


Condensed Matter Physics
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Lecture - 14
Lattice Vibrations (Continued) Phonon Thermal Conductivity

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$$\omega = \sqrt{\frac{4f}{m}} \sin\left(\frac{qa}{2}\right)$$
$$\omega = \omega_{\max} \sin\left(\frac{qa}{2}\right) \quad (14.1)$$

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




So, last time we discussed the case of vibration of the crystal lattice in particular, and infinite 1 dimensional lattice of identical atom, and consider what would be the normal modes and the frequencies of the modes of vibrations.

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Vibrations of infinite one dimensional lattice.

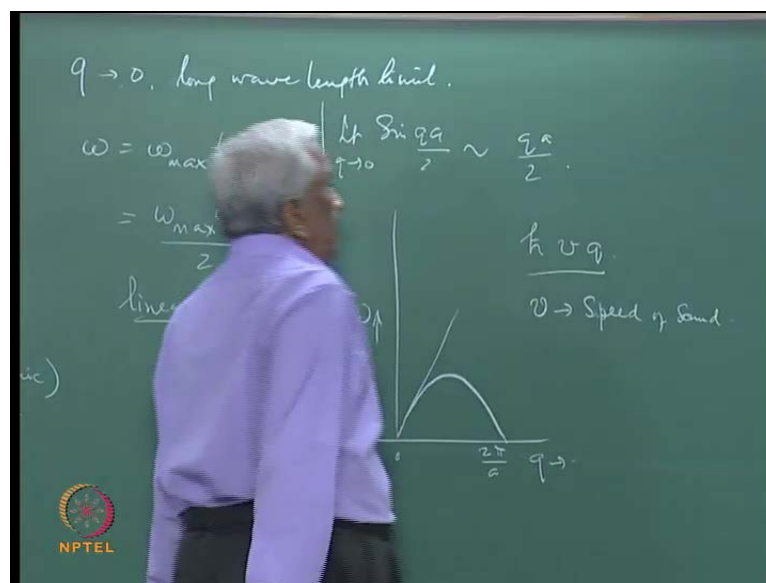
$$\omega = \omega_{\max} \sin\left(\frac{qa}{2}\right)$$
$$\omega_{\max} = \sqrt{\frac{4f}{m}}$$

$q \rightarrow$ wave number
 $f \rightarrow$ force constant (harmonic)
 $m \rightarrow$ mass of (identical) atoms
 $a \rightarrow$ repeat distance.



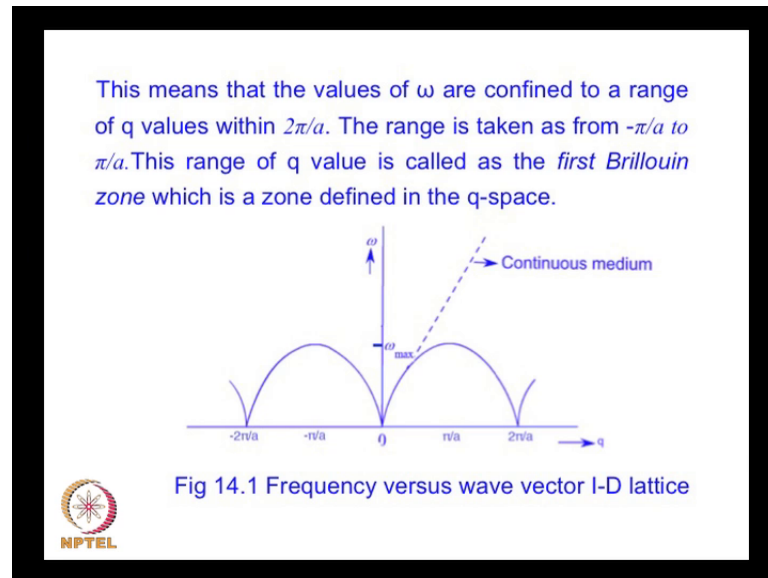
We got the basic what are known as the dispersion relation, which has the form $\omega = \omega_{\max} \sin qa/2$, where ω_{\max} is a maximum angular frequency which is $\sqrt{4f/m}$ here we just recall q is the wave vector of the periodic wave which propagates. And then or wave number, this is the 1 dimensional infinite 1 dimensional lattice vibrations of... So, f is the force constant between adjacent atoms which are identical and each of mass m identical atoms, which are vibrating and this is taken to be a harmonic simple harmonic vibrations, a is the repeated distance or periodicity along the line of atoms.

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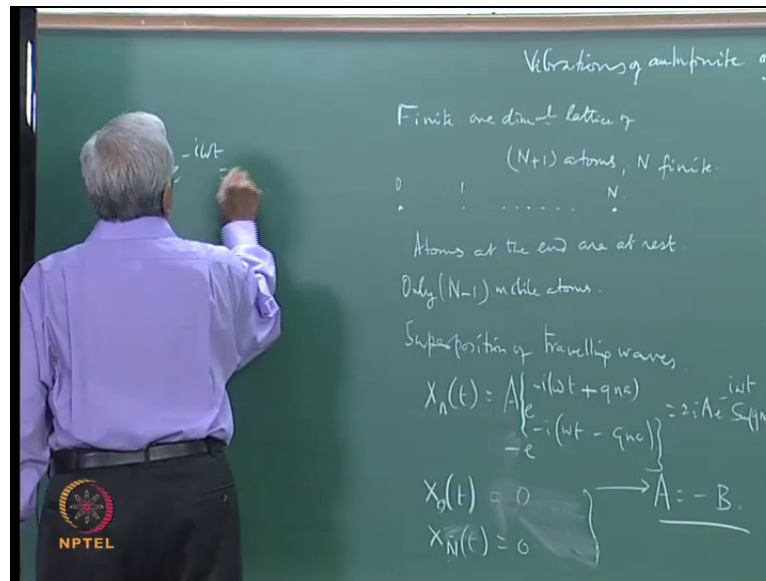
So, that for q in the q tending to 0, which means wavelength is long wavelength then we know this dispersion relation becomes because $\sin qa/2$ in the limit q tending to 0 is $qa/2$. So, this is ω_{\max} into $a/2$ times q . So, a constant ω q relationship is a linear relationship very much like the standard sound waves.

