Micro and Nanoscale Energy Transport

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Lecture – 14
Fundamentals of Solid State Physics Part 3

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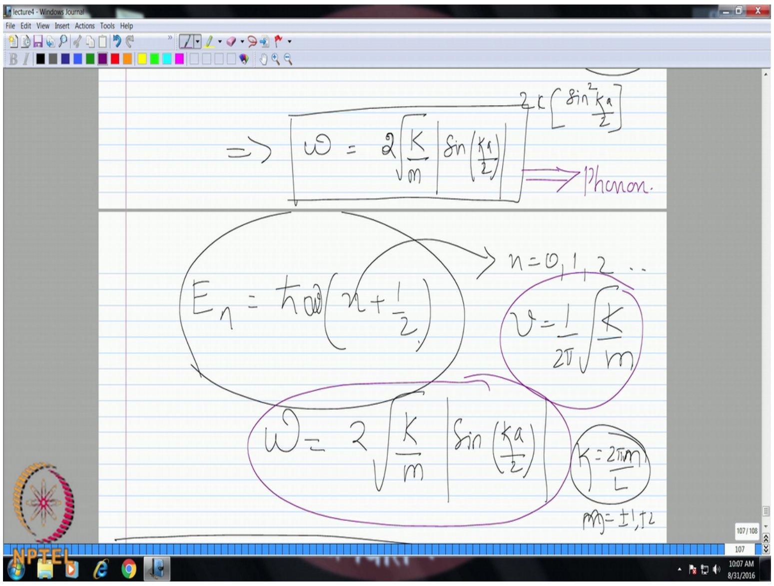

$2K\left[\sin^2\frac{\kappa a}{2}\right]$

$$\Rightarrow \boxed{\omega = 2\sqrt{\frac{K}{m}}\left|\sin\left(\frac{\kappa a}{2}\right)\right|} \Longrightarrow \text{Phonon.}$$

$$E_n = \hbar\omega\left(n+\frac{1}{2}\right) \rightarrow n = 0, 1, 2 \ldots$$

$$\nu = \frac{1}{2\pi}\sqrt{\frac{K}{m}}$$

$$\omega = 2\sqrt{\frac{K}{m}}\left|\sin\left(\frac{\kappa a}{2}\right)\right|$$

$$\kappa = \frac{2\pi m}{L}$$

$m = \pm 1, \pm 2$

Good morning, we will continue our discussion with respect to the vibration of atoms in a lattice, which is the phonon energy vibrational energy. So, yesterday we had derived the relationship between the vibrational frequency, this omega and the wave number kappa right. So, this is the dispersion relation that we had derived for with the respect to the phonons and we see that this is related to the spring constant the mass of the atom we have only 1 monatomic lattice here and this kappa here is the crystal wave vector which is 2 and pi by the length of the crystal.

So, this is discretize now because of the discrete values of kappa that it can take and we relate now this to the we actual quantum mechanical phonon vibrational energy. The vibrational energy derived for simple harmonic motion from quantum mechanics now only difference being there we had a simple relationship for the frequency now we going to substitute this with the dispersion relation that we had obtained. So, the dispersion relation itself has been obtained from just simple classical mechanics and substituting a wave solution into that and finally, discretizing the wave solution correct.

This is basically how we are approaching this vibrational energy level calculation for the phonons if you plot it I think probably if you tried yesterday to see how this dispersion relation looks; that means, we have omega on the vertical axis.

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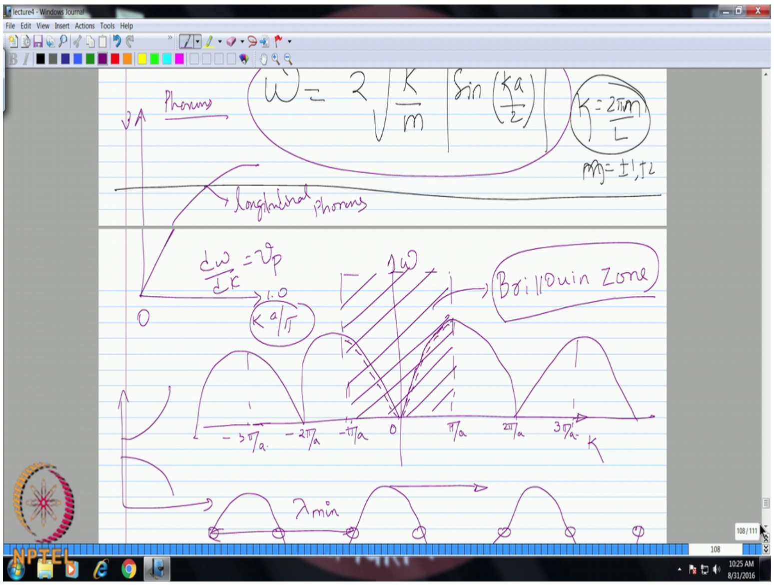

$$\omega = 2\sqrt{\frac{K}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

$$k = \frac{2\pi m}{L}$$

$$m = \pm 1, \pm 2$$

$$\frac{d\omega}{dk} = v_p$$

And once again you can plot either a non dimensional kappa or just kappa as it is if you plot kappa a by pi also that should be fine. So, how these are basically sin functions, but and these are absolute values. So, only will see everything in the positive values of omega right, therefore, if you vary your kappa let us say this is here, 0 you have minus pi by a to plus pi by a. So, these are values of kappa I am just varying by changing the values of m for example. So, on then you have 2 pi by a 3 pi by a and so on.

