
UNIT 7 LATTICE DYNAMICS

Structure

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7.1 INTRODUCTION

In Unit 6, you studied about the propagation of elastic waves in a solid and found that the corresponding dispersion relation (relation between angular frequency and wave vector) is linear. We assumed that solid is homogeneous and behaves as a continuous medium. This is a valid assumption so long as the wavelength of the elastic waves is much greater than interatomic separation. A more general analysis of wave propagation in a solid must consider it as a collection of discrete atoms arranged along a periodic lattice.

From your school physics, you are familiar with the phenomenon of wave propagation. You may recall that when a mechanical wave travels through a fluid, its (fluid's) constituent molecules begin to vibrate about their respective equilibrium positions. Moreover, since a wave transports energy, propagation of wave essentially means propagation of phase. A similar situation is observed in solids. When mechanical, thermal or electrical energy is supplied to a solid, its constituent atoms are set into vibration about their respective equilibrium sites resulting into wave propagation.

In this unit, you will learn about wave propagation through monatomic and diatomic crystals made of discrete atoms. As such, these are 3-D systems. However, it is instructive to first consider vibrations of particles arranged in a straightline. Can you say why? It involves simpler mathematics and leads to better physical understanding. That is, a 1-D system exhibits all essential features of a 3-D system. In Sec. 7.2, you will learn to obtain and analyse the dispersion relation and characteristics of a linear chain of identical atoms and would thus be able to identify the different modes of vibration. In Sec. 7.3, you will study the vibrations of a chain of two different types of atoms, i.e., 1-D Bravais lattice with a basis. You will discover that the dispersion relation of the diatomic lattice exhibits some unique features, in addition to those exhibited by the dispersion curve of a monoatomic lattice. The vibrations of atoms in a crystal determine its thermal properties, X-ray scattering, neutron scattering etc.

As such, the atomic vibrations in a crystal require quantum mechanical formulation. The quantum of these vibrations is called *phonon*. You will learn about phonons in your post-graduate classes and discover that neutron scattering from a crystal is analysed in terms of the number of phonons exchanged with the lattice. Such studies gives us vital information about crystal structure and lattice dynamics.

Objectives

After studying this unit, you should be able to:

- obtain dispersion relations for monoatomic and diatomic crystal lattices;
- identify acoustic and optical branches;

- discuss the characteristics of acoustic and optical branches of the dispersion curve; and
- solve numerical problems based on these concepts.

7.2 DYNAMICS OF A CHAIN OF IDENTICAL ATOMS: SIMPLE BRAVAIS LATTICE

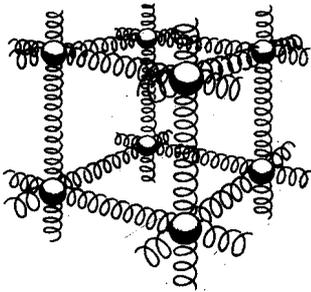


Fig 7.1: A solid modelled as a system of balls connected by springs

Before you start studying this section we would like you to go through the relevant units of the Oscillations and Waves (PHE-02) course.

A solid can be modelled as a 3-D coupled spring-mass system (Fig. 7.1). However, for simplicity, we consider a lattice shown in Fig. 7.2. Note that it consists of a large number of equally spaced, identical particles of mass M held together by elastic springs, each of force constant K , in a linear array. These atoms can vibrate along the chain or at right angle to the chain. That is, the motion can be longitudinal or transverse. We first consider longitudinal motion. Let us choose n^{th} atom as the origin.