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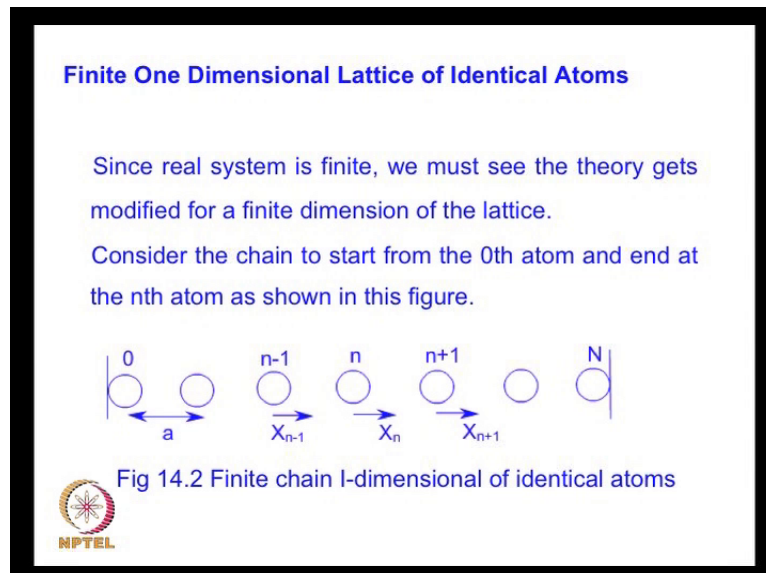
So, in the long wavelength limit the dispersion relationship gives you a dispersion relationship which is shown in the figure. So, where you have ω as a function of q . So, it goes like this in close to this, but beyond for larger as the wave vector this changes this deviates, and given by this dispersion relationship a sinusoidal relationship. So, this is the basic content of this 1 lattice dimensional vibrations, and these are the excitation of the quantize excitation of energy $h \times v \times q$, where v is the velocity of sound wave sound speed, speed of sound gives you the this gives you the energy of energy quantum of energy of this phonons which are quantize excitation of this lattice vibrations of discuss to lattice. Of course, we have made an approximation we have made the harmonic approximation, we have also taken this line to be a lattice to be infinite lattice and so on.

(Refer Slide Time: 05:42)



So, we would like to consider a real situation where these assumptions are slowly removed. So, that we have a finite 1 dimensional lattice of $n + 1$ atoms that is the zeroth atom and then 1 and so on, then you have n . So, counting from 0 to n you have $n + 1$ atoms in this as shown in the figure and where n is finite.

(Refer Slide Time: 06:19)



So, we are considering this again the model is the same we are considering the restoring force is which are simple harmonic and the 2 atoms at the end the zeroth atom and n atom at the end are addressed, there are held health bound. So, there are only $n - 1$

mobile atoms. And now because this is the boundary bounded chain which goes which is the has the boundary at the ends. So, it will be the solution is taken and not as travelling waves, but as a superposition of 2 travelling waves in general. So, we take for example, x_n of T the displacement of the n atom is taken to be $a e^{i(\omega T + qna)}$ plus $b e^{i(\omega T - qna)}$ where n is the n 'th atom.

(Refer Slide Time: 08:30)

A and B are the amplitudes of the two waves traveling from left to right and right to left respectively. The phase difference between the two waves may be assumed to be zero.

The two boundary conditions are:

(i) $x_0(t) \equiv 0$ and (ii) $x_n(t) \equiv 0$,

$$x_n(t) = A(e^{-i(\omega t - qna)} - e^{-i(\omega t + qna)})$$

$$x_n(t) = A e^{-i\omega t} (e^{jqna} - e^{-jqna})$$

$$x_n(t) = 2iA e^{-i\omega t} \sin(qna)$$

NPTEL 97

Now, that is a progressive wave which is going from left to right this is the wave like solution moves from right to left. So, the general solution is taken to be super position of these 2. So, that you get kind of standing waves in the system, because the n is fixed. So, the boundary conditions or x of T for an equal to 0 and n equal to n is 0 there are no there is no net displacement for any 1 of them. So, x_0 of T and is 0 and x_n of T is also 0 the atoms at the end are here fixed. So, if you consider such a situation then in general this superposition with this boundary condition we get a is equal to minus b as you can readily verify therefore, this becomes, and that is nothing but $2iA e^{i(\omega T - qna)}$ because at this boundary condition.

(Refer Slide Time: 10:35)

$$\text{Re } X_n(t) = 2A \sin \omega T \sin(nqa)$$

$$X_n(t) = 0$$

$$= 2A \sin \omega T \sin(nqa)$$

$$Nqa = m\pi,$$

$$m \text{ integer.}$$

Atoms at the end are
 Only $(N-1)$ mobile atoms.
 Superposition of travelling

$$X_n(t) = A \left\{ \begin{array}{l} e^{-i(\omega t + \dots)} \\ e^{-i(\omega t - \dots)} \end{array} \right.$$

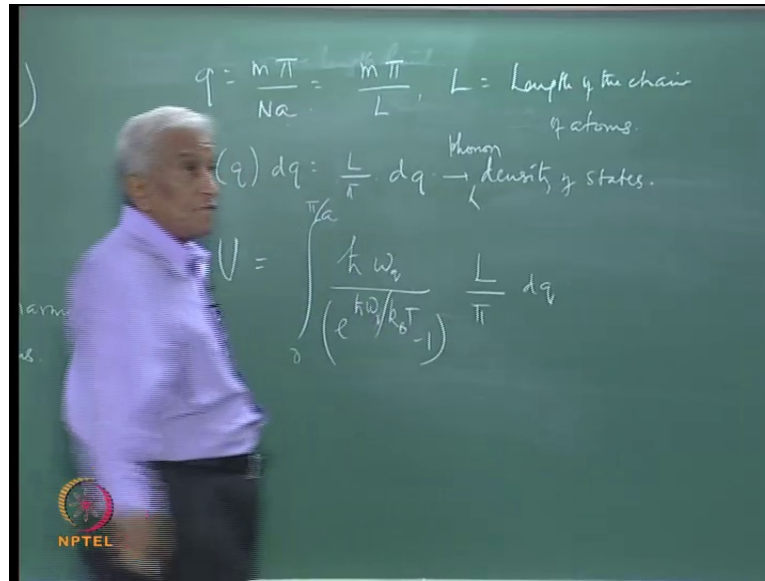
$$X_0(t) = 0$$

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So, that sense e to the power $i\omega T$ is nothing, but $\cos \omega T$ minus $\sin \omega T$ therefore, the real part of the solution really is just, if you take this this will become I times this. So, this will be $2a \sin \omega T \sin nqa$ that will be the real part now using this as the solution the equations of the motions. Of course, are the same therefore, applying this equation motion we get the same dispersion relationship as for the infinity chain. So, now that is the same.

So, we arrive at the identical I do not want to prove this it is just it can readily verify solution and with the equation motion which we consider already in the last lecture. Now we apply the second boundary condition namely x_n of T also is zero. So, the n 'th atom is also at rest. So, when I substitute this this becomes $2a \sin \omega T \sin nqa$ and that is equal to 0 giving immediately nqa equal to $m\pi$ where m is an integer. So, the allowed modes corresponding to different q value are restricted by this condition, that is the second boundary condition.

