



Dr. Avradip Pradhan,
Assistant Professor,
Department of Physics,
Narajole Raj College, Narajole.

C12T (Solid State Physics)

Topic – Elementary Lattice Dynamics (Part – 1)

Introduction:

The basis of crystal structures is often described in terms of ions for the interpretation of the properties of solids. The valence electrons are considered to have been placed in the force field of the lattice of ions. The word “ions” stands for ions in ionic crystals, ion cores in metals and covalent crystals and atoms in a rare gas solid. The roles of ionic and electronic motions are crucial to the determination of the properties of solids. While some properties depend heavily on the electronic motion, several others are closely linked to the ionic dynamics. Lattice heat capacity, thermal expansion and hardness are some examples of properties that belong to the latter class. In this e-report, a classical theory will be developed to describe small vibrations of atoms in crystalline solids in terms of normal modes (independent motions of characteristic frequency) of motion of constituent ions. In a normal mode all the ions move with well-defined amplitude and phase. A normal mode has the same amplitude in each cell, but varies from one unit cell to the other across the crystal like a wave with a certain wave vector. Such kind of elastic wave is called a *lattice wave* and the vibration with which it is associated is commonly known as *lattice vibration*.

It can be seen that, no meaningful error can be introduced by assuming that the electrons remain in their ground state at any moment for the respective ionic configuration, because the ions move so slowly on the scale of velocities of relevance to electrons. This simplifies the calculation of the potential energy of ions, enabling us to write the equations of motion of ions that are crucial to the determination of the normal modes of vibration.

Vibration of a 1-dimensional Monatomic Lattice Chain:

Let us consider the simplest crystal which can be a 1-dimensional infinite linear chain of crystal with one atom in the primitive cell (shown Fig. 1). This is equivalent to a linear chain of N primitive cells, with one atom in each of them. If we wish to describe the vibrations of the chain we are confronted with the

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problem of accounting appropriately the motion of ions in the middle and the motion of two ions at the ends. The broad feature of the motion may still be obtained by considering only the nearest neighbour interactions and ignoring the ends. The results of such a calculation are most acceptable when the number of atoms is large. If we denote the displacement of an ion at any moment from its site s in the static lattice by u_s , the effective potential energy of a chain of inter-ionic separation a , in the harmonic approximation is given by

$$U_{eff} = \frac{1}{2} C \sum_s (u_s - u_{s+1})^2$$

Here C is the force constant between nearest-neighbour atoms and will differ for longitudinal and transverse waves. So, the restoring force on the ion sitting at site s will be given by $F_s = -C[(u_s - u_{s+1}) + (u_s - u_{s-1})]$. Therefore the equation of motion of the atom having mass m will be

$$m \frac{d^2 u_s}{dt^2} = F_s = -C[(u_s - u_{s+1}) + (u_s - u_{s-1})] = C(u_{s+1} + u_{s-1} - 2u_s)$$

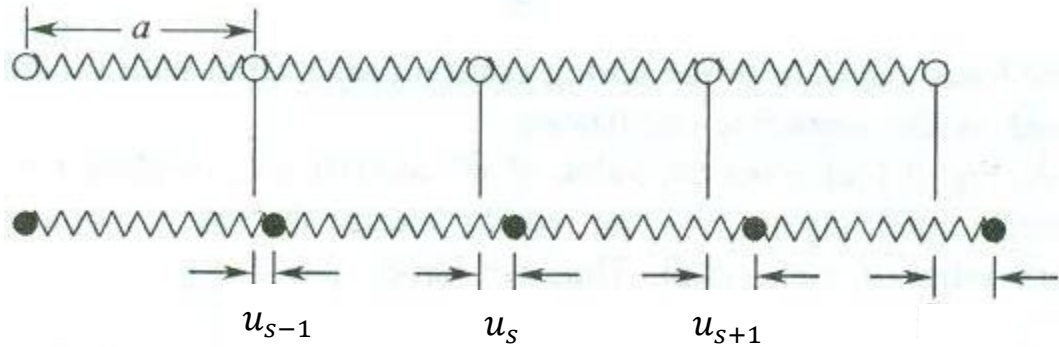


Fig. 1

We are looking for solutions with all displacements u having the time dependence as $\sim e^{-i\omega t}$, where ω is the frequency of the lattice wave or elastic wave. This gives us $\frac{d^2 u_s}{dt^2} = -\omega^2 u_s$. So, the equation of motion becomes

