Introduction to Solid State Physics
Prof. Manoj K. Harbola
Prof. Satyajit Banerjee
Department of Physics
Indian Institute of Technology, Kanpur

Lecture – 49
Displacements of atoms for the acoustic and the optical phonons

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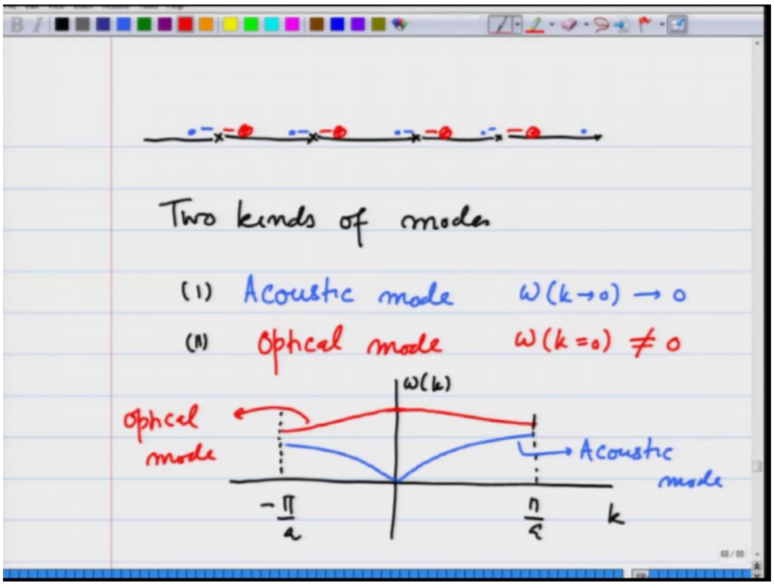

What you have learned in the previous lecture is that when I have crystal with a basis that means I have atoms two coins on each lattice point, then there are two kinds of modes that exists. And the two kinds of modes that exist are one acoustic mode, and in this case omega k tending to 0 goes to 0. And the other one is the optical mode where omega k equal to 0 is not equal to 0.

And when I show it graphically, if I plot omega k versus k, the optical mode has nonzero value at k equals 0 and goes slightly down, where I am plotting this in the first blowing zone. And the acoustic mode goes linearly near k equals 0 and then becomes flat near the Brillouin zone. So, this is acoustic mode. And the orange one is the optical mode. This is what I have shown you in the previous lecture, and graphically I have just plotted it.

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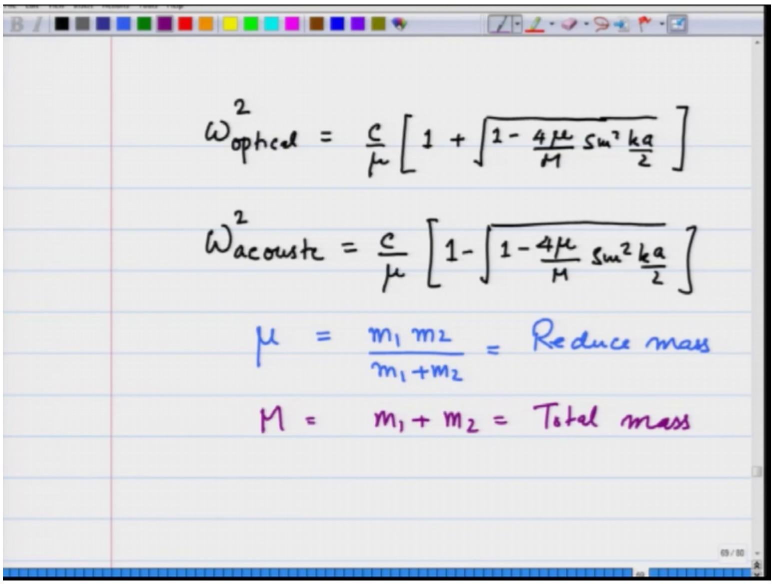

And the frequencies mathematically are given like this. For the optical mode the frequency is c over mu 1 plus square root of 1 minus 4 mu over m sine square k a by 2. And for acoustic mode, the frequency this is square of it, this is square of it, a c over mu 1 minus square root of 1 minus 4 mu over m sine square k a by 2. Where mu is m 1 m 2 over m 1 plus m 2 which is the reduced mass; and M is m 1 plus m 2 this is the total mass.

