Subject: Physics

Lesson: Lattice Vibrations

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Lattice vibration

To get into the deeper knowledge of Lattice Vibrations first we should understand what do the "vibrations in a lattice" means. It is well known that the Heisenberg's uncertainty principle accounts for the vibration of atoms (in a real crystal) around their equilibrium position even at absolute zero temperature. At this temperature the energy of each atom is known as zero point energy with the amplitude of vibrations known as zero point amplitude. The amplitude of vibrations of the atoms around their equilibrium position starts increasing when the temperature of the crystal is increased. The atoms gain more thermal energy at higher temperatures and thus start oscillating with greater amplitude as shown in Fig.1.

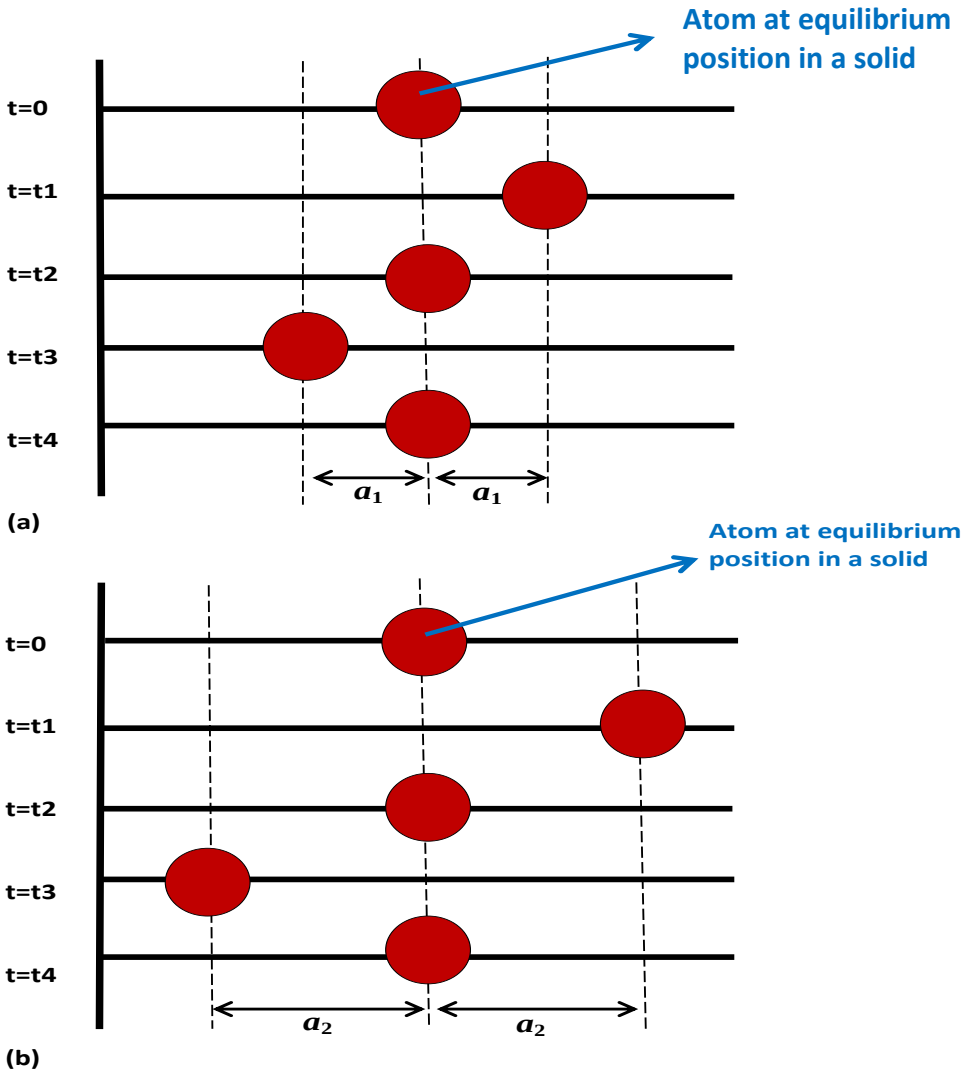


Fig.1. (a) The atoms in a crystal at absolute zero temperature with zero point motion of atoms with displacement from the equilibrium position as a_1 (b) The atoms in a crystal at room temperature with increased amplitude of vibrations of atoms with displacement from the equilibrium position as a_2.

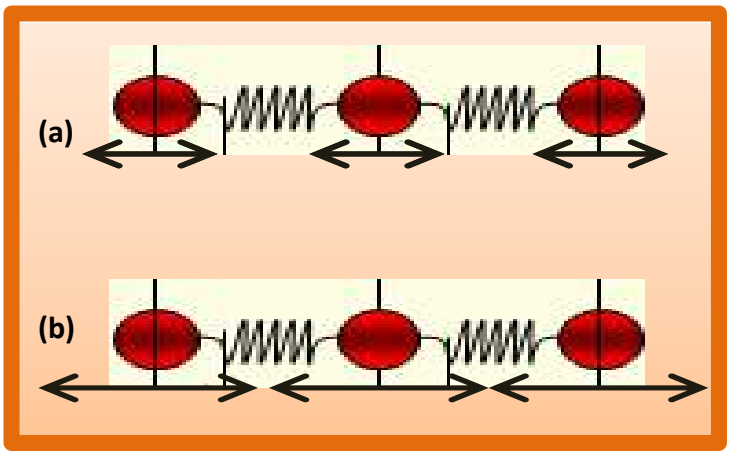


Fig.1'. (a) The atoms in a crystal at absolute zero temperature with zero point motion of atoms with displacement from the equilibrium position as a_1 (b) The atoms in a crystal at room temperature with increased amplitude of vibrations of atoms with displacement from the equilibrium position as a_2.

In a real crystal atoms are not bounded to their equilibrium positions only, but the motion of one atom also affects the motion of neighbouring atom. Thus when one atom of a crystal vibrated about the equilibrium position the neighbouring atom also start vibrating and so the next neighbouring atom. In this way when an entire group of atoms vibrate in a coordinated way it is referred to as a Lattice vibration. The forces which lock the atoms in a crystal to their equilibrium position are directly proportional to their displacements from equilibrium position in the elastic limit and therefore we assume that atoms are being bound by elastic springs between them as shown in Fig.2. This assumption is known as Harmonic approximation where we have assumed the particles (atoms) of a crystal being coupled by an ideal elastic spring. In this approximation atoms vibrate about the equilibrium position under a simple harmonic oscillation (like a simple harmonic oscillator). One important point to mention is that, the lattice vibration character is highly dependent on the –

(a) Number of atoms in one unit cell of crystal (Monoatomic, Diatomic, Triatomic etc.),

(b) Symmetry of the crystal,

(c) Type of chemical bond between the atoms,

(d) Crystal defect concentration.

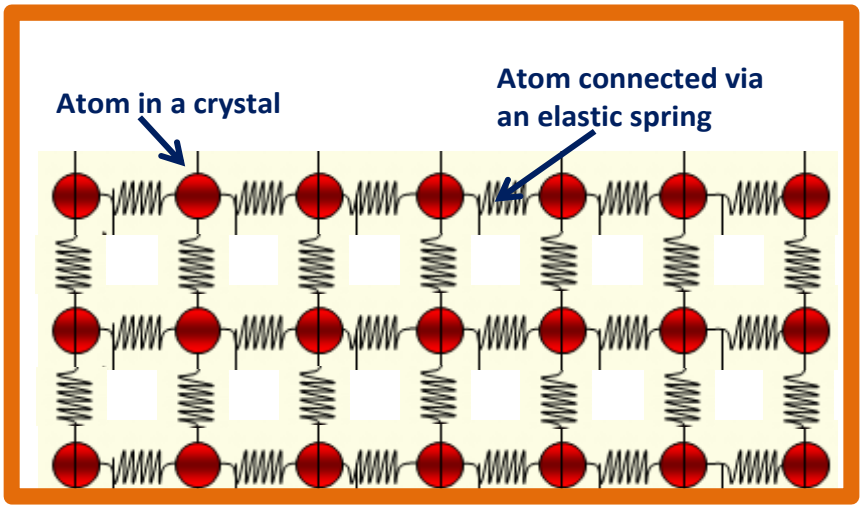


Fig.2. The model of a simplest lattice showing the elastic coupling between the neighbouring atoms.

Lattice vibrations as explained above accounts for the thermal properties of the crystals and contribute to the heat capacity of metals. In our further discussion we want to study the traits of elastic vibrational motion of the crystal lattices by considering the case of one dimensional monoatomic and di-atomic chain of atoms first. In reality the crystal is a 3D structure but to simplify the problem we have reduced the system to lower dimension (1D) and if required then we can generalize the results to 2D and 3D.