(Refer Slide Time: 12:42)




So, we have finally, we have q equal to $m \pi$ by na , which we can write na is the total length of the chain there are n atoms which a apart. So, this is nothing but $m \pi$ by l , where l is the length of the chain chain of the atom. So, we have this and the modes of the vibration the density of states can all be found using the same conditions as for as we did earlier.

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There is one mode for every change in q value by $\frac{\pi}{L}$. So the number of modes in a range dq is $\frac{L}{\pi} dq$, i.e the density of modes:

$$D(q) dq = \frac{L}{\pi} dq \quad (14.5)$$

Expression (14.5) is different from Equation(13.3) because the periodic boundary condition (Eq 13.1) for an infinite one dimensional solid is different from the cyclic boundary condition for a one dimensional solid of finite number of atoms.




And we get the density of modes d of q $d q$ which will be 1 by π times $d q$ 1 by π is number of modes per unit unit q value length in q square. So, if you take an interval $d q$ around the q value it is 1 by $\pi d q$.

(Refer Slide Time: 14:20)

With this expression for density of modes, the energy of the system of vibrating atoms in a one dimensional lattice can be evaluated by

$$U = \int_0^{\pi/a} \frac{h\omega}{e^{h\omega/k_B T} - 1} D(q) dq = \frac{L}{\pi} \int_0^{\pi/a} \frac{h\omega}{e^{h\omega/k_B T} - 1} dq \quad (14.6)$$

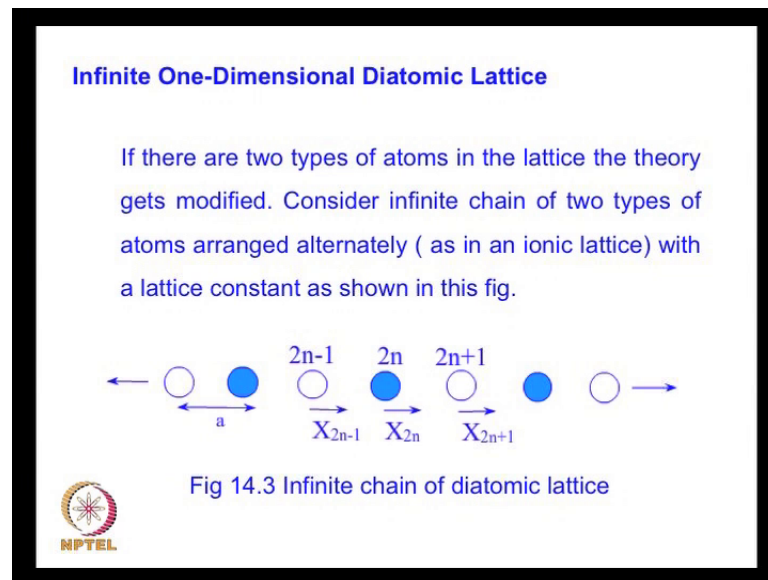
The integral may be evaluated by expressing q in terms of ω using Equation (14.4) we get

$$U = \frac{2L}{\pi a} \int_0^{\omega_{\max}} \frac{h\omega d\omega}{(e^{h\omega/k_B T} - 1)(\omega_{\max}^2 - \omega^2)^{1/2}} \quad (14.7)$$


So, this is the density of states phonon density of states using this we can again calculate because we know the internal energy. For example, the specific heat how does this get modified, because via have done that what have done here. We have departed from the d by assumption of a continuous medium they continue and replace it by a discrete finite 1 dimensional lattice of atoms taking into account's periodicity and the discreteness of such a lattice.

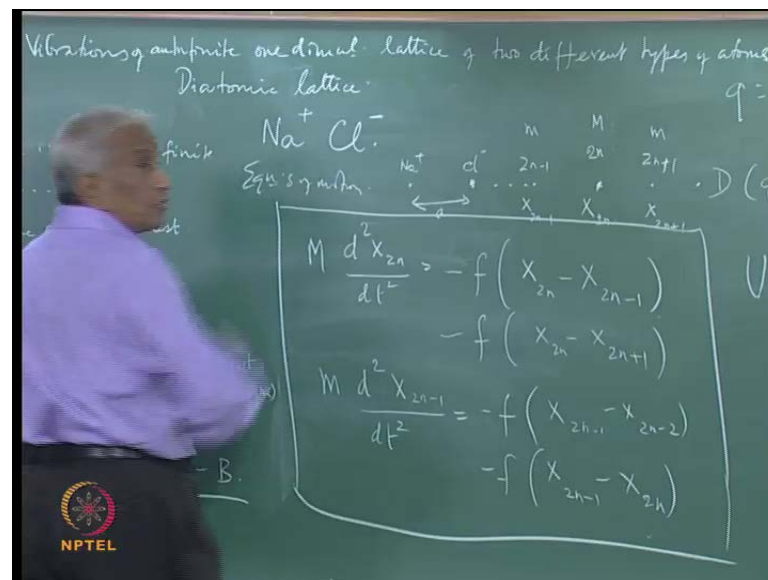
So, again we find h cross ω by e to the power h cross ω by $a b T$ minus 1 is the average energy, we discussed already in connection with the d by solid and then multiply by 1 by $\pi d q$ integrated from 0 to π by a . And that would give me this is a ωq their ωq is related to the dispersion by this therefore, replacing that. So, that would be the corresponding expression and the specific heat is got by differentiating the specific heat $d u$ by $d T$ as before. So, this is the modification to Debye theory which which brought about by removing the model of a continue and replacing it with a discrete 1-dimensional the extensional to 3-dimensional is a straightforward will not go through that now.

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But let us consider while we are talking about lattice vibration which gave rise to phonons with the different modes.

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We will consider extend this model that we have just discussed to the case of an infinite 1 dimensional lattice, but of 2 different types of atoms it is called diatomic lattice not a monatomic lattice for why is this important. The reason for the importance comes from the fact that many solids are diatomic in nature many common solids like sodium chloride for example. So, you have an infinite lattice of atoms in a 3-dimensional lattice, but

we will consider for simplicity and infinite 1 dimensional chain consisting of sodium ion and negative chloride ions. So, there are different masses.

So, they have arranged alternatively. So, you have a lattice of n plus 1 minus again n plus 1 minus like that. So, again we consider an infinite lattice the spacing is the same. So, let us consider the $2n$ 'th atom they this is $2n$ 'th atom. So, you have many such. So, you have its neighbor $2n - 1$ and another neighbor next neighbor we consider only the next neighbor interaction. So, the displacement is taken of the $2n$ 'th atom is taken as x_{2n} and the corresponding displacement of this atom is $x_{2n - 1}$ and this is $x_{2n + 1}$. Now, this is the atom of mass M while this is another atom these 2 atoms are of mass m . So obviously, the equations of motion are going to be different from that for the monatomic lattice.