$$-m\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s)$$

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We incorporate the spatial part of the wave as $u_s = u_0 e^{i(kx_s - \omega t)}$ where x_s is the equilibrium position of the atom situated at site s . Therefore, $x_s = sa$, $x_{s\pm 1} = (s \pm 1)a$ and so on, and we obtain

$$\begin{aligned} -m\omega^2 e^{iksa} &= C(e^{ik(s+1)a} + e^{ik(s-1)a} - 2e^{iksa}) \\ \text{or } m\omega^2 &= C(2 - e^{ika} - e^{-ika}) = 2C(1 - \cos(ka)) \\ \text{or } \omega^2 &= \frac{2C}{m}(1 - \cos ka) = \frac{4C}{m} \sin^2\left(\frac{ka}{2}\right) \end{aligned}$$

Therefore, we obtain $\omega(k) = \sqrt{\frac{4C}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$. Here modulus has been used just to avoid the negative value of the root since the frequency cannot be negative.

The maximum frequency $\omega_0 = \sqrt{\frac{4C}{m}}$ is observed at $k = \pm \frac{\pi}{a}$. It is important to note that s has not appeared in the final expression of $\omega(k)$ indicating that the equation of motion of every atom gives the same algebraic relation between ω and k . This relation is known as the *dispersion relation* and the plot of ω vs k is called as the *dispersion curve* (shown in Fig. 2).