Dynamics of one dimensional infinite monoatomic chain of atoms

To investigate the dynamics of the vibrational motion in an infinite 1D-chain of identical atoms (each having the same mass *m*), we assume that the distance between the equilibrium position of nearest-neighbouring atoms is *a* such that the total number of atoms *N* in the chain is very large . The system we have considered is non-homogeneous as atoms are separated from one another, and being bound by the ideal elastic springs between them. The 1D-chain of atoms is assumed to be lying along *x*-axis (Fig.3).

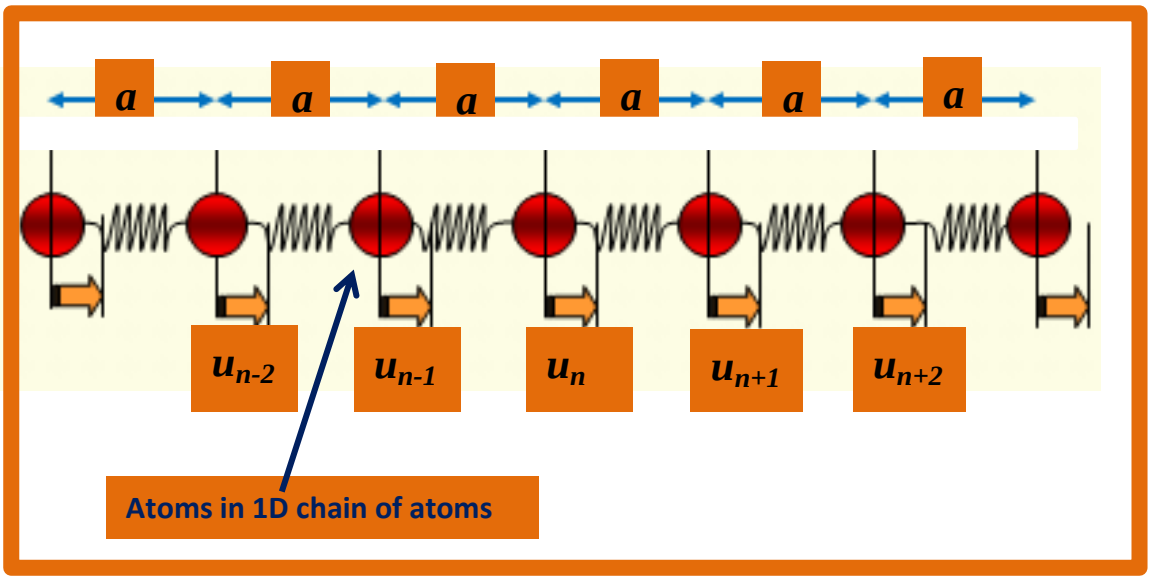


Fig.3. The model of a linear (1D) monoatomic lattice

The *x*-coordinates of the atoms present in the 1D-chain at $(n+2)^{th}$, $(n+1)^{th}$, n^{th}, $(n-1)^{th}$, $(n-2)^{th}$, …….sites are at $x_{n+2}=(n+2)a$, $x_{n+1}=(n+1)a$, $x_n=na$, $x_{n-1}=(n-1)a$, $x_{n-2}=(n-2)a$ ……. Similarly the symbols u_{n+2}, u_{n+1}, u_n, u_{n-1}, u_{n-2}, …… represents the displacements of the atoms present at $(n+2)^{th}$, $(n+1)^{th}$, n^{th}, $(n-1)^{th}$, $(n-2)^{th}$, …….sites in the 1D-chain within the elastic limits. These displacements arises due to excitation in vibrational motion of the atoms, otherwise the atoms execute only zero-point oscillations around their mean positions (or more or less stay at the equilibrium positions). In the elastic limit it is assumed that the restoring forces acting between the nearest-neighbour atoms are linear. Under these assumptions we can write the force equation for the n^{th} atom as –

$$\begin{aligned} F_n &= f_1 - f_2 \\ &= \eta\left(u_{n+1} - u_n\right) - \eta\left(u_n - u_{n-1}\right) \\ &= \eta\left(u_{n+1} + u_{n-1} - 2u_n\right) \end{aligned} \qquad \ldots(1)$$

In the above equation we have assumed that η is the spring constant or force constant (or force of interaction per unit displacement), F_n is the net force acting on the n^{th}

atom, and (u_{n+1}-u_n), (u_n-u_{n-1}) are the extensions produced in the springs connected with the n^{th} atom. The force $f_1 = \eta\left(u_{n+1} - u_n\right)$ acts in the right direction, while the force $f_2 = \eta\left(u_n - u_{n-1}\right)$ acts in the left direction. In writing the above force equation we have strictly neglected the effect of atoms other than nearest ones on n^{th} atom. According to Newton's second law of motion Eqn.(1) can be rewritten as –

$$m\frac{d^2x_n}{dt^2} = m\ddot{x}_n = \eta\left(u_{n+1} + u_{n-1} - 2u_n\right) \qquad \ldots(2)$$

The solution of above equation of motion can be assumed as travelling waves (i.e. the displacements produced in atoms are in the form of travelling waves) as –

$$u_n = u_0 e^{i(\omega t - Kna)} \qquad \ldots(3.1)$$

$$u_{n+1} = u_0 e^{i(\omega t - K(n+1)a)} \qquad \ldots(3.2)$$

$$u_{n-1} = u_0 e^{i(\omega t - K(n-1)a)} \qquad \ldots(3.3)$$

where, K is the wave-vector, u_0 is amplitude of oscillation of an atom, ω is the frequency of oscillations which is same for each atom (i.e. all atoms in lattice vibration oscillate with the same frequency). Substituting the Eqns.(3.1), (3.2), (3.3) in Eqn.(2) we arrive at the following equation –

$$\begin{aligned} -m\omega^2 &= \eta\left(e^{iKa} - 2 + e^{-iKa}\right) \\ &= \eta\left(e^{iKa/2} - e^{-iKa/2}\right)^2 \end{aligned} \qquad \ldots(4)$$

Substituting the, $\sin(x) = \left(\frac{e^{ix} - e^{-ix}}{2i}\right)$ and $\sin^2(x) = -\frac{1}{4}\left(e^{ix} - e^{-ix}\right)^2$ in the above equation we can again rewrite it as –

$$-m\omega^2 = -4\eta\sin^2\left(\frac{Ka}{2}\right) \qquad \ldots(5)$$

$$\begin{aligned} \Rightarrow \omega &= \left|\sqrt{\frac{4\eta}{m}}\sin\left(\frac{Ka}{2}\right)\right| = +\frac{2}{a}\sqrt{\frac{c}{\rho}}\left|\sin\left(\frac{Ka}{2}\right)\right| \\ &= \omega_{\max}\left|\sin\left(\frac{Ka}{2}\right)\right| \end{aligned} \qquad \ldots(6)$$

where the maximum value or cut-off value of frequency is $\omega_{\max} = 2v_s / a$, with $v_s = \sqrt{c/\rho}$, $\rho = m/a$ being the mass per unit length and $\eta = c/a$ is the longitudinal stiffness per unit length. As frequency is a positive quantity therefore we have neglected the negative solution in Eqn.(6) and have considered only magnitude. Above relation in Eqn.(6) is known as Dispersion relation. This dispersion curve is shown in Fig.4, which is periodic in nature with a period of 2π and symmetric about the origin at K=0.

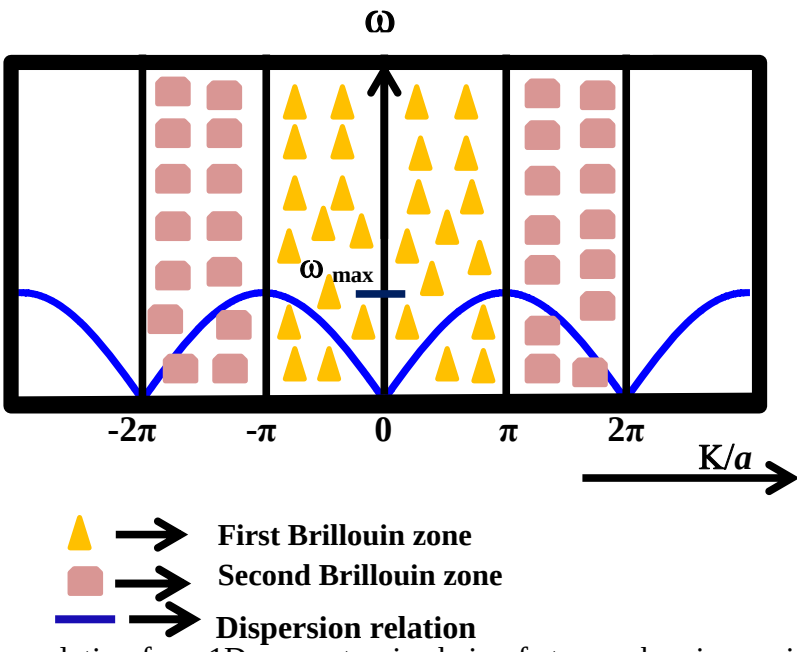


Fig.4. Dispersion relation for a 1D monoatomic chain of atoms, showing periodic curve.