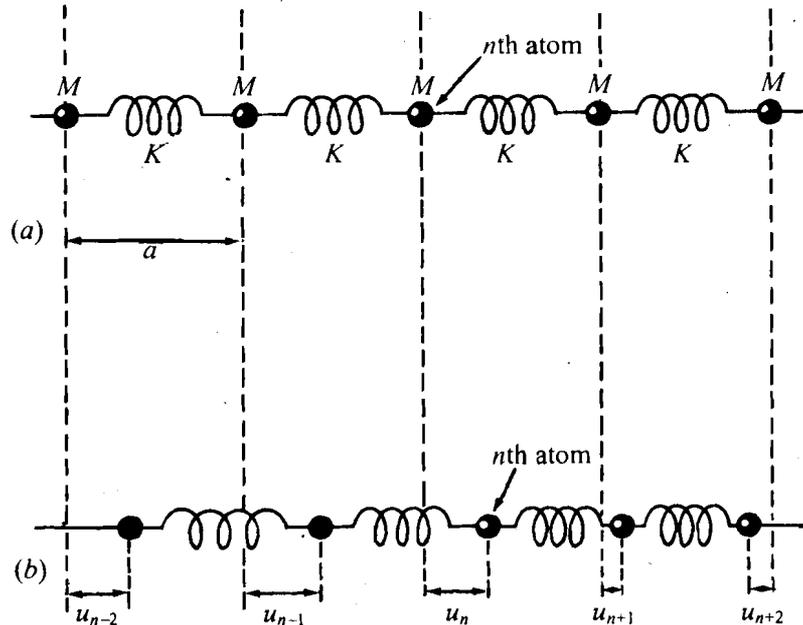


Fig. 7.2: A chain of masses M connected by springs a) at equilibrium positions $x_n^0 = na$; and b) at displaced positions $x_n = na + u_n$

The mathematical analogy of spring mass system suggests that forces between atoms obey Hooke's law and the energy of interaction between any two atoms will be a function of the interatomic distance. You may recall that this type of interaction is known as the central force interaction.

We assume that the last atom is joined to the first so as to form a closed loop. This enables us to visualize the linear chain as endless and thereby all atoms have identical environment. We denote the equilibrium spacing between the atoms by a .

From Unit 5 of Oscillations and Waves (PHE-02) course, you may recall that if the n^{th} atom is displaced from its equilibrium position, its equation of motion can be written as

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

or

$$M \frac{d^2 u_n}{dt^2} = K(u_{n+1} - 2u_n + u_{n-1}), \quad (7.1)$$

where u_n denotes the displacement of the n^{th} atom from its equilibrium position. It is small compared to the interatomic distance. Note that at any instant of time, the

coordinate of the n^{th} atom will be given by $x_n = na + u_n$. Further note that in writing the equation of motion of the n^{th} atom (Eq. (7.1)), we have assumed that the force on the n^{th} atom is proportional to its relative displacements from the nearest neighbours only. This is known as *harmonic approximation* and holds well so long as $u_n \ll a$.

To solve Eq. (7.1) we take a solution in the form of progressive wave:

$$u_n = A \exp[-i(\omega t - kx_n^0)] \quad (7.2)$$

where A is amplitude of the wave, $x_n^0 (= na)$ denotes the equilibrium coordinate of the n^{th} atom, k is wave number and ω is angular frequency. You must note that solution given by Eq. (7.2) is possible only because of the translational symmetry of the lattice and is valid for longitudinal wave propagation along the linear array of atoms.

Substituting Eq. (7.2) in Eq. (7.1), we get:

$$-\omega^2 M \exp[-i(\omega t - kna)] = K \left\{ \exp[-i(\omega t - k(n+1)a)] - 2 \exp[-i(\omega t - kna)] + \exp[-i(\omega t - k(n-1)a)] \right\}$$

$$\frac{du_n}{dt} = -Ai\omega \exp[-i(\omega t - kx_n^0)]$$

and

$$\frac{d^2 u_n}{dt^2} = -A\omega^2 \exp[-i(\omega t - kx_n^0)]$$

On dividing throughout by $\exp[-i(\omega t - kna)]$, this expression simplifies to

$$\begin{aligned} -\omega^2 M &= K(e^{ika} - 2 + e^{-ika}) \\ &= 2K(\cos ka - 1) \end{aligned}$$

or

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

$$\frac{e^{ika} + e^{-ika}}{2} = \cos ka$$

so that the expression relating angular frequency and wave vector k of longitudinal wave is given by

$$\omega = \omega_{0L} \left| \sin \left(\frac{ka}{2} \right) \right| \quad (7.3)$$

where $\omega_{0L} = 2\sqrt{\frac{K}{M}}$. Eq. (7.3) gives the dispersion relation for a linear array of same type of atoms. Note that we have taken modulus of the sine function to ensure that angular frequency is always positive. Let us pause for a while and see what can be inferred from Eq. (7.3).