Similarly, here you have minus 2 pi by a minus 3 pi by a and so on. So, typically you will have the maximum at quad points suppose you substitute pi by a for kappa. So, this becomes sin pi by 2 which is equal to 1. So, that is the maximum value of omega that you will get. So, you get a maximum here and from there you will be again dipping down at 2 pi by a what happens if you substitute 0. So, similarly you have symmetry about this therefore, for the negative values of the wave number also you will be. So, this now it is going to be periodic and it is going to repeat. So, this will reach maximum here and so on.

So, this is how the dispersion looks in this case, now as you can see the values kappa or also now discrete right. So, these are not actually continuous bands again, but these are cos a continuous or discrete value s of m these kappa values have now discrete and you have corresponding values of omega. So, you can actually to be more accurate you have to denote this by means of the cos a continuous bands. Now we will see why we have drawn in this particular units minus pi by a and what is the significance of this block here. So, the block between minus pi by a to plus pi by a and as you can see from between this minus pi by a to plus pi by a it is looks like a unit cell you have the dispersion and about which it is periodic and repeating.

So, again if you say minus then you go from pi by a to 2 pi by a or 3 pi by a. So, now, this becomes repeating in structure. So, about the center line between minus pi by a and pi by that is totally for the width of 2 pi by a. So, it is 1 unit cell and then it keeps repeating every 2 pi by a correct. So, we will see what is this to do with 2 pi by a. So, to understand, so this will be actually the unit cell of the crystal itself. So, this I will just give you the name right now. So, this is called the brillouin zone. So, let me right down the exact spelling brillouin zone.

So, this brillouin zone is nothing, but the unit cell of the crystal and about which you can say your dispersion or your energy relationship with wave vector keeps self repeating. So, your analysis more or less can be confined only to one periodic brillouin zone. So, you do not have to do is for the entire crystal just 1 brillouin zone and the solution will also be periodic and repeating. So, in crystals in solid state physics in crystal crystalline material usually these analysis are confined to only 1 brillouin zone width. So, which spans from the wave vector of minus pi by a to plus pi by a. So, we will also show that. So, another thing I want to talk about is the vibration of these phonon waves if you if you look at these atoms.

So, we are talking about atoms which are periodically space. So, this was our one dimensional monatomic chain of atoms in a crystal. So, these were separated by the lattice constant a right. So, if you look at the wave length of these phonon vibrations. So, what will be the minimum wave length that you can minimum wave length let us say lambda min for this phonon vibrational waves that is possible. So, you can imagine the minimum wave lengths to take this form here like this understand. This is the minimum wave length that is possible when you talk about this phonon vibrational ways which are propagating may be as a right running wave correct. So, if you therefore, look at lambda min what is the minimum wave length possible 2 a right. So, you cannot have wave length which are smaller than 2 a, because there are no atoms.

So, physically it does not make sense if you are having phonon vibrational wave length smaller than the separation between the atoms correct. So, this is the minimum wave length. So, therefore, your wave lengths are now constraint due to the positioning of these atoms.

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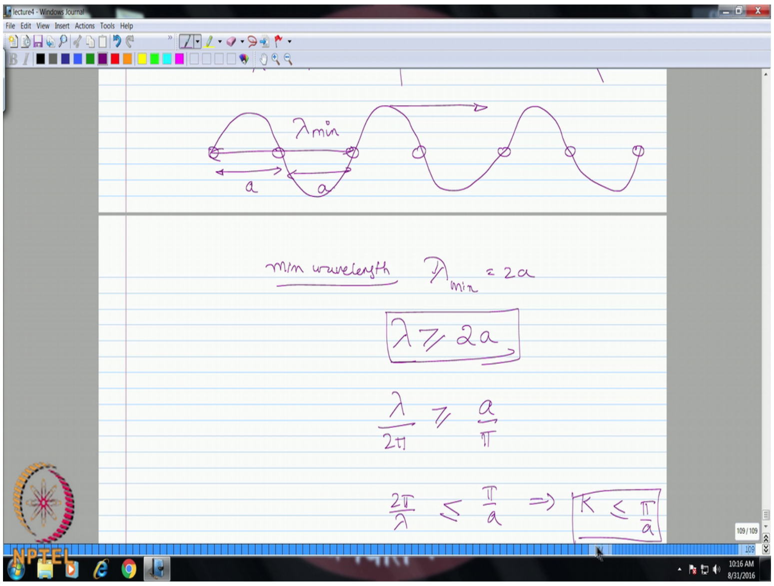

min wavelength $\lambda_{min} = 2a$

$$\boxed{\lambda \geq 2a}$$

$$\frac{\lambda}{2\pi} \geq \frac{a}{\pi}$$

$$\frac{2\pi}{\lambda} \leq \frac{\pi}{a} \Rightarrow \boxed{K \leq \frac{\pi}{a}}$$

