Introduction to Solid State Physics

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Lecture – 48
Lattice with two – atom basis: Optical phonons

In the previous week, we looked at the vibrations of atoms in a crystal.

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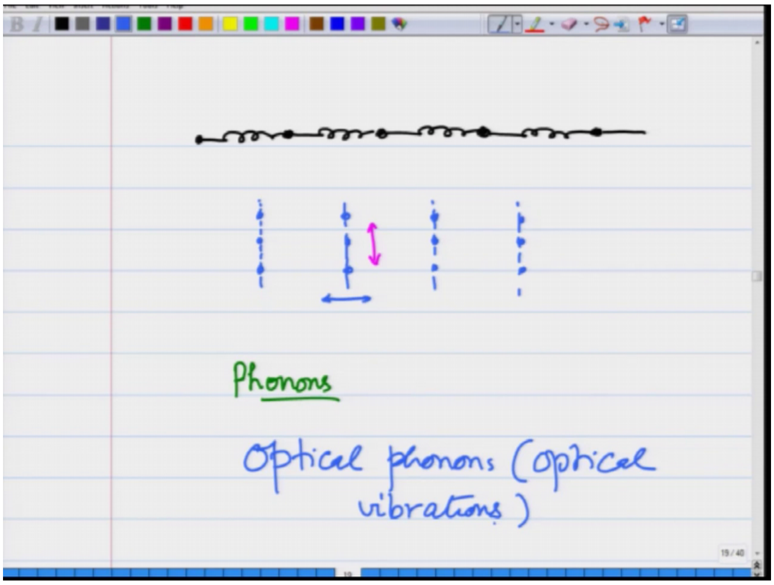

So, what we considered was these atoms in one-dimensional crystal and obtained the omega versus k for these systems and then we related these two the planes of crystals vibrating in particular directions. And I gave you examples of these towards the end of those lectures. So, these are vibrating either like this or like this, transverse and longitudinal vibrations. And then we said that the quantum of these vibrations is known as phonons and we gave the concept of phonons, and then what energy phonons carry and consider the crystal as a collection of phonons when these atoms are vibrating.

We are going to take it to further in this week's lecture. And see what all happens when these phonons are excited and carry energy or the temperature of the crystal is raised, but before that I need to also tell you about a different kind of phonon and that is known as optical phonons or optical vibrations, I keep writing vibrations so that you realize that phonons are nothing but these quanta of these vibrations.

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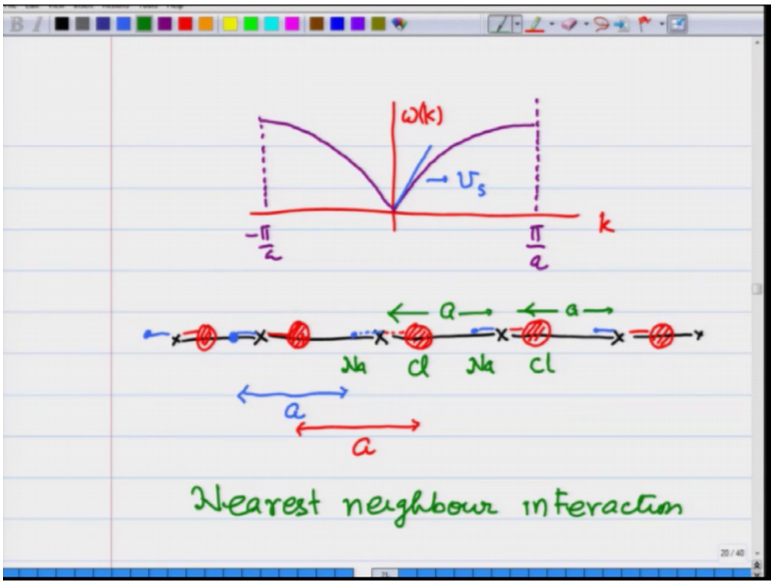

So, just to recap what we had seen in the previous weeks lectures was when I plotted omega k versus k, I got a curve which was like this, all the way up to the Brillouin zone boundary. And the slope of these phonons at k equals 0 was related to velocity of sound. When we go further and consider more kinds of atoms in a lattice, then we get some different kinds of vibrations in the crystal and that is what we would discuss now.

So, consider a crystal again we will focus on one dimensions first, consider a crystal with these crystal sides shown by crosses. And at each side, there are two kinds of atoms attached to each side let us say the blue one and the red one the blue one and the red one, the blue one and the red one and so on.

