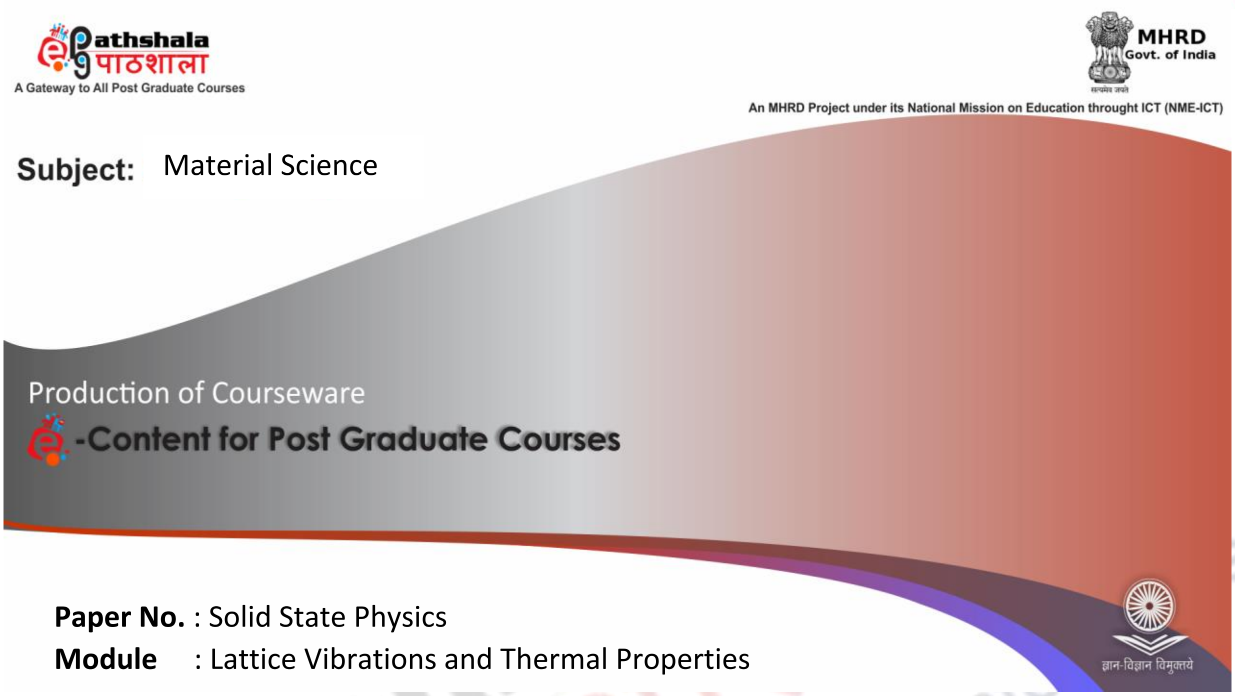


A Gateway to All Post Graduate Courses

An MHRD Project under its National Mission on Education throught ICT (NME-ICT)

Subject: Material Science

Production of Courseware

-Content for Post Graduate Courses

Paper No. : Solid State Physics

Module : Lattice Vibrations and Thermal Properties

Development Team

Principal Investigator	**Prof. Vinay Gupta, Department of Physics and Astrophysics, University of Delhi.**
Paper Coordinator	Prof. Mahavir Singh, Professor , Department of Physics, Himachal Pradesh University, Shimla
Content Writer	Prof. Mahavir Singh, Professor , Department of Physics, Himachal Pradesh University, Shimla
Content Reviewer	Prof. P. N. Kotru, Jammu University , India

Description of Module	
Subject Name	Material science
Paper Name	Solid State Physics
Module Name/Title	Lattice Vibrations and Thermal Properties
Module Id	M10

Contents of this Unit

1. Lattice Vibrations
    - 1.1Vibrations in One Dimensional Mono-atomic lattice
    - 1.2 Vibrations in One Dimensional Di-atomic lattice
    - 1.3 Dispersion in 3 dimensional crystal
2. Summary

Learning Outcomes

The objective of the module is to

- Visualise the lattice dynamics with the help of simple lattice model
- Understand the basic phenomenon of lattice vibrations and extending the study to mono atomic and diatomic lattice chains.
- Mathematically analyse the waves for displacements and frequency response.
- Relate the idea of dispersive and non dispersive media and consequence as acoustic and optical branch.

