Condensed Matter Physics
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Lecture - 13
Debye Theory of Specific Heat, Lattice Vibration

In the previous lecture, we saw how the thermal vibrations of the crystal lattice gave raise to lattice waves, lattice vibrations which set into motion, the acoustic or elastic waves whose quantized excitations are known as phonons.

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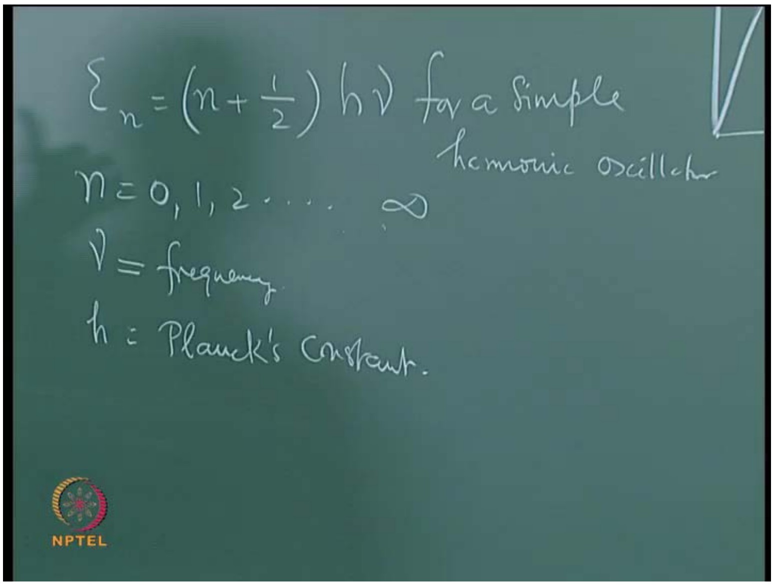

$\varepsilon_n = (n+\frac{1}{2})h\nu$ for a simple harmonic oscillator

$n = 0, 1, 2 \ldots \infty$

ν = frequency

h = Planck's constant.

And we saw how the classical theory of specific heat by Dulong and Petit, which did not taken into account anything except the bad idea of the equiv partition theorem due to Boltzmann, which determined the kinetic the internal energy of the solid. Considered as an assembly of three an atoms and how this lead to specific heat which is 3 R per mole, a constant specific heat which does not change with temperature and this is not in accordance with experimental observations. Because, the experimentally this specific heat of typical solid goes as from 3 R from the value 3 R at high temperatures, it designs down like this.

So, while the Dulong-Petit theory, correctly predicts and accounts for the molar specific heat reaching this constant value of 3 R, it did not give was not able to explain why there is a decrease at lower temperatures, and this was the experimental fact namely here reduction of the specific heat at lower temperatures till the specific heat vanishes at absolute zero. This is the experimental observation which was successfully explained by Einstein by assuming making the rather artificial assumption that all the three n atoms, we are mind you we are talking about something like 10 to power 24 atoms, trillions and quadrillions of atoms.

All vibrating in unison at one characteristic frequency that is something like an artificial assumption which is not likely to be born out cannot be substantiated by theory also. But still as a first step he made this assumption that all these three an atoms all these vibrate harmonically, simply harmonically at one given frequency. And assuming this frequency was taken by him to be given or given the corresponding energy associated with this mode of this the frequency was taken by him to be given by the quantum theory as n plus half h nu for a harmonic oscillator. Where n is an integer, and nu is the frequency of the oscillator which is assumed to be the same for all the oscillator and h is the Planck's constant.

We saw that based on this assumption, calculating the average energy of an assembly of such oscillators he could arrive at the total internal energy as some to infinity of a progression. And this give raise to a specific heat which goes at high temperatures the Dulong-Petit value of 3 R at sufficiently high temperatures and which is also predicts qualitatively not quantitatively. A qualitatively decrease has at low temperatures till it reaches zero at absolute zero.

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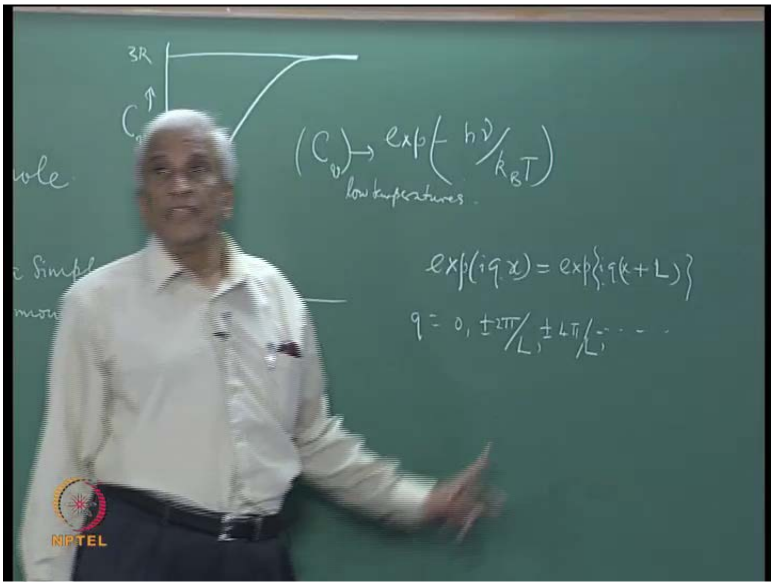

The qualitative variation was accounted for in terms of a theoretical dependent an exponential decrease at low temperatures. This was low temperature, but such an exponential variation was not observed by experiment, there was considerable deviation from this exponential curve predicted by the Einstein theory. So, this is we have already pointed out one shot coming of the Einstein theory namely that all the oscillators vibrate at the same frequency which is a rather drastic simplification.

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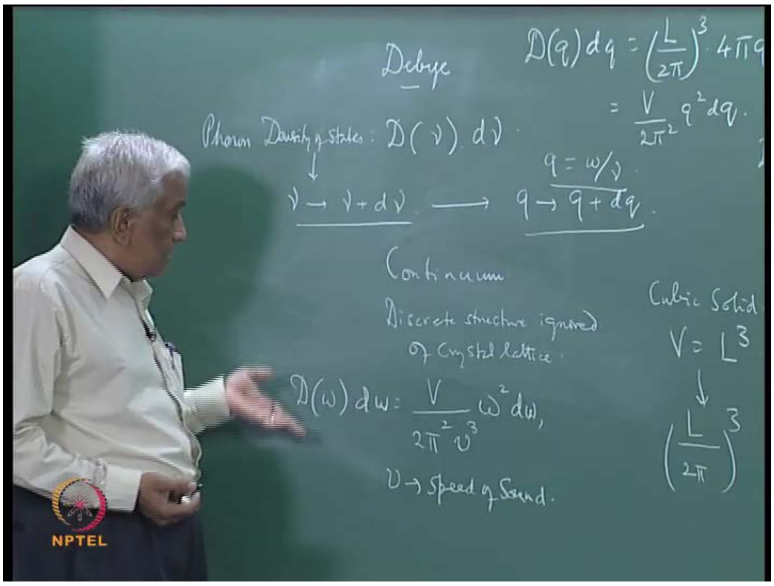

So, this is the point, which are addressed by the Debye theory specific heat. So, we are going to discuss the Debye theory of specific heat today, it is an improvement over the Einstein theory, and in this we assume a range of frequency of the phonons.

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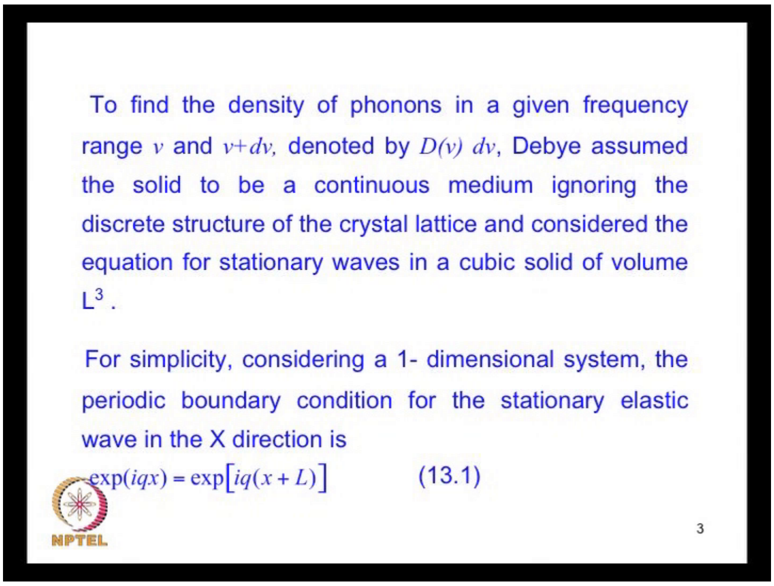

To find the density of phonons in a given frequency range ν and $\nu+d\nu$, denoted by $D(\nu)\, d\nu$, Debye assumed the solid to be a continuous medium ignoring the discrete structure of the crystal lattice and considered the equation for stationary waves in a cubic solid of volume L^3.

For simplicity, considering a 1- dimensional system, the periodic boundary condition for the stationary elastic wave in the X direction is

$$\exp(iqx) = \exp\left[iq(x+L)\right] \qquad (13.1)$$

And how in this range determinate, we assume that within a given frequency range, we have the phonons which are described by the number of phonons in this range are describe again by a density of states function d nu this is the density of states of phonons. This is very similar to what discussed in the case of the electrons in this solid - the conduction electrons. So, this is the density of states in the frequency range nu to nu plus d nu in a very small interval. The Debye assumed that the actual solid is a continuum is a continuous medium. In other words, he assumed the solid to be a continuum which means that heat grow with a discrete structure due to the atoms in the lattice this discrete structure is ignored. So, this is again in turn a short coming on the Debye theory we will come to latter. So, this solids is regarded as one continuous medium ignoring, the discrete structure of the crystal lattice; ignoring this we can consider stationary waves elastic waves which has set up in a cubic solid of volume v equal to the l cube; considering a cubic solid; volume v is l cube that means, that the cube as a ideal.