So, let me just complete the picture. It is as if a molecule made up of two different atoms is sitting at each side. Now, example this could be Na Cl, Na Cl or some other kind of atoms. So, this is like Na Cl molecule sitting at each side shown by this cross. The distance between these sides is again a, so that the distance between the blue atoms is also a and so is the distance between the red atoms.

So, imagine this one-dimensional crystal, where these molecules are sitting here at each side and now the vibration takes place. Again I am going to assume nearest neighbor interaction that means the atoms from one side interact with atoms only to the next side or the atoms nearest to them and nothing else. This itself brings out many features of the vibrations of this kind of system as it did in the case of single kind of atom on a lattice.

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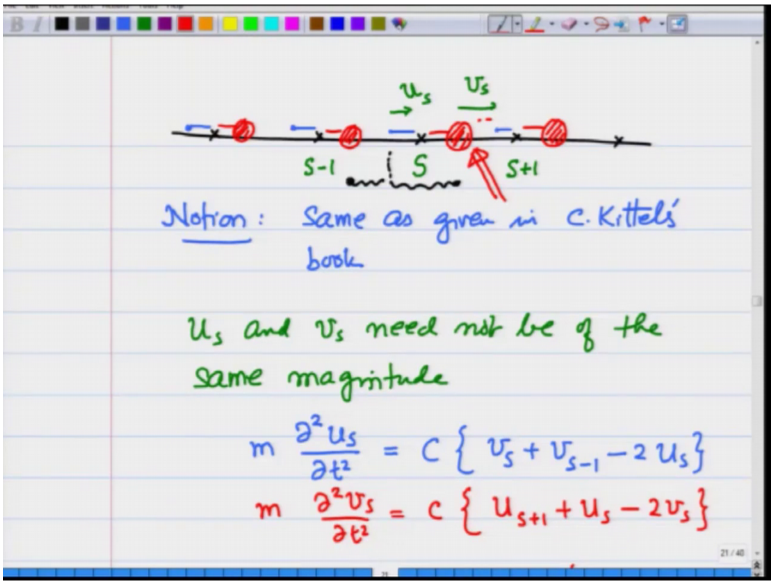

So, let us see now what happens in this case. So, I have these molecules sitting at these sides with different kind of atoms which we can also call that now I have a basis at each side with two different kinds of atoms. I am just making three or four of them, because that is all I need to derive my equations etcetera for the nearest neighbor. So, let me take this side to be Sth side, next one is S plus 1th side and the previous one is S minus 1 side. And I am going to follow the notation or the book prescribed that is notation same as given in Charles Kittle's book.

So, one of these displacements I am going to call u. So, let us say at Sth side the blue one shifts by u s, and the red one shifts by v s. So, that on the next side it will be v s plus 1 u s plus 1 and the previous side it will be u s minus 1 and v s minus 1 now these v and u u s and v s need not be of the same magnitude. Why, because one atom could be heavier than the other the heavier atom would move less lighter atom would move more and so on.

So, these are two different kinds of atoms two different kinds of motion, and now we write the equation of motion. Let us look at the blue atom and for the blue atom the acceleration will be d 2 u s by d t square, the force will be m, and this would be given by assuming the nearest neighbor interaction c, where c is the coefficient of the force or the spring constant times the blue atom in the Sth side is interacting with the orange atom in its own side and one with the previous side.

So, the force and I will leave it for you to kind of work out because we have we have been working this out for the one atom case is going to be v s plus v s minus 1 minus to u s because if you look at the picture I am going to make some wiggles this atom at the Sth side is interacting with this atom and this atom the previous atom. So, it is interacting with atom at the Sth side itself with the other atom and the other atom in the previous side.

Similarly, for the orange atom or the red atom, the acceleration is going to be d 2 v s by d t square is equal to c. Now, this atom out here the orange atom I am showing it by an arrow is interacting with the blue atom on the next side, and the same the blue atom on the Sth side. So, the force is going to be u s plus 1 plus u s minus 2 v s, these are the equations of motion.