So, let me write the equation of motion for example, for the atom of mass M that will be $M d^2 x_{2n} / dt^2$. This is the mass times acceleration is given by minus f times $x_{2n - 1} - x_{2n}$ minus f times $x_{2n} - x_{2n + 1}$ at a similar equation there are 2 equations, now 1 for the mass capital M and the other for the small m . So, this will be minus f times $x_{2n - 1} - x_{2n}$ minus f times $x_{2n} - x_{2n + 1}$ that would be the neighbor here on this side, and minus f times $x_{2n + 1} - x_{2n}$. So, these are the equations of motion in the harmonic approximation these are the equations which we you have to solve using the identical procedure.

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Let the mass of the even numbered atoms (*i.e.* $2n^{\text{th}}$) be M and the mass of odd numbered atoms be m . The $2n^{\text{th}}$ atom of mass M is surrounded by the $(2n + 1)^{\text{th}}$ and the $(2n - 1)^{\text{th}}$ atoms of mass m . Let the force constant of interaction between the two types of atoms be f . The equations of motion of the $2n^{\text{th}}$ and the $(2n + 1)^{\text{th}}$ atoms are

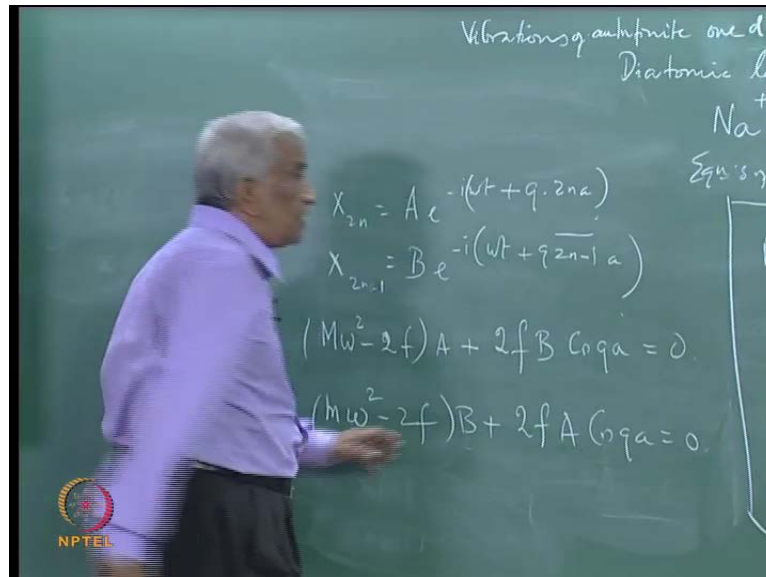
$$M \frac{d^2 x_{2n}}{dt^2} = -f(x_{2n} - x_{2n+1}) - f(x_{2n} - x_{2n-1}) \quad (14.8)$$

$$m \frac{d^2 x_{2n+1}}{dt^2} = -f(x_{2n+1} - x_{2n+2}) - f(x_{2n+1} - x_{2n}) \quad (14.9)$$



So, we have since it is an infinite lattice, we can assume travel waves solutions.

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So, we assume x_{2n} equals $A e^{-i(\omega t + q \cdot 2na)}$ and x_{2n-1} for example, is not necessarily $B e^{-i(\omega t + q \cdot (2n-1)a)}$. So, A and B are the amplitude of the vibration of the atoms of mass capital M and small m substituting this in the equation of motion and doing the different situation et cetera and solving them, we arrive at a detrimental solution which is the solution for the resulting for simultaneous equation. So, this times A plus $2fB \cos qa = 0$. And similarly $m\omega^2 - 2f$ plus $2fA \cos qa = 0$, these are the simultaneous equation which results from this.

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The solutions are taken as the running wave of the type:


$$x_{2n} = Ae^{-i(\omega t + q \cdot 2na)} \text{ and } x_{2n-1} = Be^{-i(\omega t + q \cdot 2n-1a)} \quad (14.10)$$

Where A and B are the amplitudes of vibration of atoms of mass M and m respectively.

On substituting Eq.(14.9) in (14.7) and (14.8), we get the two equations:

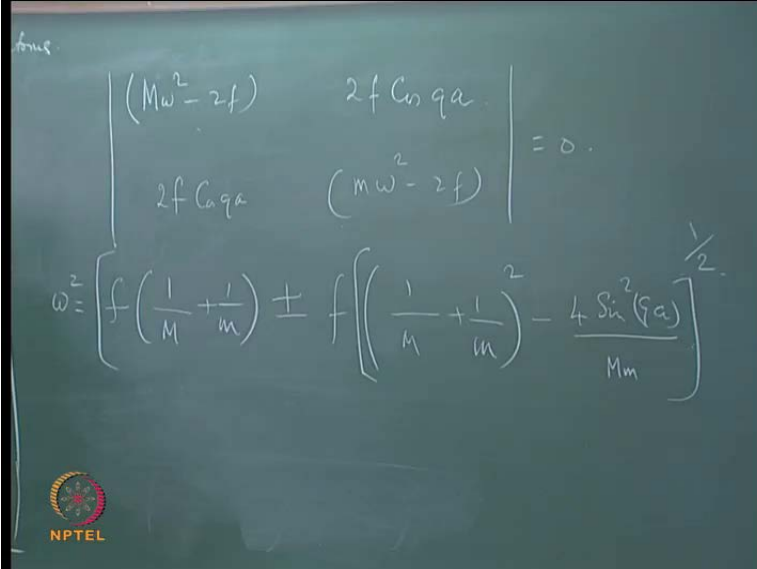
$$(M\omega^2 - 2f)A + 2fB \cos qa = 0 \quad (14.11)$$

and

$$(m\omega^2 - 2f)B + 2fA \cos qa = 0 \quad (14.12)$$



So, solution of this requires the determinant of coefficient to vanish for nontrivial solution. So, setting this determinant equal to 0, and solving the result in quadratic equation is a 2 by 2 determinant which has the form.