- Since the maximum value of $\sin\left(\frac{ka}{2}\right)$ is 1, we have $\omega = \omega_{0L} = 2\sqrt{\frac{K}{M}}$. How does it compare with the value of ω for a spring-mass system?
- ω is independent of n , which means that all atoms would lead to the same algebraic relation between ω and k . Moreover, this relation is unique, i.e. corresponding to each k , there is a definite ω . It means that the oscillations are uncoupled and correspond to normal modes. (Recall from PHE-02, Block-1.)
- For $\omega = 0$, we have $k = 0$ and $\omega = \omega_{\text{max}}$ for $k = \pm \frac{\pi}{a}$. This shows that the frequencies of all the normal modes lie in the range $-\pi/a \leq k \leq \pi/a$. This range of k values defines the boundaries of the first *Brillouin zone* for a 1-D crystal lattice.

You may now like to answer an SAQ.

Spend 3 min.

SAQ 1

Determine the number of normal modes i.e. possible number of k -values in the range $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$ for a linear chain of N identical atoms.

[Hint: Start from the fact that all atoms are identical, i.e. $u_n = u_{n+N}$.]

For transverse motion, you can write the equation of motion in the nearest neighbourhood interaction and solve it to obtain the dispersion relation. We will only quote the result, without going into details:

$$\omega = \omega_{0T} \left| \sin \frac{ka}{2} \right|, \quad (7.4a)$$

where

$$\omega_{0T} = \left(\frac{4K}{aM} \right)^{1/2} \quad (7.4b)$$

Note that the dispersion relation for transverse mode is similar to that for the longitudinal mode. However, $\omega_{0T} < \omega_{0L}$.

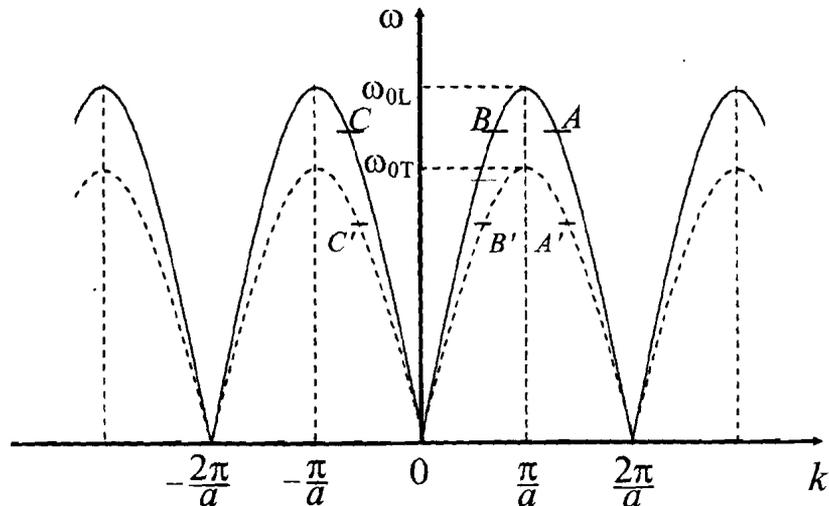


Fig.7.3: Normal mode frequencies for a linear chain of atoms

Now refer to Fig. 7.3, which depicts the dispersion relations for transverse as well as longitudinal modes. You will note that

- the transverse branch lies below the longitudinal branch; and
- wave numbers corresponding to points A, B, C on longitudinal branch correspond to the same frequency. The same holds for transverse waves.

Before proceeding further, we would like you to solve an SAQ.

Spend 5 min.

SAQ 2

The group velocity and phase velocity are defined as $v_g = \frac{d\omega}{dk}$ and $v_p = \frac{\omega}{k}$. Starting from Eq. (7.3), show that for $ka \ll 1$,

$$\frac{\omega}{k} = \frac{d\omega}{dk}$$

What is the significance of the above relation?

In general, for a linear chain of identical particles, there will be one longitudinal and two transverse branches corresponding to two independent mutually perpendicular directions of vibrations of the constituent particles.