1. Lattice vibrations :-

To understand crystal lattice dynamics, it is assumed that a crystal consists of a regular arrangement of atoms (or molecules) which are fixed at equilibrium positions at absolute zero. But when there is a rise in temperature these particles execute simple harmonic motion and vibrate at mean positions. The atoms are connected with each other by elastic springs such that each atom exerts a force on its neighboring atoms and the vibrations so produced in the whole crystal are termed as lattice vibrations.

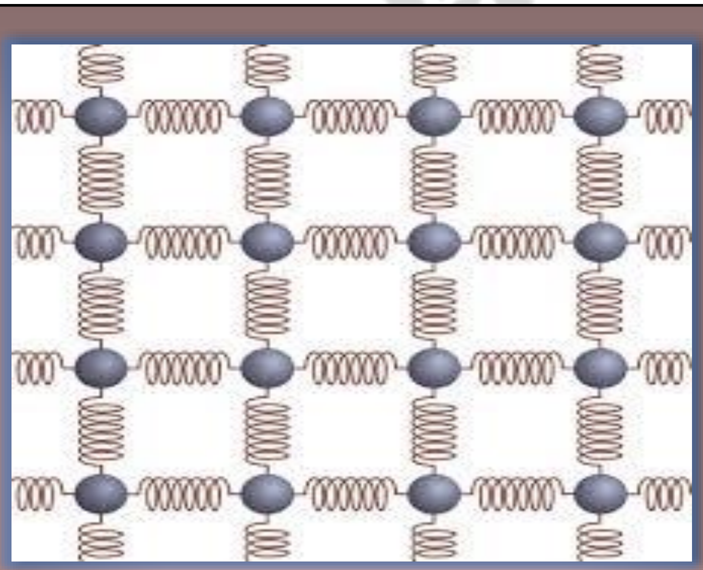


Fig (1) Simple model of a lattice depicting atoms attached to neighboring atoms through mass less springs.

The energy of each oscillator is quantized and is given as

$$E_n = \left(n + \frac{1}{2}\right) \hbar\nu \qquad \text{\_\_\_\_\_\_\_\_\_\_\_\_\_\_(1)}$$

With $E_o = \frac{1}{2}\hbar\nu$,called zero point energy .

The energy change corresponding to transition from state n_1 to n_2 is

$$\Delta E = (n_{2-}n_1)\,\hbar\nu$$

It is accompanied by either emission or absorption of *quantized thermal energy* called *phonon*.

So the lattice vibrations are thermally excited phonons that are the smallest energy of vibration, which require a medium to propagate and exhibit elastic wave behavior. Phonons behave like a mass less particle with energy hν , it does not carry any physical momentum, but it appears to interact as if carrying a momentum $\hbar\boldsymbol{k}$ more precisely called the crystal momentum, where $\vec{k}$ is the wave vector of phonon.

1.1 Lattice vibrations in one – dimensional mono atomic crystal:

To understand the dynamics of lattice behavior, a simple model is proposed to make the relevant studies. It is assumed that

1) Lattice is a periodic arrangement of particles (atoms, ions or molecules) in three dimensions connected to each other through mass less springs executing simple harmonic motion.
2) Particles are identical spheres of same mass m and there is no interaction between these particles except for nearest neighbours.
3) The system obeys Hooke's law essentially and for the sake of simplicity, the system is worked within harmonic approximation.

It is known fact that atoms in solids vibrate because of their thermal energies. Let us consider a one dimensional chain of atoms forming a ring so that all atoms have similar environment. With the vibration of one atom, the disturbance travels through the chain and say the displacement of *nth* atom from equilibrium position be X_n. and X_{n-1} & X_{n+1} be the displacements of *(n-1)th* atom and *(n+1)th* atom respectively from their mean positions.