Let us to start with consider simple one-dimensional system in which we will write the phonons waves. The acoustic wave the spatial part as exponential i q x were q is the phonon wave vector. The periodicity requires that this should be equal to exponential i q x plus l; where l is the size of the length of one-dimensional solid say in the x-direction.

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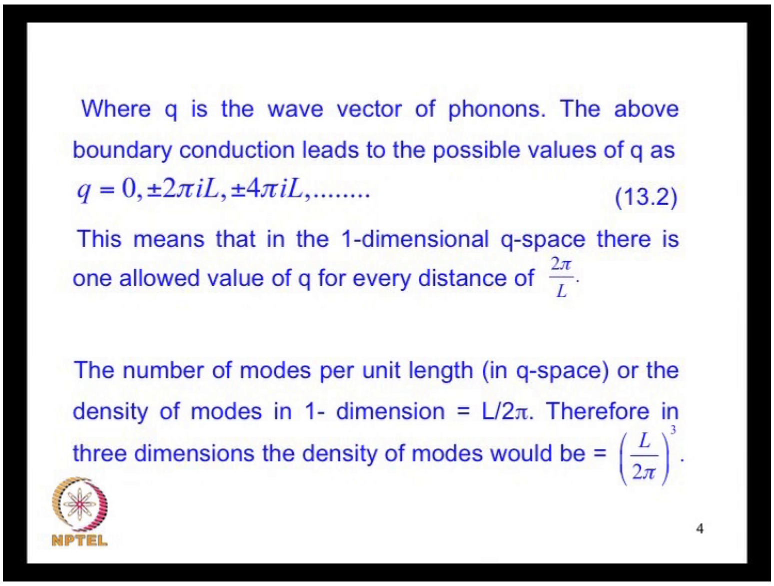

Where q is the wave vector of phonons. The above boundary conduction leads to the possible values of q as

$$q = 0, \pm 2\pi i L, \pm 4\pi i L, ... \quad (13.2)$$

This means that in the 1-dimensional q-space there is one allowed value of q for every distance of $\frac{2\pi}{L}$.

The number of modes per unit length (in q-space) or the density of modes in 1- dimension = L/2π. Therefore in three dimensions the density of modes would be = $\left(\frac{L}{2\pi}\right)^3$.

So, this immediately imposes a condition on the vector, the possible values of q can only be 0 plus minus pi plus minus 2 pi plus minus 4 pi by etcetera by l. The argument must become 2 pi, 4 pi etcetera. So, these are the allowed values in one-dimensional space and there is one allowed value for a distance 2 pi l that mean the number of vibrational modes per unit length in q space which is known as the density of modes is the reciprocal of this which is density of modes in one-dimensional. It is just reciprocal of this, reciprocal of 2 pi by l which is l by 2 pi, and the density of states of three dimensions in for a three dimensional solid will be l by 2 pi cube. This is in this is the number of modes per unit dimensions in a cubic solids in three dimensions.

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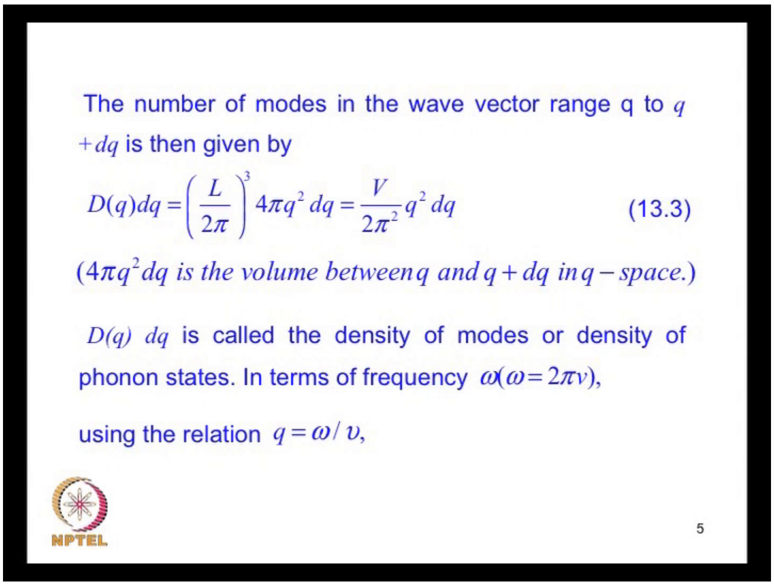

The number of modes in the wave vector range q to $q + dq$ is then given by

$$D(q)dq = \left(\frac{L}{2\pi}\right)^3 4\pi q^2\, dq = \frac{V}{2\pi^2} q^2\, dq \qquad (13.3)$$

($4\pi q^2 dq$ *is the volume between* q *and* $q + dq$ *in* $q-$*space.*)

$D(q)\ dq$ is called the density of modes or density of phonon states. In terms of frequency $\omega(\omega = 2\pi v)$,

using the relation $q = \omega / \upsilon$,

So, the number of modes in the wave vector range q to q plus dq, this is per unit length in q vector space. Now we want to calculate the number of modes in the frequency interval nu to nu plus d nu, which corresponds to a wave vector interval from q to q plus dq. So, this will be given by this is what will be given by D of q dq that will be L by 2 pi whole cube into 4 pi q square dq. So, this will be were L cube is V - the volume, so v by 8 pi cube and 4 pi. So, this will be 2 pi square q square dq. Therefore, we can find the corresponding this density of state function in omega space or nu space in frequency space.

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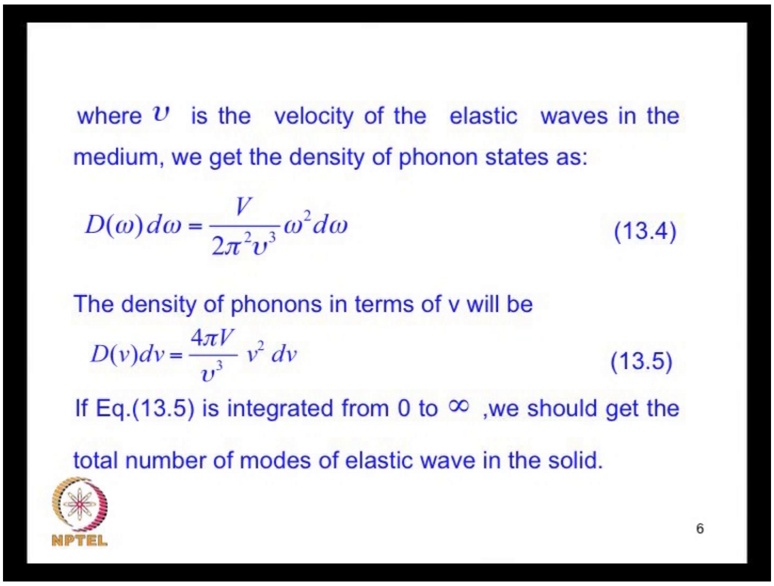

where υ is the velocity of the elastic waves in the medium, we get the density of phonon states as:

$$D(\omega)\,d\omega = \frac{V}{2\pi^2 \upsilon^3}\omega^2 d\omega \qquad (13.4)$$

The density of phonons in terms of v will be

$$D(v)dv = \frac{4\pi V}{\upsilon^3} v^2\, dv \qquad (13.5)$$

If Eq.(13.5) is integrated from 0 to ∞ ,we should get the total number of modes of elastic wave in the solid.

So, it turns out that the frequency space it will be just be D of omega d omega is correspondingly given by V by 2 pi square into v cube omega square d omega. Where v is the speed of sound, because these are sound waves, the phonons correspond to elastic waves, excitation of the elastic waves. So, this should give you the density of states. So, this is the phonons density of states

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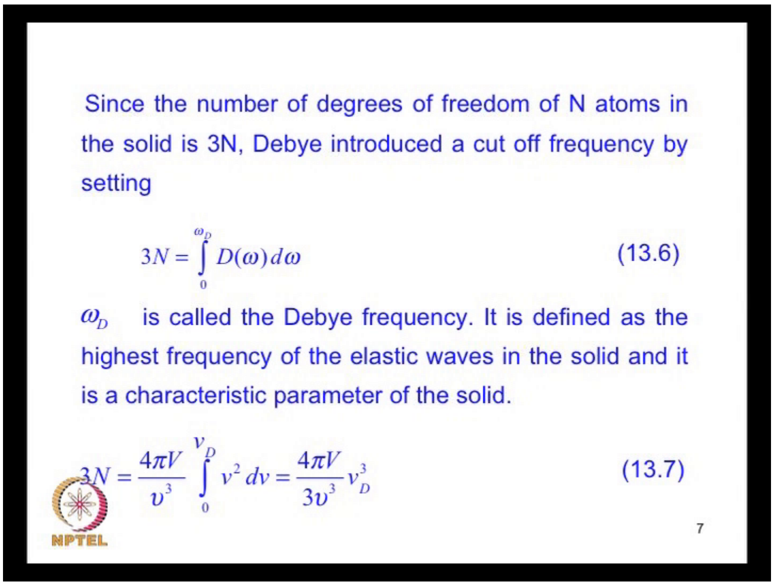

Since the number of degrees of freedom of N atoms in the solid is 3N, Debye introduced a cut off frequency by setting

$$3N = \int_0^{\omega_D} D(\omega)\,d\omega \qquad (13.6)$$

ω_D is called the Debye frequency. It is defined as the highest frequency of the elastic waves in the solid and it is a characteristic parameter of the solid.

$$3N = \frac{4\pi V}{\upsilon^3}\int_0^{v_D} v^2\,dv = \frac{4\pi V}{3\upsilon^3}v_D^3 \qquad (13.7)$$

Now, we have to calculate the total number of modes in correspondingly, accordingly we can define D of nu d nu. So, we define Debye define a cut off frequency because the number of degrees of freedom is not be infinite, the number of degrees freedom is, if N is number of atoms in the cubic solid then the number of degrees of freedom is just 3 N.