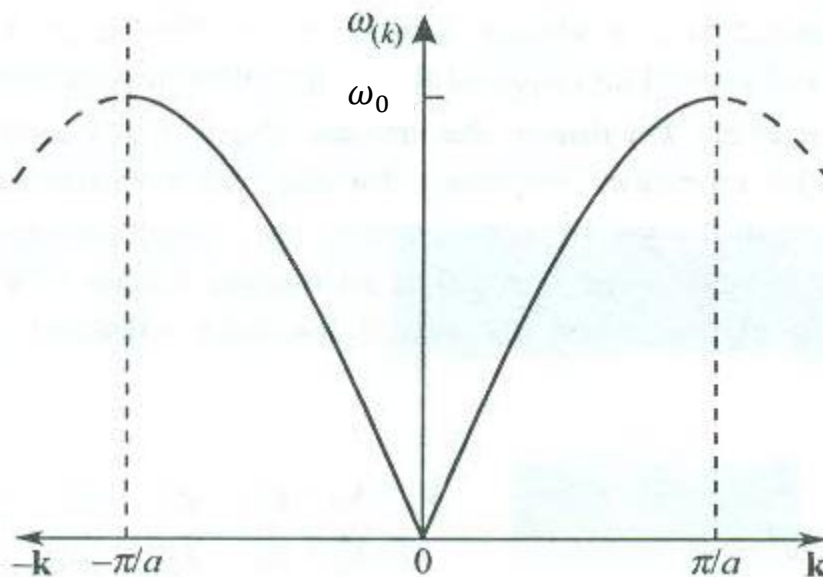


Fig. 2

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Features of the Dispersion Curve. We are interested in the range of k that is physically significant for elastic waves. The range of independent values of k is specified by $-\pi < ka < \pi$ or $-\frac{\pi}{a} < k < \frac{\pi}{a}$. This range is the *first Brillouin Zone* of the linear lattice, as we have seen before. We may treat a value of k outside these limits by subtracting the integral multiple of $\frac{2\pi}{a}$ that will give a wavevector inside these limits. Let us suppose k lies outside the first zone, but a related wave vector k' defined as $k' = k - \frac{2\pi n}{a}$ lies within the first zone, where n is an integer. Then the displacement ratio between two successive atoms becomes $\frac{u_{s+1}}{u_s} = e^{ika} = e^{i(k'a+2\pi n)} = e^{ik'a}$. We notice that $\frac{2\pi n}{a}$ is nothing but a reciprocal lattice vector G . Thus by subtraction (or addition) of an appropriate reciprocal lattice vector from k , we always obtain an equivalent wave vector in the first zone.

At the Brillouin Zone boundaries, the solution of u_s does not represent a travelling wave, rather a standing wave. At $k = \pm \frac{\pi}{a}$, u_s is given by $u_0(-1)^s$. This is a standing wave, as $u_s = \pm 1$ according to whether s is an even or an odd integer. The wave moves neither to the right nor to the left. This situation is equivalent to Bragg's diffraction of X-rays. When Bragg's condition is satisfied a travelling wave cannot propagate in a lattice, through successive reflections back and forth, a standing wave is set up at the Brillouin Zone boundaries.

The transmission velocity of a wave packet is the *group velocity*, given by the expression $v_g = \frac{d\omega}{dk}$ which is the gradient of the frequency with respect to k . This is the velocity of energy propagation in the medium. So, from the dispersion, we obtain the group velocity as $v_g = \sqrt{\frac{ca^2}{m}} \left| \cos\left(\frac{ka}{2}\right) \right|$. This is zero at the zone boundary where $k = \pm \frac{\pi}{a}$. Here the wave is a standing wave and we expect zero net transmission velocity for a standing wave.

Long Wavelength Limit. In the limit of small k values ($ka \ll 1$), more often referred to as the *long wavelength limit*, $\sin\left(\frac{ka}{2}\right)$ in the dispersion relation may

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be replaced with $\frac{ka}{2}$ in the first approximation. The dispersion relation would then read as

$$\omega(k) = \sqrt{\frac{c}{m}} ka$$

We infer that the frequency varies linearly with the wave vector for small values of the wave vectors. This behaviour is clearly evident in Fig. 2. The behaviour of elastic waves in continuum is of exactly similar nature. In the long wavelength limit of the waves where the wavelength is much larger than the interatomic spacing or the lattice constant a , the medium behaves as an elastic continuum since these waves pass smoothly through the medium with a constant group velocity $v_g = \sqrt{\frac{c}{m}} a$. The chain of atoms under this condition acts like a heavy elastic string.

Vibration of a 1-dimensional Diatomic Lattice Chain:

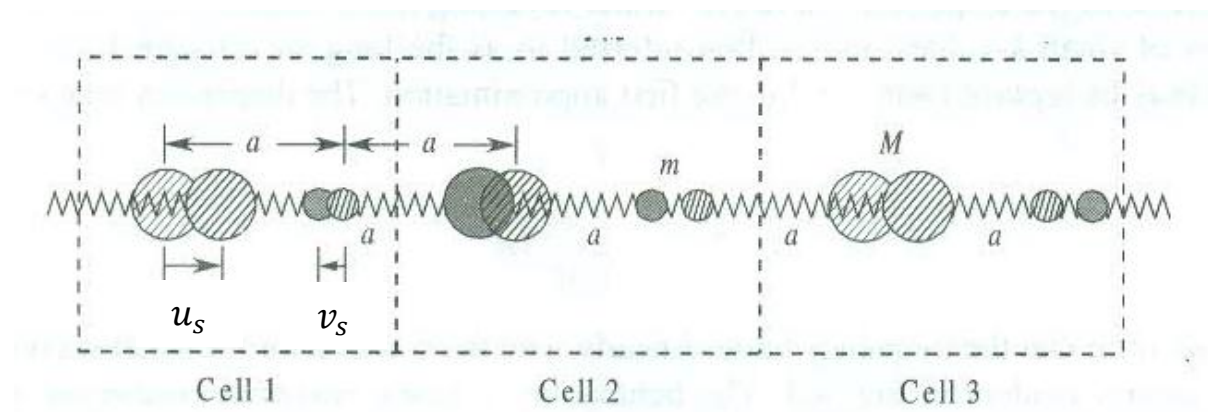


Fig. 3

We consider a crystal where atoms of mass M lie on one set of planes and atoms of mass m , lie on planes interleaved between those of the first set (shown in Fig. 3). It is not essential that the masses be different, but either the force constants or the masses will be different if the two atoms of the basis are in non-equivalent sites. Let a denote the repeat distance of the lattice in the direction normal to the lattice planes considered. We treat waves that propagate in a



Dr. Avradip Pradhan,
Assistant Professor,
Department of Physics,
Narajole Raj College, Narajole.

symmetry direction such that a single plane contains only a single type of ion. This situation creates a basis with two non-identical atoms.

We write the equations of motion again under the assumption that each atom interacts only with its nearest-neighbour atoms and that the force constants C are identical between all pairs of nearest-neighbour atoms. The displacements of atoms M are denoted by $u_{s-1}, u_s, u_{s+1} \dots$ and of atoms m , by $v_{s-1}, v_s, v_{s+1} \dots$ etc.

Therefore the equations of motion of the two atoms will be written as

$$M \frac{d^2 u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s)$$
$$m \frac{d^2 v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s)$$

Again we look for travelling wave solutions of the type $u_s = u_0 e^{i(ksa - \omega t)}$ and $v_s = v_0 e^{i(kx_s - \omega t)}$. So, the equations of motion now become

$$-M\omega^2 u_0 = C v_0 (1 + e^{-ika}) - 2C u_0$$
$$-m\omega^2 v_0 = C u_0 (e^{ika} + 1) - 2C v_0$$

These are two homogeneous linear equations with two unknowns u_0 and v_0 . These unknowns are basically the amplitudes of the two atoms. Now from elementary linear algebra, we know that these equations will have a solution, only if the determinant of the coefficients of u_0 and v_0 vanishes. We therefore need

$$\begin{vmatrix} 2C - M\omega^2 & -C(1 + e^{-ika}) \\ -C(1 + e^{ika}) & 2C - m\omega^2 \end{vmatrix} = 0$$

$$\text{or } Mm\omega^4 - 2C(m + M)\omega^2 + 2C^2(1 - \cos(ka)) = 0$$

We can solve this equation exactly for ω^2 , but it is simpler to examine the limiting cases near the zone centre ($ka \ll 1$) and at the zone boundary $k = \pm \frac{\pi}{a}$.

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For small values of ka we approximately write $\cos(ka) \approx 1 - \frac{k^2 a^2}{2}$ and the two roots are given by

$$\omega^2 \approx 2C\left(\frac{1}{M} + \frac{1}{m}\right)$$

$$\text{and } \omega^2 \approx \frac{C}{2(M+m)} k^2 a^2$$

So, looking for the dispersion relation for a diatomic chain, we obtain two different solutions known as “branches”. The first solution is called the *Optical Branch* and the second solution is called as the *Acoustical Branch* (shown in Fig. 4). The Acoustical Branch gives $\omega = 0$ at $k = 0$.