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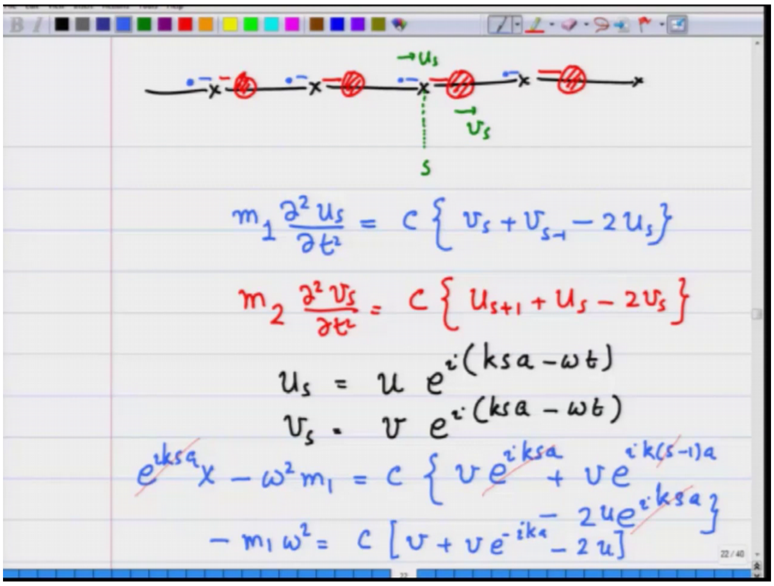

So, let us write them again what I have done is I have taken this crystal with a basis at each point. So, blue atoms and the orange atoms and at the Sth side the displacement is u s for the blue one and v s for the orange one. And then we have written the equations of motion is m d 2 u s by d t square is equal to c v s plus v s minus 1 minus 2 u s and m d 2 v s by d t square is equal to c u s plus 1 plus u s minus 2 v s.

Now, in writing these equations you may have noticed so far I made a mistake and the mistake was that I have taken the masses of the atoms to be the same they are actually different that is why there are different kinds of atoms. So, I am going to put m 1 and m 2 here. So, these two atoms of different masses follow this equation considering only nearest neighbor interaction. And now we again assume solutions like u s is equal to some amplitude u e raised to i k s a minus omega t; and v s is equal to some amplitude v e raised to i k s a minus omega t this is a wave like solution that we consider for one atom basis.

And substitute these in the equations, when we do that, I am going to get minus omega square m 1 is equal to c v s is going to be v e raised to i k s a e raised to minus i omega t is common and that gets cancelled from all the sides plus v e raised to i k s minus 1 a minus 2 u s which is going to be e raised to i k s a; and on the left hand side also I have a raised to i k s a. So, this term is going to cancel from all sides, this s term will cancel. And you end up getting minus m 1 omega square is equal to c v plus v e raised to minus k a minus 2, there should be a u, u.

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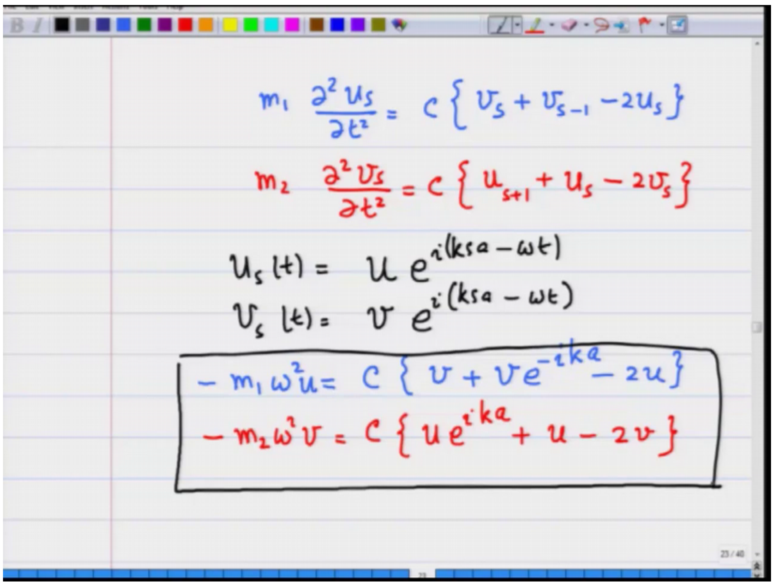

So, taking the equations to be m 1 d 2 u s over d t square is equal to c v s plus v s minus 1 minus 2 u s and m 2 d 2 v s over d t square is equal to c u s plus 1 plus u s minus 2 v s and assuming the solution u s t to be of the form some u e raised to i k s a minus omega t, and v s to be of the same form, that is wave like form v times e raised to i k s a minus omega t. When I substitute this in the equations, I get minus m 1 omega square u is equal to c v plus v e raised to minus i k a minus 2 u. And for the orange one, minus m 2 omega square v is equal to c u e raised to i k a plus u minus 2 v. These are the two equations that I need to solve to get omega versus k graph.