You may also note that the dispersion curve is periodic in k -space and it exhibits reflection symmetry around the origin. Can you guess what might be the cause of these features? If you are thinking of translational symmetry of the 1-D lattice, you are right. To investigate the role of translational symmetry, if we replace k by

$$k_m = k + \frac{2\pi m}{a}, \tag{7.5}$$

with $m = \pm 1, \pm 2, \dots$, in Eqs. (7.3) and (7.4), we find that these equations remain the same. That is, the state of vibration of a linear array of identical atoms corresponding to a wave vector k will be identical to the state corresponding to the wave vectors k_m specified by Eq. (7.5). In other words, waves specified by k and k_m are generated by the same kind of atomic motion. It implies that to have one-to-one correspondence between the states of vibration of a lattice and the wave vector k , the latter must be confined to a range of values of width $2\pi/a$ and this range is invariably taken as

$$-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}. \tag{7.6}$$

Note that positive values of k correspond to waves propagating in the +ve x -direction. Similarly, negative values of k specify waves moving in the negative x -direction. As pointed out earlier, the range of the k specified by Eq. (7.6) is known as the *first Brillouin zone*. The *second Brillouin zone* is defined by

$$-\frac{2\pi}{a} < k \leq -\frac{\pi}{a}, \text{ and} \\ \pi/a < k \leq \frac{2\pi}{a}. \tag{7.7}$$

Higher order Brillouin zones can be similarly specified. However, note that the total width of any one zone is the same (Fig. 7.4).

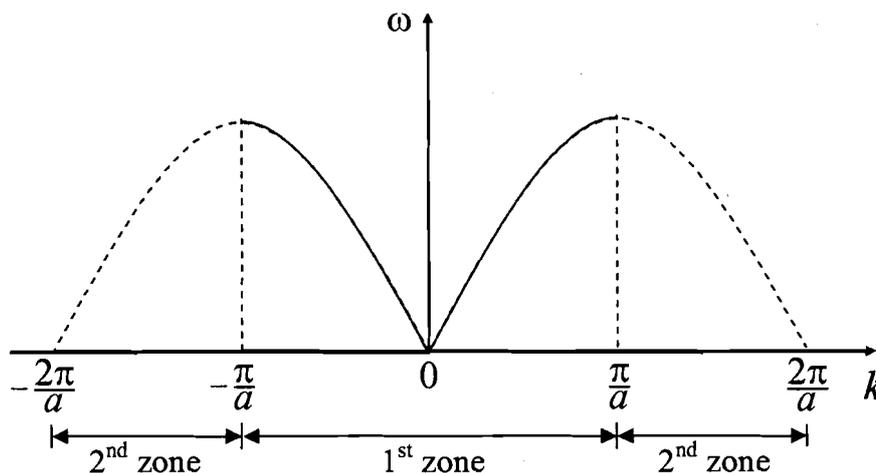


Fig.7.4: First two Brillouin zones in the dispersion curve due to monatomic lattice

Yet another interesting feature of the dispersion relation (Eq. (7.3)) is that no wave propagating in a linear chain can have frequency greater than ω_{0L} for the longitudinal mode. To convince yourself about this statement, solve the following SAQ.

SAQ 3

A longitudinal wave is propagating along a linear monatomic chain. Calculate the group velocity and phase velocity of this wave if its frequency is $\omega = \omega_{0L} = 2\sqrt{\frac{K}{M}}$.

Spend
7 min.

Comment on the results.

Solving SAQ 3, you must have noted that in a monatomic chain, waves only with frequencies less than ω_{0L} can propagate. In other words, waves having frequencies greater than ω_{0L} (or wavelength shorter than $2a$) cannot propagate down a monatomic linear chain. It means that linear chain behaves as a low pass filter because it can only transmit waves whose frequencies are in the range $0 < \omega < \omega_{0L}$.

So far we have discussed vibrational modes of a linear lattice of equally spaced identical atoms. This signifies a simple Bravais lattice. However, as you know, a large number of solids are defined by a Bravais lattice with a basis. And the results obtained in Sec. 7.2 do not hold for this slightly complex case. You will now learn how a chain with basis can be described.

7.3 VIBRATIONS OF A CHAIN OF TWO DIFFERENT TYPES OF ATOMS: BRAVAIS LATTICE WITH A BASIS

In the 1-D case, there are two possible ways to create a chain with a basis:

- The atoms are placed at equal distances but alternate atoms have different masses;
- All atoms are of equal mass but the distances between them are not uniform.

A simple Bravais lattice can be generated by the translation of a unit cell – containing one particle. A Bravais lattice with a basis is generated by a simple translation when two different atoms are translated together.