Above dispersion curve clearly shows that for one value of ω there are several values of wave-vector *K*. Therefore we have defined the brillouin zones as –

First Brillouin zone : $-\pi < \frac{K}{a} < \pi$

Second Brillouin Zone : $-2\pi < \frac{K}{a} < -\pi$ and $\pi < \frac{K}{a} < 2\pi$

Now in first brillouin zone each value of frequency correspond to a unique value of wave-vector. The above dispersion curve also indicates the mirror symmetry as $\omega(-K) = \omega(K)$. The mirror symmetry implies that +*K*,-*K* represents a plane wave propagating in the positive, negative direction through the monoatomic lattice. Now we will examine some simple cases of this Dispersion relation, of which first is –

If the Frequency of oscillations is very low – This case is often regarded as Long wavelength limit also. In this limit $K \to 0$ which implies that, $\sin\left(\frac{Ka}{2}\right) \to \frac{Ka}{2}$. This reduces the Dispersion relation in Eqn.(6) to –

$$\omega = \omega_{\max} \left|\frac{Ka}{2}\right| \qquad \ldots(7)$$

$$\Rightarrow \qquad \omega = \frac{2v_s}{a}\frac{|K|a}{2} = v_s|K| \qquad \ldots(8)$$

Using the dispersion relation in above equation we can calculate the,

Phase velocity v_p as, $v_p = \frac{\omega}{K} = v_s$ …(9)

Group velocity v_g as, $$v_g = \frac{d\omega}{dK} = v_s \quad \ldots(10)$$

Above shows that in this limit, phase velocity and group velocity are equal to v_s and the dispersion relation is linear. This is the case where discrete chain of atoms behaves as if it is continuous and approaches continuum. In fact, long wavelengths in the system do not respond to discreteness of the system. Here a very large number of atoms contribute to the displacements, which is very much similar to the case of homogeneous line. The system here follows the dynamical behaviour, neglecting the effect of atomic nature of chain.

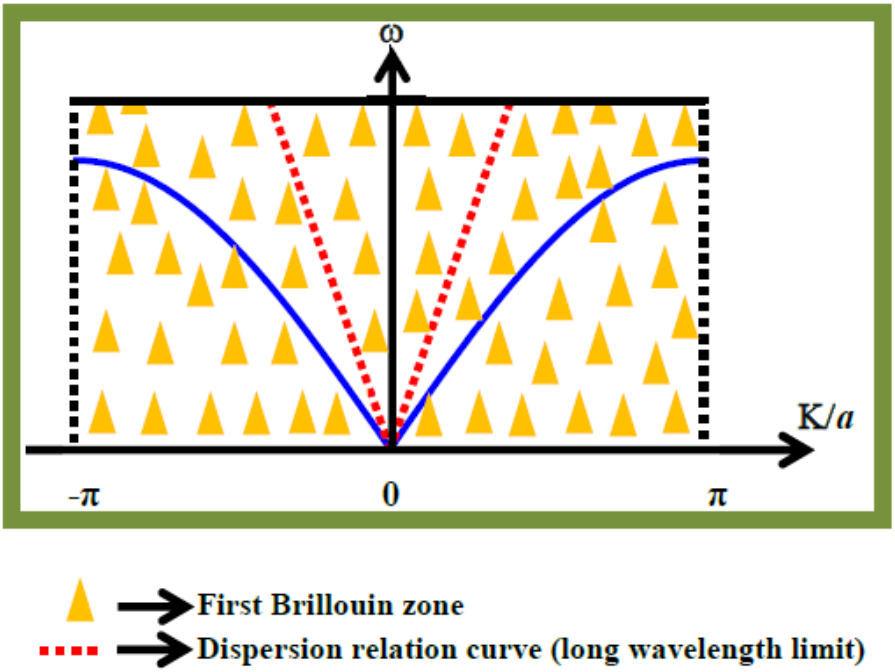


Fig.5. Dispersion relation for a 1D monoatomic chain of atoms (low frequency case).

If the Frequency of oscillations is high – In the high frequency limit, the phase velocity and group velocity are no longer equal as compared to the previous case. Using the Eqn.(6) we obtain,

Phase velocity v_p as, $$v_p = \frac{\omega}{K} = \frac{\omega_{\max}}{K}\left|\sin\left(\frac{Ka}{2}\right)\right| \quad \ldots(11)$$

Group velocity v_g as, $$v_g = \frac{d\omega}{dK} = \omega_{\max}\frac{a}{2}\left|\cos\left(\frac{Ka}{2}\right)\right| \quad \ldots(12)$$

It is clear from the above equations that both group and phase velocities are a function of frequency ω_{max}. This kind of medium is highly dispersive in nature. In the previous case the medium was not dispersive and it follows the characteristics of a homogenous continuous medium. **(**Note: Dispersion refers to a phenomenon in which group/phase velocity of a wave travelling through a medium is dependent on its own frequency and such a medium is known as Dispersive medium.**)**

If the Frequency of oscillations is maximum – In this limit the atoms in monoatomic chain of vibrate with the maximum frequency which is –

$$\omega = \omega_{\max} = 2\frac{v_s}{a} \qquad \ldots(13)$$

Using above the group and phase velocities are calculated as,

Phase velocity v_p as, $$v_p = \frac{\omega}{K} = 2\frac{v_s}{aK} \qquad \ldots(14)$$

Group velocity v_g as, $$v_g = \frac{d\omega}{dK} = 0 \qquad \ldots(15)$$

Zero group velocity refers to no propagation of energy or signal. In this condition only standing wave is produced as shown in Fig.(6).

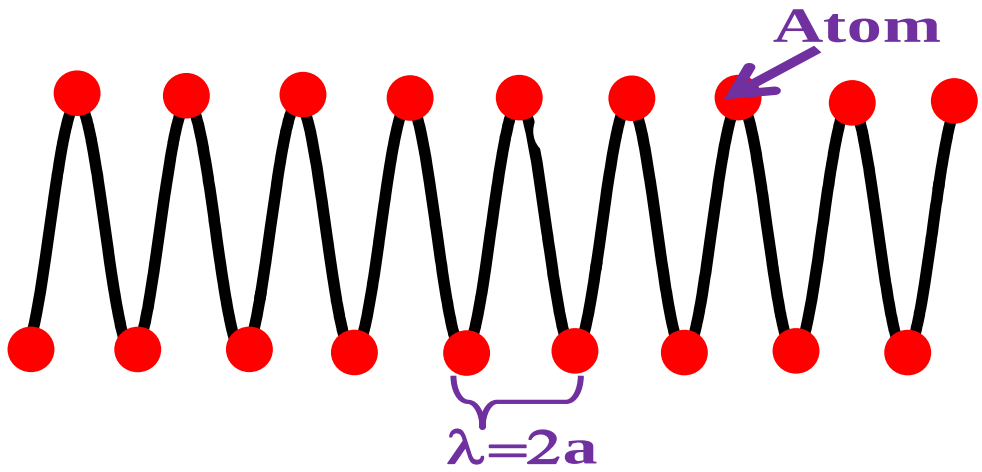


Fig.6. Standing wave produced in lattice when each atom vibrates with the same maximum frequency.

At $K=\pi/a$, wavelength is equal to $2a$. This situation is parallel to Bragg's reflection (According to Bragg reflection of X-rays by the atomic planes in a crystal $n\lambda=2d\sin(\theta)$, where n is the order of reflection. Here for the 1st order reflection with normal incidence $n=1$, which implies that $\lambda=2d\sin(90)=2d$).

Dynamics of one dimensional finite monoatomic chain of atoms

(a) In the previous case we considered the infinite length of the chain but now we want to examine the normal modes of vibration when the length of chain is finite. We assume that the length of chain is L and is fixed at both the ends as shown in Fig.(7) with zero displacement at the two fixed atoms.