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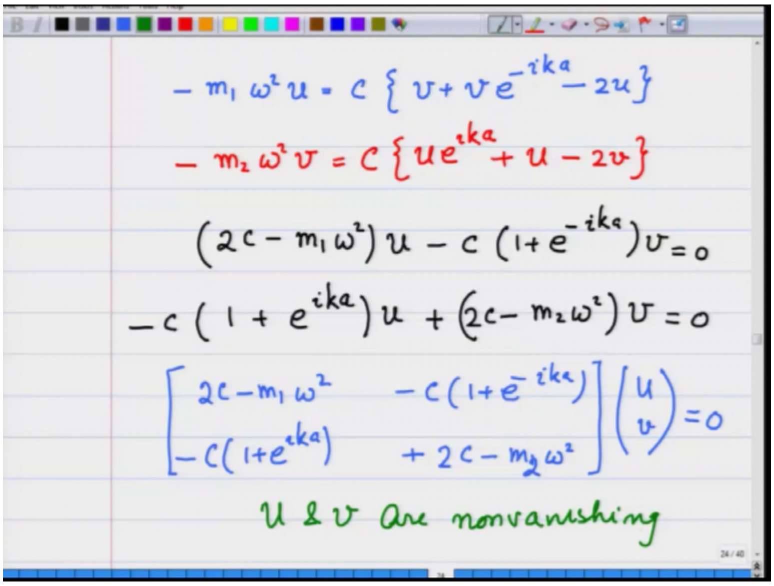

So, I am getting minus m 1 omega square u is equal to c v plus v e raised to minus i k a minus 2 u and minus m 2 omega square v is equal to c u e raised to i k a plus u minus 2 v. I rearranged the terms, collect them all together, and I get these equations as 2 c minus m 1 omega square u minus c 1 plus e raised to minus i k a v is equal to 0 that is equation 1.

And I get minus c one plus e raised to i k a u plus 2 c minus m 2 omega square v is equal to 0, which I can write in the matrix form as 2 c minus m 1 omega square minus c 1 plus e raised to minus i k a minus c 1 plus e raised to i k a and 2 c minus m 2 omega square times u v is equal to 0. And the solution I want is where u and v are non-vanishing in such kind of cases either the case is that u v both are 0 and that is a solution. But we do not want that solution, because u and v we want to be non vanishing then only the wave is propagating.

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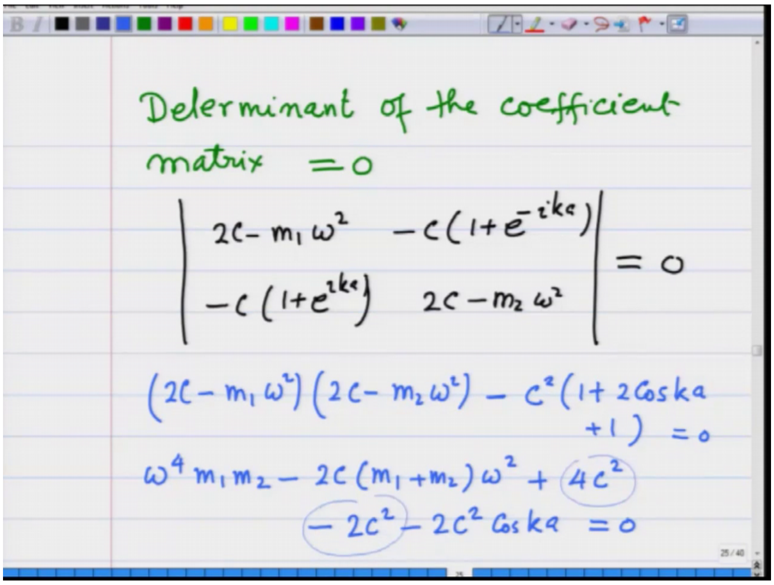

And to have that solution I must have the determinant of the coefficient matrix to be equal to 0. And therefore, for the solution to exist nonzero solution to exist, I should have 2 c minus m 1 omega square minus c 1 plus e raised to minus i k a minus c 1 plus e raised to i k a and 2 c minus m 2 omega square determinant must be 0 for the case, when this wave exists. And that gives me 2 c minus m 1 omega square times 2 c minus m 2 omega square minus c square 1 plus two cosine of k a plus 1 is equal to 0 or omega raised to 4 m 1 m 2 minus 2 c m 1 plus m 2 omega square plus 4 c square minus 2 c square minus 2 c square cosine of k a is equal to 0. I collect the terms 4 c square and 2 c square here.