You are lambda has to be what greater than or equal to 2 a. So, this is important condition that these phonon vibrational waves have to have to satisfy right. So, if we therefore, based on this if you divide by pi on both sides. So, you will have a lambda by 2 pi greater than or equal to a by pi or if you take reciprocal of this you have 2 pi by lambda pi by a and what should the sin wave less than or equal to. So, which means what is two pi by lambda wave number K should be less than or equal to pi by a, or in other wards.

So, what we are saying is this is basically the boundary of the brillouin zone. So, therefore, your plus or minus pi by a that we have chosen. This is because of the facts that pi by a, marks the boundary of the brillouin zone beyond which it does not make any sense to look at the solution. So, we are confining our entire solution to this brillouin zone because of the fact that your K is less than or equal to pi by a. So, this is one thing now we can continue this analysis a little further and we can also substitute now this k here is nothing, but kappa. So, I am just going to use kappa here. So, that you do not confuse with the other K this is your spring constraint.

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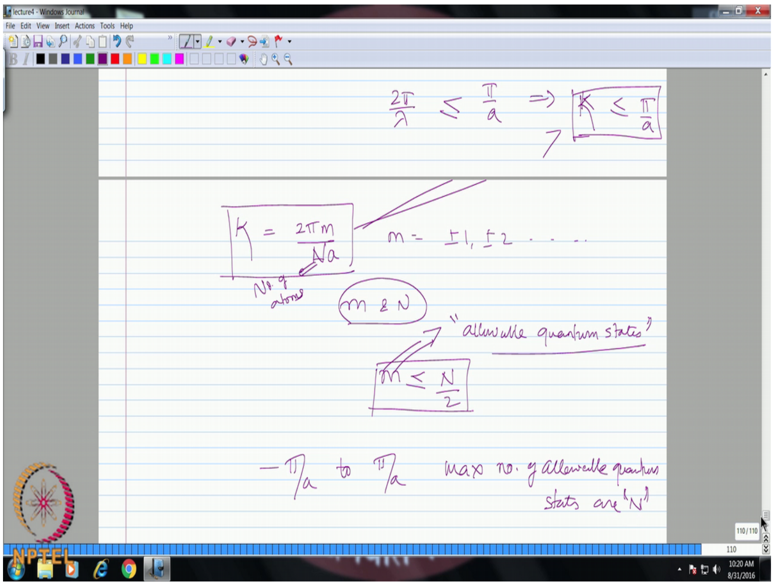

$\frac{2\pi}{\lambda} \leq \frac{\pi}{a} \Rightarrow \boxed{K \leq \frac{\pi}{a}}$

$\boxed{K = \frac{2\pi m}{Na}}$ $m = \pm 1, \pm 2 \ldots\ldots$

No. of atoms

m & N

"allowable quantum states"

$\boxed{m \leq \frac{N}{2}}$

$-\pi/a$ to π/a max no. of allowable quantum states are 'N'

So, we are also having a constraint in the crystal that K is equal to two pi m by l where m is equal to plus or minus 1 plus or minus 2 and. So, on therefore, from this can you derive a relationship between your m and this l is nothing, but capital n times a where n is the number of atoms and a is the lattice basic and you derive a relationship between m and n. So, now, you have this constraint here for the crystal and you also have this constraint for the phonon vibrational waves. So, equating these 2 derive a relationship between m and capital N. M is Less than or equal to n by 2.

So, what do you understand from this m is less than or equal to n by 2. So, if there are n numbers of atoms and what is m here you can, these you can interpret this as allowable quantum state right because these are discrete. So, these are representing the quantum states or the separation in K discretize due to the crystal structure itself. So, these allowable quantum states should always be less than or equal to n by 2. So, now, therefore, the maximum no of quantum states that are possible from 0 to pi by a how many are possible n by 2. So, therefore, if you go about the unit cell I have drawn here from minus pi by a to less pi by a. So, therefore, how many numbers of maximum possible quantum states are allowed n capital n between 0 to pi by a you have n by 2 number of quantum states.

So, therefore, from minus pi by a to plus pi by a, the maximum allowable number of allowable quantum states are basically nothing, but capital n; that means, what. So, if you are drawing this the number of these discrete points are basically if you count them they will be capital n between minus pi by a to plus pi by a right. So, this is how they are discretized. So, because these kappa is now discretize for different values of m and then we have seen for this case there are maximum allowable values of m between minus pi by a to plus pi by a is capital n therefore, when you are drawing this discrete representation you can break this into n discrete points between minus pi by a. So, within this brillouin zone you have therefore, n number of quantum states maximum number of quantum states possible.