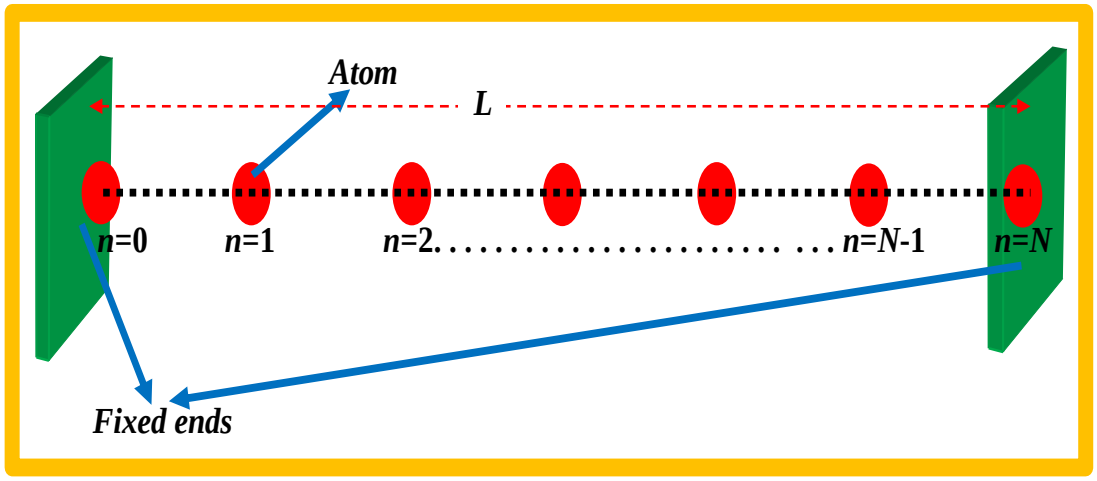


Fig.7. One dimensional finite monoatomic chain of length L having N+1 atoms fixed at both the ends.

We number the atoms in the chain in such a way that 0^{th} atom is fixed at the left end and N^{th} atom is fixed at right end of the chain. Therefore total number of atoms present in the lattice is N+1 with $L=Na$. We assume that (due to fixed boundary conditions a standing wave is produced in the lattice) the symbol u_n is given as –

$$u_n = u_0 \sin(Kna)\sin(\omega t) \qquad \ldots(16)$$

such that, $u_0 = u_N = 0$ which ensures the normal mode of vibration of the lattice. For this we must have $\sin(Kna)=0$ giving,

$$K = \frac{m\pi}{L} \qquad \text{where} \quad m = 1, 2, 3, 4, \ldots\ldots N\text{-}1$$

We have not included m=0, N values as they correspond to u_n=0 (zero displacement of the atom). This clearly indicates that in the N+1 number of atoms we have fixed the two atoms and thus there are N-1 normal modes of vibration where each mode corresponds to one atom which is free to move.

(b) Now we consider the case where the one dimensional monoatomic chain is bent in form of a circular ring and 0^{th} atom is joined with N^{th} atom. In this situation when a vibrational mode is excited then both joined atoms suffer the same displacement and are free to move (shown in Fig.8), which is unlike the previous case where the two end atoms were fixed.

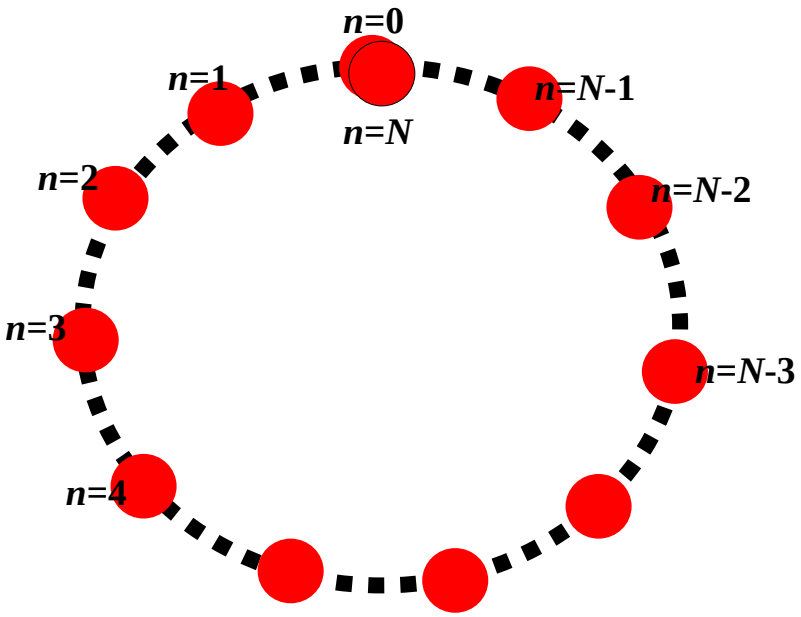


Fig.8. One dimensional finite monoatomic chain of length L having N+1 atoms aligned along a circular ring with first and last atoms being superimposed on each other.

The running wave solution for this case can be written as –

$$u_n = u_0 e^{i(\omega t - Kna)} \qquad \ldots(17)$$

The boundary condition for this case is $u_n = u_{n+N}$, as the amplitude is same after every N number of atoms. To satisfy this boundary condition (Born and Von Karman cyclic boundary conditions) we must have –

$$\exp(-iKNa) = 1 \qquad \ldots(18)$$

Above implies that,

$$K = 0, \pm\frac{2\pi}{Na}, \pm\frac{4\pi}{Na}, \pm\frac{6\pi}{Na}, \ldots\ldots \pm\frac{N\pi}{Na} \qquad \ldots(19)$$

It means that there is total number of N independent K values which makes the frequency spectrum discrete. The dispersion relation curve is no longer a continuous curve for this case.

♦ Assuming a linear monoatomic lattice, through which a maximum frequency of $5x10^{12}$ Hz can propagate through lattice, calculate the velocity of the wave in solid. (Given a=10 A^0)

Ans : It is known that frequency $f = v/\lambda$ *where* λ *is the wavelength at maximum frequency condition. We have seen that maximum frequency occurs at first brillouin zone boundary at* $\pm\pi/a$ *in a monoatomic linear lattice, where wavelength is 2a. Therefore,*

$$f = v/\lambda = v/2a = \frac{v}{2\times10^{-10}\,m} = 5\times10^{12}\,\text{Hz}$$

$$\Rightarrow \qquad v = 10^3\,m/s$$

Dynamics of one dimensional diatomic linear chain of atoms

Next we consider a linear diatomic chain of atoms as shown in Fig.9. We assume that it is a one dimensional lattice with two different kinds of atoms having masses M_1 and M_2 in one unit cell of the lattice. We also assume that the separation between any two consecutive M_1 and M_2 atoms is a and symbol u_r represents the displacement of r^{th} atom from its equilibrium position. In this case also we restrict the interactions between the atoms to nearest neighbours only within the consecutive atoms M_1 and M_2. In the Fig.9 all M_1 atoms are present at the even sites (…2n-4, 2n-2, 2n, 2n+2, 2n+4…..) and all M_2 atoms are present at the odd sites (…2n-5, 2n-3, 2n-1, 2n+1, 2n+3…..).

We can write the equations of motion for both the kind of atoms as –

$$F_{2n,M_1} = M_1\ddot{u}_{2n} = \eta\left(u_{2n+1} - 2u_{2n} + u_{2n-1}\right) \qquad \ldots(20)$$

$$F_{2n+1,M_2} = M_2\ddot{u}_{2n+1} = \eta\left(u_{2n+2} - 2u_{2n+1} + u_{2n}\right) \qquad \ldots(21)$$

In the above equations of motion, η is again the spring constant or force of interaction per unit displacement which is equal between any two consecutive atoms M_1 and M_2. If we assume that all the atoms vibrate with same frequency ω, then the solutions of Eqns.(20) and (21) can be written as –

$$u_{2n} = A_1 e^{i(\omega t - 2Kna)} \qquad \ldots(22)$$

$$u_{2n+1} = A_2 e^{i(\omega t - (2n+1)Ka)} \qquad \ldots(23)$$

In the above running wave type solutions K represents a particular vibrational mode. An important point to note here is that we have taken the same frequency of oscillations for both the kinds of atoms, irrespective of their different masses. This makes them oscillate with different amplitudes. On substituting Eqns.(22) and (23) in Eqns.(20) and (21) we get –

$$-M_1\omega^2 A_1 = \eta A_2\left(e^{-iKa} + e^{iKa}\right) - 2\eta A_1 \qquad \ldots(24)$$

$$-M_2\omega^2 A_2 = \eta A_1\left(e^{-iKa} + e^{iKa}\right) - 2\eta A_2 \qquad \ldots(25)$$

$$\Rightarrow \quad \left(2\eta - \omega^2 M_1\right)A_1 - \left(2\eta\cos\left(Ka\right)\right)A_2 = 0 \qquad \ldots(26)$$

$$\left(-2\eta\cos\left(Ka\right)\right)A_1 + \left(2\eta - \omega^2 M_2\right)A_2 = 0 \qquad \ldots(27)$$

The above system of equations is known as “constant coefficient linear homogeneous system”.