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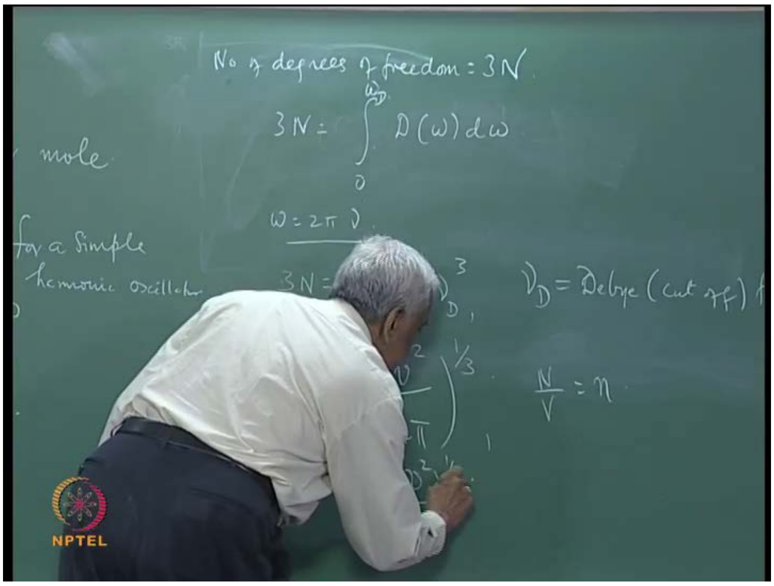

And this should be equal to the integral of since D of omega d omega, the density of state function integrated from zero up to a cutoff frequency omega d. So, this gives me where omega is 2 pi nu. So, putting all this in, we get where nu d is known as the Debye cutoff frequency. This means that you cannot assume that the phonons have all frequency some zero to infinity, in state the finite number of degrees have freedom imposes that cut off in the frequency spectrum given by the Debye frequency. So, only frequencies up to that are allowed and if you integrate the phonon density of states over that frequency interval, we get the total number of degrees of freedom.

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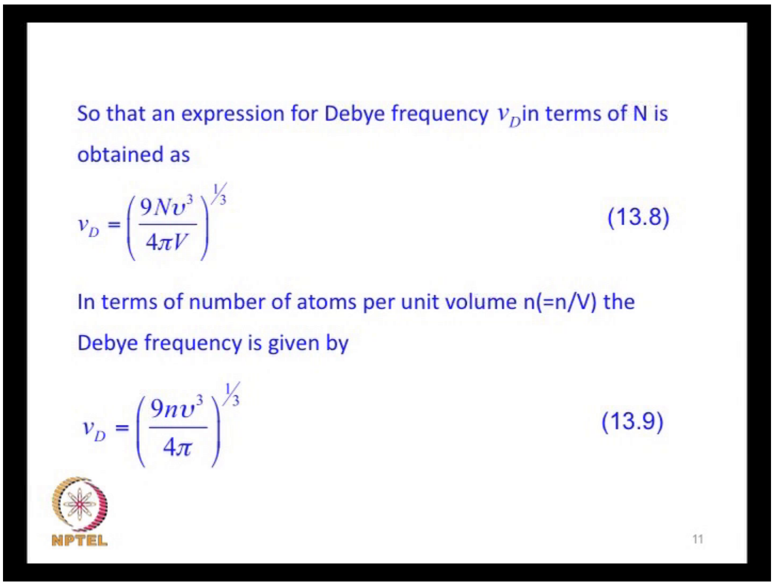

So that an expression for Debye frequency v_D in terms of N is obtained as

$$v_D = \left(\frac{9N\upsilon^3}{4\pi V}\right)^{1/3} \qquad (13.8)$$

In terms of number of atoms per unit volume n(=n/V) the Debye frequency is given by

$$v_D = \left(\frac{9n\upsilon^3}{4\pi}\right)^{1/3} \qquad (13.9)$$

Using this, we can write the Debye frequency in nu d, so that gives an expression for this Debye frequency. Here this is nu D cube, so this power becomes one-third I made a mistake.

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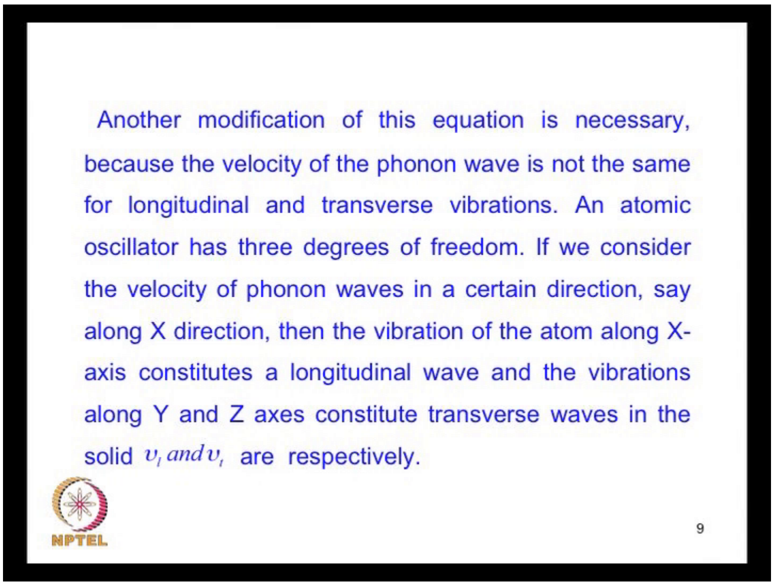

Another modification of this equation is necessary, because the velocity of the phonon wave is not the same for longitudinal and transverse vibrations. An atomic oscillator has three degrees of freedom. If we consider the velocity of phonon waves in a certain direction, say along X direction, then the vibration of the atom along X-axis constitutes a longitudinal wave and the vibrations along Y and Z axes constitute transverse waves in the solid $\upsilon_l \, and \, \upsilon_t$ are respectively.

Now, we also have to remember that sound waves or not just propagating in one dimensional alone. You have longitudinal sound waves and also transverse modes, if the x direction, in the direction of the vibration then the longitudinal sound waves propagate along the x-direction. But along the y and z directions, there will be a transverse sound waves and the speed of sound need not be the same in all the three directions even for a cubic solid because of the anisotropy. So, we have to distinguish between the speed of sound for longitudinal waves, and the speed of sound for transverse sound waves. There will be two sets of modes for transfer waves corresponding to one mode each longitudinal mode, because there are two directions at right angles plane.

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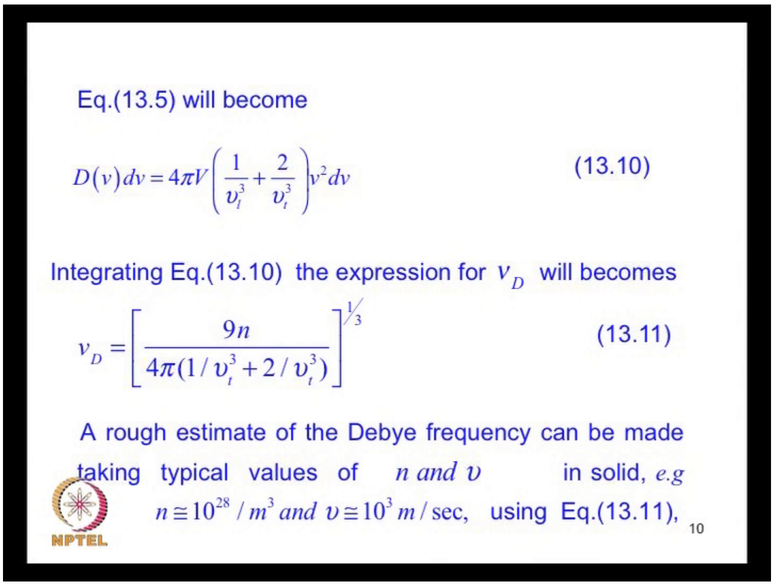

Eq.(13.5) will become

$$D(\nu)d\nu = 4\pi V\left(\frac{1}{\upsilon_l^3}+\frac{2}{\upsilon_t^3}\right)\nu^2 d\nu \qquad (13.10)$$

Integrating Eq.(13.10) the expression for ν_D will becomes

$$\nu_D = \left[\frac{9n}{4\pi(1/\upsilon_l^3+2/\upsilon_t^3)}\right]^{1/3} \qquad (13.11)$$

A rough estimate of the Debye frequency can be made taking typical values of n and υ in solid, e.g $n \cong 10^{28}/m^3$ and $\upsilon \cong 10^3\ m/\sec$, using Eq.(13.11),

So, we have to count price as many modes in the transverse waves taking that into account we can finally, write this expression for the Debye cutoff frequency as nu d for a real solid with which vibrating which has transfer as well as longitudinal frequencies.