So, this is a very important concept. So, 1 thing is you have for the phonon vibrational waves you have a constraint on the minimum wave length of this phonon waves. It cannot be smaller than the lattice spacing for sure and at the same time we also have a constraint on the wave number for the crystals for from this we know what is the maximum number of quantum states allowable within this brillouin zone, right. So, now, what we will do is a few therefore, draw the representation of this just like we did for the electrons you know in the electrons also, since it was symmetric we draw about the you know vertical axis only one half this energy bands the same way usually for the phonons also you draw the K a by pi on the vertical axis you have the omega and you just only draw this part. So, this is spanning from 0 to K a by pi what should the maximum value or K pi by s it becomes 1.

So, this is the dispersion curve that is generally plotted for phonons because they know that this is symmetric and therefore, they avoid the other side, but do not thing that this is the only 1 its actually symmetric about the vertical axis just like the wave we plot it for the electrons the electrons can be plotted like this, but this is also symmetry right. So, this is the dispersion curve that we get now in the case of 1 dimension we get only 1 dispersion curve and this is corresponding to what kind of vibration it is only in the x direction. So, these are called longitudinal phonons these are longitudinal vibrations right. And the slope of this dispersion curve that is basically d omega by d K will give you what? It will give the wave velocities. So, that is nothing, but the speed of sounder the lattice, because the longitudinal waves are corresponding to basically the acoustic waves. So, that is how this sound will propagate within the particular crystal. So, if you want to calculate the acoustic velocity you have to take basically the slope of this dispersion curve and that will give you the speed of a propagation of the acoustic waves which is also the speed of the longitudinal phonons right you understand now, this is only 1 kind of mode that we are getting in the one-dimensional picture.

So, if you are now translating this into the three dimensions. So, right now we talked about only longitudinal vibrational modes.

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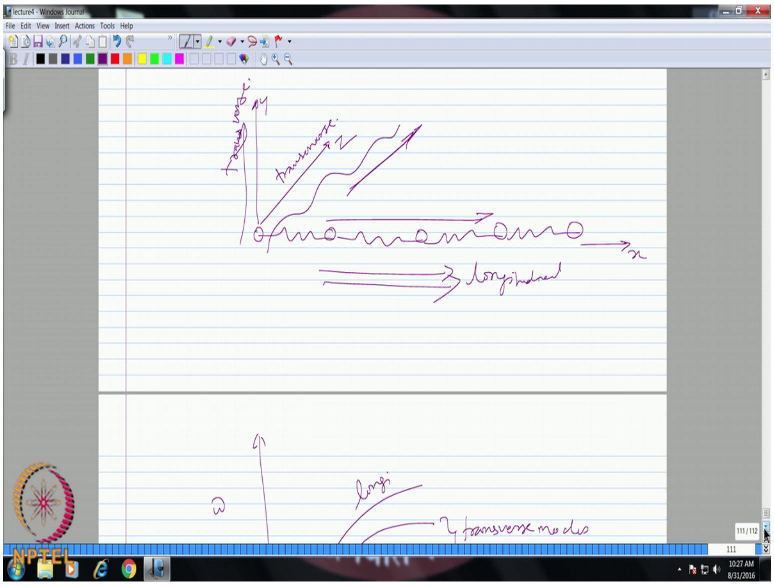

So, if you are extending this to 3 dimensional systems where you have the longitudinal vibration along the X and you have a similar structure along Y and similar structure along Z. So, this is going to be your longitudinal mode and what are these? These are going to be transverse mode. So, the perpendicular directions to the longitudinal mode you have the transverse modes.

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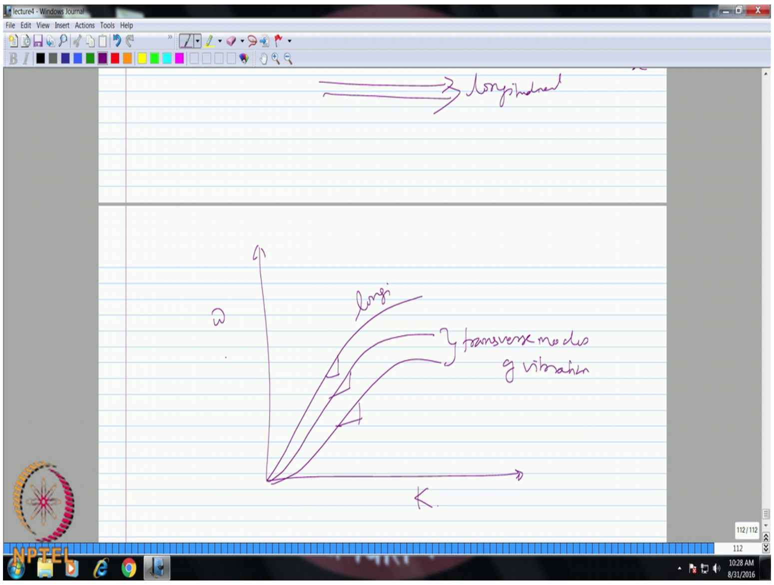

So, therefore, for this 3 dimensional system if you plot the dispersion curve omega versus K. So, now, you will be able to see this longitudinal mode and also you will have transverse modes, this was this were your transverse modes of vibration understand. So, you are talking about now vibration in the longitudinal direction and also vibrational waves which can travel like these.