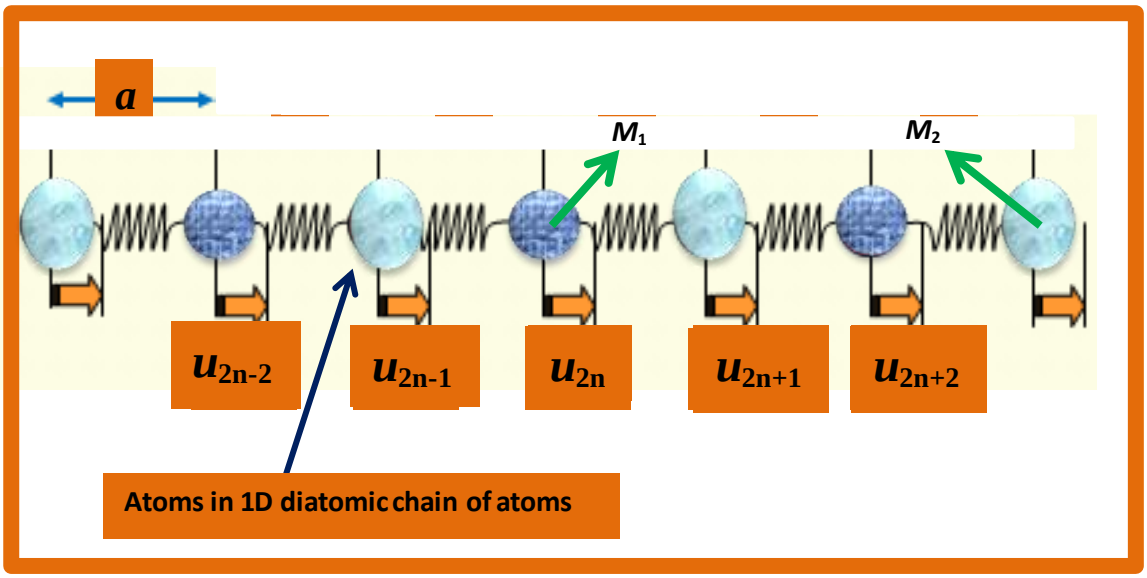


Fig.9. The model of a diatomic linear lattice showing the elastic coupling between the neighbouring atoms having two kinds of atoms with masses M_1 and M_2.

Now we put the determinant of the system in equations (26) and (27) equal to zero to get the solution of this system as –

$$\begin{vmatrix} 2\beta-\omega^2 M_1 & -2\beta\cos(Ka) \\ -2\beta\cos(Ka) & 2\beta-\omega^2 M_2 \end{vmatrix} = 0 \qquad \ldots(28)$$

On solving the above determinant the dispersion relation for the diatomic linear chain of atoms is obtained as follows –

$$\omega^2 = \eta\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \pm \eta\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2(Ka)}{M_1 M_2}} \qquad \ldots(29)$$

It is clear from the above dispersion relation that even if we have single value of wavevector, it corresponds to two different values of ω as –

$$\omega_+ = \left(\eta\left(\frac{1}{M_1}+\frac{1}{M_2}\right)+\eta\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2(Ka)}{M_1 M_2}}\right)^{1/2} \Rightarrow \textbf{Optical Branch}$$

$$\omega_- = \left(\eta\left(\frac{1}{M_1}+\frac{1}{M_2}\right)-\eta\sqrt{\left(\frac{1}{M_1}+\frac{1}{M_2}\right)^2 - \frac{4\sin^2(Ka)}{M_1 M_2}}\right)^{1/2} \Rightarrow \textbf{Acoustical Branch}$$

Using the above frequencies we can plot the Dispersion relation for the diatomic linear chain of atoms as shown in Fig.10 below. It is clear from the Fig.10 above that the only range of frequencies that can be excited in a diatomic linear chain of atoms gets

broken up into two branches, where top branch is called optical and lower one is called acoustical branch. It means that for each value of *K* there are two types of vibration in which a lattice can go or we can say that there are two different modes for each *K*. Also in between these two branches there exists a band gap of frequencies corresponding to no lattice vibrations. It means that this range of frequencies cannot be excited in a diatomic linear chain of atoms.

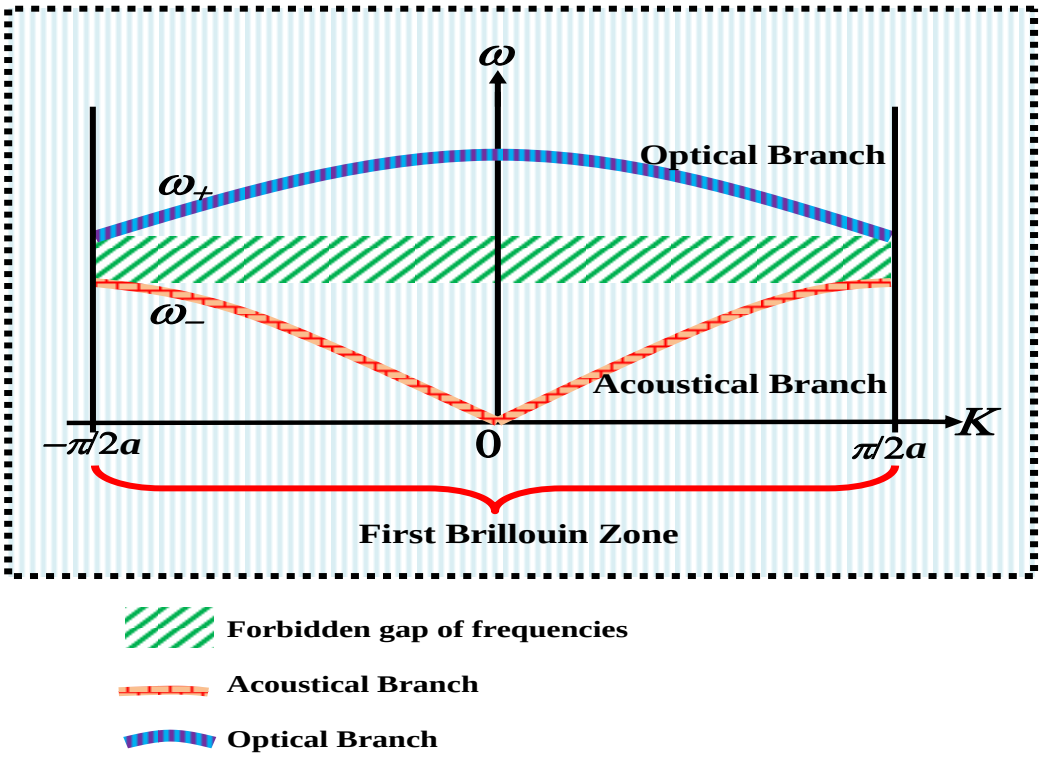


Fig.10. The optical and acoustical branches and forbidden frequency band gap in the frequency spectrum for a linear diatomic chain of atoms (for the first brillouin zone only).

(1) Optical Branch

In this case, the atoms undergo a lattice vibration such that both the kinds of atoms move in the opposite directions as shown in Fig.11. To excite these kinds of vibrations a force is needed such that, it incorporates the opposite motions on two kinds of atoms such that the center of mass (of the unit cell) is at rest with the amplitude of vibration of atoms being inversely proportional to their masses. Using the expression of ω_+ we get the optical branch frequency as –

$$\lim_{K\to 0}\omega_+ = \left(2\eta\left(\frac{1}{M_1}+\frac{1}{M_2}\right)\right)^{1/2} \qquad \ldots(30)$$

$$\lim_{K\to \pm\frac{\pi}{2a}}\omega_+ = \left(\frac{2\eta}{M_1}\right)^{1/2} \qquad \ldots(31)$$

where we have assumed M_1 to be less than M_2. Hence in the Fig.[] above the maximum value of ω_+ is given at the point where K=0 and minimum at the K=±π/2a at the first brillouin zone boundary. Using the Eqns.(26) and (27) at K=0, we get –

$$\left(2\eta - \omega^2 M_1\right) A_1 - \left(2\eta\right) A_2 = 0 \qquad \ldots(32)$$

$$\left(-2\eta\right) A_1 + \left(2\eta - \omega^2 M_2\right) A_2 = 0 \qquad \ldots(33)$$

On solving the above we get, $\frac{A_1}{A_2} = -\frac{M_2}{M_1}$ which also shows that atoms move in opposite directions.