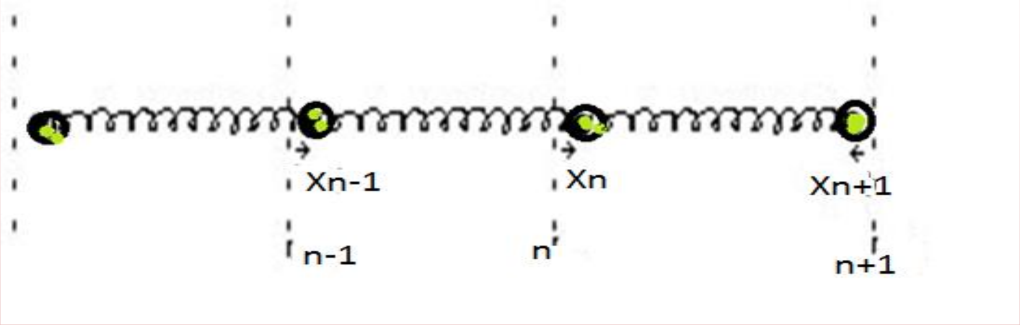


Fig (2) One dimensional linear chain of identical atoms at equilibrium.

Let F_n be the force on *nth* atom after displacement due to its adjacent atoms and S be the spring constant.

$$F_n = S[(X_{n+1}-X_n)-(X_n-X_{n-1})] \qquad \_\_\_\_\_\_\_(2)$$

$$M\frac{d^2X_n}{dt^2} = S\,[(X_{n+1}-2X_n-X_{n-1})] \qquad \_\_\_\_\_\_\_(3)$$

Let the solution of this equation be of the form

$$X_n = A \exp i\,(nka-\omega t)$$

This represents a travelling wave with atoms oscillating at frequency **ω** and amplitude **a** with substitutions from eqn (3) in eqn (2) we get

$$-\,\omega^2M = 2S\,(\cos ka-1)$$ which further reduces to

$$\omega = [4S/M]^{1/2}\left|\sin\frac{ka}{2}\right| \qquad \_\_\_\_\_\_\_\_\_(4)$$

equation (4) is a relation between angular frequency ω and wave vector k and is called ***dispersion relation*** for one dimensional periodic lattice. The variation of ω w.r.t k is studied as under,

1) For small frequencies, i.e, when k→ 0, $\sin\frac{ka}{2} \approx \frac{ka}{2}$

Therefore,

$$\omega = \left[\frac{S}{M}\right]^{1/2} ka$$

expression for phase velocity is

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

and that of group velocity is

$$v_g = \frac{d\omega}{dk} = \left[\frac{S}{M}\right]^{1/2} ka$$

so it is evident that for long wavelengths or small frequencies the lattice behaves as a continuum or non dispersive and no dispersion takes place as shown by dotted line in fig (3).

2) When the frequency is high, the phase velocity is

$$v_p = \frac{2}{k}\left[\frac{S}{M}\right]^{1/2} \sin\frac{ka}{2}$$ and the group velocity is

$$v_g = a\left[\frac{S}{M}\right]^{1/2} \cos\frac{ka}{2}$$

the medium behaves dispersive in nature.

3) The maximum value of ω is when $\frac{ka}{2} = \frac{\pi}{2}$

$\omega_{max} = 2\left[\frac{S}{M}\right]^{1/2}$ which is called the cut-off frequency.

4) When k→ $\frac{\pi}{2}$, $v_g = 0$ and there is no transfer of energy and the wave is a standing wave.
So one dimensional mono-atomic lattice allows frequencies lying between 0 to ω_{max} only.

5) From the above discussion it is concluded that the only waves that can propagate are the ones satisfying the following condition,

$$-1 \leq \sin\frac{ka}{2} \leq 1$$

Or $$-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$$

The region of k values represented here is first brillouin zone.