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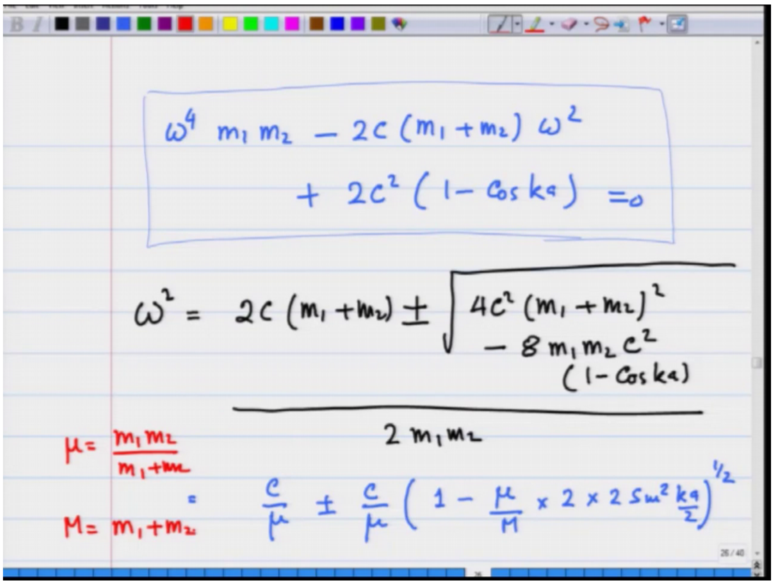

And then write this equation as omega raised to four m 1 m 2 minus 2 c m 1 plus m 2 omega square plus 2 c square 1 minus cosine of k a is equal to 0. This is the equation to be solved to get omega versus k. So, this is a quadratic equation in omega square. And therefore, I can write the solution as omega square is equal to 2 c m 1 plus m 2 plus or minus square root of 4 c square m 1 plus m 2 whole square minus 8 m 1 m 2 c square 1 minus cosine of k a, this whole thing divided by 2 m 1 m 2 which can be simplified to c over mu plus or minus I will take 4 c square out from there and you get 2 c.

So, I can write this as c over mu again and inside I get I have taken out 4 c square m 1 plus m 2 square. So, I get 1 minus mu upon m 1 minus cosine k a is 2 sine square k a and there was a 2 left from when I took 4 out so times 2 sine square k a by 2 raised to one half where let me write for completeness on the left hand side mu is the reduced mass m 1 m 2 over m 1 plus m 2, and m is the total mass of the molecule.

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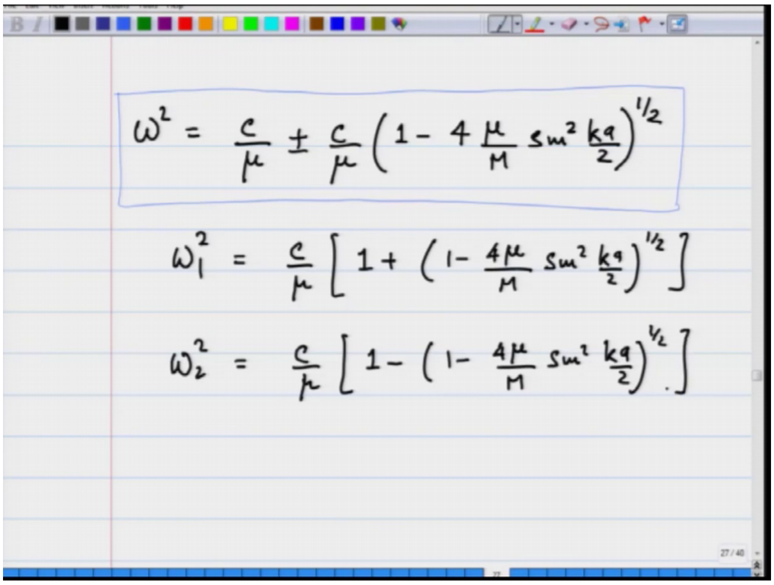

So, I get omega square is equal to c over mu plus or minus c over mu times 1 minus 4 mu over m sine square k a by 2 raised to one-half that is the solution for omega square as a function of k. Notice that it has two solutions, there is 1 omega 1 square, which is c over mu 1 plus 1 minus 4 mu over m sine square k a by 2 raised to one-half, and omega 2 square which is equal to c over mu 1 minus 1 minus 4 mu over m sine square k a by 2 raised to one-half.