(Refer Slide Time: 23:02)



Handwritten derivation on a chalkboard:

$$\begin{vmatrix} (M\omega^2 - 2f) & 2f \cos qa \\ 2f \cos qa & (m\omega^2 - 2f) \end{vmatrix} = 0$$

$$\omega^2 = \left[f \left(\frac{1}{M} + \frac{1}{m} \right) \pm f \left[\left(\frac{1}{M} + \frac{1}{m} \right)^2 - \frac{4 \sin^2(qa)}{Mm} \right]^{\frac{1}{2}} \right]$$


So, that would be the detrimental solution. So, solving this resulting quadratic equation we get omega square equals f times 1 by m plus 1 by m plus or minus f times 1 by m plus 1 by m square minus four sin square q a by m times m. So, that would be to power half is we are looking for real solution for the frequencies, we take only the less sign here

and then write the solution, and so we will have 2 solutions corresponding to the plus and minus sign. So, you will have ω_1 and ω_2 . So, we will have dispersion curve which will have 2 branches corresponding to ω_1 and ω_2 or ω_+ and ω_- .

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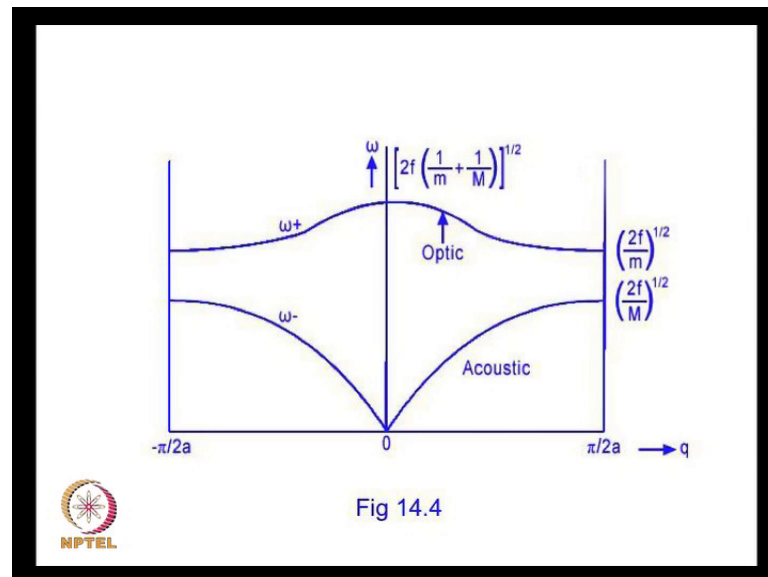
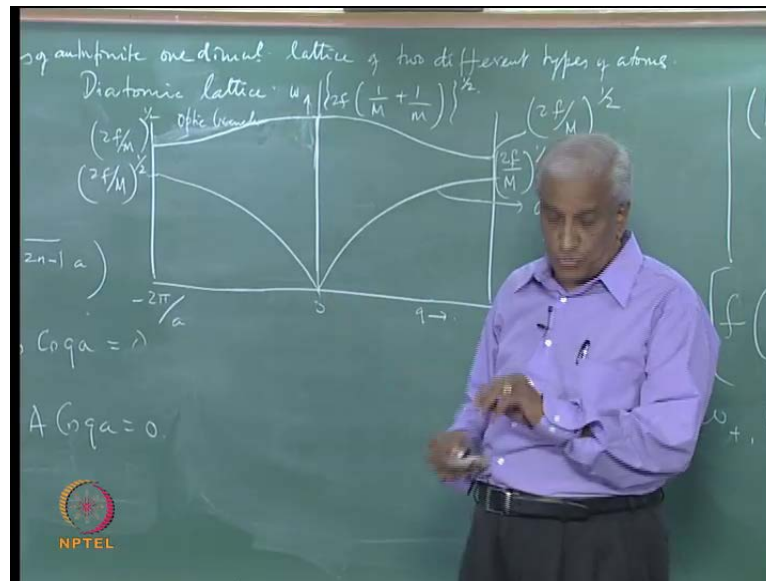


Fig 14.4

So, this can be plotted just like in the case in the monatomic solid. So, this gives me modes of vibration normal modes of vibration of a diatomic lattice, and infinite 1-dimensional diatomic lattice. So, that is the essential difference between these 2 cases and the previous case.

(Refer Slide Time: 25:37)




So, you have the acoustic and optical branches these are allowed phonon modes, which must be used in calculating the characteristics of the of such a lattice.

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It is seen that the greater the ratio between the masses M and m , the greater will be the separation between the optical and the acoustic branches.

By substituting the value of ω_+ and ω_- , at $q = 0$, in Eq (14.10) and (14.11), we get the following results:

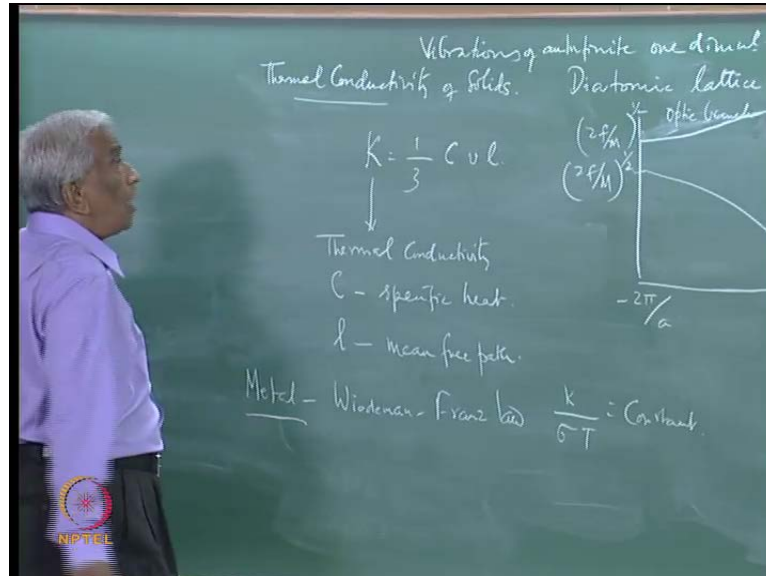
For optic mode: $\frac{A}{B} = -\frac{m}{M}$



For example sodium chloride and despairingly other alkali atom, so having discussed the properties of phonon modes the allowed phonon modes for simple models of the solid. We can try to see what it means for the thermal properties that we discussed already we already talked about specific heat to some extent, but let us now go back to thermal conductivity. So, in the case of thermal conductivity we have already discussed the

thermal conductivity of metallic solid, and the thermal conductivity allows mainly from the conduction by the electrons considered as a gas.

(Refer Slide Time: 27:01)




And we use the kinetic theory expression for the conductivity namely k equals $\frac{1}{3} c v l$ now here c is a thermal conductivity. So, v is the c is a specific heat or heat capacity v the speed and l is the mean free path this is the expression that we have already used in connection with the electron gas. And how the thermal conductivity contribution due to that we have already seen that the Wiedemann Franz law. In the case of a metal we have already considered how you have so-called theoretical description leads to Wiedemann Franz law $\frac{k}{\sigma T} = \text{constant}$ where k is the thermal conductivity, and σ is the electrical conductivity and T is the absolute temperature. So, we have seen this part metals. Now we are going to consider what happens when the thermal conduction takes place in an insulator in an insulators, there are no electrons there are no conduction electrons.