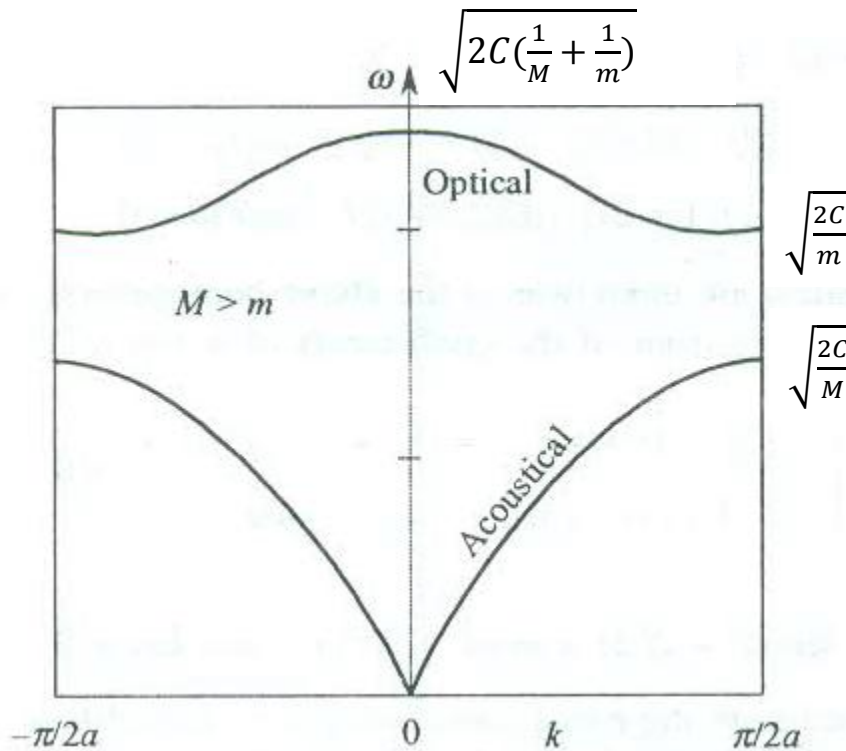


Fig. 4

At the zone boundaries $k = \pm \frac{\pi}{a}$, we get $\omega^2 = \frac{2C}{m}$ for Optical Branch and $\omega^2 = \frac{2C}{M}$ for Acoustical Branch.

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Features of the Dispersion Curve. The most prominent feature of the dispersion curves shown in Fig. 4 is the manifestation of a *frequency gap* $\Delta\omega$ between the acoustical and optical branches. This brings out the fact that a diatomic linear chain acts as a *band pass filter*. It contrasts the behaviour of a monatomic linear chain which was shown to act as a low pass filter. Other features of the observed two branches representing two different types of normal modes are discussed below.