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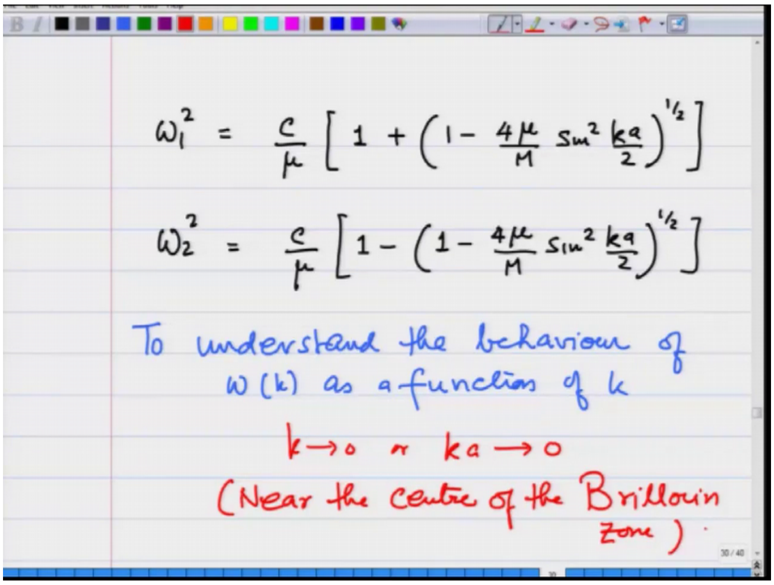

So, let me collect terms and write again omega 1 square is equal to c over mu 1 plus 1 minus 4 mu over m sine square k a by 2 raised to one-half, and omega 2 square is c over mu 1 minus 1 minus four mu over m sine square k a by 2 raised to one-half understand that these two omegas which are there as a function of k. So, for each k, I am getting two omegas, what do they mean and how do they look. So, let us to understand the behavior of omega k as a function of k let me study them in the limit of k going to 0 or k a going to 0 that is very small near the center of the Brillouin zone.

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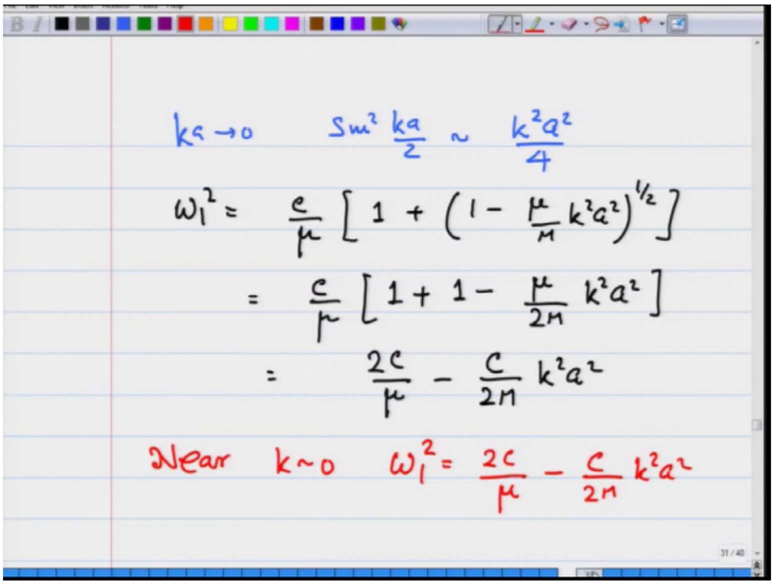

When I do that for k a going to 0, I get sine square k a by 2 as k square a square by 4, and therefore, I can write omega 1 square as equal to c over mu 1 plus 1 minus mu over m k square a square raised to one-half which is equal to c over mu 1 plus I can do the binomial expansion 1 minus mu over 2 m k square a square which is equal to 2 c over mu minus c over 2 m k square a square. So, near k equal to 0 omega 1 square is equal to 2 c over mu minus c over 2 m k square a square. How does it look? So, let us plot this.