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The total thermal conductivity K is given by

$$\frac{1}{K_{total}} = \frac{1}{K_{Umklapp}} + \frac{1}{K_{impurity}} + \frac{1}{K_{boundary}} \quad (14.12)$$


To explain the temperature dependence of thermal conductivity, the expression for thermal conductivity of gases obtained from the classical kinetic theory of gases may be extended to solids. The expression for thermal conductivity of gases is

$$K = \frac{1}{3} C v l \quad (14.13)$$


So, if you have insulating solid like a plastic or a ceramic or any such. So, there are no conduction electrons. So, the thermal conduction cannot take place through the electrons. So, the thermal conduction mechanism is by a phonon. So, the carriers of heat in insulators are the phonons, and there is exchange of energy and momentum between the phonons, namely the phonon-phonon interactions that give rise to thermal conduction in insulators. So, this is the reason why we consider the nature of the lattice vibration.

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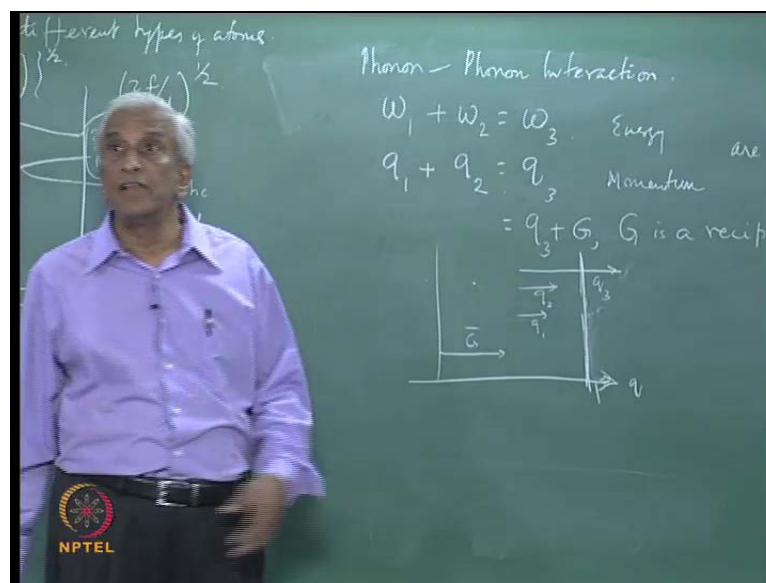
In a material, at temperature T , there will be a certain equilibrium distribution of phonons. When there is a temperature gradient in the material, the phonon distribution will be disturbed. Phonon-phonon collisions occur in the system to restore the equilibrium distribution. The rate of the restoring process decides the thermal resistance of the material. In a poor thermal conductor, the rate of restoration of equilibrium is very slow. The process of restoration is through phonon-phonon interaction.



54

So, you have certain equilibrium distribution of phonons at any finite temperature t , and when there is a temperature gradient in the material the phonon distribution will be disturbed. Phonon-phonon interaction will occur. And this will tend to restore the equilibrium distribution. Now this restoration will take place with a characteristic relaxation time. So, the rate of the restoring process is what determines thermal resistance of the material. In a poor thermal conductor the rate at which the restoration of equilibrium takes place is very slow. So, basically this is entirely due to phonon-phonon interaction.

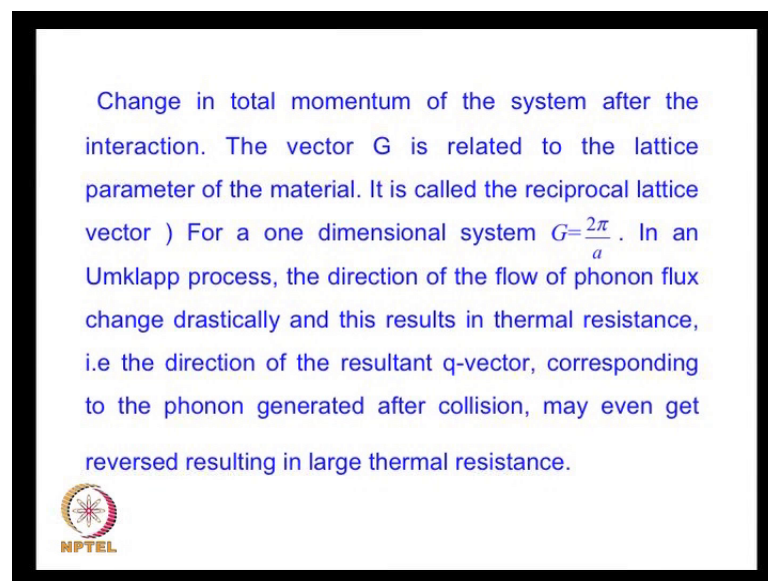
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So, the interaction is described by equations which conserve energy $\omega_1 + \omega_2 = \omega_3$. So, multiplied throughout by \hbar it becomes $\hbar\omega_1 + \hbar\omega_2 = \hbar\omega_3$, this gives you energies of 2 phonons of frequencies ω_1 and ω_2 resulting in a third phonon of frequency ω_3 angular frequency. There is also the conservation of momentum which is described by the equation $q_1 + q_2 = q_3$. So, the momentum and the energy are conserved in such a process. So, this is known as a normal or n process. You can also have a situation where this is the same, but this becomes $q_3 + G$, where G is what we have seen already is a reciprocal lattice vector. q is a reciprocal space vector.

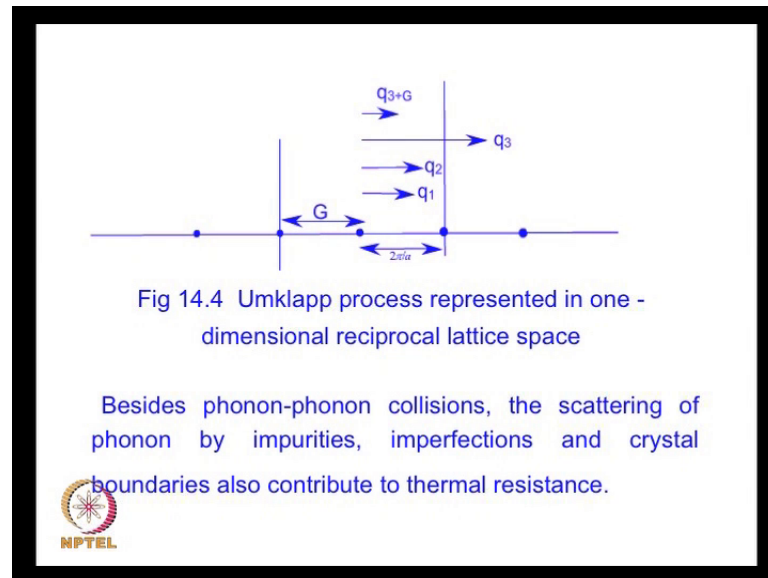
So, this such a where this is also allowed and this is known as umklapp process known in short as a u process. So, both this processes are possible in in phonon phonon interaction both will contribute to the conductivity. So, this tells you a phonon of energy $\hbar \omega_1$ interacts with another phonon in track energy $\hbar \omega_2$ resulting in a creation of a phonon of energy $\hbar \omega_3$. So, the total energy of the phonon system is conserved this tells you the corresponding conservation of the momentum of the corresponding q_1 and q_2 $\hbar q_1$, and $\hbar q_2$ or the momentum of the interacting phonons result in the creation of phonon with momentum $\hbar q_3$.