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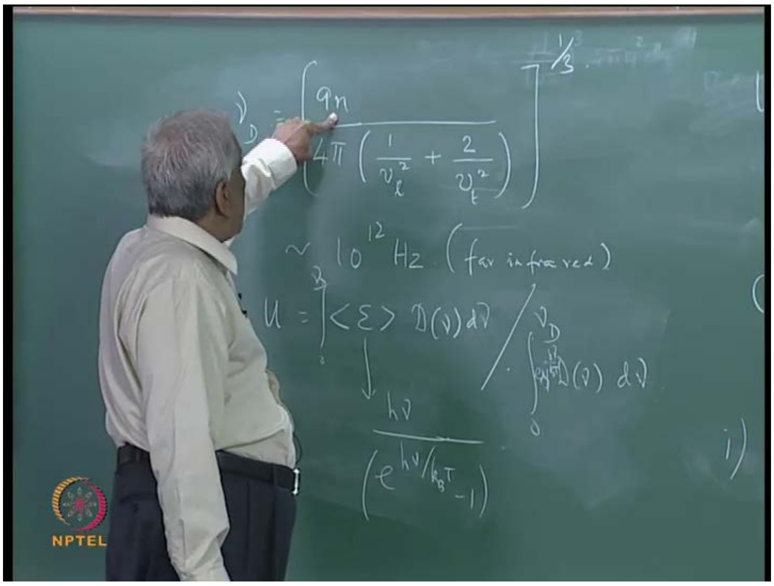

This will be just 9 n as before times divided by 4 pi and we will have this whole thing raised to the power one-third that will be the correct expression for the Debye frequency and putting in the typical values of n and the speed of sound in ordinary solid.

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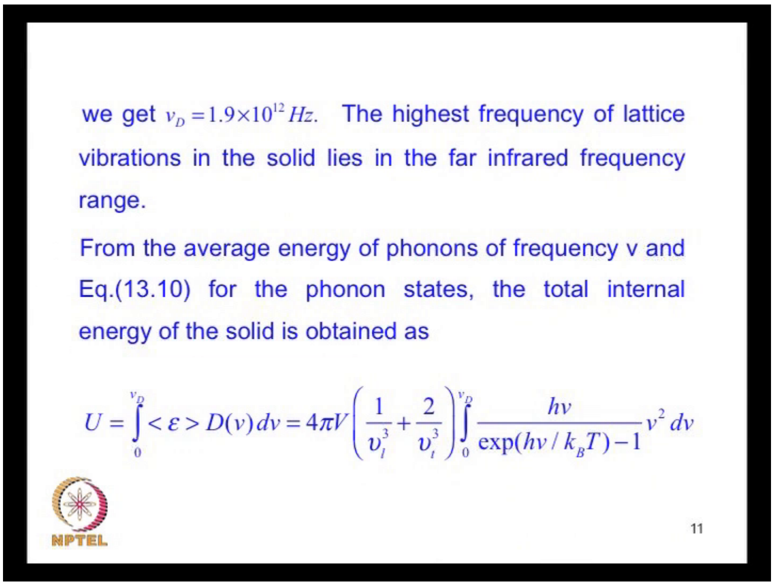

we get $\nu_D = 1.9\times10^{12}\,Hz.$ The highest frequency of lattice vibrations in the solid lies in the far infrared frequency range.

From the average energy of phonons of frequency v and Eq.(13.10) for the phonon states, the total internal energy of the solid is obtained as

$$U = \int_0^{\nu_D} < \varepsilon > D(\nu)\,d\nu = 4\pi V\left(\frac{1}{\upsilon_l^3}+\frac{2}{\upsilon_t^3}\right)\int_0^{\nu_D}\frac{h\nu}{\exp(h\nu/k_BT)-1}\nu^2\,d\nu$$

We get Debye frequency as something like 10 to power typically 10 to power 12 hertz which is in the far infrared. So, the Debye cutoff frequency life in the for a solid for a typical solid, lights in the infrared frequency. Modes above these are really high frequency wave which are not the solid is not responding to this. Once we have this expression we can find the internal energy as before by calculating the average energy of the phonon different modes and multiply by the density of states function and then integrated from zero to nu d. So, borrowing the other ideas that the average energy, the average energy we have already seen is of the firm h nu by e to the power h nu by k B T minus 1.

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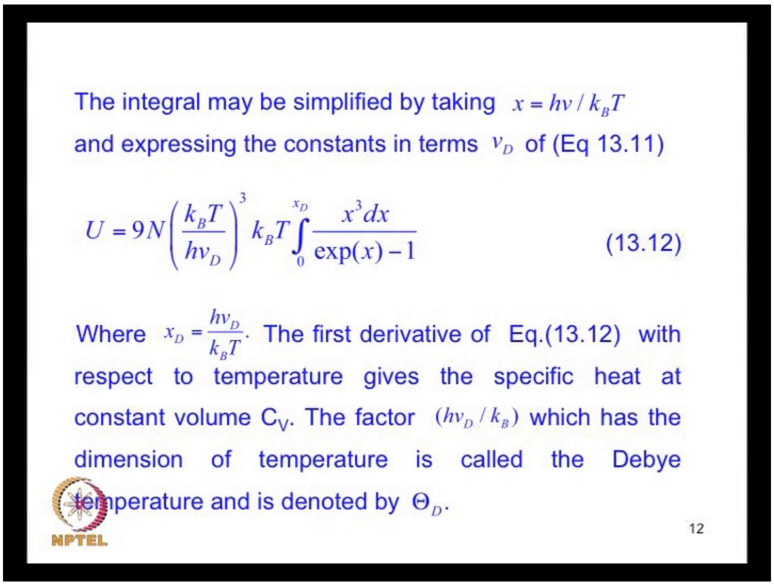

The integral may be simplified by taking $x = h\nu / k_B T$ and expressing the constants in terms ν_D of (Eq 13.11)

$$U = 9N\left(\frac{k_B T}{h\nu_D}\right)^3 k_B T \int_0^{x_D} \frac{x^3 dx}{\exp(x) - 1} \qquad (13.12)$$

Where $x_D = \frac{h\nu_D}{k_B T}$. The first derivative of Eq.(13.12) with respect to temperature gives the specific heat at constant volume C_V. The factor $(h\nu_D / k_B)$ which has the dimension of temperature is called the Debye temperature and is denoted by Θ_D.

So, if we take this and calculate the internal energy and differentiated with respect to temperature, we get the Debye expression for specific heat.

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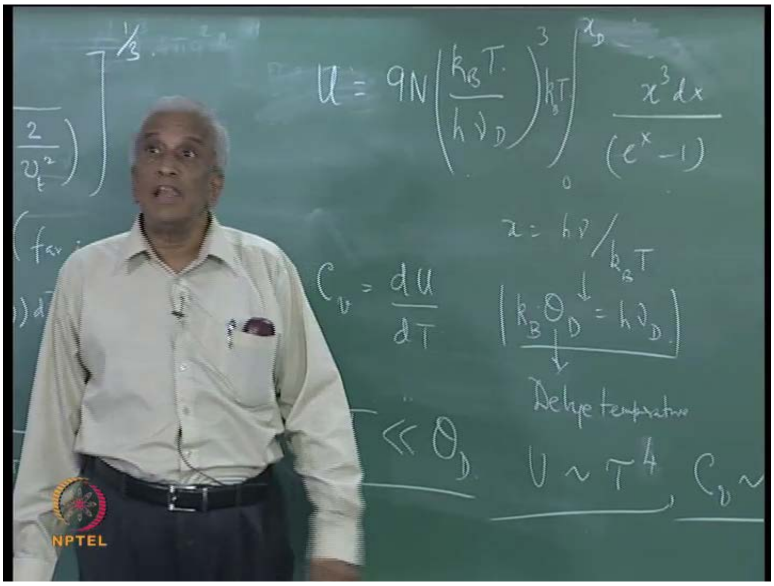

So, we get the average energy turns out to be r which we can write the as the internal energy that is nothing but 9 n k B T by h nu d times whole cube integral zero times zero h nu d by k d T x cube dx by e to power x minus 1. So, this is written as x d taking x equal to h nu by k B T, there is also another k B T value, so that is the internal energy and differentiating it, we get this persecute is the d u and d t.

So, if we take again, we consider the high temperature limit and the low temperature limit. Since the low temperature limit as great interest, let us take that first. So, corresponding this I can define also a temperature k B theta d equal to h nu d; where theta d is the known as the Debye temperature. So, if the Debye, the temperature is very small compare to the Debye temperature then that is the low temperature limit and in this we get U as a constant, which is got easily from the this.

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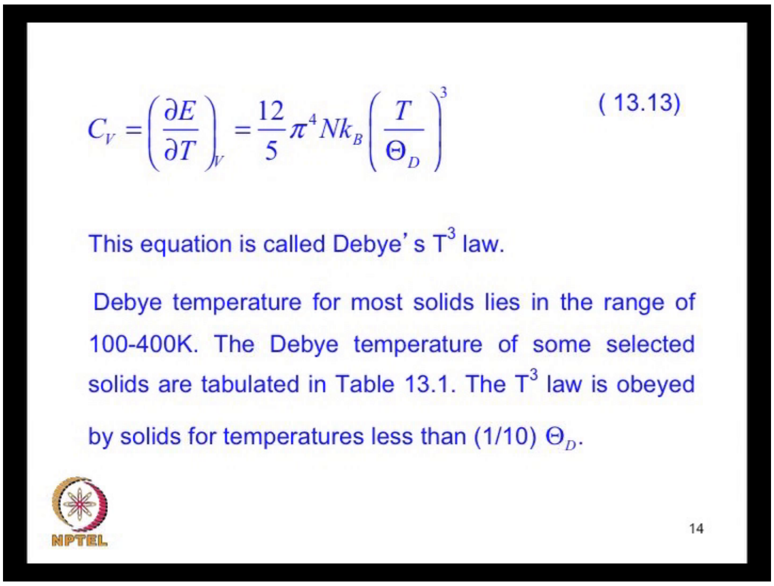

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = \frac{12}{5}\pi^4 N k_B \left(\frac{T}{\Theta_D}\right)^3 \qquad (13.13)$$

This equation is called Debye's T^3 law.

Debye temperature for most solids lies in the range of 100-400K. The Debye temperature of some selected solids are tabulated in Table 13.1. The T^3 law is obeyed by solids for temperatures less than (1/10) Θ_D.