So, these are your right running waves these waves can also propagate in this direction and also in vertical direction. So, these transverse waves will also contribute to the dispersion and they will have a separate set of dispersion curves is a point clear. So, they will also have suppose you take the slope of the transverse modes to they will also correspond to certain velocities. So, that those are not the speed of sound, but they are the speed of the transverses the phonons. So, they are also important when you talk about the contribution of heat transports, the heat transport all the 3 modes will contribute to heat transport the phonons which are propagating in the longitudinal direction as well as in the transverse there. So, we have to have the information of the velocity of phonons for all 3 modes from the dispersion curve the dispersion curve is important in the sense that not only to you understand how frequency angle of frequency varies with wave vector, but also to do any analysis of E transverse the velocity respective phonon velocities are obtained from this curve.

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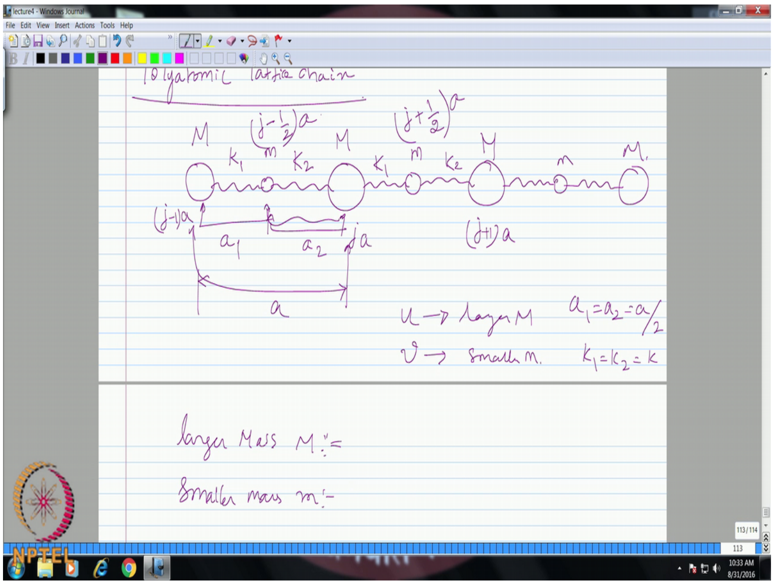

So, now let us consider a slightly more complex structure of atoms. So, we have assumed monatomic atoms in crystal, now let us do a polyatomic lattice chain. So, where in you have 1 large mass large atom 1 smaller atom let taken be a different masses. So, we will call the mass of the large atom with the capital M mass of the small atom with the small m. So, this is a polyatomic structure and you can have many of this now repeating to form a crystal.

So, the next one will be again a large 1 and again you have a smaller one and now this keeps self repeating. So, the interaction between the larger atom and the smaller atom this is a polyatomic structure. So, this could be some K 1 and the interaction between. So, this is K1 and then you can have the neighboring once between this and this to be K2. You can have 2 different lattice constants in principle and this can be self repeating again we have K1 K2 and so on. So, you can have therefore, the entire lattice form with these larger and smaller atoms and again the separation between the 2 atoms can be a 1 and the separation between these 2 here is a 2.

So, this total this is the entire lattice space a. So, this a is broken down into the spacing between the larger 1 and the smaller 1 a 1 and between the smaller 1 and the next larger 1 a 2 and also we can number these notes for example, the larger once we will call these with notation j a then this is j plus 1 a. So, we are using the conventional notation we used earlier for the larger once and this is going to be j minus 1 a, and for the smaller once we will use slightly different convention for example, we will call this with half integer location because it is between j and j plus 1 will cal this j plus half a is it. So, what we are assuming now is that a 1 is equal to a 2 is equal to a by 2.

So, let us just say that they are equidistant and also the fact that K1 is equal to K2 is equal to K2 is equal to K. We are also assuming that this spring constants are equal. So, this is your half integer atom the smaller 1 and what about this j minus half a. So, with this kind of a notation now you can go back to the earlier case where we wrote down the force balance right and rewrite it now for 1 for the larger mass M and the other for the smaller mass small m.