For $-\frac{2\pi}{a} \leq k \leq \frac{2\pi}{a}$, the region is second brillouin zone and so on

Fig (3) One dimensional monoatomic dispersion curve for ω versus k

1.2 Lattice vibrations in one dimensional diatomic crystal:-

In case of a one dimensional diatomic (two atoms per primitive cell) linear chain, the underlying principle for describing vibrational modes is more or less same as that of monoatomic lattice but the only difference is the different masses of the two atoms, see figure (4).

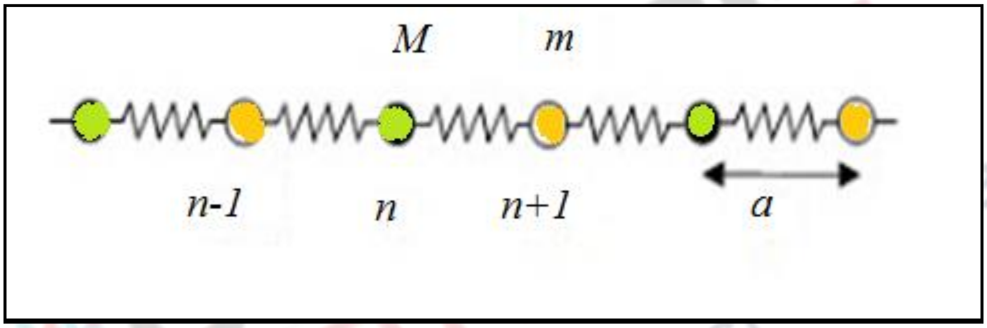


Fig (4) One dimensional diatomic linear crystal chain

Let the two masses be m and M, m be the mass of odd numbered atoms and M the mass of even numbered atoms, such that m$<$M and ‘a’ is the distance between immediate neighbors.

The distance between immediate atoms is same as in linear monoatomic lattice i.e ‘a’ but it is assumed that the distance between similar atoms is ‘2a’, see figure (5).

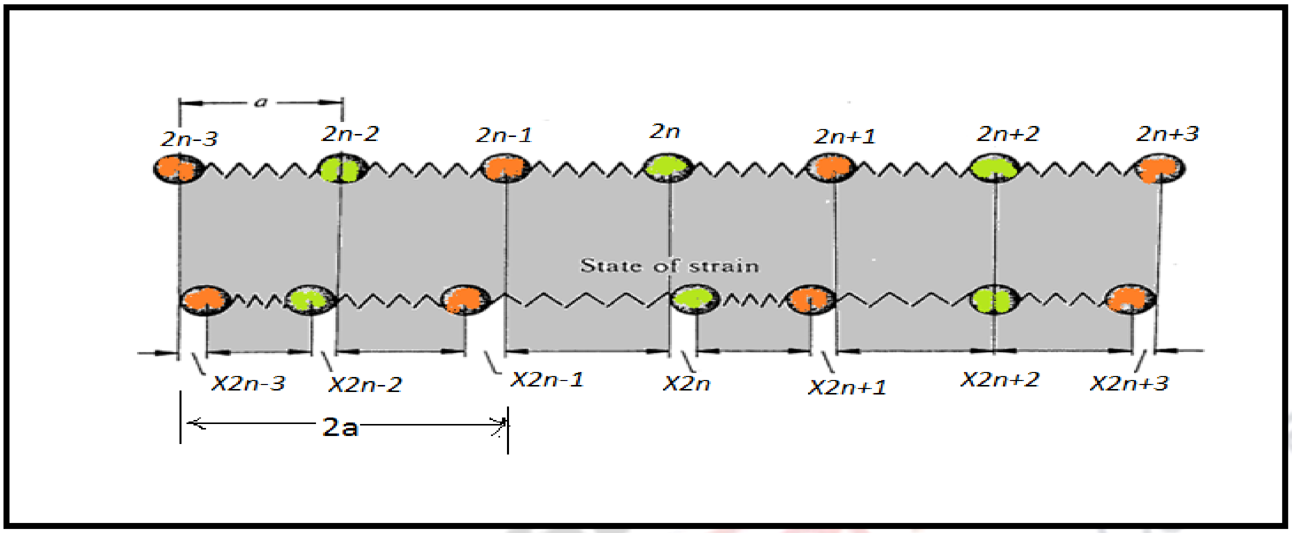


Fig (5) Displacement of atoms in linear diatomic lattice. Distance between immediate neighboring atoms is ‘a’ while that between atoms of same kind is ‘2a'.