But the important thing is the temperature dependence is T to the power four behaviors for the internal energy, and this specific heat goes as T cube. So, the Debye theory predicts at T cube dependence on this specific heat of the specific heat from the temperature. And this is what is experimentally observed at sufficiently low temperature for all solids, which specific heat at constant volume goes as the T cube, the cube as the absolute temperature. So, this is elevated to a law and is usually know as the Debye T cube law.

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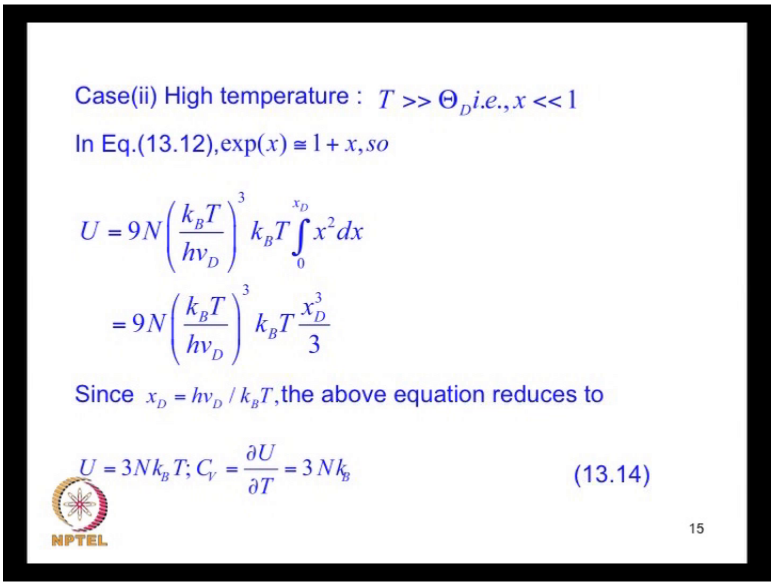

Case(ii) High temperature : $T >> \Theta_D i.e., x << 1$

In Eq.(13.12),$\exp(x) \cong 1 + x, so$

$$U = 9N\left(\frac{k_BT}{h\nu_D}\right)^3 k_BT\int_0^{x_D} x^2 dx$$

$$= 9N\left(\frac{k_BT}{h\nu_D}\right)^3 k_BT\frac{x_D^3}{3}$$

Since $x_D = h\nu_D / k_BT$,the above equation reduces to

$$U = 3Nk_BT; C_V = \frac{\partial U}{\partial T} = 3Nk_B \qquad (13.14)$$

The second case of course, is the high temperature case, this is one then we have the second case of high-temperature where T is very large compared to theta d.

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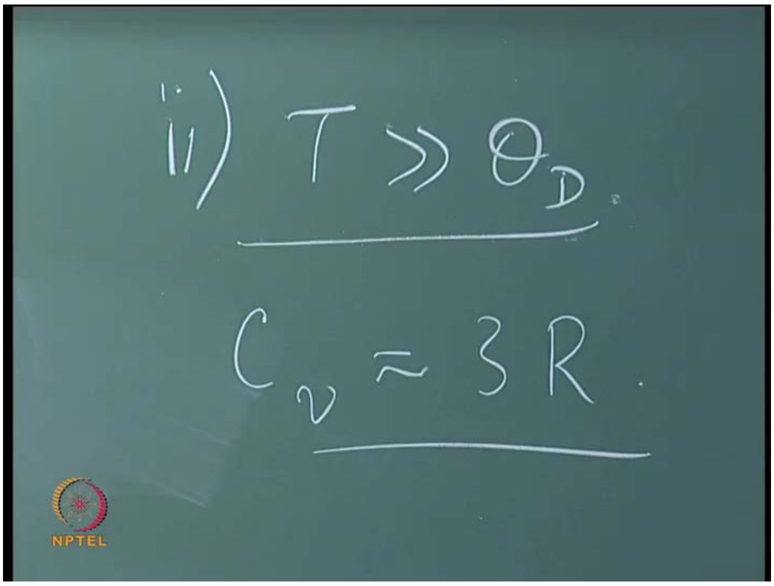

ii) $T \gg \Theta_D$

$C_v \approx 3R$

And it is found that the specific heat goes to 3 R as at sufficiently high temperature you get back the Dulong petit values. Intermediate temperature, you have to numerically integrate and obtain this specific heat values.

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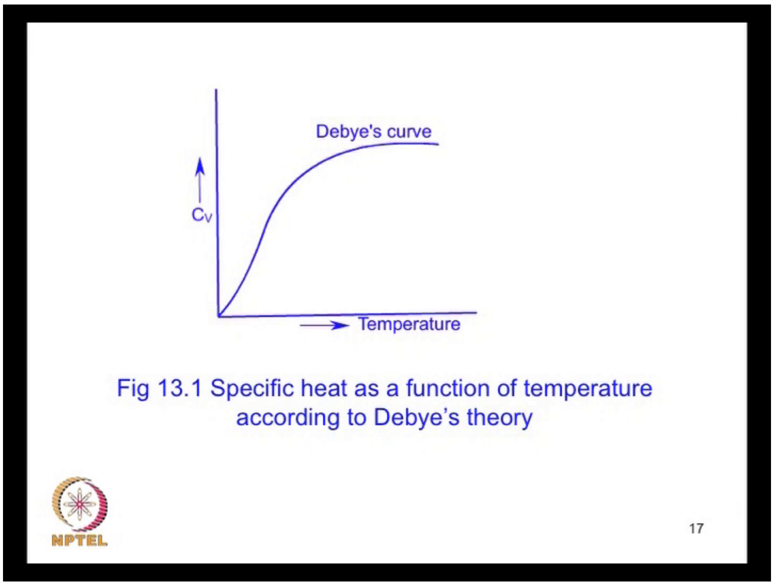

Fig 13.1 Specific heat as a function of temperature according to Debye's theory

The next figure gives you the Debye variation of the specific heat it temperature. In fact, many solids you find a very good corresponds between the experimental data and the theoretical calculations.

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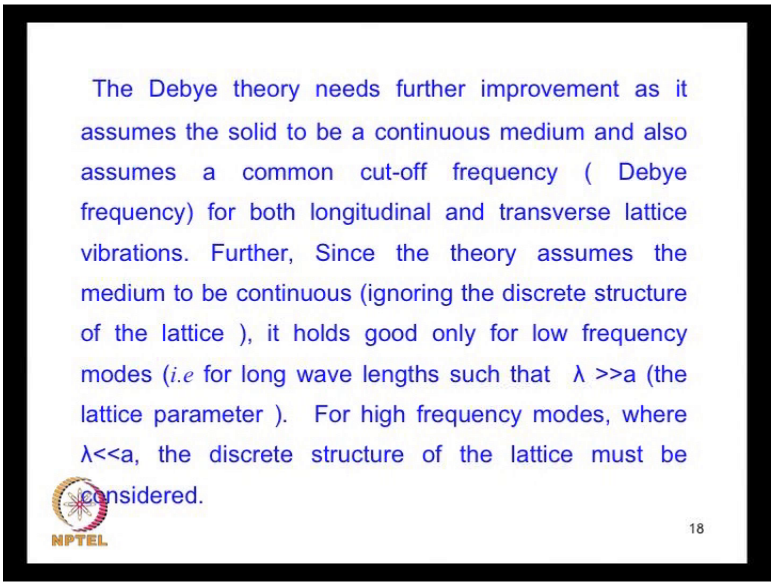

The Debye theory needs further improvement as it assumes the solid to be a continuous medium and also assumes a common cut-off frequency (Debye frequency) for both longitudinal and transverse lattice vibrations. Further, Since the theory assumes the medium to be continuous (ignoring the discrete structure of the lattice), it holds good only for low frequency modes (*i.e* for long wave lengths such that $\lambda >> a$ (the lattice parameter). For high frequency modes, where $\lambda << a$, the discrete structure of the lattice must be considered.

However, there are deviation and we know and these are because the Debye theory needs other improvement as it is assumed the solid to be continuous medium and it ignores the discrete atomic structure the solid, also it assume a common cutoff frequency nu d for the entire solid of both the longitudinal and transverse vibration. So, this is when is this good theory was because when the assumption that the solid is continuum is the correct one, this will be correct only when the discrete structure of the lattice can be ignored that mean if the wave length is very long only for long wave length or low-frequency modes of phonons. For high-frequency modes the wave length becomes smaller and smaller and then the discrete structure of the lattice can no longer be ignored. So, because of that there will be a deviation this problem has to be rectified.

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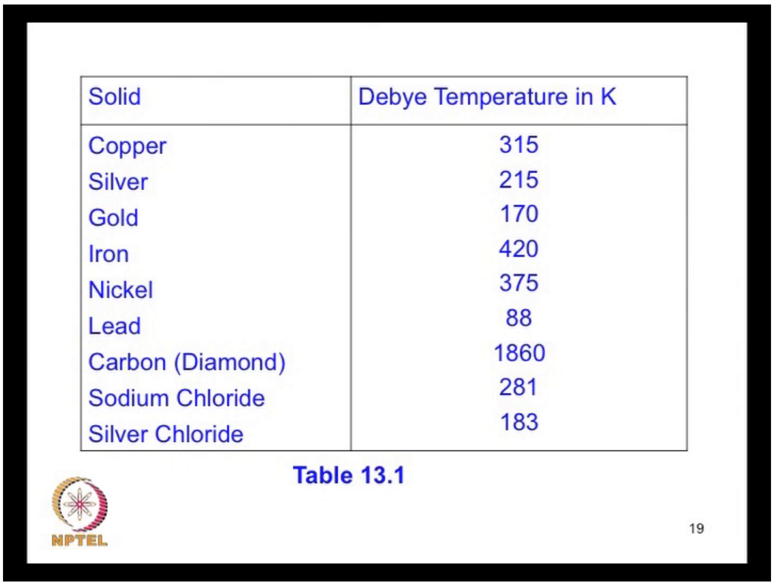

Solid	Debye Temperature in K
Copper	315
Silver	215
Gold	170
Iron	420
Nickel	375
Lead	88
Carbon (Diamond)	1860
Sodium Chloride	281
Silver Chloride	183

Table 13.1

List typical Debye temperatures given by this calculated because they had the expression for nu d which can be calculated, once you know the number of atoms per unit volume and then the speed of sound in a cubic solid. So, you can calculate this theoretically and the Debye temperature calculated in this way for different materials is given in table, for example, in copper it is close to room temperature 315; whereas in diamond, it is very high 1860 Kelvin. So, you can see there is considerable variation. As we already discussed in connection with the conduction electron theory in metals, we have in addition to the phonon contribution to the specific heat, there is also an electronic contribution due to the free-electron.