(2) Acoustical Branch

In this case, the atoms undergo a lattice vibration such that both the kinds of atoms move in the same direction with the same amplitude irrespective of their different masses as shown in Fig.12. The motion of the center of mass is also in the same direction. To excite these kinds of vibrations a force is needed such that, it incorporates the motions in two kinds of atoms in the same direction with equal amplitudes such that the center of mass (of the unit cell) also moves in same direction. Using the expression of ω_- we get the optical branch frequency as –

$$\lim_{K \to 0} \omega_- = 0 \qquad \ldots(34)$$

$$\lim_{K \to \pm \frac{\pi}{2a}} \omega_- = \left(\frac{2\eta}{M_2}\right)^{1/2} \qquad \ldots(35)$$

Hence in the Fig.[] above the minimum value of ω_- is given at the point where K=0 and maximum at the K=±π/2a at the first brillouin zone boundary. Using the Eqns.(31) and (35) we can calculate the width of the forbidden band gap of frequencies in Fig.[]. This gap depends on the ratio of two masses as –

$M_2 / M_1 \rightarrow$ Increases $\Rightarrow$ Forbidden frequency bandgap also increases

$\rightarrow$ Decreases $\Rightarrow$ Forbidden frequency bandgap also decreases

$\rightarrow$ 1 $\Rightarrow$ Forbidden frequency bandgap disappear

(The two spilt branches join at $K = \pm\frac{\pi}{2a}$)

At θ =0, we can replace sin(θ) by θ only, therefore in the limit of K→0, we can also substitute, $\omega_- = \left(\eta\left(\frac{1}{M_1} + \frac{1}{M_2}\right) - \eta\sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4}{M_1 M_2} K^2 a^2}\right)^{1/2}$ …(36)

$$\Rightarrow \qquad \omega_- = Ka\sqrt{\frac{2\eta}{M_1 + M_2}} \qquad \ldots(37)$$

Substituting the $\cos(Ka) \simeq \left(1-\sin^2(Ka)\right)^{1/2} \simeq \left(1-(Ka)^2\right)^{1/2} \simeq 1-\frac{(Ka)^2}{2}$ and using Eqns.(37), (26) and (27) we get –

$$\left(2\eta - \left[Ka\sqrt{\frac{2\eta}{M_1+M_2}}\right]^2 M_1\right)A_1 - 2\eta\left(1-\frac{(Ka)^2}{2}\right)A_2 = 0 \qquad \ldots(38)$$

$$-2\eta\left(1-\frac{(Ka)^2}{2}\right)A_1 + \left(2\eta - \left[Ka\sqrt{\frac{2\eta}{M_1+M_2}}\right]^2 M_2\right)A_2 = 0 \qquad \ldots(39)$$

On solving the above we get, $\frac{A_1}{A_2} = +1$ which also shows that atoms move in same directions with equal amplitudes.

- Do you know why we call these branches as Optical & Acoustical ????.....

Ans : An ionic crystal consists of two kinds of ions which are oppositely charged. When this kind of crystal comes under the influence of light beam, the oppositely charged ions are forced in the different directions, and the optical branch kinds of vibrations are excited in the system. From this, the term Optical branch has been derived.

Similarly when sound waves strike any crystal surface then it forces all the atoms to vibrate in the same direction and produces acoustical branch vibrations. Thus these kinds of vibrations are called Acoustical branch vibrations.

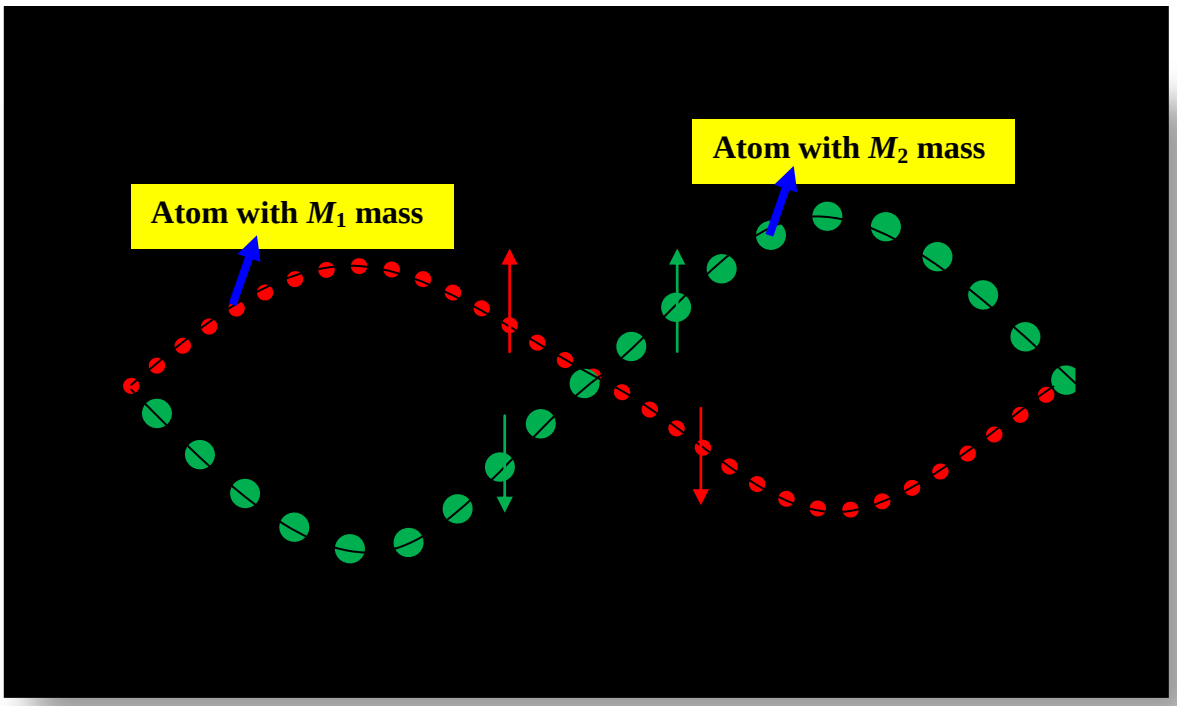


Fig.11. Motion of atoms (neighbouring atoms out of phase) in a diatomic linear chain of atoms when the optical branch vibrations are excited.

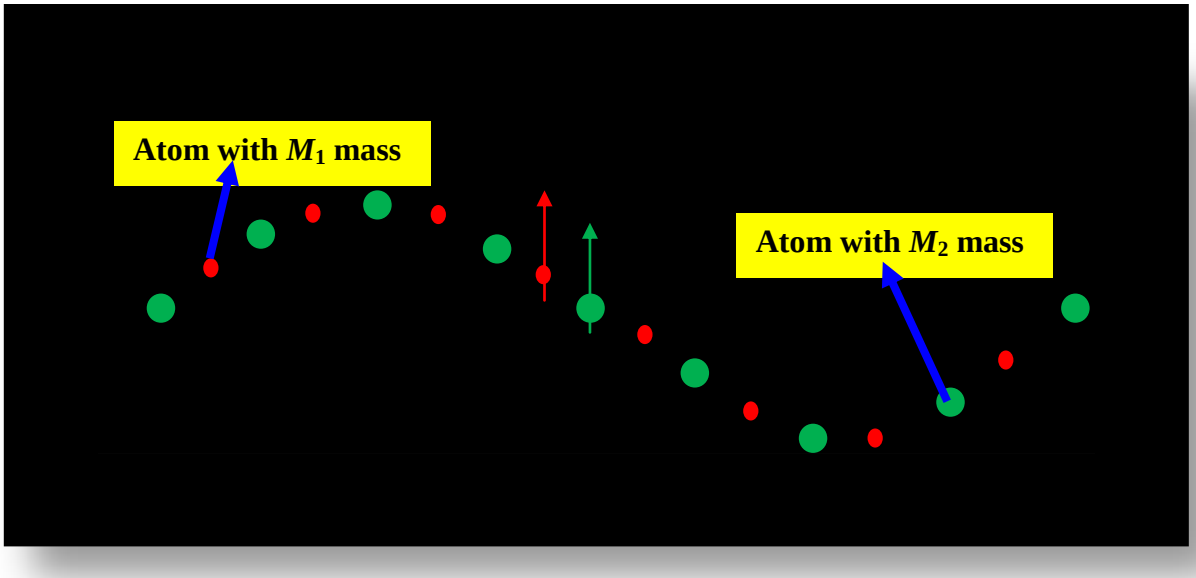


Fig.12. Motion of atoms (neighbouring atoms in phase) in a diatomic linear chain of atoms when the acoustical branch vibrations are excited.