Here we will consider the first case as it provides a model for ionic crystals. Let atomic masses with a basis be denoted by M and m ($m < M$) as shown in Fig. 7.5. As before, we suppose that the distance between the nearest neighbours is a . We can write down the equation of motion for longitudinal vibrations for the masses M and m as

$$M \frac{d^2 u_n}{dt^2} = K(u_{n+1} - 2u_n + u_{n-1}) \quad (7.8)$$

and

$$m \frac{d^2 u_{n-1}}{dt^2} = K(u_n - 2u_{n-1} + u_{n-2}) \quad (7.9)$$

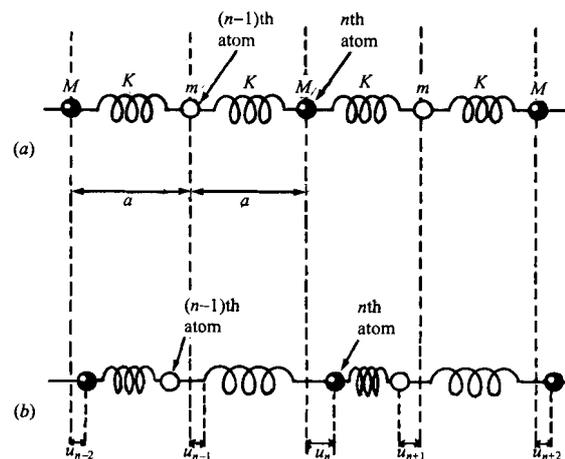


Fig.7.5: A chain of unequal masses connected by springs a) at equilibrium position $x_n^0 = na$; and b) at displaced positions $x_n = na + u_n$

The general solution of Eqs. (7.8) and (7.9) can be assumed to be of the form

$$u_n = A\alpha e^{-i(\omega t - kx_n^0)},$$

where α is a complex number giving relative amplitude and phase. For a diatomic chain of atoms consisting of two different types of atoms, this solution can be written as

where α is a complex number giving relative amplitude and phase. For a diatomic chain of atoms consisting of two different types of atoms, this solution can be written as

$$u_n = Ae^{-i(\omega t - kx_n^0)} \quad \text{for mass } M$$

and

$$u_{n\pm 1} = A\alpha e^{-i(\omega t - kx_{n\pm 1}^0)} \quad \text{for mass } m.$$

Note that the first expression represents a wave of amplitude A propagating only through particles of mass M . The second equation represents a wave (of same frequency and wavelength) of different amplitude propagating through particles of mass m .

Substituting these solutions in Eqs. (7.8) and (7.9) respectively, we get

$$-\omega^2 Me^{-i(\omega t - kna)} = K \left\{ \alpha e^{-i[\omega t - k(n+1)a]} - 2e^{-i(\omega t - kna)} + \alpha e^{-i[\omega t - k(n-1)a]} \right\}$$

and

$$-\alpha\omega^2 me^{-i[\omega t - k(n-1)a]} = K \left\{ e^{-i(\omega t - kna)} - 2\alpha e^{-i[\omega t - k(n-1)a]} + e^{-i[\omega t - k(n-2)a]} \right\}.$$

On simplification, we get

$$-\omega^2 M = 2K(\alpha \cos ka - 1) \quad (7.10a)$$

and

$$-\alpha\omega^2 m = 2K(\cos ka - \alpha). \quad (7.10b)$$

These can be rewritten as

$$2K - \omega^2 M = 2K\alpha \cos ka \quad (7.11a)$$

and

$$\alpha(2K - \omega^2 m) = 2K \cos ka. \quad (7.11b)$$

On rearranging terms and using Eq. (7.11a) in Eq. (7.11b), we get

$$\frac{2K \cos ka}{2K - \omega^2 m} = \frac{2K - \omega^2 M}{2K \cos ka}. \quad (7.12)$$

On cross-multiplication, we obtain a quadratic equation in ω^2 :

$$mM\omega^4 - 2K(M+m)\omega^2 + 4K^2(1 - \cos^2 ka) = 0$$

or

$$mM\omega^4 - 2K(M+m)\omega^2 + 4K^2 \sin^2 ka = 0.$$

The roots of this equation are given by

You should note that in a diatomic chain, solutions of equations of motion of two masses differ by a factor α , which accounts for the relative amplitude and phases of the vibration of two types of atoms. In other words, this takes care of the fact that two different atoms have different amplitudes of vibration.