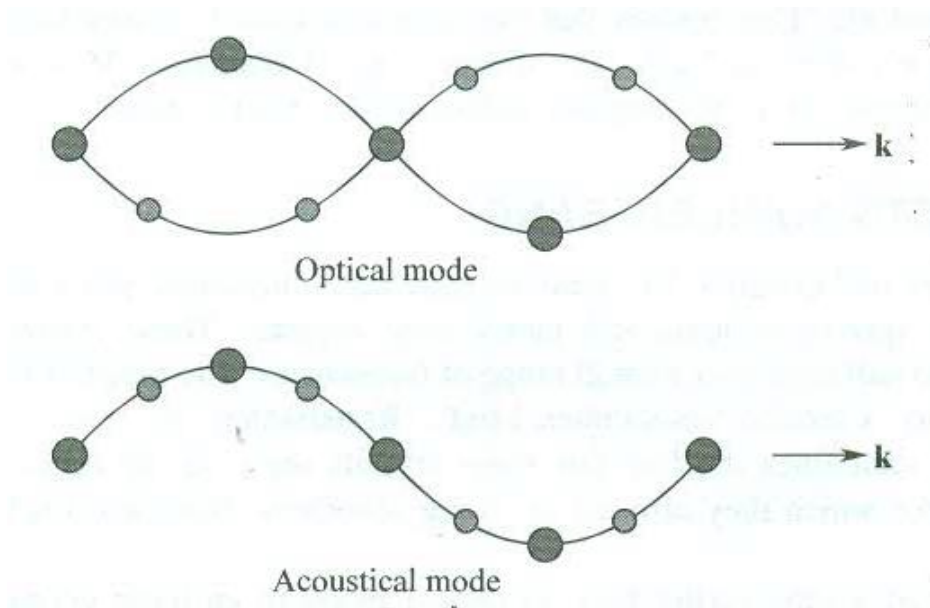


Fig. 5

The frequency of the optical branch is nearly constant in the limit $k \rightarrow 0$ as made out by the approximate nature of ω . But it decreases slowly as k increases, dropping to the value $\sqrt{\frac{2C}{m}}$ at the zone boundary. The acoustic branch corresponds to the single branch, obtained for the linear chain of monatomic atoms. The linear behaviour of ω vs k in the limit of small k (or long wavelength) is in the limit of sound waves which are longitudinal and treat the crystal as elastic continuum. We may, further, exploit the above treatment to derive the state of ionic motions in the two branches, again for the same two limiting cases. Substituting ω^2 at $k = 0$, we have for the optical branch,

$$\frac{u_0}{v_0} = -\frac{m}{M}$$



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This relation shows that the movements of the heavy and light ions are out of phase, i.e. they move towards each other or away from each other such that their centre of mass remains at rest. This refers to the situation in ionic crystals where such a motion of positive and negative ions may displace the centre of positive charges with the centre of negative charges creating an electric dipole. The oscillating electric dipole on interaction with the electromagnetic radiation may absorb the radiation. From a rough calculation we can find that the frequency of vibration of ionic crystals (e.g. NaCl, KBr, LiF) lies in the infrared region. That is why ionic crystals are known to absorb infrared light. The results can be only instructive as we have allowed the linear chain to produce only longitudinal waves. In real crystals, there can be two transverse waves for each longitudinal wave. Generally, the frequencies of all the modes are different with the exception that the two transverse modes along directions of high symmetry in the crystal are degenerate. The longitudinal and transverse vibrational modes of a crystal can be clearly separated only in certain symmetry directions of crystals. The modes for any arbitrary direction are mixed in character.

For acoustical branch at $k = 0$, we obtain $\frac{u_0}{v_0} = \frac{m}{M}$, which shows that the two atoms move in phase.

The state of motions of the ions in the optical and acoustical branches is illustrated for a transverse wave in Fig. 5. The example of a transverse wave is chosen since the difference between the motions of ions in the two branches is more striking in appearance for the transverse motion. Though this motion is not allowed in the linear chain, it is present in all real crystals.

The variation of the amplitude ratio $\frac{u_0}{v_0}$ with the wave vector k can be seen in Fig. 6. The state of motion at the zone end ($k = \pm \frac{\pi}{a}$, the maximum k) can be interpreted with the help of this figure. The light ions are at rest in the acoustical mode while the heavy ions are at rest in the optical mode.

As we will see next, these two branches are called as Optical Phonons and Acoustical Phonons in quantized picture of lattice vibration.

