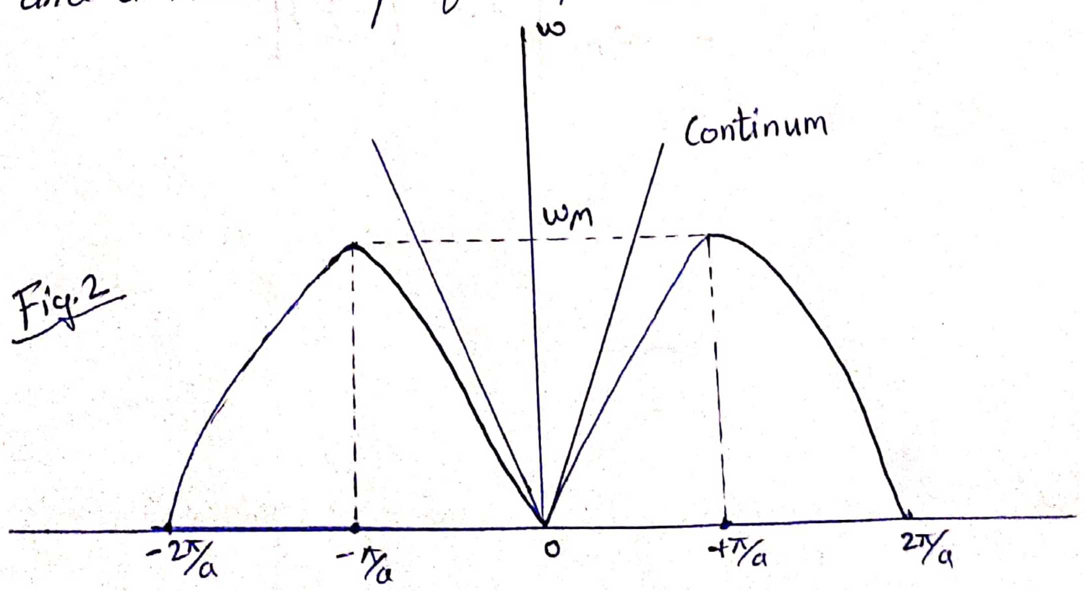
This equation can be further simplified by canceling the common factor e^{iqna} and making use of Euler's formula $e^{iy} + e^{-iy} = 2\cos y$. After a simple trignometric simplification, we can write the result as

$$\omega = \omega_m |\sin(qa/2)| \quad (6)$$

where, $\omega_m = (4\alpha/M)^{1/2}$ and where we have restricted ω to positive values only because of the physical meaning of the frequency.

Eq.(6), which is the dispersion relation for the one-dimensional lattice, is the result we have been seeking. It is sketched in following figure, in which the dispersion curve is seen to be a sinusoid with a period equal to $2\pi/a$ in q-space, and a maximum frequency equal to ω_m.

Fig. 2



The dispersion relation eq^n (6) has several important and intriguing properties which we will now examine in details, as they apply not only to one but two and three dimensional lattices as well.

(1) The long wavelength limit:

Since, the dispersion curve is periodic and symmetric around the origin, we may confine to the range $0 < q < \pi/a$

These frequencies cover the continuous range
$$0 < \omega < \omega_m.$$

These frequencies are only transmitted by the lattice, while other frequencies will be strongly attenuated. The lattice therefore acts as a low-pass mechanical filter.

In the long wavelength limit as $q \to 0$ ($\sin\theta \approx \theta$ for small θ), the dispersion relation (6) may be approximated by
$$\omega \approx \left(\frac{\omega_m a}{2}\right) q \quad \text{--- (7)}$$

which is a linear relation between ω and q. In this limit the lattice behaves as an elastic continum.

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