The roots of a quadratic equation of the form

$$ax^2 + bx + c = 0$$

are given by

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

$$\omega_{\pm}^2 = \frac{K(M+m) \pm \left[K^2(M+m)^2 - 4K^2 mM \sin^2 ka \right]^{1/2}}{mM}$$

$$= \frac{K(M+m)}{mM} \left\{ 1 \pm \left[1 - \frac{4mM}{(m+M)^2} \sin^2 ka \right]^{1/2} \right\}. \quad (7.13)$$

Since we consider only positive value of ω , we have two values of ω for a given value of k . Therefore, Eq. (7.13) gives two dispersion relations for a 1-D Bravais lattice with a basis. You would recall that for a simple 1-D lattice, we obtained only one value of ω for a given value of the wave vector. So, if we plot angular frequency as a function of wave vector, we will obtain two branches (Fig. 7.6).

If we replace k by

$$k_j = k + \frac{j\pi}{a},$$

where $j = \pm 1, \pm 2, \dots$, the displacements and dispersion relations remain unchanged. That is, the state of vibration of the lattice corresponding to a wave vector k is

identical to the state corresponding to any of the wave vectors $k + \frac{j\pi}{a}$. Therefore, for

one to one correspondence between the state of vibration of the lattice and the wave vector k , the latter must be restricted to a range of values π/a . The range of the first Brillouin zone in this case is

$$-\frac{\pi}{2a} < k \leq \frac{\pi}{2a}$$

Note that width of Brillouin zone for a lattice with a basis is half of that for a simple lattice.

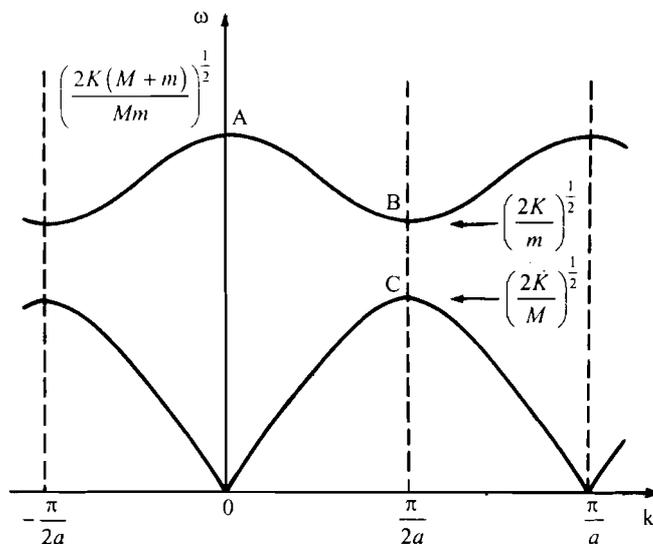


Fig.7.6: Normal mode frequencies of a chain of two types of atom. At A the two types of atoms are oscillating in opposite phases with their centre of mass at rest; at B the lighter mass m is oscillating and M is at rest; and at C, M is oscillating and m is at rest

Further for $k = 0$,

$$\omega_+^2 = \frac{2K(M+m)}{mM} \quad (7.14)$$

and

$$\omega_-^2 = 0. \quad (7.15)$$

The branch which correspond to a non-zero value of ω for $k = 0$ is called *optical branch*. Can you guess the genesis of this nomenclature? It is because the frequencies in this branch are of the order of infrared frequencies. The branch corresponding to $\omega = 0$ for $k = 0$ is called *acoustical branch* because the corresponding frequencies are of the order of acoustical or supersonic vibrations.

For small values of k , that is, for $k \rightarrow 0$, we have $\sin ka \approx ka$ and frequencies corresponding to optical and acoustical branches are obtained by simplifying Eq. (7.13):

$$\omega_o = \sqrt{\frac{2K(M+m)}{mM}} \left(1 - \frac{1}{2} \frac{mMk^2 a^2}{(m+M)^2} \right) \quad (7.16)$$

and

$$\omega_a = \sqrt{\frac{2K}{M+m}} ka. \quad (7.17)$$

Note that for the acoustical branch, the angular frequency is proportional to the wave vector, as in case of the simple lattice. However, for optical branch, angular frequency is maximum for $k = 0$ and decreases parabolically as $|k|$ increases.

Note that in-between the *optical branch* and the *acoustic branch*, there is a band of frequencies which cannot propagate in a diatomic chain. However, you may also note that for $m = M$, this forbidden band disappears and we get ω versus k curve similar to monoatomic chain (Fig. 7.3).