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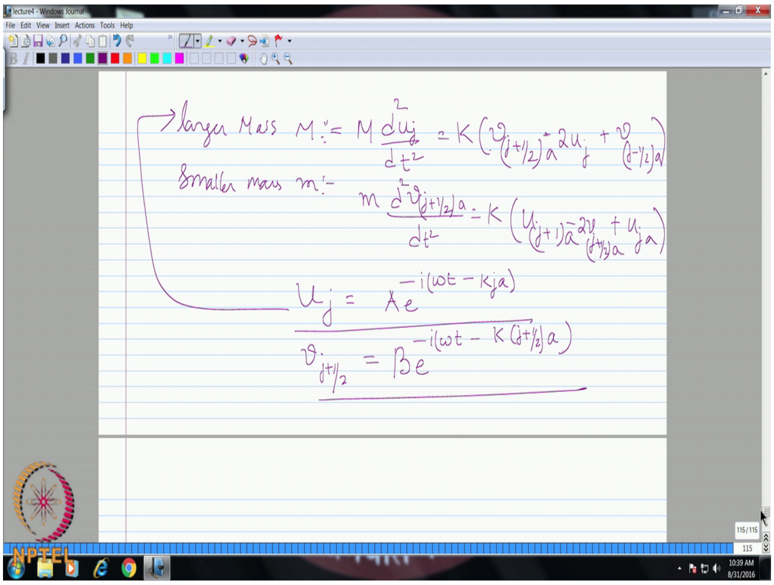

larger Mass M :- $M\frac{d^2u_j}{dt^2} = K\left(v_{(j+1/2)a} - 2u_j + v_{(j-1/2)a}\right)$

Smaller mass m :- $m\frac{d^2v_{(j+1/2)a}}{dt^2} = K\left(u_{(j+1)a} - 2v_{(j+1/2)a} + u_{ja}\right)$

$$u_j = Ae^{-i(\omega t - kja)}$$

$$v_{j+1/2} = Be^{-i(\omega t - K(j+1/2)a)}$$

So, we will also call the relative displacement from equilibrium for the larger atoms to be u this is for the larger mass and will use the notation v as the relative displacement for this smaller mass or the half integer atoms. So, we will have therefore, two sets of equations 1 for the larger mass and 1 for the smaller mass; that means, whatever we have written down here. So, what we call this as equation 1 a or even 1 step before that.

So, 1 a you can rewrite this 1 a for both the larger and smaller atoms, you know the neighbours now we have use the corresponding convention. So, the larger mass what will be the equation of motion M into d square you let us write it for the atom j u j by d t square will be equal to K times. Now this will be influenced by this moral atom on the right and the left right. So, therefore, we have relative displacement of the smaller 1 which is v j plus half a and then what do we have plus j minus half a and then minus 2 times u j right. So, the relative displacement from equilibrium of the present atom the neighbouring atoms has the smaller once. The similarly for the smaller mass we have d square v let us write this for j plus half write it d t square. So, this will be K of what do we have for this j plus half this atom we have j plus 1 and we have j. So, you can write this in terms of u j plus 1 plus you have u j a and we have minus 2 v j plus half.

So, with this you can once again assume the wave solution to this problem. So, we will substitute the assume solution for u j to be once again a e power minus i omega t minus k j a. This is the discrete wave solution for u j what we assume and this can be substituted into this equation here and the other solution what we will assume for v j plus half will be sum b e power minus i omega t minus k into j plus half a right. So, both are right running waves. So, the net displacement is resulting in right running waves for both the larger atom displacement in the smaller displacement.

So, we have therefore, 2 sets of waves 1 due to the motion displacement of the larger atoms 1 due to the displacement of the smaller atoms. And I will just give you the solution you can actually continue this you can put it into that equation and get the dispersion relation for this case also only that it looks a little bit bigger I will just give you the final solution for omega.

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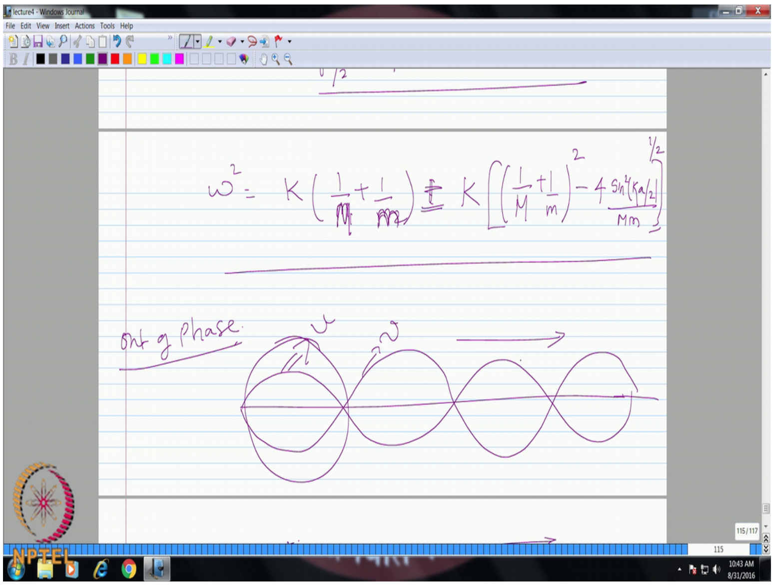

$$\omega^2 = K\left(\frac{1}{M}+\frac{1}{m}\right) \pm K\left[\left(\frac{1}{M}+\frac{1}{m}\right)^2 - 4\frac{\sin^2(ka/2)}{Mm}\right]^{1/2}$$

So, you will have omega square will be spring constant will call this kappa here. So, distinguish this from K. So, we have 1 by M 1 plus 1 by M 2. So, this is the larger mass small mass this is the harmonic mean between the 2 plus or minus you have again spring constant into 1 by capital M plus 1 by small m the whole square minus 4 times sin square kappa a by 2 by capital M times small m the whole raise to the power 1 by 2.