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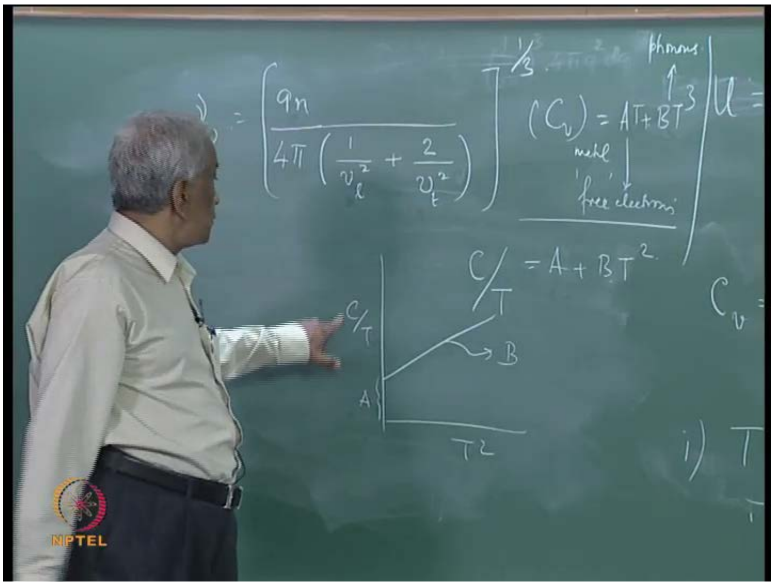

And we have as we already discussed this specific heat in metal and good metal is goes as A T plus B T cube the electronic contribution is proportional to T and the phonon contribution, this is the electron contribution - free electrons, and this is due to the lattice vibration or phonons. So, there are contribution of specific heat from both and observed the measured specific heat is a combination of these two. So, if you take the experimental value, and then divided by T is gives you A plus B T square. So, if you plot C by T as a function of T square, it should be a linear curve like this.

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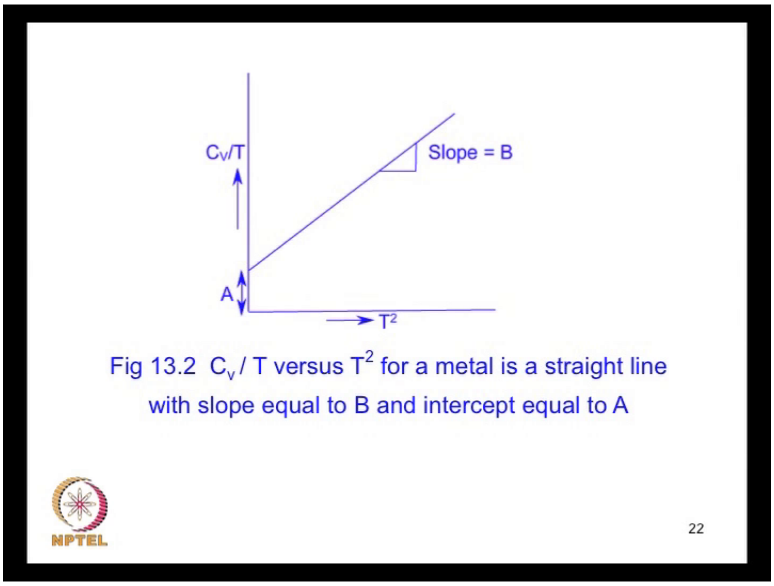

Fig 13.2 C_v / T versus T^2 for a metal is a straight line with slope equal to B and intercept equal to A

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So, this is actually observed and if you can shows how this is. So, this slope of this the slope gives you constant b which is occurs in the phonon contribution and the intercept is equal to a which gives you the electronic heat capacity equation. So, both electronic heat capacity equation and the phonon contribution which involves the db frequency can also be calculate the from the observed experimental data on specific heats by making a plot of C by T versus T square for metals.

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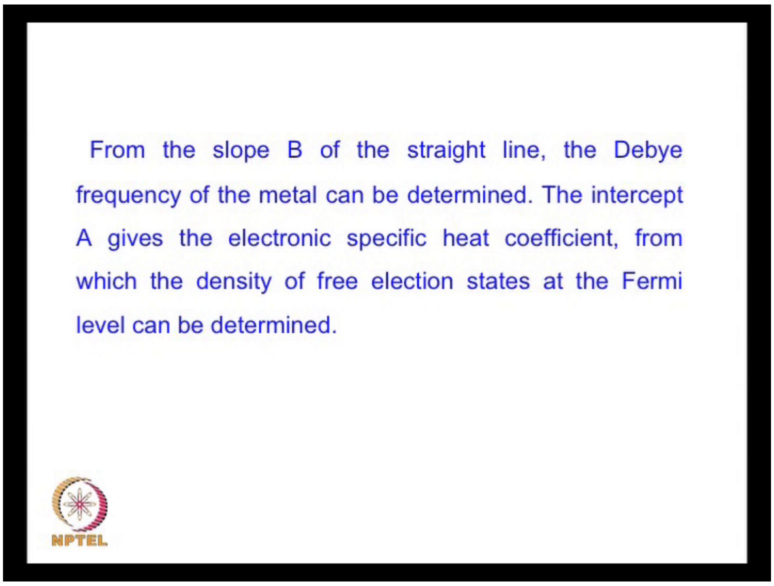

From the slope B of the straight line, the Debye frequency of the metal can be determined. The intercept A gives the electronic specific heat coefficient, from which the density of free election states at the Fermi level can be determined.

So, from the slope B, can be determined and hence the Debye frequency are the Debye temperature can determine. Actually the values in the table which we discussed already are obtain in this way.

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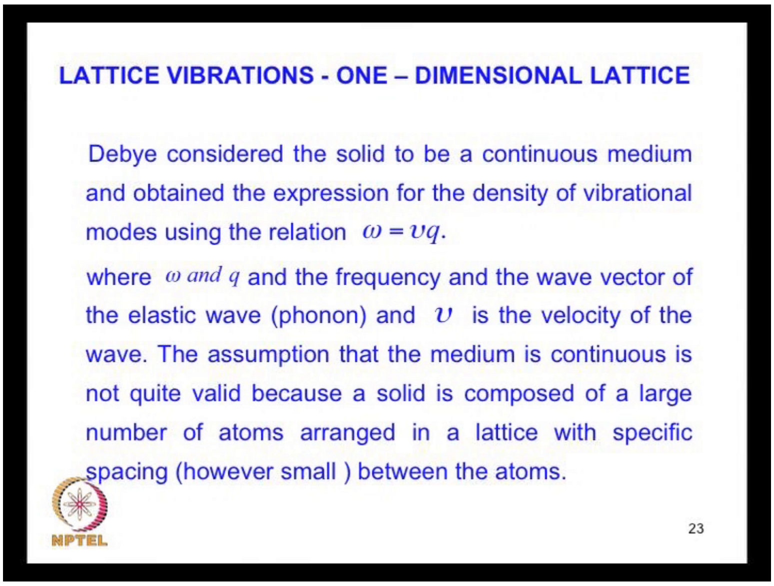

LATTICE VIBRATIONS - ONE – DIMENSIONAL LATTICE

Debye considered the solid to be a continuous medium and obtained the expression for the density of vibrational modes using the relation $\omega = \upsilon q$.

where ω *and* q and the frequency and the wave vector of the elastic wave (phonon) and υ is the velocity of the wave. The assumption that the medium is continuous is not quite valid because a solid is composed of a large number of atoms arranged in a lattice with specific spacing (however small) between the atoms.

But in order to take into account, the discrete nature of the lattice structure, we have to reconsiders among these issues and consider lattice vibrations in a discrete crystal lattice of atoms, so to start with the considered the one-dimensional lattice.

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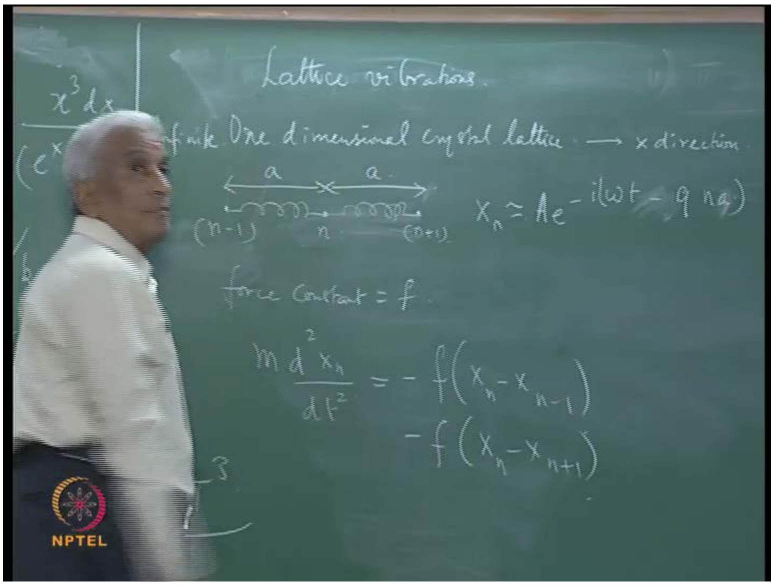

So, we plan to consider the lattice vibration in some detail in order to see how the Debye theory can be further improved. So, in this again we start with the simply case of a one dimensional crystal lattice of an atoms. So, we have now an atom a large line of atoms on a microscopic scale and we consider an infinite two start with we consider an infinite one-dimensional lattice as shown in figure.