The solution (7.16) corresponds to point *A* in Fig. 7.6; M and m oscillate out of phase with respect to each other. Their centre of mass is at rest and the frequency is given by the spring constant $2K$ and the reduced mass, $\mu = Mm/(M+m)$.

The solution (7.17) represent long wavelength sound waves in the neighbourhood of the point *O* in Fig. 7.6 and the velocity of sound is

$$v_s = \frac{\omega}{k} = \sqrt{\frac{2k}{M+m}} a \quad (7.18)$$

In this case, both types of atoms oscillate with the same amplitude and phase and the result is essentially the same as for a chain of single type of atom.

Let us now sum up what you have learnt in this unit.

7.4 SUMMARY

- The arrangement of atoms in a solid may be visualised as a microscopic spring-mass system.
- A monoatomic linear chain of N atoms can be considered equivalent to a system of N coupled harmonic oscillators and the resulting ω vs k characteristics shows that ω is independent of the position of the atom and corresponding to each k there is a definite ω .
- The range $-\pi/a \leq k \leq \pi/a$ includes all possible values of the frequency ω and defines first Brillouin zone.

For small values of k , we use binomial expansion for the expression under radical sign in Eq. (7.13) and retain only linear term in $k^2 a^2$. This gives

$$\omega^2 \cong \frac{K(M+m)}{mM} \left\{ 1 \pm \left[1 - \frac{2mMk^2 a^2}{(m+M)^2} \right] \right\}$$

This gives, on simplification,

$$\omega^2 \cong \frac{2K(M+m)}{mM} \left[1 - \frac{mMk^2 a^2}{(m+M)^2} \right]$$

Since $ka \ll 1$, we can neglect the second term in the parenthesis to obtain

$$\omega_o^2 = \frac{2K(M+m)}{mM}$$

The root corresponding to negative sign gives

$$\omega_a^2 = \frac{2Kk^2 a^2}{M+m}$$

For two types of atom, corresponding to Eq. (7.16), what matters is the mean density.

- For a diatomic linear chain, the ω vs k characteristic has two distinct branches; optical and acoustic branches and the width of the Brillouin zone is half of that for a simple Bravais lattice.

7.5 TERMINAL QUESTIONS

· Spend 15 min.

1. The maximum value of the frequency of longitudinal wave propagating in a linear monatomic chain is 10^{14} Hz. The mass of an atom in the chain is 30×10^{-27} kg and interatomic separation is 1.2 \AA . Calculate Young's modulus of the chain.
2. The unit cell size of NaCl is 5.6 \AA , and Young's modulus, Y in [100] direction is $5 \times 10^{10} \text{ Nm}^{-2}$. Estimate the wavelength at which electromagnetic radiation is strongly reflected by a NaCl crystal. (Atomic weight: Na = 23, Cl = 37).

7.6 SOLUTIONS AND ANSWERS

Self-Assessment Questions (SAQs)

1. We have

$$u_n = A \exp[-i(\omega t - kna)] \quad (i)$$

Since all atoms are identical, we can write $u_n = u_{N+n}$ so that

$$A \exp[-i(\omega t - kna)] = A \exp[-i\{ka - \omega t(n + N)\}]$$

This expression simplifies to

$$e^{ikNa} = 1 \quad (ii)$$

so that we have

$$kNa = 2\pi p$$

or

$$N = \frac{2\pi p}{ka}, \quad (iii)$$

where p is an integer.

We know that the spread of k is $\frac{2\pi}{a}$ from $-\pi/a \leq k \leq \pi/a$. Using this result in (iii), we get $p = N$. It means that there are N possible values of k .

2. From Eq. (7.3), we get

$$\omega = \omega_{0L} \sin \frac{ka}{2}$$

For $ka \ll 1$, we have $\sin \frac{ka}{2} \approx \frac{ka}{2}$. Therefore, we have

$$\omega = \omega_{0L} \cdot \frac{ka}{2}$$

or

$$\frac{\omega}{k} = \omega_{0L} \frac{a}{2}$$

Since ω_{0L} and a are constant, we have

$$\frac{d\omega}{dk} = \omega_{0L} \frac{a}{2} = \frac{\omega}{k}$$

or,

$$v_g = v_p$$

It means that for small k , a linear chain of atoms acts as a dispersionless medium. Moreover, in the long wavelength sound limit, group velocity ($d\omega/dk$) is equal to the phase velocity. This is expected because long wavelengths would not be sensitive to discreteness of atomic arrangement.