Assuming immediate neighbor interaction alone, the equation of motion will be

$M\frac{d^2x_n}{dt^2} = S\,[(X_{2n+1} - 2X_{2n} + X_{2n+1})]$ ___________(5)

$m\frac{d^2x_{2n+1}}{dt^2} = S\,[(X_{2n} - 2X_{2n+1} + X_{2n+2})]$ ____________(6)

the probable solutions of these equations are given as

$X_{2n} = A \exp[-i(\omega t-2nka)]$

And, $X_{2n+1} = B \exp[-i\{\omega t-(2n+1)ka\}]$

A and B are amplitudes of different masses M and m. solving for eqn (5) & (6) using their solutions we get

$(M\omega^2-2S)A + 2BS \cos ka = 0$ __________(7)

and $(m\omega^2-2S)A + 2BS \cos ka = 0$ ____________(8)

Eqn (7) & (8) have non trivial solutions if

$$\begin{vmatrix} M\omega^2 - 2S & 2Scoska \\ 2Scoska & m\omega^2 - 2S \end{vmatrix} = 0$$

Solving for ω^2 we get two possibilities,

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

This is dispersion relation for one dimensional diatomic lattice. It is observed that unlike mono atomic lattice , the frequency here obtained has two components ω_+ and ω_- For ka $\ll$ 1 (k=0),

$$\omega_+ = \left[2S\left(\frac{1}{m}+\frac{1}{M}\right)\right]^{\frac{1}{2}} \quad \text{and} \quad \omega_- = 0 \qquad \text{--------------(9)}$$

for k = $\pm\frac{\pi}{2a}$

$$\omega_+ = \left[\frac{2S}{m}\right]^{\frac{1}{2}} \quad \text{and} \quad \omega_- = \left[\frac{2S}{M}\right]^{\frac{1}{2}} \qquad \text{\_\_\_\_\_\_\_\_\_\_\_\_\_(10)}$$

The solutions obtained from above equations are plotted in fig (6)