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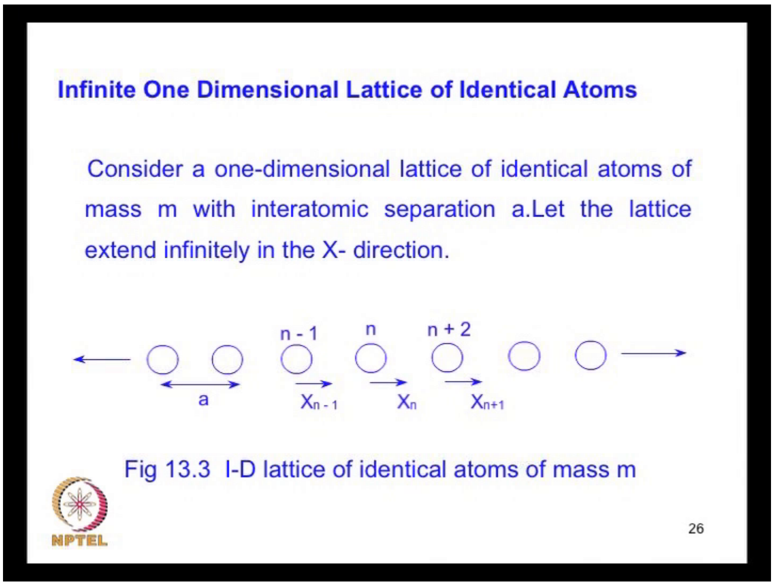

Infinite One Dimensional Lattice of Identical Atoms

Consider a one-dimensional lattice of identical atoms of mass m with interatomic separation a.Let the lattice extend infinitely in the X- direction.

Fig 13.3 I-D lattice of identical atoms of mass m

So, this lattice we take to be extending along the x-direction. So, we have the various atom situated at regular intervals at regular spacing on this one-dimensional lattice of identical atoms.

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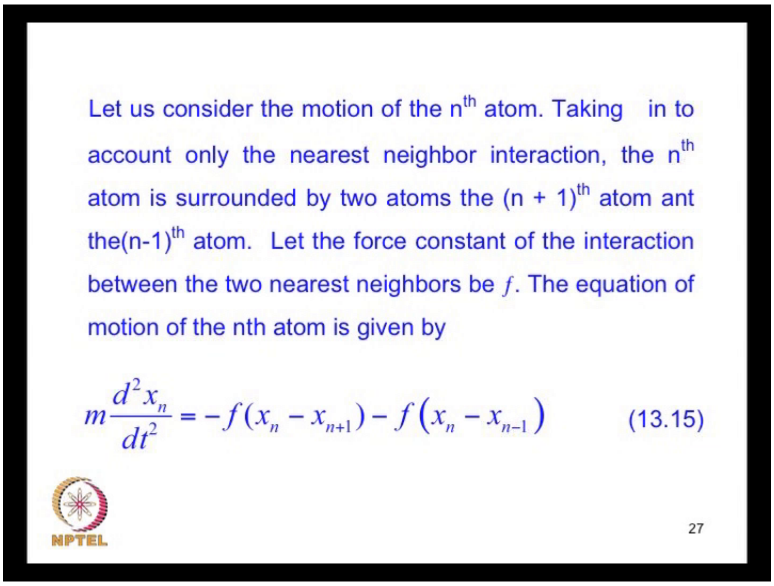

Let us consider the motion of the nth atom. Taking in to account only the nearest neighbor interaction, the nth atom is surrounded by two atoms the $(n + 1)^{th}$ atom ant the$(n-1)^{th}$ atom. Let the force constant of the interaction between the two nearest neighbors be f. The equation of motion of the nth atom is given by

$$m\frac{d^2x_n}{dt^2} = -f(x_n - x_{n+1}) - f(x_n - x_{n-1}) \qquad (13.15)$$

Let us consider the n th atom and consider its vibration; considered as a simple harmonic oscillator have to connected with its neighbors on either side the n minus one th atom. So

I have an atom here and atom here, and an atom here. This is n, this is n plus one, this is n minus one. So, there are this is a simple harmonic oscillator which means that we can think of springs of the same spring constant. So, let the force constant be f in which case if equation of motion of this n th atom can be written as m d square x n by dt square where x n is the displacement from equilibrium position of the n th atom, and that is given by minus f and this force constant then the net displacement is x n minus x n minus 1. And similarly, for the other atom x n minus x n plus one, so force constant time the displacement, the net extension are contractions. So, that gives the equation of motion and so we now assume, that these or these displacements are given by the running waves. So, a periodic solid in simple harmonic vibration, so you get the propagation of elastic waves of the form A e to the power minus i omega t plus q n x that will be the X n, where A is the amplitude.

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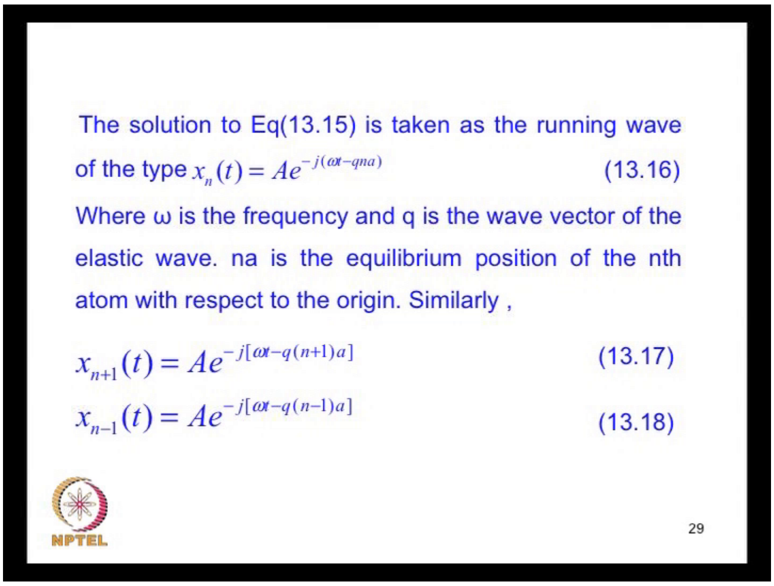

The solution to Eq(13.15) is taken as the running wave of the type $x_n(t) = Ae^{-j(\omega t - qna)}$ (13.16)

Where ω is the frequency and q is the wave vector of the elastic wave. na is the equilibrium position of the nth atom with respect to the origin. Similarly ,

$$x_{n+1}(t) = Ae^{-j[\omega t - q(n+1)a]} \quad (13.17)$$

$$x_{n-1}(t) = Ae^{-j[\omega t - q(n-1)a]} \quad (13.18)$$

I should write the repeat distance. So, this is the repeat distance, the regular spacing in the lattice. We have similar expressions for x and minus 1, and x n plus 1, wherever n occurs you replace it with n minus 1 or n plus 1 respectively.

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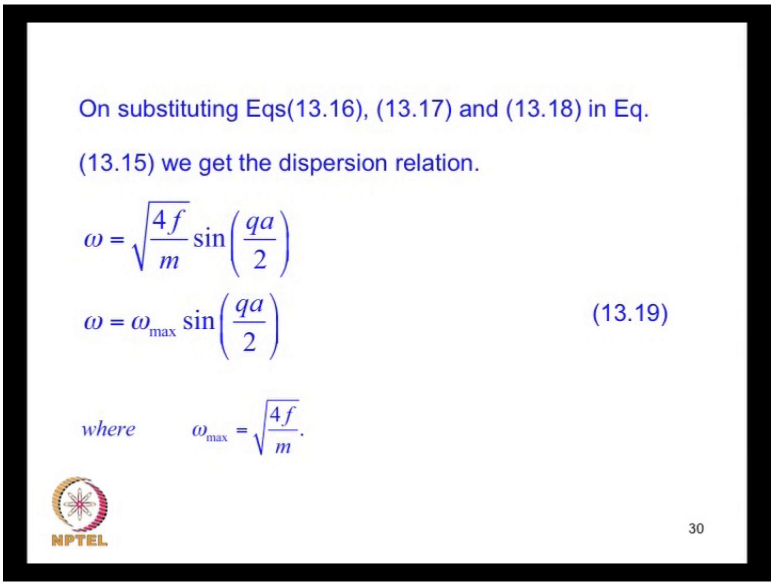

On substituting Eqs(13.16), (13.17) and (13.18) in Eq. (13.15) we get the dispersion relation.

$$\omega = \sqrt{\frac{4f}{m}}\sin\left(\frac{qa}{2}\right)$$

$$\omega = \omega_{\max}\sin\left(\frac{qa}{2}\right) \qquad (13.19)$$

where $\omega_{\max} = \sqrt{\frac{4f}{m}}$.

Once you have this and substitute this and substitute this in this equation of motion that we have written here, so d square extended simply give minus m omega square x n.