- If $M_2 \rightarrow \infty$, then acoustical branch frequency becomes single valued at zero and optical branch frequency at $\sqrt{2\eta / M_1}$.

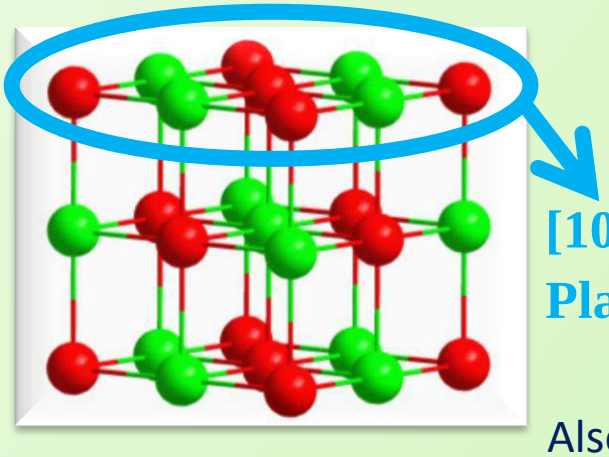
- If $M_1 \rightarrow 0$, the diatomic case reduces to monoatomic case with lattice constant being $2a$. Here optical branch does not appear without affecting the acoustical branch.

- If $M_1 = M_2$ then lattice vibration frequency range lies between 0 and $\sqrt{4\eta / M_1}$. The only difference then between monoatomic and diatomic case is that, for monoatomic case whole range of this frequency accounts for acoustical branch and for diatomic case this range of frequency splits into two branches acoustical one corresponding to frequency from 0 to $\sqrt{2\eta / M_1}$ and $\sqrt{2\eta / M_1}$ to $\sqrt{4\eta / M_1}$ corresponding to optical branch.

- For a crystal with N number of atoms per unit cell, the frequency range will split up into N number of bands.

- For a fixed length L the periodic boundary condition is, $u_{2n}(x) = u_{2n}(x + L)$ which ensures, $K = \pm\frac{\pi}{L}, \pm\frac{2\pi}{L}, \pm\frac{3\pi}{L}, ... \pm\frac{N\pi}{2L}$. Here N is the total number of allowed K values representing N normal modes for vibration.

♦ For a KCl crystal the unit cell parameter is $6.3A^0$.



[100] Plane

And the young's modulus of elasticity along [100] direction is 29.67GPa. Calculate the maximum value of the optical branch frequency and the corresponding wavelength. Also estimate the forbidden frequency band gap.

Ans : The parameters we know for this problem are :

$$a = 6.3A^0 = 6.3\times10^{-10}\,m$$
$$Y = 29.67GPa = 2.967\times10^{10}\,N/m^2$$
$$K\ (\text{At. Wt.}) = 39amu\ ,\quad Cl\ (\text{At. Wt.}) = 37amu$$
$$1amu = 1.67\times10^{-27}\,Kg$$

Using the above parameters we can calculate :

(a) Maximum value of optical branch frequency as -

$$\omega_+(\max) = \lim_{K\to0}\omega_+ = \left(2\eta\left(\frac{1}{M_1}+\frac{1}{M_2}\right)\right)^{1/2}$$

Here $\eta = aY$, therefore on substituting these values we get –

$$\omega_+(\max) = \left(2\times6.3\times10^{-10}\times2.967\times10^{10}\left(\left(\frac{1}{37}+\frac{1}{39}\right)\times\frac{1}{1.67\times10^{-27}}\right)\right)^{1/2}\ \text{rad/sec}$$

$$=3.4336\times10^{13}\ \text{rad/sec}$$

(b) Forbidden frequency band gap is estimated as –

$$\text{Forbidden gap} = \lim_{K\to\pm\frac{\pi}{2a}}\omega_+ - \lim_{K\to\pm\frac{\pi}{2a}}\omega_- = \left(\frac{2\eta}{M_1}\right)^{1/2} - \left(\frac{2\eta}{M_2}\right)^{1/2}$$

$$=\left(\sqrt{\frac{2\times6.3\times10^{-10}\times2.967\times10^{10}}{37\times1.67\times10^{-27}}} - \sqrt{\frac{2\times6.3\times10^{-10}\times2.967\times10^{10}}{39\times1.67\times10^{-27}}}\right)\text{rad/sec}$$

$$=0.0638996380\times10^{13}\ \text{rad/sec}$$

Note : If instead of K atom we take Na atom this band gap will increase.

♦ If $v_0=10^5$ cm/sec, compare the frequencies of sound waves of λ=10-7 cm for (a) Homogeneous line (b) Acoustic waves (c) Optical waves on a linear lattice containing two identical atoms per primitive cell of interatomic spacing $2.5A^0$ (d) Light waves of same wavelength

Ans :

(a) Frequency in case of homogeneous line is given by ω_0 *given by -*

$$\omega_0 = v_0 K = v_0 \frac{2\pi}{\lambda} = 10^5\, cm/\sec \times \frac{2\pi}{10^{-7}\, cm} = 2\pi \times 10^{12}\, rad/\sec$$

(b) For acoustic waves in a diatomic lattice the frequency varies from $\omega = 0$ *to for* $K = 0$ *to* $\omega = \sqrt{\frac{2\eta}{M}}$ *for* $K = \frac{\pi}{2a}$ *where* η *is the force constant. In case of diatomic lattice,* $v_0 = \sqrt{\frac{2\eta}{M}}a$

$$\Rightarrow \quad \omega = \frac{v_0}{a} = \frac{10^5\, cm/\sec}{2.5\times 10^{-8}\, cm} = 4\times 10^{12}\, rad/\sec$$

(c) For optical waves in diatomic lattice the frequency varies from $\omega_1 = \sqrt{\frac{4\eta}{M}}$ *for* $K = 0$ *to* $\omega_2 = \sqrt{\frac{2\eta}{M}}$ *for* $K = \frac{\pi}{2a}$ *. Since the lattice has two identical atoms per primitive cell hence there will be no forbidden gap in frequencies. Therefore,*

$$\omega_1 = \sqrt{\frac{4\eta}{M}} = \sqrt{2}\sqrt{\frac{2\eta}{M}} = 4\sqrt{2}\times 10^{12}\, rad/\sec \text{ and } \omega_2 = \sqrt{\frac{2\eta}{M}} = 4\times 10^{12}\, rad/\sec$$

(d) For light waves of wavelength 10^{-7}*cm, the velocity we have c=3x*10^{10}*cm/sec.*

We have, $\omega = 2\pi\nu = 2\pi\frac{c}{\lambda} = 2\pi\frac{3\times 10^{10}\, cm/\sec}{10^{-7}\, cm} = 6\pi\times 10^{17}\, rad/\sec$.

♦ A cubic cell consists of two atoms of masses m_1 and m_2 ($m_1 > m_2$) with m_1 and m_2 atoms situated on alternate planes. Assuming only nearest neighbour interaction the center of mass of the two atoms :

(a) Moves with the atoms in the optical mode and remains fixed in the acoustic mode

(b) Remains fixed in the optical mode and moves with the atoms in the acoustic mode

(c) Remains fixed in both optical and acoustic mode

(d) Moves with the atoms in both optical and acoustic modes

Ans : Option 'd'

♦ Consider the energy E in the first brillouin zone as a function of the magnitude of wavevector k for a crystal of lattice constant a. Then

(a) Slope of E vs. k is proportional to the group velocity

(b) Slope of E vs. k has its maximum value at $|k|=\pi/a$

(c) Plot of E vs. k will be parabolic in the interval $(-\pi/a) < k < (\pi/a)$

(d) Slope of E vs. k is non-zero for all k in the interval $(-\pi/a) < k < (\pi/a)$

Ans : Option 'c'

Concept of Phonons

The concept of photons is well known. A photon is basically a quantum of light (or all forms of EM radiations). The energy of a single photon is given by $\hbar\omega$ where ω is the photon frequency. If we have an EM radiation with a particular mode (having photons of single frequency) then its energy can be expressed as $n\times\hbar\omega$ where n is the number of photons. Similar is the concept of phonons. Basically a phonon is a quantum of vibrational motion. Whenever a lattice (all atoms in a lattice) vibrates with single frequency, then the energy of this particular mode is given by –

$$E_{LatticeVibration} = n\times\hbar\omega \qquad \ldots(40)$$

Here n is the number of Phonons and ω is a single frequency at which all the atoms in lattice vibrate. This is known as the quantization of lattice vibrations. A particular mode of lattice vibrations represents an average number of phonons given by –

$$n_{AVERAGE} = \left(e^{\hbar\omega/K_BT} - 1\right)^{-1} \qquad \ldots(41)$$

A phonon is sometimes referred to as a quasiparticle also. Phonons also follow the Bose-Einstein distribution function. There could be different types of phonons as shown in Fig.13 below.