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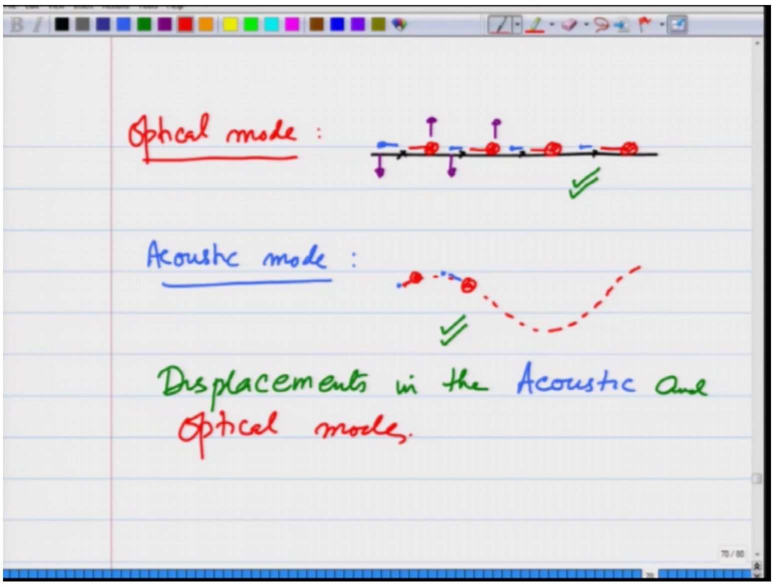

And what I had also discussed is that in the optical mode because there is a reduced mass coming and we had argued that the motion is such that suppose I look at a few of these units, this is my orange atom and this is the blue atom. In the optical mode, the motion is such that it is relative motion between the particles. And in the acoustic mode, the motion is as if this whole unit is acting like one system and so on.

Then I had argued why optical mode is called the optical mode, because it may be excited by light because the frequency is nonzero even at k equals 0, and light being a very large wave c is the lattice as almost continuous, and the large wavelength means that k is almost 0. And therefore, it can excite in a mode the optical mode in the system. Acoustic mode is the sound wave. And we have shown this again and again that is slope at k equals 0 is the velocity of sound, and it has a sound wave propagating, it has sound like properties.

In this lecture, I want to show more clearly how these displacements arise. So, what we want to see in this lecture is displacements in the acoustic and optical modes, and that will give you a further feel for what these modes are like and what kind of motion do these modes represent.

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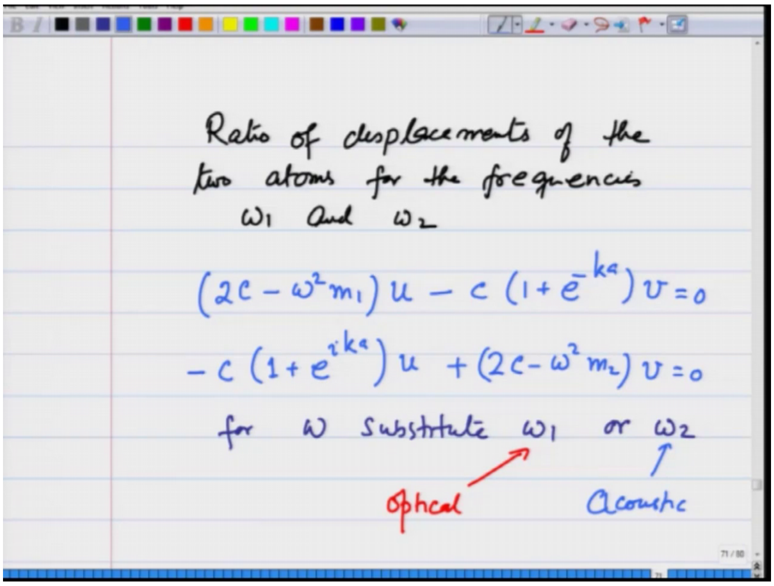

So, for that what we are going to do is look at the ratio of displacements of the two atoms for the frequencies, omega 1 and omega 2. And how do we do that? We do that by writing the equation of motion again. And if you recall the two equations of motion that we had were 2 c minus omega square m 1 u minus c 1 plus e raised to minus k a v equals 0. And the other equation was minus c 1 plus e raised to i k a u plus 2 c minus omega square m 2 v is equal to 0. So, what we want to do is now substitute for omega we substitute omega 1 or omega 2; omega 1 corresponds to the optical mode and omega 2 corresponds to acoustic mode. And see what the ratios of u and v are, and they will give you an idea what the displacements are in these modes.