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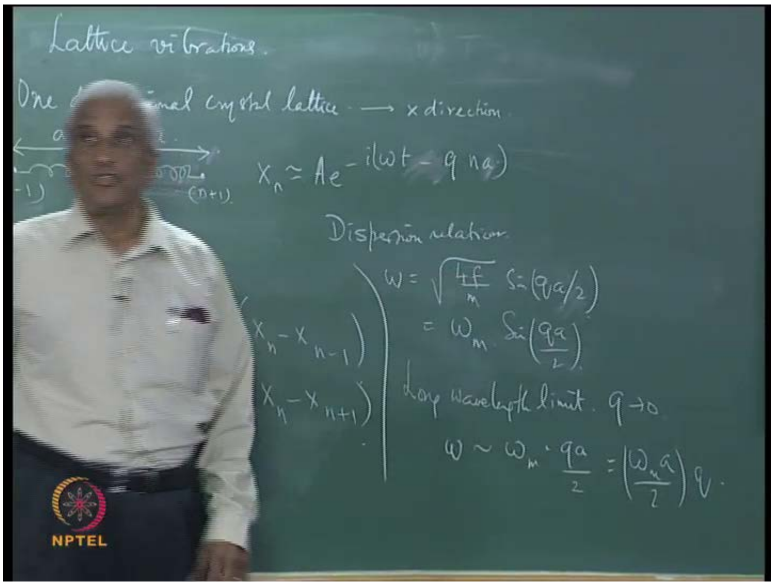

So, that will gives the so we will simplifying this, we have arrive at the so-called dispersion relation which relates the omega to the wave vector the angular frequency to wave vector and that is given by omega as root 4 f by m sign q a by two. This is a kind of we can call this omega maximum, so that gives the relation between omega and q the angular frequency and the wave vector. So, this is called the dispersion relation of the elastic wave propagating in a discrete medium. So, we have something like this and we can see that for a long waves, long wavelength limit which mean the phonon wave vector wave number is to pi by lambda.

So, if the wavelength is long the q becomes smaller and smaller. So, we can take the limit q tends into zero in that case we can write replace sign q a by two as omega goes as omega m into q a by 2 are equal to omega m a by 2 into q. So, you see a omega and q these are all constant; omega m means root four f by m; where m is the mass of the atom and f is the force constant, so a is lattice periodicity. So, all these are constant of the given lattice. So, you can see that omega is a linear function of the wave vector as indeed be known for sound waves. So, this is what we have assumed for the continuum model of the Debye model.

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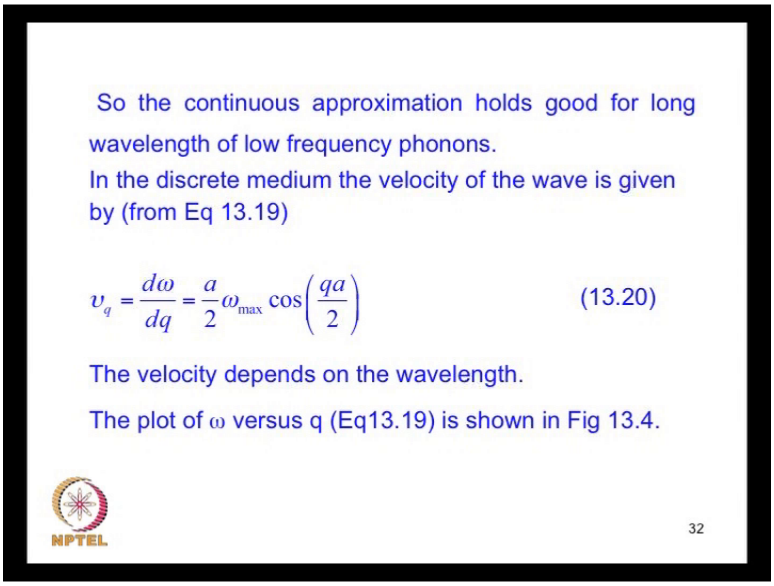

So the continuous approximation holds good for long wavelength of low frequency phonons.

In the discrete medium the velocity of the wave is given by (from Eq 13.19)

$$v_q = \frac{d\omega}{dq} = \frac{a}{2}\omega_{\max}\cos\left(\frac{qa}{2}\right) \qquad (13.20)$$

The velocity depends on the wavelength.

The plot of ω versus q (Eq13.19) is shown in Fig 13.4.

Whereas for high frequencies, when q is no longer 0, and q become sufficiently large, we have to consider the actual dispersion relationship of this kind.

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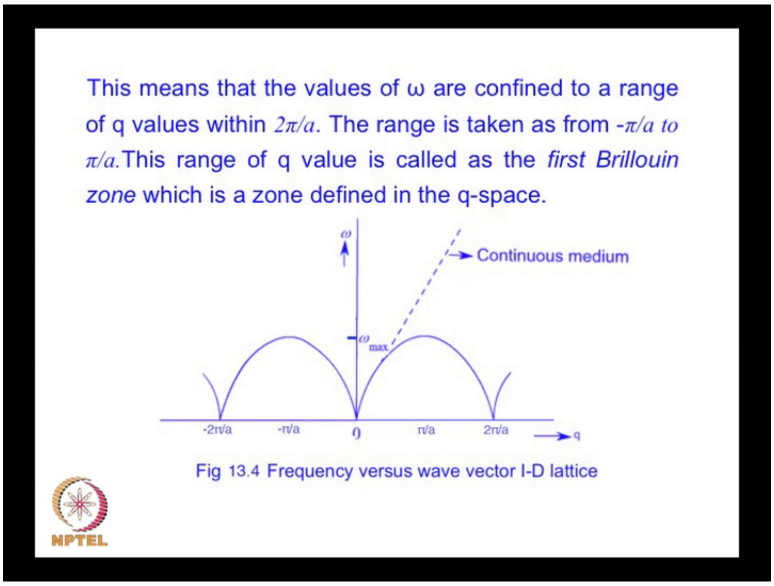

This means that the values of ω are confined to a range of q values within $2\pi/a$. The range is taken as from $-\pi/a$ *to* π/a. This range of q value is called as the *first Brillouin zone* which is a zone defined in the q-space.

Fig 13.4 Frequency versus wave vector I-D lattice

So, the figure gives you the actual variation figure nine eight gives the frequency versus wave vector for a one-dimensional lattice. In this you can see, it is a periodic repeating pattern the function is periodic therefore, it is enough if we consider the range of q values from minus pi by a to plus by a minus pi by a to plus pi by a that will you have something like this.

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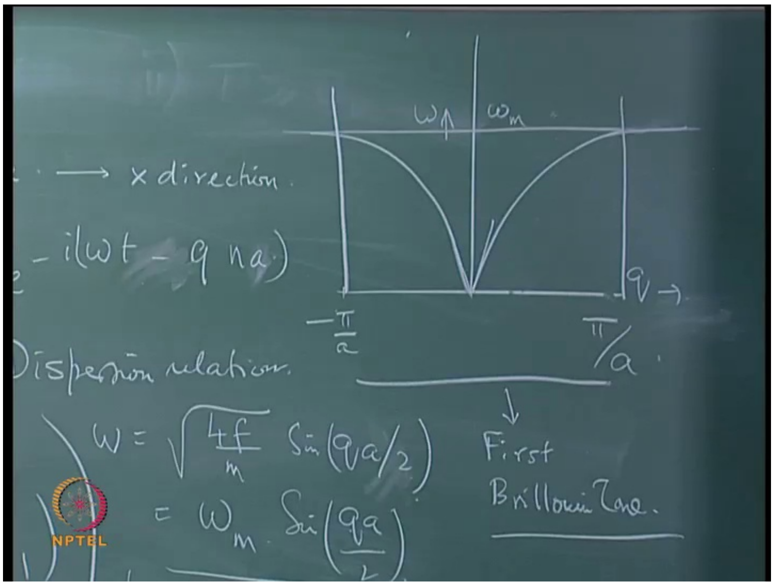

→ x direction.

$- i(\omega t - q\, na)$

Dispersion relation.

$\omega = \sqrt{\frac{4f}{m}} \sin(qa/2)$

$= \omega_m \sin\left(\frac{qa}{2}\right)$

So, this is omega m at very small values of q this is a linear function; beyond that at higher q values it deviate from the linearity and become a sinusoidal function which is a periodic function. So, we can consider it is enough if we can consider the behavior within this range of q values from minus pi by a to plus pi by a, this zone this range of values defines this is. So, called first brilloum zone. So, the phonon density of state can be considered within this. We next go on to the case of finite one-dimensional lattice of identical atoms, because we know that any crystal lattice is not infinite, even though it is periodically convenient assume that it is infinite, but it is not infinite. And so we must relief this assumption and considered the finite nature of this lattice. We will do this in the next lecture.

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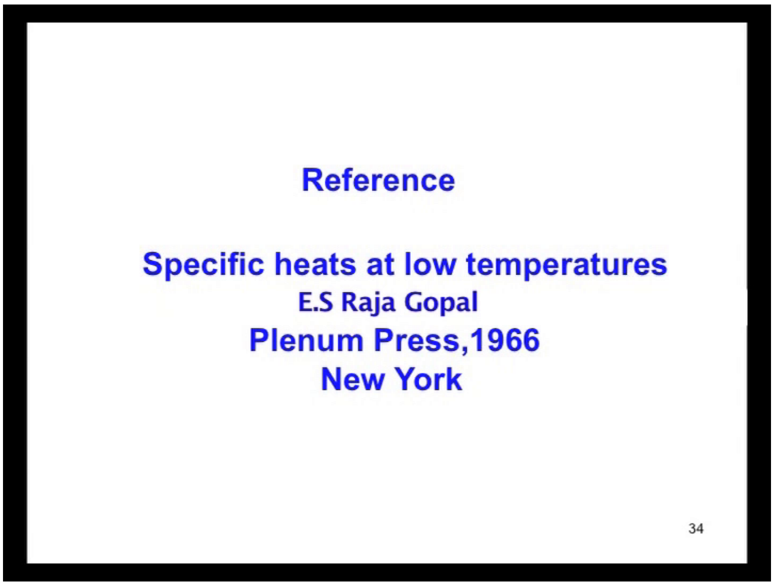

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