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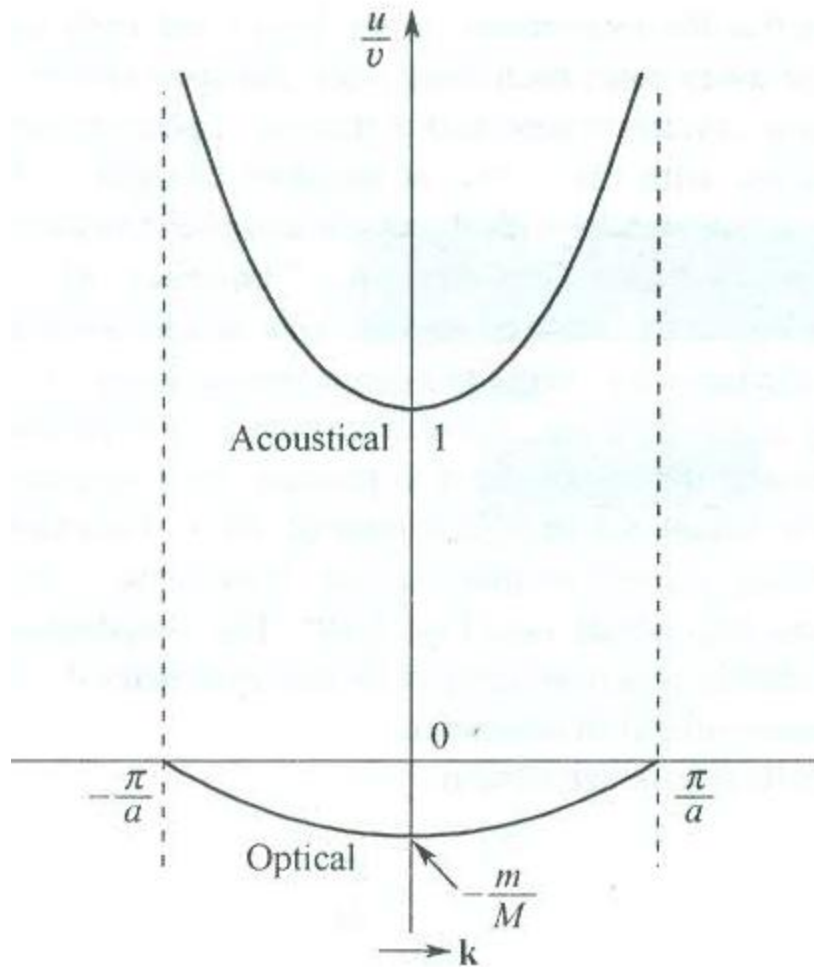


Fig. 6

Quantum of Lattice Vibration or Phonons:

The energy of a lattice vibration is quantized. The quantum of this energy is called a *phonon* in analogy with the photon of the electromagnetic wave. In a harmonic crystal, the atomic oscillators are treated analogous to the Planck's radiation oscillator. The energy of an elastic mode of angular frequency ω is given by $\varepsilon_n = (n + \frac{1}{2})\hbar\omega$, when the mode is excited to a quantum number n , which means that the mode is occupied by n phonons. The term $\frac{1}{2}\hbar\omega$ is called the *zero point energy* of the mode (for $n = 0$). It occurs for both phonons and photons as a consequence of their equivalence to a quantum harmonic oscillator of frequency ω .

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We can quantize the phonon amplitude. Let us consider the standing wave mode of amplitude $u = u_0 \cos(kx) \cos(\omega t)$. Here u is the displacement of a volume element from its equilibrium position at x in the crystal. The energy in the mode, as in any harmonic oscillator, is half kinetic energy and half potential energy, when averaged over time. The kinetic energy density is therefore $\frac{1}{2}\rho\left(\frac{du}{dt}\right)^2$, where ρ is the mass density. In a crystal having a volume V , the volume integral of the kinetic energy is given by $\frac{1}{4}\rho V \omega^2 u_0^2 \sin^2 \omega t$. The time averaged kinetic energy is $\frac{1}{8}\rho V \omega^2 u_0^2$. So,

$$\frac{1}{8}\rho V \omega^2 u_0^2 = \frac{1}{2}\left(n + \frac{1}{2}\right)\hbar\omega$$

$$\text{or } u_0^2 = \frac{4\left(n + \frac{1}{2}\right)\hbar}{\rho V \omega}$$

This relates the displacement in a given mode to the phonon occupancy n of the mode.

This concludes part 1 of this e-report.

The discussion will be continuing in the part 2 of this e-report.

Reference:

Introduction to Solid State Physics, Charles Kittel, Wiley

Elements of Solid State Physics, J.P. Srivastava, PHI Learning

(All the figures have been collected from the above mentioned reference)

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