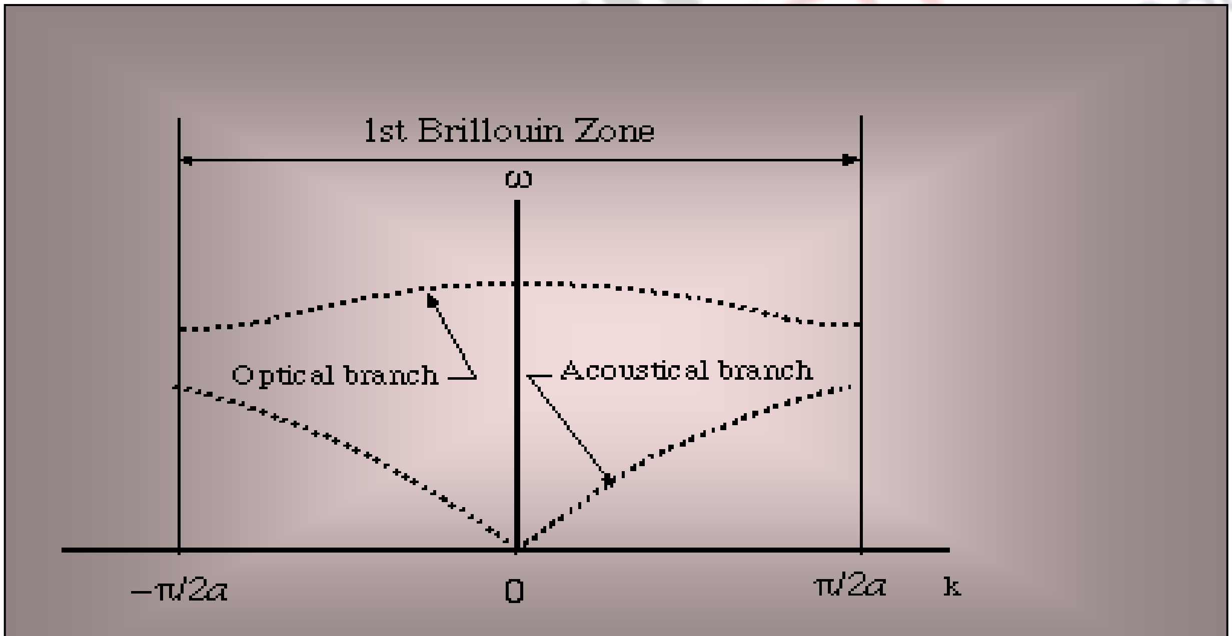


Fig (6) One dimensional diatomic dispersion curve for ω versus k

The allowed frequencies are split into two branches as shown in fig (6). The lower branch is called acoustical branch and the upper one is termed as optical branch.

Considering equations (7) & (8) the amplitude ratio A/B for k→0, implies *cos ka* =1 we get

$$\frac{A}{B} = -\frac{M}{m}$$

For m=M , $\frac{A}{B} = -1$

Indicating that the two masses move opposite to each other as in transverse waves , hence termed optical branch.

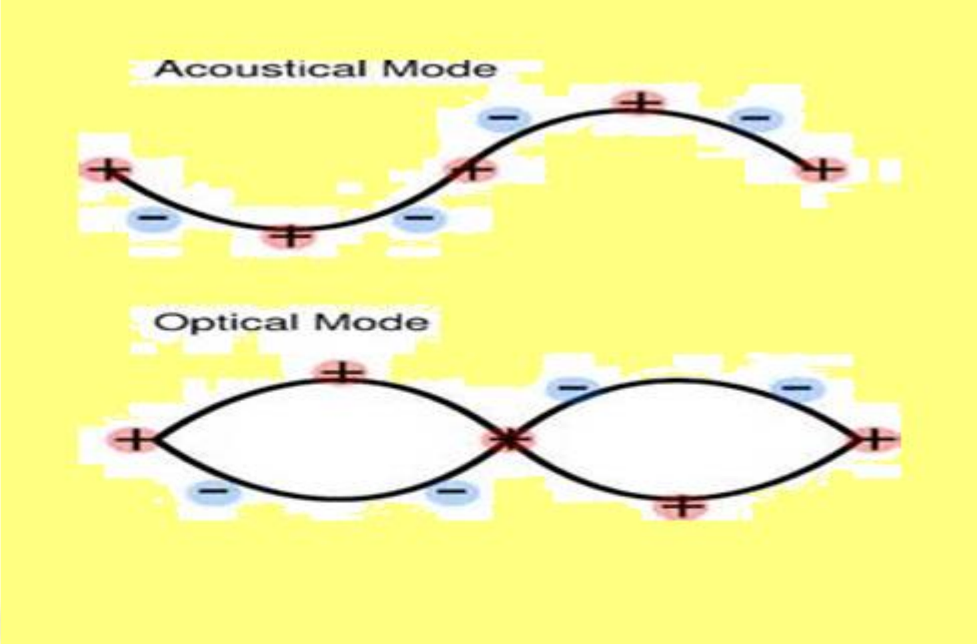


Fig (7) Two modes of vibration of masses (M and m) corresponding to acoustical branch and optical branch

In acoustical waves for longer wavelengths k→0, implies that

$coska \approx 1 - (k^2a^2)/2$, hence the ratio

$\frac{A}{B} = \frac{M}{m}$

for M = m , $\frac{A}{B} = 1$

Indicating that the neighbouring atoms vibrate in same direction as in longitudinal waves, so for this reason this branch is termed acoustical branch

Also we notice that between two branches there exists a band gap (forbidden gap) where there are no possible solutions in this frequency range as shown in fig (8). The width of this band depends on the ratio of two masses such that larger the ratio, wider is the forbidden gap.