3. From Eq. (7.3), we have

$$\sin\left(\frac{ka}{2}\right) = 1$$

for longitudinal wave propagating at frequency ω_{0L} . Thus we can write, $\frac{ka}{2} = \frac{\pi}{2}$.

Now, the group velocity,

$$v_g = \frac{d\omega}{dk} = \omega_{0L} \frac{a}{2} \cos \frac{ka}{2} \quad (\text{from Eq. (7.3)})$$

$$= 0 \quad (\text{since } \frac{ka}{2} = \frac{\pi}{2})$$

And phase velocity,

$$v_p = \frac{\omega}{k} = \frac{\omega_{0L}}{k} \sin\left(\frac{ka}{2}\right)$$

$$= \frac{\omega_{0L}}{k} = \text{finite}$$

Thus, the group velocity and phase velocity of the longitudinal wave is not the same when the value of its frequency is maximum. Further, the zero value of the group velocity implies that, at this frequency, no energy is transported by the wave. That is, the condition gives rise to a standing wave.

Terminal Questions (TQs)

1. For longitudinal wave propagating in a linear monatomic chain, the maximum frequency is given as

$$\omega_{0L} = 2\sqrt{\frac{K}{M}} \quad (i)$$

where K is the force constant and M is the mass of the atom. Further, the Young's modulus for a linear chain is given as

$$Y = \frac{K\delta a/a^2}{\delta a/a}; \quad (\text{where } a \text{ is the interatomic separation})$$

or

$$K = Ya \quad (\text{ii})$$

Substituting (ii) in (i), we get

$$\begin{aligned} (\omega_{0L})^2 &= 4 \frac{K}{M} \\ &= \frac{4Ya}{M} \end{aligned}$$

or

$$Y = \frac{M(\omega_{0L})^2}{4a} \quad (\text{iii})$$

Given that $M = 30 \times 10^{-27} \text{ kg}$; $\omega_{0L} = 10^{14} \text{ s}^{-1}$; $a = 1.2 \times 10^{-10} \text{ m}$.

Substituting these values in (iii), we get

$$\begin{aligned} Y &= \frac{(30 \times 10^{-27} \text{ kg}) \times (10^{14} \text{ s}^{-1})^2}{4 \times 1.2 \times 10^{-10} \text{ m}} \\ &= 6.25 \times 10^{10} \text{ Nm}^{-2}. \end{aligned}$$

2. The extension of NaCl along [100] may be considered as a set of linear chains in parallel where lateral forces have been ignored. With this assumption, Young's modulus, Y is related to the atomic spacing d as

$$\begin{aligned} Y &= \frac{K\delta d/d^2}{\delta d/d} \quad (\because K\delta d/d^2 \text{ is force per unit area and } \delta d/d \text{ is the linear strain}) \\ \therefore Y &= \frac{K}{d} \end{aligned}$$

The situation corresponds to the optical mode ($k = 0$) for which

$$\begin{aligned} \omega &= \frac{2\pi c}{\lambda} = \left[\frac{2K(M+m)}{Mm} \right]^{1/2} \\ \therefore \lambda &= 2\pi c \left[\frac{Mm}{2Yd(M+m)} \right]^{1/2} \quad (\text{i}) \end{aligned}$$

Given that $M = 37 \times 1.66 \times 10^{-27} \text{ kg}$, $m = 23 \times 1.66 \times 10^{-27} \text{ kg}$, $c = 3 \times 10^8 \text{ ms}^{-1}$, and $d = 2.8 \times 10^{-10} \text{ m}$.

On substituting these values in (i) above, we get

$$\begin{aligned} \therefore \lambda &= 6\pi \times 10^8 \left[\frac{(37 \times 1.66 \times 10^{-27} \text{ kg}) \times (23 \times 1.66 \times 10^{-27} \text{ kg})}{(2 \times 5 \times 10^{10} \text{ Nm}^{-2}) \times (2.8 \times 10^{-10} \text{ m}) \times \{(23 + 37) \times 1.66 \times 10^{-27} \text{ kg}\}} \right]^{1/2} \\ &= 55 \times 10^{-6} \text{ m} \end{aligned}$$