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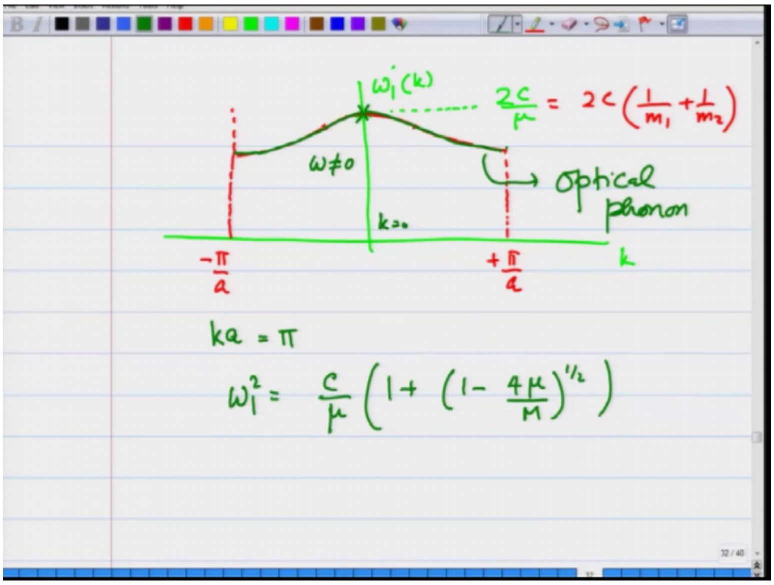

If I plot omega 1 k versus k, you will see that it has value out here which is 2 c over mu which I can also write as 2 c 1 over m 1 plus 1 over m 2, and then it goes down. And then if you plot it fully, it comes down and comes to the Brillouin zone boundary minus pi by a and plus pi by a like shown in the figure. You can also figure out what the value is near the Brillouin zone, because at k a equals pi I am going to have omega 1 square is equal to c over mu 1 plus 1 minus 4 mu over m raised to one-half.

So, this is going to be slightly less than 2 c over mu. So, it goes down. So, this is how so omega 1 square looks like. So, I have this mode which is has frequency omega naught equal to 0 at k equal to 0, and then it is almost flat, this is known as optical phonon for reasons will I explain a bit later let us look at omega 2.

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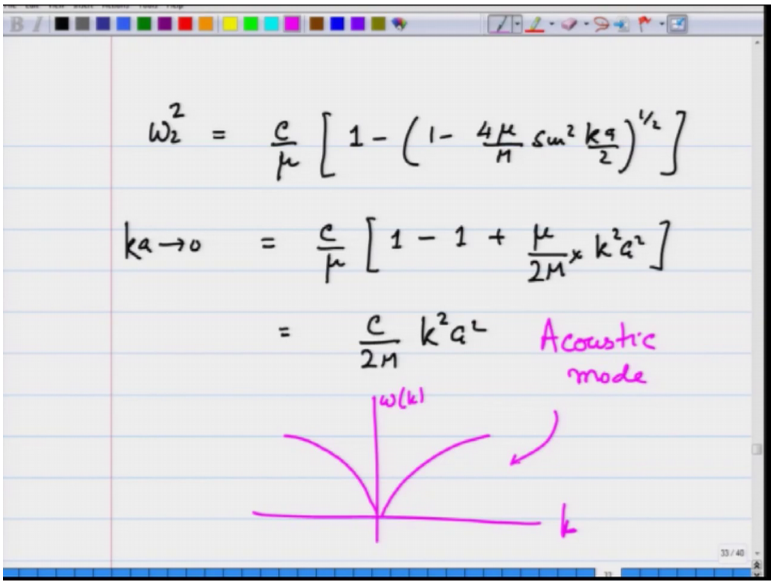

Now, when I look at omega 2, omega 2 square is equal to c over mu 1 minus 1 minus 4 mu over m sine square k a by 2 raised to one-half. And this for k a going to 0 goes to c over mu 1 minus 1 plus mu over 2 m k square a square. So, this is equal to c over 2 m k square a square. This is exactly like what we had earlier in the acoustic mode that we studied last week for a single atom system. So, this is the acoustic mode. And in this case omega k versus k goes exactly like to single atom mode. So, this is known as the acoustic mode.