So, this is the dispersion solution for this case where we have a polyatomic that is to be have 2 atoms now, 1 larger mass 1 smaller mass and this is how. Now, therefore, if you look at the dispersion you have plus or minus here so; that means, not just 1 branch, but we have 2 branches of waves. So, effectively what is happening is you have a wave from the larger atom displacement wave from the smaller atom displacement, they can either be out of phase or they can be in phase with each other. So, the out of phase waves will correspond to a motion like this. So, you have 1 wave from the larger atom displacement like this the out of phase will be? This is from the smaller atom displacement. You can call this as u and this as v, these are the waves coming from the 2 respective displacement and they can be out of phase like this or they can finally, be in phase like this so this is your out of phase component.

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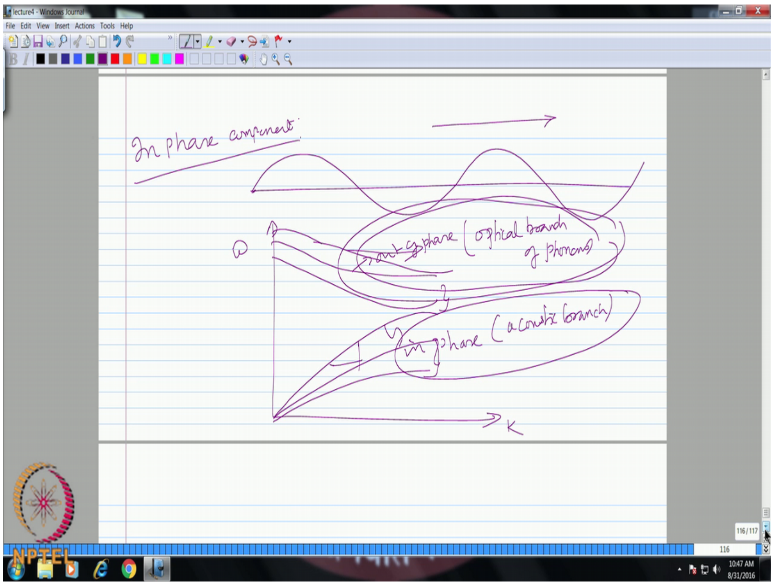

So, which 1 of these require more energy to vibrate, the out of phase component or the in phase component. Why in phase component? But the out of phase one actually consumes more energy.

One is trying to basically move in 1 phase the other in the opposite phase. So, this actually consumes more energy than the in phase components if you look at it. So, therefore, if you draw the dispersion curves now what happens let us still stick to 1 d now. So, you have you are in phase component which is giving to an effective right running waves, which is your longitudinal phonon vibration and on top of that you have an out of phase wave, which is also running effectively in the right, but this 1 is going to consume more energy than the in phase 1 because they are trying to you know be of out of phase with each other. So, therefore, if you plot this value will come out to be something like this. So, this is your out of phase. So, therefore, the positive sign here should correspond to the out of phase wave and the negative to the in phase.

So, this out of phase wave is also called optical mode or optical branch of phonons and the in phase is called the acoustic branch because as we said that this slope of this will give you the speed of sound in the lattice. So, this is your longitudinal vibration corresponding to the speed of sound propagation whereas, the other 1 the out of phase 1 corresponds to this is the higher energy mode of the phonon vibration which is usually associated with interaction with the electromagnetic waves for example. So, 1 phenomena that we can observe with these optical? why it is call optical is they you can interact with the photons. So, when you have a photon and phonon interaction the optical branch of phonons are the once which will gets the energy from the photons they are that once which can directly interact with these electromagnetic waves and from there transverse and d k into finally, the in phase or acoustic branches.

So, you see. So, this is how the photon phonon coupling can happen you understand. So, for example, if you have a semiconductor solar cell and you expose it to u v variation. So, you have absorption of the photons some heat generation is also happening within the semiconductor material. So, how this is happening is because of the photon phonon interaction and that is coming from the optical branch which is basically first interacting with the photons light waves and transferring that energy to the acoustic branch which is now dissipating this has heat. So, this is a very complex process it is not been very clearly understood, but from the dispersion relation you know that there are 2 branches possible, but it is not very clearly the mechanism of how the optical branch can interact with photon and then how it can degenerated to an acoustic branch all right. So, this is from a relatively simple analysis you know from the analytical solution we could reach this point.