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So, if you take these equations. So, you have changing the total momentum let spend a little time on this umklapp umklapp is a German word which tells which means folding up.

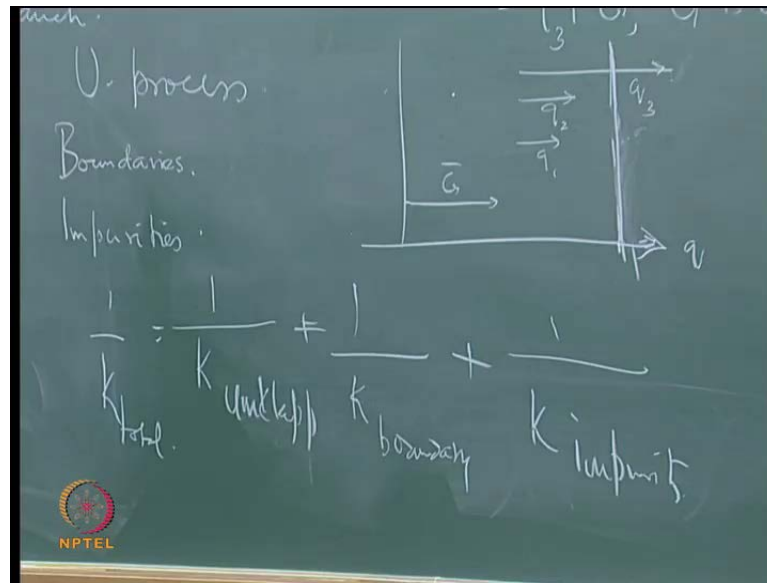
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So, let us just look at what this means. So, you have q space let me just plot it in 1-dimension. So, this is that and I have q_1 . So, this is its own boundary I have q_1 and q_2 and now I have q_3 the result of this addition gives you same q_3 now this take it outside this own boundary. And there have already talked about how we considered state within this own boundary for all our discussion because of the periodism, but this wave vector takes it the combination of q_1 and q_2 takes it outside this. So, what do we do we bring it back into this by adding a g 's a reciprocal lattice a reciprocal lattice vector.

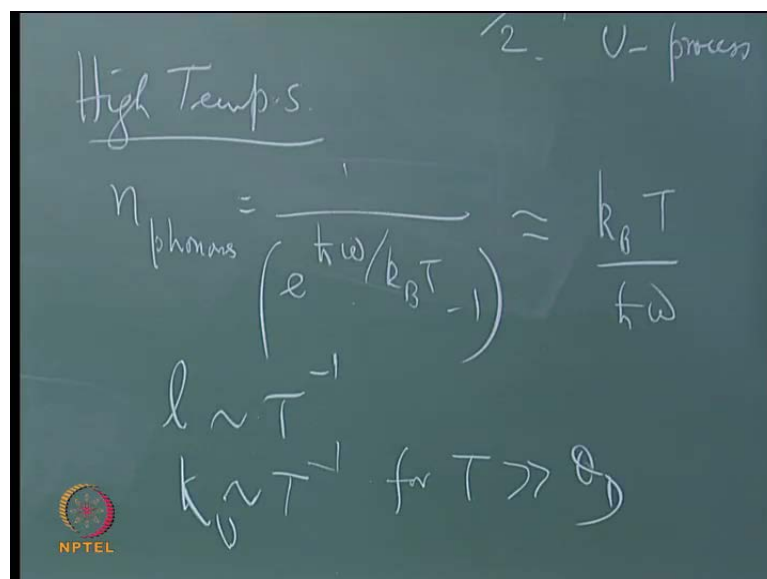
So, this comes back into the first zone in this case the course g will be in the opposite direction then this will be q_3 plus g where g is in this direction therefore, this will this result and vector will come back into the first zone. So, that is how this is this process take place and this makes this reversal and bringing it back means that the scattering at the phonon can reverse its direction its moment. So, the thermal resistance can be appreciable because of this. So, these are the processes which can contribute to thermal resistance in addition you can also have boundaries like grain boundaries.

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And then they can be impurities it is the unclad process which is dominant in thermal conduction due to phonons. So, each 1 gives a contribution and the net conductivity is 1 by k unclad plus 1 by k boundary plus 1 by k impurity. So, the each 1 contributes. So, that that gives you them f k. So, this is the total conducting conductivities add in this way this is the resistivity which are in series and conductivities which are reciprocals add this way. So, this is how we calculate over all thermal conduction just let us spend a little time to talk about what is the temperature dependence, now if I consider this kinetic expression kinetic theory.

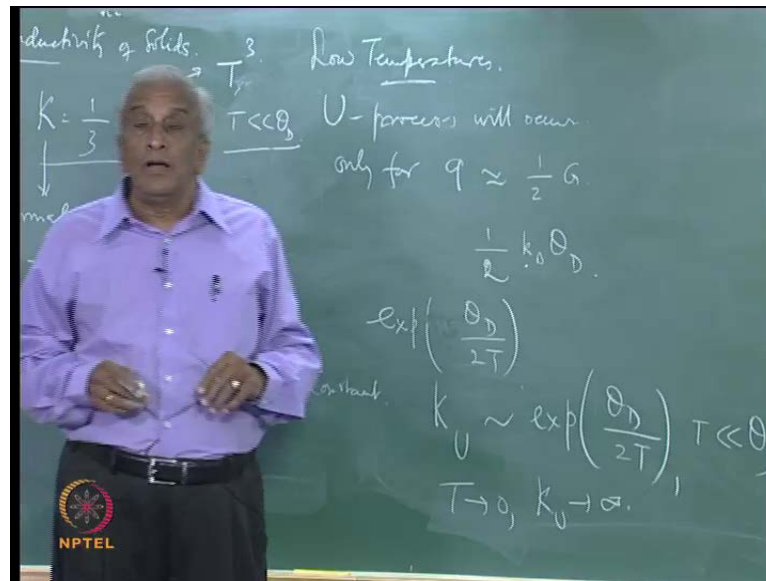
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Suppose consider high-temperatures thermal conductivity at a high-temperatures we know that the specific heat is independent of temperature at a high-temperature because of due long petitions law we are already consider, so the temperature dependence as the thermal connectivity you going to mainly depend on thermal temperature dependence of the mean free path. So, that is what will give you the net over all thermal temperature dependence of the conductivity. Now the mean free path is the average distance travelled by the phonons between successive collisions, therefore it will be the mean free path will become smaller if there are more number of phonons, and there are more collisions in other words mean free path for given phonon is inversely proportional to the density of all the other phonons.