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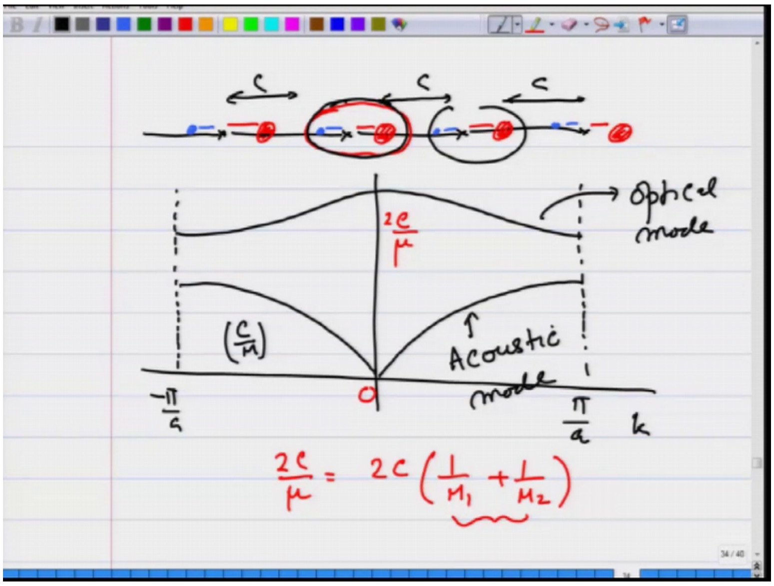

So, in general when I have these two atoms per lattice side, let me make them completely they have these two frequencies, and let me plot the frequencies versus k within the Brillouin zone, because that is the only k that matters and we have really understood it last week. One mode is like this almost flat omega k versus k, and one is like this. This is known as the acoustic mode and the upper one has the optical mode. At k equals 0, the values for the omega for optical mode is 2 c over mu, and this is 0.

So, you see that when I look at 2 c over mu which is 2 c 1 over m 1 plus 1 over m 2. It is the vibration as if the atoms are vibrating within themselves right, it is as if it is a vibration of this atom with itself that is why the reduced mass is coming. And c is the strength of this is this interaction between the atoms.

Whereas, the acoustic mode is carries c over m, and then it is as if this whole molecule is acting like one system, and they are connected with this c interaction strength, and this whole molecule is vibrating like a single unit. So, optical mode is where the constituents of the basis vibrate against each other mainly, and in acoustic mode is where this whole thing vibrates as a unit.

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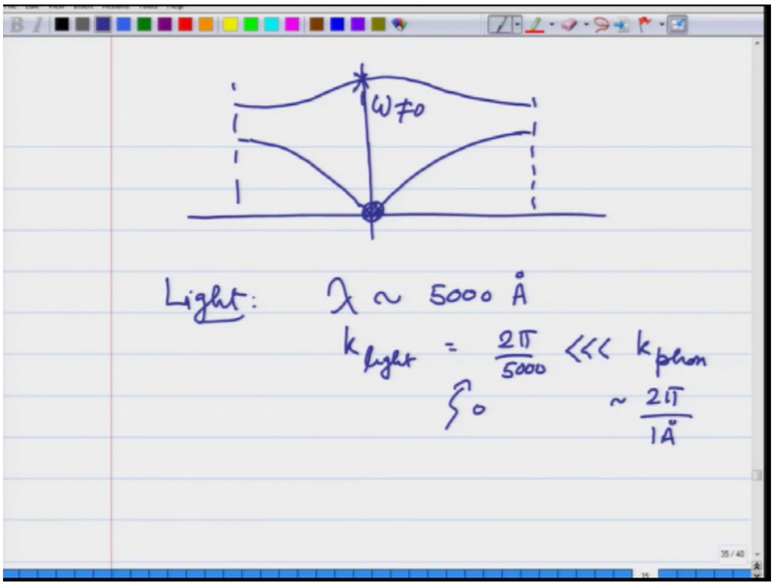

Now, you may ask why I am calling this in an optical mode recall from the previous week that if I want to excite these modes using some external excitation the last time we studied last week we studied how neutrons are used or other particles or interactions are used when we considered light we found that lambda for light is almost of the order of

5000 angstrom, and k light is 2 pi over 5000 which is much much much much much less than k phonon which is more like 2 pi over 1 angstrom, so it is almost 0. So, light does not really transfer any momentum to the phonons.

For the acoustic mode, if it does not transfer any momentum it will hardly transfer any energy also, because for acoustic mode as k goes to 0, there is no energy absorbed. On the other hand, for k equals 0, the optical mode does have an omega which is nonzero. And if therefore, it can absorb energy.

So, these can be excited using light and that is why these are called optical modes. Now, in the next lecture, we will study how these modes then can be counted, and how the energy is stored by them at temperature t, then gives you the specific heat and other properties of solids.

Thank you.