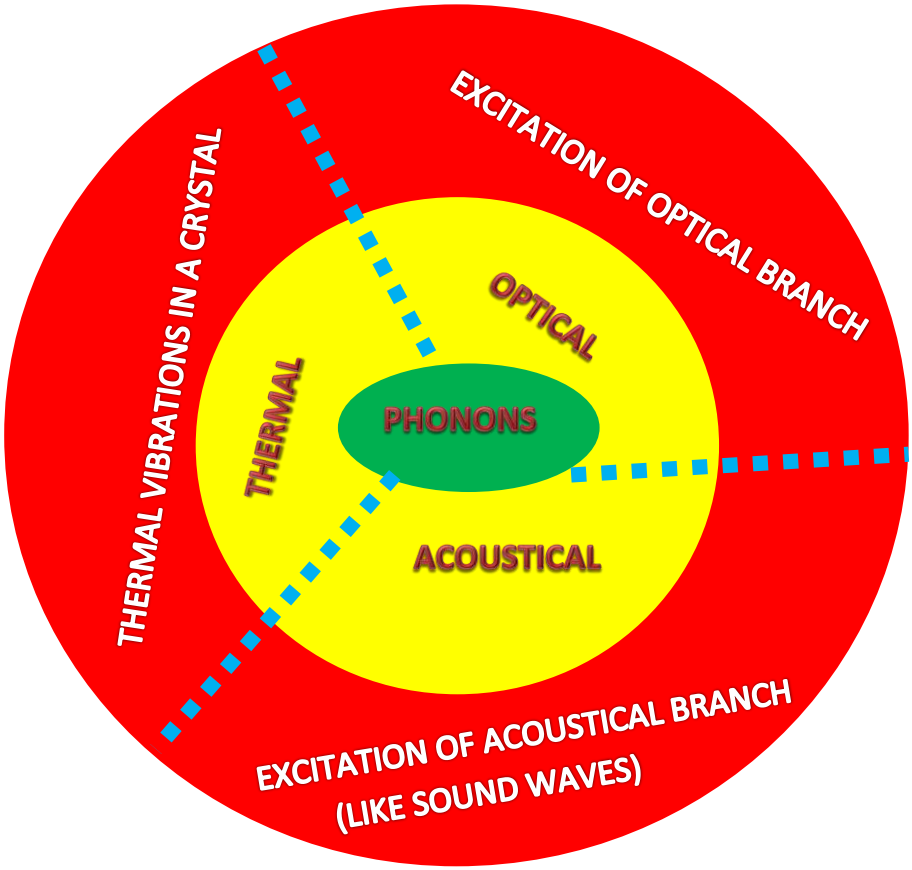


Fig.13 : Three types of phonons optical, acoustical and thermal.

The change of energy in the lattice vibrations is also quantized, for example whenever the energy of a lattice vibration is increased or decreased it has to be –

$$\Delta E_{LatticeVibration} = \pm\hbar\omega \ , \ \ \Delta n = \pm 1 \qquad \ldots(42)$$

Because we assume that up to the first order approximation only, the energy of lattice vibration changes by the gain or loss of one phonon only. Similar to the photons, phonons also have momentum related to them known as the Phonon Momentum. For the phonons also we can use the De-Broglie relation as –

$$p = \hbar K \qquad \ldots(43)$$

where, K is the wavevector for a particular phonon.

♦ Evidence for phonons????

Ans : *Inelastic scattering of neutrons and X-rays by crystals*

&

Zero lattice heat capacity at absolute zero temperature

CONCLUSION

The theory of lattice vibrations discussed above mainly aims at indicating that, the atoms in a crystal cannot vibrate with all frequencies. There are some definite frequencies with which a lattice vibration can exists and these frequencies exist in form of allowed band of energies. There are some frequencies also which cannot propagate in a crystal and these frequencies occur in the forbidden frequency band gap. Also the lattice vibrations are quantized, which are explained in terms of phonons. As a summary we can go through the following points –

- For a one dimensional monoatomic chain of atoms, the dispersion relation is linear in the long wavelength limit whereas in the higher frequency region the medium behaves as dispersive one.

- A linear monoatomic lattice is equivalent to a low pass filter as it allows only the frequencies less than equal to $\sqrt{4\eta / m}$, to pass through it.

- Any lattice wave propagating through a linear monoatomic lattice can be reduced to a corresponding wave which represents a wavevector lying in the first brillouin zone from $-\pi / a$ to $+\pi / a$.

- In the finite length of linear monoatomic lattice the number of normal modes of vibration is N-1 when the atoms at the end are fixed and N modes when the chain is bent in form of circular ring.

- For a diatomic linear chain of atoms the frequency range if split up into two frequency branches known as optical and acoustical branches where the frequency of acoustical branch is less than the optical branch.

- The region between the optical and acoustical branches in the spectrum is known as the forbidden frequency gap whose width increases with the increase in the mass of atom (having higher mass).

- The first brillouin zone for diatomic case lies in the region from $-\pi / 2a$ to $+\pi / 2a$.

- There is N number of normal modes for a diatomic case.

- The lattice vibrations are quantized where a quantum of lattice vibration energy is known as phonon.

- A phonon acts like as if, it is having a momentum $\hbar K$ but in reality there is no such thing like a phonon momentum on a lattice in physical sense.

Unit-2

Elementary lattice Dynamics: lattice vibrations & phonons, linear mono. & diatomic chains, Acoustical / optical phonons, Qualitative description of phonon spectrum in solids, Dulong & Petit's law, Einstein & Debye theories of specific heat of solids, T^3 law (10 lec)

A phonon is a quantum of vibrational motion. Whenever a lattice vibrates with single frequency, then the energy of this particular mode is given by —

$$E_{(\text{lattice vibration})} = n \times \hbar\omega$$

n ↓ No of phonons

ω → single freq. at which all atoms in lattice vibrate.

This is called quantization of lattice vibrations. A particular mode of lattice vibrations represents an average no of phonons given by —

$$n_{average} = \left(e^{\hbar\omega/k_B T} - 1\right)^{-1}$$

(1) At any temp crystal is full of phonons.
As temp ↑ ⇒ No of phonons ↑
As temp ↓ ⇒ " " " ↓

(2) Phonons travel with vel' of sound in solid medium.
$\hbar\omega_k = \hbar v_s k$

(3) Vibration Spectrum of phonon waves occupy wide range of freq. from $10^4 - 10^{12}$ cps. Low freq part of spectrum is in the acoustic range & higher freq part in infrared range.

(4) Physically a lattice phonon does not carry any momentum, but it interacts with other particles & fields as if it has a momentum $\hbar\vec{K}$, where $\vec{K}$ represents wave vector of phonon.

from De-broglie relation $\Rightarrow$ $p = \frac{\hbar}{\lambda} = \hbar K$ (2)

Quantity $\hbar\vec{K}$ is called crystal momentum.

(5) $\boxed{k' = k + G}$ (All vectors)

$\Downarrow$ Bragg diff. of x-ray photon by a crystal.

If scatt. of photon is inelastic, with creation of phonon of wavevector $\vec{K}$, then

$$k' + \vec{K} = k + G$$

If phonon is absorbed, $\vec{k}' = k + \vec{K} + G$

(6) Acoustic phonons: They are coherent movements of atoms of lattice out of their equillibrium positions. If displacement is in the direction of propagation, then in some ~~cases~~ areas atoms will be closer and in others farther apart, as in sound wave in air (hence the name acoustic)

If wavelength of acoustic phonons goes to ∞, this means simple displacement of whole crystal & this costs zero deformation energy. They exhibit a linear relation b/w freq & phonon wavevector for long wavelengths. The freq. of acoustic phonons tend to 0 with longer wavelength. Longitudinal & transverse acoustic phonons are often called LA & TA phonons.

⑦ Optical phonons : These are out of phase movements of atoms in lattice, one atom moving left & neighboring to right. This occurs if lattice basis consist of two / more atoms. They are called optical because in ionic crystals, like NaCl, they are excited by infrared radiation.

They have a non-zero freq at B.Z. Center & show no dispersion near that long wavelength limit.