

Lattice Vibrations: One Dimensional Monoatomic Lattice

Dr. Manish Kumar Verma
Assistant Professor, Department of Physics
Magadh Mahila College, Patna University

Elastic waves in crystals are said to be composed of phonons. Phonon is the quantum of energy of lattice vibration. Photons are boson particles and are not conserved; they can be created or destroyed in a collision. The energy of each phonon is given by

$$\epsilon = h\nu \quad (1)$$

where h is Planck's constant (6.626×10^{-34} J-s). Indirect evidences in support of phonons:

- i) Lattice contribution to specific heat of solids always approaches zero as the temperature approaches zero; this can be explained only if the lattice vibrations are quantized, implying the existence of phonons.
- ii) X-rays and neutrons are scattered inelastically by crystals, with energy and momentum changes corresponding to the creation and annihilation of one or more phonons. By measuring the recoil of scattered X-ray or neutron, it is possible to determine the properties of individual phonons.

1 Dynamics of one dimensional monoatomic lattice

Suppose a system of identical atoms elastically coupled to each other by springs. Let us assume that the system has a cubic arrangement of atoms of mass M joined by springs of force constant K , the interatomic spacing is a . The elastic couplings provide a restoring force on the atoms when they are displaced from equilibrium position. To simplify the system, we consider a one dimensional chain of atoms. This can be achieved if we assume that

longitudinal waves are parallel to the cube edge along [1 0 0] direction. In this direction transverse springs have no effect and results in 1-D approximation.

Now we assume that we have a long chain of N atoms with the last atom connected to the first atom to form a ring. This approximation is made to make the environment of each atom as equivalent to each other. Now the system is allowed to vibrate. If one atom starts vibrating, it does not continue to vibrate with a constant amplitude because it interacts with its neighbours.

If u_n is the displacement of the n^{th} atom from its equilibrium position then force on n^{th} atom due to $(n + 1)^{th}$ and $(n - 1)^{th}$ atoms will be:

- a) $K(u_n - u_{n-1})$ to the left from the springs on its left
- b) $K(u_{n+1} - u_n)$ to the right from the springs on right

The net force on n^{th} atom is

$$F_n = K[(u_{n+1} - u_n) - (u_n - u_{n-1})]$$

$$M \frac{d^2 u_n}{dt^2} = K(u_{n+1} - 2u_n + u_{n-1}) \quad (2)$$

Let the solution of the equation is

$$u_n = A \exp i(nka - \omega t) \quad (3)$$

Equation 3 represents a travelling wave, in which all atoms oscillate with the same frequency ω and have the same amplitude A . Substituting eqn. 3 in eqn. 2 we get

$$-\omega^2 M u_n = K(e^{ika} - 2 + e^{-ika})u_n$$

$$-\omega^2 M = K(e^{ika} + e^{-ika} - 2)$$

$$-\omega^2 M = 2K(\cos ka - 1)$$

$$\omega^2 M = 4K \sin^2 \frac{ka}{2}$$

$$\omega = \sqrt{\frac{4K}{M}} \left| \sin \frac{ka}{2} \right| \quad (4)$$

From eqn 4, the maximum (natural cutoff) frequency is given by

$$\omega_m = \sqrt{\frac{4K}{M}} \quad (5)$$

$$\therefore \omega = \omega_m \left| \sin \frac{ka}{2} \right| \quad (6)$$

Equation 6 is a dispersion relation between angular frequency ω and wave vector k for a one dimensional periodic lattice.

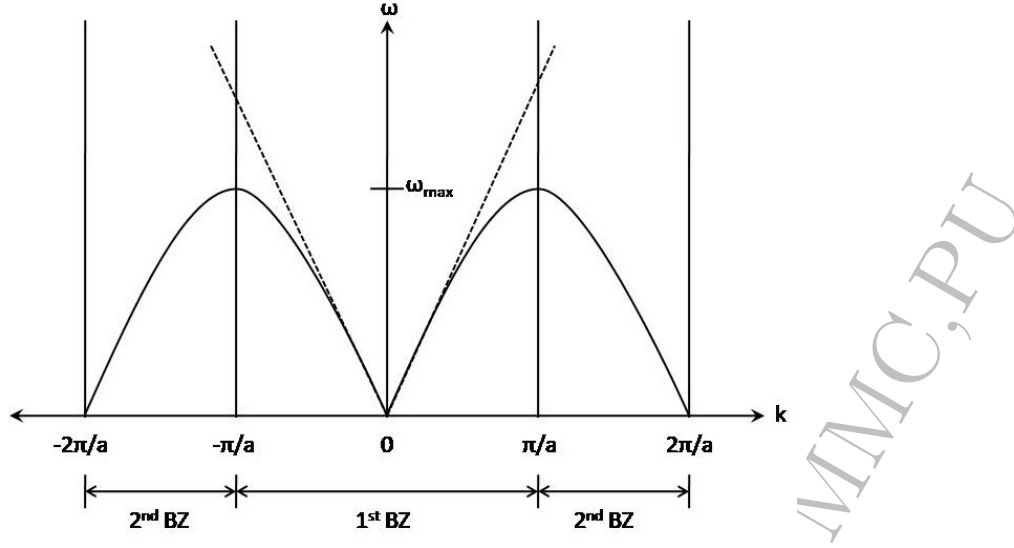


Figure 1: Dispersion Curve ω vs k for a one dimensional monoatomic lattice with nearest neighbour interaction

