DEBYE'S MODEL OF LATTICE HEAT CAPACITY

Main assumptions of Debye's Model

- ***Debye was the one who first took over simplified assumption into the account which was assumed by the Einstein's theory in his theory of lattice heat capacity.***
- ***So, instead of independent quantum harmonic oscillator, Debye chosen the lattice of atoms as the coupled harmonic oscillators***
- ***Debye proposed that crystal can propagate elastic waves of wavelengths ranging from low frequency (sound waves) to high frequencies (infrared ranges)***

So, what to do now ?

This simply means that a crystal can have a number of modes of vibration. These number of vibration modes per unit frequency range is called density of modes i.e. $Z(v)$. Thus, the most interesting thing here is to determine such mode of vibrations by treating crystal as a continuous medium

We simply starts from the general from of wave equation

or

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{v_s^2} \frac{\partial^2 u}{\partial t^2} \tag{4.69}$$

where $v_s = \sqrt{\frac{Y}{\rho}}$ represents the velocity of propagation of the wave along the string. It is independent of frequency. The Eq. (4.69) is the well known one-dimensional wave equation. Since the string is fixed at both the ends, the solutions of Eq. (4.69) should correspond to standing waves. These types of solutions are given by

$$u(x, t) = A \sin\left(\frac{n\pi}{L} x\right) \cos 2\pi\upsilon_n t \tag{4.70}$$

where n is a positive integer ≥ 1. Using Eq. (4.70) in (4.69), we get

$$\lambda_n = \frac{2L}{n}$$

and

$$\upsilon_n = \frac{v_s}{\lambda_n} = \frac{n v_s}{2L} \tag{4.71}$$

i.e.,

$$\upsilon_1 = \frac{v_s}{2L}, \upsilon_2 = \frac{v_s}{L}, \upsilon_3 = \frac{3v_s}{2L}, \text{ etc.} \tag{4.72}$$

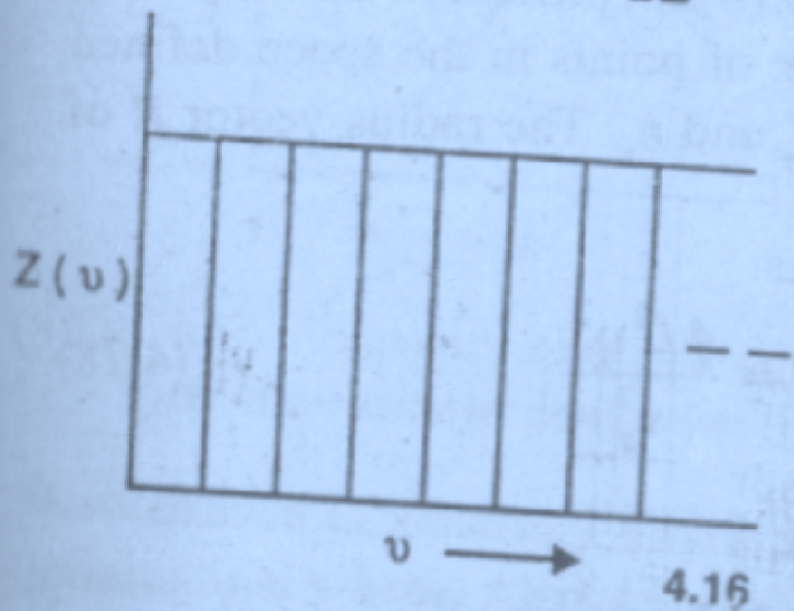

Fig. 4.16. *Frequency spectrum of a continuous string.*

This shows that the frequency of the string can have discrete values only and is an integral multiple of $\frac{v_s}{2L}$. It implies that the frequency spectrum of a continuous string is discrete and contains an infinite number of parallel lines equidistant from each other as shown in Fig. 4.16.

From Eqs. (4.71), we have

$$n = \frac{2L}{v_s}\upsilon_n$$

$\therefore$

$$dn = \frac{2L}{v_s}d\upsilon \tag{4.73}$$

This gives the number of possible modes of vibration in the frequency interval $d\upsilon$.

We simply starts from the general from of wave equation in 3D

Considering now the three-dimensional case; the wave equation (4.69) can be written as

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = \frac{1}{v_s^2}\frac{\partial^2 u}{\partial t^2} \tag{4.74}$$

The three-dimensional continuous medium can be taken as a cube of side L whose faces are fixed. In analogy with Eq. (4.70), the standing wave solutions of the wave equation (4.74) are

$$u(x, y, z, t) = A\sin\left(\frac{n_x\pi}{L}x\right)\sin\left(\frac{n_y\pi}{L}y\right)\sin\left(\frac{n_z\pi}{L}z\right)\cos 2\pi\upsilon t \tag{4.75}$$

where n_x, n_y, n_z are positive integers ≥ 1. Substituting this solution into (4.74) and simplifying, we obtain

$$\frac{\pi^2}{L^2}(n_x^2 + n_y^2 + n_z^2) = \frac{4\pi^2\upsilon^2}{v_s^2} \quad (4.76)$$

or

$$n_x^2 + n_y^2 + n_z^2 = \frac{4L^2\upsilon^2}{v_s^2} \quad (4.77)$$

This equation gives the possible modes of vibration. The integers n_x, n_y and n_z determine the possible frequencies or wavelengths. In order to determine the number of possible modes of vibration, $Z(\upsilon)d\upsilon$, present in the frequency range υ and $\upsilon + d\upsilon$, we consider a network of points in the space defined by three positive integral coordinates n_x, n_y and n_z. The radius vector R of any point from the origin is given by

$$R^2 = n_x^2 + n_y^2 + n_z^2 = \frac{4L^2\upsilon^2}{v_s^2} \quad (4.78)$$

This is the equation of a sphere of volume

$$V' = \frac{4}{3}\pi R^3$$

Differentiating it, we get

$$dV' = 4\pi R^2 dR$$

The number of modes present in the frequency range υ and $\upsilon + d\upsilon$ should be the same as number of points lying in the volume interval V' and $V' + dV'$ or in the range R and $R + dR$ of the radius vector. Since each point occupies, on an average, a unit volume in the space of integers, the number of points present in the volume dV' of the spherical shell is numerically equal to the volume of the shell, i.e.,

$$dn = 4\pi R^2 dR$$

But since a mode of vibration is always determined by the positive values of n_x, n_y and n_z only, we must consider the number of points lying in the octant defined by these positive integers only. Thus the number of possible modes of vibraton is

$$Z(\upsilon)d\upsilon = \frac{1}{8}\left(4\pi R^2 dR\right)$$

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$$= \frac{1}{8}4\pi \frac{4L^2\upsilon^2}{v_s^2}\frac{2L}{v_s}d\upsilon = \frac{4\pi L^3\upsilon^2}{v_s^3}\,d\upsilon$$

$$= \left(\frac{4\pi V}{v_s^3}\right)\upsilon^2 d\upsilon \tag{4.79}$$

The velocity of propagation, v_t, of transverse waves is generally different from the velocity of propagation, v_l, of longitudinal waves. Also, for each frequency or direction of propagation, the transverse waves have two vibrational modes perpendicular to the direction of propagation whereas the longitudinal waves have only one mode which lies along the direction of propagation. For such a case, the total number of vibrational modes is expressed as

$$Z(\upsilon)d\upsilon = 4\pi V\left(\frac{2}{v_t^3} + \frac{1}{v_l^3}\right)\upsilon^2 d\upsilon \tag{4.80}$$