Now, what happens in a 3 dimensional crystal structure now how many modes of out of phase waves can exist how many modes of in phase waves can exist? So, you can now extend this to another 2 corresponding to the transverse in plain or transverse in plain or acoustic branches and similarly you will have 2 more sets. So, the highest 1 will be corresponding to the longitudinal optical phonons and the other 2 branches will be the transverse optical phonons.

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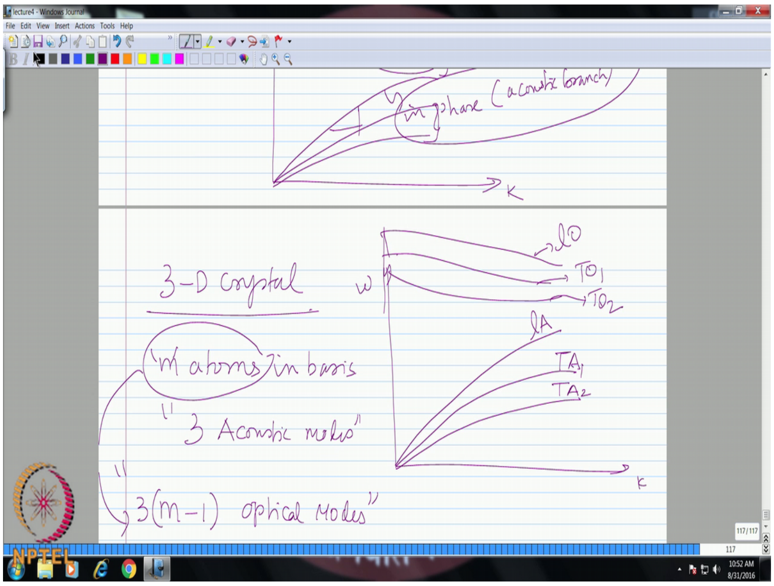

So, for a real 3-D crystal, you can therefore, end up with so many branches. So, one is your acoustic branch and you will have first the longitudinal once and you will have the transverse.

So, this is your longitudinal acoustic phonons. So, people use this convention l a means longitudinal acoustic, then you can have transverse acoustic you can have TA1 then you can have TA2 and in many crystals like silicon for example, is a common semiconductor material the 2 transverse acoustic branches exactly overlap on top of each other. So, similarly if you look at the optical phonons, you can have different branches, you can have longitudinal optical phonons, you have transverse optical phonon 1 transverse optical phonon 2. So, in general if you have m atoms in a basis in a monatomic chain you have only 1 atom in a diatomic you have 2 diatomic 3. So, if you have m atoms in basis.

So, how many acoustic modes are possible. So, you have m minus 1 the suppose m is equal to 1. So, in this case it should be just. So, 3 you should have 3 acoustic modes and in the case of optical modes you have 3 into m minus 3, this is your general thumb rule. So, therefore, if you put m equal to 1 into this for a monatomic lattice chain you have 3 acoustic waves in 3 dimensions and 0 optical modes and then if you have a diatomic it should simply 3. It should simply 3, because the m atoms are only influencing the optical modes by default you will have 3 acoustic modes, but if you are having m number of atoms say 2 atoms diatomic chain then you will have 3 optical modes this is what we see here. If we have 3 atoms in the basis, you have optical modes. So, this is your general thumb rule calculation you know if you want to understand how many modes of acoustic phonons optical phonons are there. So, you have to apply this someone is it clear?

So, in a 3-D crystal, we will kind of I thing we have given broad over view about the dispersion of phonons in a crystal and also the fact that you have the branching of this phonon dispersion. So, due to the vibration in 1 direction in the other and in the other directions and also due to in phase and out of phase phonon waves, what we will do is you just right now you just have to understood this, but when we solve the heat transport you will understood how these dispersion curves are used for the transport of heat.

So, in the next class tomorrow we will complete the solid state physics. So, we will focus on the last part which is called the density of states. So, this density of states is now the bridge when we go from the quantum mechanics to statistical thermodynamics. Because now we have seen that whether it is a simple system or whether it is real crystal structure you have quantization of the wave vector space quantization of the energy or the omega whatever. So, now, we have if you plot therefore, the 3 dimensional a wave vector map that is k x k y k z you are going to plot all discrete points corresponding to the these values of m L and n right.

So, therefore, how useful is this. So, many random discrete points for us, we cannot keep track of the variation of the each and every quantum state there are. So, many quantum states and in three dimensions all 3 dimension are discrete quantum state. So, how useful is bookkeeping all these discrete quantum states, so we cannot have all these information with us. So, what will finally, do is take a band continuous band and then average out these discrete states. So, this is called density of states. So, we need to do this before we slowly transition to the macro scale to calculate the properties. So, somehow we have to average out the individual quantum states by taking bands and within these bands we will count how many of these quantum states are existing and then directly use the density of states for calculating the macro scale properties and now will slowly do away with all these micro states.

So, the next topic tomorrow will introduce the density of states for electrons and the phonons both.

Thank you.