1.1 Properties of Dispersion Relation

1.1.1 Symmetry in K space (The First Brillouin Zone)

The dispersion relation shows two types of symmetry, translational symmetry and mirror symmetry. One dimensional chain of atoms has a translational periodicity of a . Because of this the frequency ω is a periodic function of k with a period $\frac{2\pi}{a}$, giving several values of k for each value of ω below ω_m . To each value of k there is a corresponding wavelength,

$$k = \frac{2\pi}{\lambda}$$

To make a unique representation, we choose an interval in k space whose length is equal to $\frac{2\pi}{a}$. The most convenient range is

$$-\frac{\pi}{a} < k < \frac{\pi}{a} \quad (7)$$

This region is known as the First Brillouin Zone for 1D periodic lattice. In addition to the translational symmetry, the dispersion curve also has a mirror symmetry (about the origin $k=0$) in k space.

$$\omega(-k) = \omega(k) \quad (8)$$

where mode k (with $k > 0$) represents a wave travelling to the right through the lattice in the positive x direction and $-k$ represents a wave of same wavelength but travelling in the opposite direction.

1.1.2 Number of modes in the First Zone

The assumption that the last atom is joined to the first atom makes the chain endless and identical environment to all the atoms provides a basis to apply periodic boundary condition. Therefore,

$$u_n(x = 0) = u_{N+n}(x = L) \quad (9)$$

where $L = Na$ is the length of ring of atoms. substituting eqn 3 in eqn 9

$$e^{ikL} = 1 \quad (10)$$

$$kL = 2n\pi$$

$$k = \frac{2n\pi}{L} = n \frac{2\pi}{L}$$

where $n = 0, 1, 2, \dots$ Only discrete values of k are allowed which are integral multiples of $\frac{2\pi}{L}$. For large L the points form a quasi-continuous mesh along k axis. Thus the total number of points inside the first zone will be given by

$$\frac{2\pi/a}{2\pi/L} = \frac{L}{a} = N$$

where N is the total number of atoms or unit cells in the lattice and is equal to the allowed values of k inside the first brillouin zone. This is expected because the vales of k inside the zone uniquely describes the vibrational modes of the lattice. Therefore, the number of modes must be equal to the number of degrees of freedom in the latttice, which is N .

1.1.3 Long Wavelength Limit

For the part of of dispersion curve $0 < k < \frac{\pi}{a}$ the frequency of the wave varies in the range $0 < \omega < \omega_m$ (where ω_m is the natural cutoff frequency). This implies that one dimensional crystal lattice allows the propagation of frequency lying between 0 and ω_m only while strongly attenuates all other frequencies and hence behaves as a low pass filter. In long wavelength limit ($k \rightarrow 0$)

$$\omega = \omega_m \left| \sin \frac{ka}{2} \right|$$

can be approximated as

$$\omega = \omega_m \frac{ka}{2}$$

$$\omega = \left(\frac{\omega_m a}{2} \right) k = v_s k$$

This shows a linear relationship between ω and k an expected result, because in this limit lattice behaves as an elastic continuum.

$$\frac{\omega_m a}{2} = v_s = \text{velocity of sound in solid medium.}$$

$$\frac{\omega_m a}{2} = \sqrt{\frac{Y}{\rho}} \quad (11)$$

where Y is Young's modulus and ρ is density of solid material.

$\therefore \omega_m = \left(\frac{4K}{M}\right)^{1/2}$ and $\rho = \frac{M}{a^3}$ from eqn. 11 we have

$$\begin{aligned} \left(\frac{4K}{M}\right)^{1/2} \cdot \frac{a}{2} &= \sqrt{\frac{Y a^3}{M}} \\ \frac{4K a^2}{M \cdot 4} &= \frac{Y a^3}{M} \\ K &= aY \end{aligned} \quad (12)$$

1.1.4 Phase and Group Velocities

The phase velocity is given by

$$v_p = \frac{\omega}{k} = \frac{\omega_m \sin\left(\frac{ka}{2}\right)}{k} = \frac{\omega_m a \sin(ka/2)}{2 \cdot ka/2} v_p = v \frac{\sin(ka/2)}{ka/2}$$

The transmission velocity of a wave packet is the group velocity, given by

$$v_g = \frac{d\omega}{dk} = \frac{\omega_m a}{2} \cos \frac{ka}{2} = v \cos \frac{ka}{2}$$

v_p is the velocity of propagation of pure wave of exactly specified ω and k . v_g is the velocity of wave packet whose average frequency and wave vector are specified by ω and k .

Since energy and momentum are practically transmitted via pulse rather than the waves, group velocity is more significant. when $k \rightarrow 0$

$$\left(\frac{\sin(ka/2)}{ka/2}\right) \rightarrow 1 \text{ and } \cos(ka/2) \rightarrow 1$$

$$v_p = v_g = v$$

As k increases v_g being the slope of dispersion curve decreases steadily and becomes zero at $k = \pm\pi/a$. At zone boundary $k = \pm\pi/a$, $v_p = 2v/\pi$ and $\lambda = 2a$. This indicates that nearest neighbours are moving in antiphase. Further at $k = \pm\pi/a$, $v_g = 0$. Means no energy is being propagated, and the wave is a standing wave. This situation is equivalent to Bragg reflection in X-ray diffraction.