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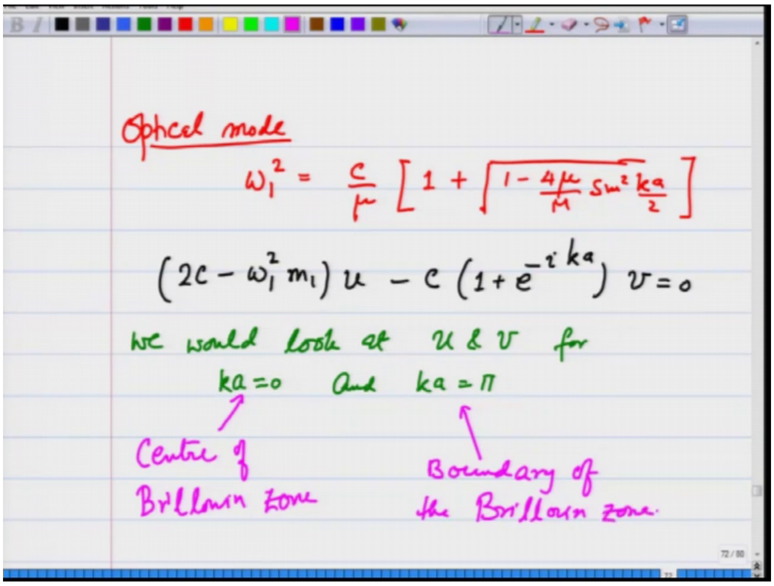

So, let us first look at the optical mode, where omega 1 square is given as c over mu 1 plus square root of 1 minus 4 mu over m sine square k a by 2. And the equation I am looking at where I can find the ratios from 2 c minus omega 1 square now m 1 u minus c 1 plus e raised to minus I k a v is equal to 0. If I substitute omega 1 square I can find out what the ratios are is best to look at it for clarity for. So, we would look at u and v for k a equals 0 and k a equals pi. Let me remind you what they correspond to k equals 0 corresponds to the center of the Brillouin zone, and this corresponds to the boundary of the Brillouin zone.

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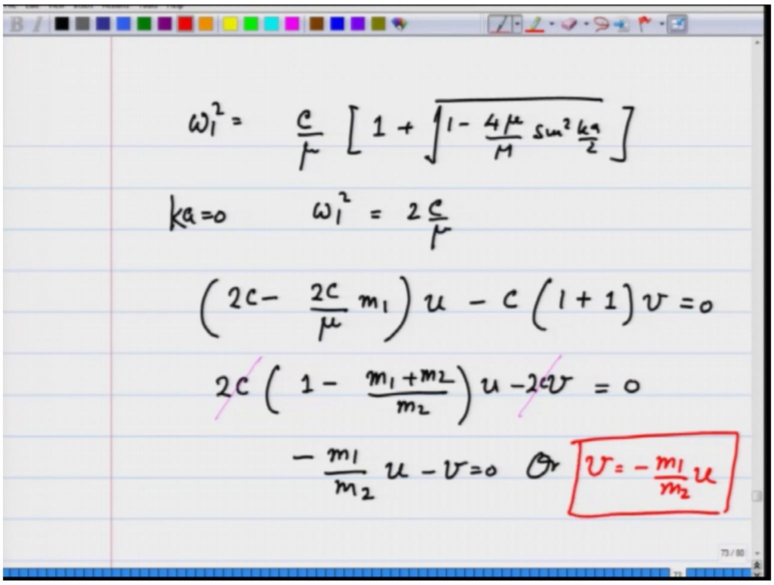

So, we look at the ratio of u and v at these two points, so omega 1 square we have already seen is c over mu 1 plus square root of 1 minus 4 mu over m sine square k a by 2. And for k a equals 0, omega 1 square becomes c over mu times 2. So, for this when I substitute this in the equation, I get 2 c minus omega 1 square which is 2 c over mu m 1 u minus c 1 plus 1 v is equal to 0. So, I get c cancels from all over the place, in fact 2, I get 2 c 1 minus m 1 plus m 2 divided by m 2, when I substitute mu times u minus v is equal to 0 to c mu. So, 2 c, 2 c cancels, and I get minus m 1 over m 2 u minus v is equal to 0 or v is equal to minus m 1 over m 2 u, that is my result.