So, a given node we know that the number of phonons number of phonons is given by $e^{-\frac{h\nu}{k_B T}}$ to the power of $h\nu$ by $k_B T$ minus 1. So, this is the factor which will give you this now this will be in the high temperature limit you can check this this will go as $k_B T$ by $h\nu$. So, the mean free path which is a inversely proportional to the number of phonons will go as 1 will go as T to the power minus 1 at high temperatures. So that means that the unit clock process the mean free path will go also as T to the power minus 1 for temperatures T very large compare to θ_D at a high temperature. If you have a pure solid, which is well and Neal, then impurity scattering can be neglected there are not any impurities, we are considering a pure specimen. And if the crystal size is fairly large then boundary effect can be neglected. So, we can forget about these the first approximation a when we have a pure large crystal. So, the thermal conductivity will essentially go by this. So, the conductivity will be proportional to the universe of the absolute temperature that is in the high temperature.

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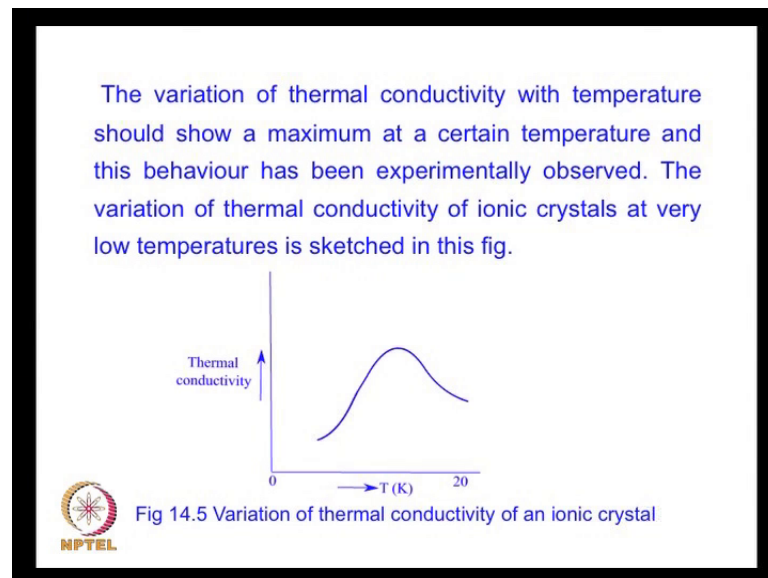


Now, let us go to the low temperature region at low temperatures the unclotche process will occur only for q of the order of half g you should be half a reciprocal lattice vector. We interacting phonon wave vector because the result an should be outside the first bellowing zone that foe that to happen? This is the condition and this wave vector corresponds to phonon energy of half $k_B T \theta_D$. So, if we take such an energy. So, what happens the number of phonons which have this is going to go as exponential minus θ_D by $2T$ this is going to be the number of because of the Boltzmann factor.

So, the temperature depends upon the phonon mean free path l due to the unclotche process must be proportional to exponential θ_D by t , because the mean free path goes as the inverse of the number density. So, the correspondingly the thermal conductivity also for the u process will go as exponential θ_D by $2T$ for T very small comparatively this means as T tens to 0 this tends to infinity, but the total thermal conductivity will not go to infinity, because it is limited by contribution for the boundary. And impurities scattering at low temperature the boundaries scattering will dominate for a pure crystal the mean free path of phonon is nearly equal to the dimensional the crystal. Because the mean free path becomes, if a if the crystal is pure the phonons have no impurities or defects are therefore the mean free path is nearly equal to the entire dimensional the crystal it becomes very large.

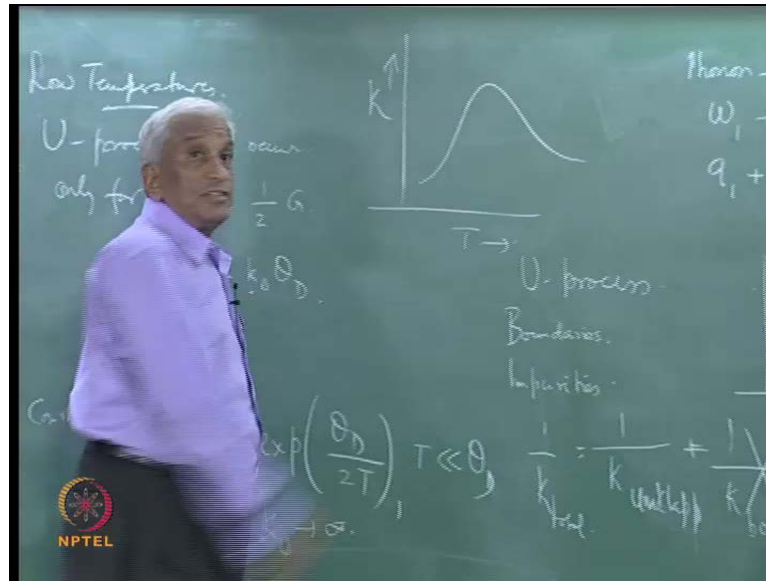
So, it will become practically independent of the temperature. So, the temperature dependence of k will be mainly due to the temperature dependence of the specific heat because this becomes temperature independent. And this goes at low temperature as T^3 for T less than 30 this is the d by specific heat the area. So, we have at these temperatures the k will go as T^3 . So, therefore, if you consider everything together the thermal conductivity of an insulator increases with increasing temperature starting from very low temperature being proportional to the cube as the absolute temperature and later unclotted process take over. And then the thermal conductivity decrease exponentially. If you change the temperature further if you increase the temperature if you increase further it vary as the T^{-1} .

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So, the overall temperature dependence is shown in a figure five. So, it goes some bottle like this you have a peak.

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So, this is the temperature dependence as the thermal conductivity of an insulator. So, such a wave an explain.