For M = m branches become degenerate as band disappears

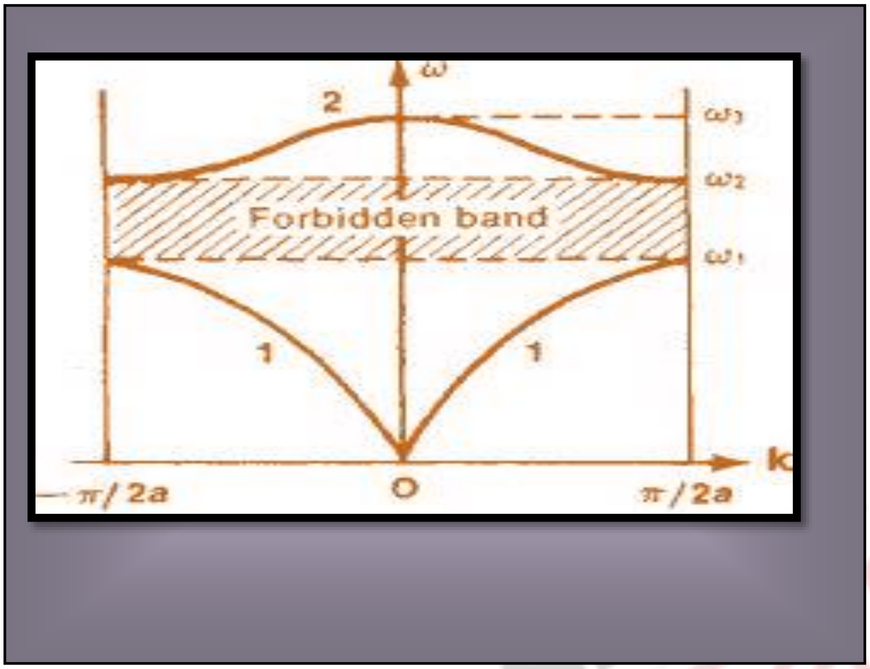


Fig (8) Forbidden band between acoustical and optical frequencies corresponding to which no waves can propagate

1.3 Dispersion Relation for 3-Dimensional Crystal.

The properties of dispersion relations(monoatomic and di atomic) corresponding to one dimensional cases are also applicable to three dimensional system.

However the only additional feature in three dimensional crystal is the polarization of lattice waves. But the basic difficulty in developing the lattice dynamics of 3-D space lattice involves very complex mathematics.

But qualitatively for a simple cubic lattice, the normal mode solution may be written as

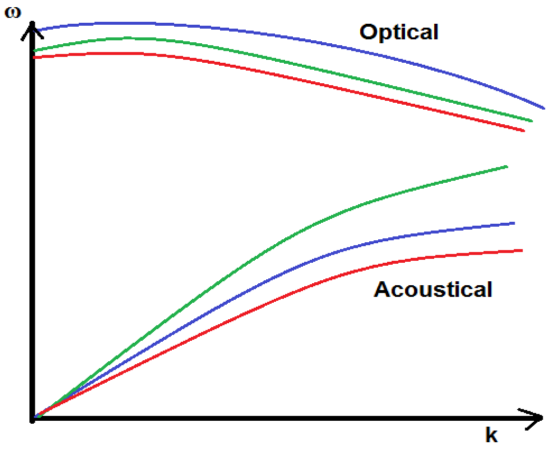
$$U_n = A\exp i(k.r-\omega t)$$

where the wave vector k specify both, the wavelength and direction of propagation.

A represents amplitude as well as the direction of vibrations of the atoms.

r is the position vector.

Correspondingly three dispersion relations are obtained for acoustic and optical branches each as shown in figure.



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2.Summary:

After the completion of this module we are able to understand the following

- The study of solids cannot be done on an isolated system of particle, but the entire crystal determines its behaviour.

- The concept of harmonic motion of atoms at their mean positions and lattice vibrations in mono-atomic and di-atomic crystal structures is also studied in detail.

- Concept of continuum and dispersive medium is understood in context to lattice dynamics and the consequence of frequency responses giving idea of acoustic and optic modes of vibrations is clear.