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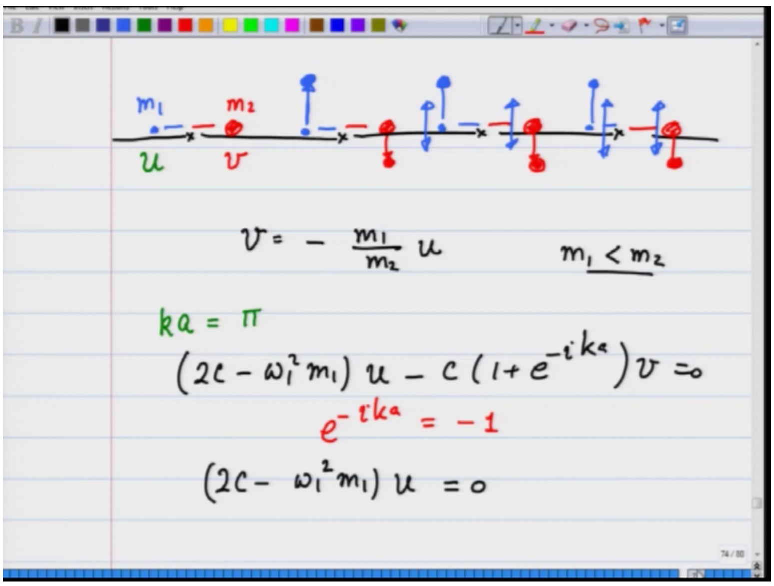

Let us see, what does it mean, let me remind you again that I am looking at this, that is where I have these atoms with different masses attached with each lattice. And we have indicated by u the displacement of mass m 1 and for mass m 2 the displacement is v. And what we have just found is that v is equal to minus m 1 over m 2 u. So, I am going to show the relative displacements in the next unit. So, now, suppose m 1 is less than m 2 then v is going to be less than u, so and in the opposite direction. So, if u suppose is this much let us say this atom gets displaced by this much I am showing even the second unit, then v would be smaller and in the opposite direction. So, I will have at k equals 0 which is like infinite wavelength. So, all the atoms would be displaced like this, and then they will be going back and forth.

So, it is as if there is a relative motion of these two atoms at each side, and this is what the optical mode is where at large wavelength the motion is relative with each other that is why that mu comes in between in the expression. Let us now look at for k a equals pi. If I look at the k a equals pi result then I am going to have 2 c minus omega 1 square m 1 u minus c 1 plus e raised to minus i k a v equals 0. I have e raised to minus i k a equals minus 1 and therefore, I am going to get 2 c minus omega 1 square m 1 u is equal to 0.

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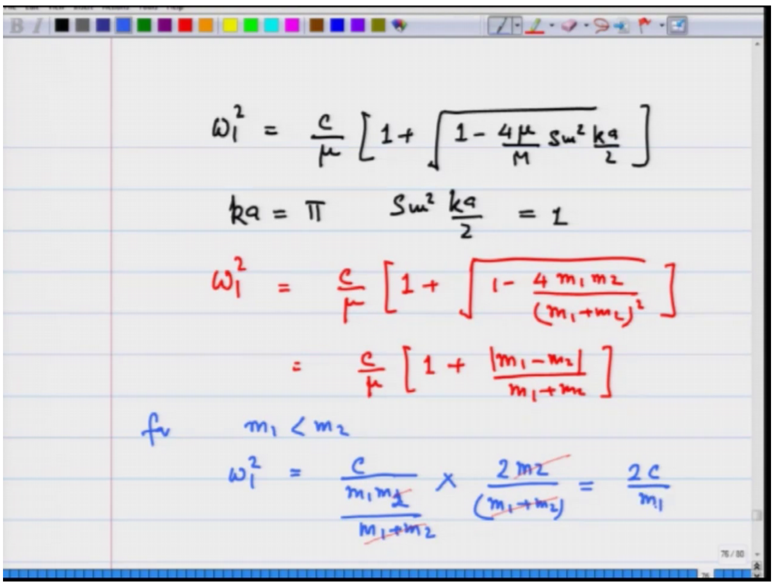

Now, let us see what is omega 1 square. So, I have omega 1 square is equal to c over mu 1 plus square root of 1 minus 4 mu over m sine square k a by 2. And for k a equals pi, I have sine square k a by 2 is equal to 1. And therefore, I get omega 1 square is equal to c over mu 1 plus square root of 1 minus 4 mu is m 1 m 2 over m 1 plus m 2, and with the m it gets a square. And this will be c over mu 1 plus m 1 minus m 2 modulus over m 1 plus m 2. Now, let us take the case for m 1 less than m 2, omega 1 square will be equal to c over m 1 m 2 divided by m 1 plus m 2 times 2 m 2 over m 1 plus m 2, and thus m 2 cancels m 1 plus m 2 cancels, and we get this equal to 2 c over m 1.

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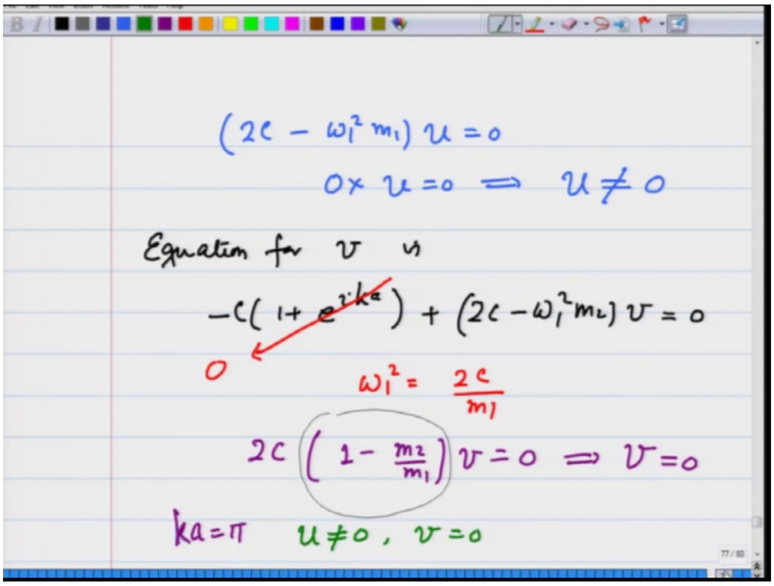

And when I substitute this in the equation 2 c minus omega 1 square m 1 u is equal to 0, I get 0 times u is equal to 0, and this implies u need not be 0 for k a equals pi. How what v the equation for v is minus c 1 plus e raised to i k a plus 2 c minus omega 1 square m 2 v is equal to 0, this we know is 0. And I also know that omega 1 square is 2 c over m 1, and therefore, I have 2 c 1 minus m 2 over m 1 v is equal to 0, and this implies v is 0 because the first term this term here is not 0. So, for the case of k a equals pi, I have u not 0, and v is equal to 0.

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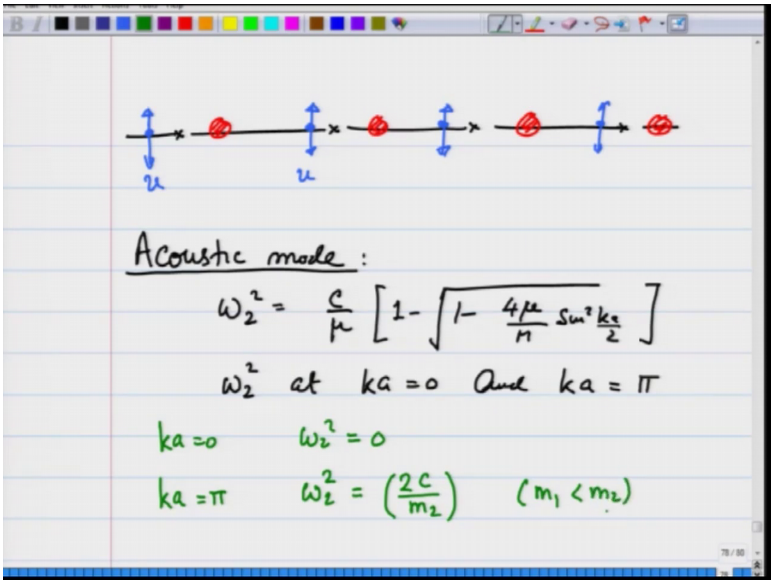

And therefore, in the optical mode, again if I make this crystal I have u nonzero and v 0. So, this heavy atom is sitting right there, and this atom is oscillating back and forth, this is u. Now, let us look at the acoustic mode. In the acoustic mode, omega 2 square is equal to c over mu 1 minus square root of 1 minus 4 mu over m sine square k a by 2. Again we do the same exercise, when you do the same exercise taking omega 2 square at k a equal to 0, and k a equals pi. For k a equals 0, we get omega 2 square is equal to 0 which is correct because at k equals 0, the frequency is 0. And for k a equals pi, we get omega 2 square is equal to 2 c over m 2 for m 1 less than m 2.

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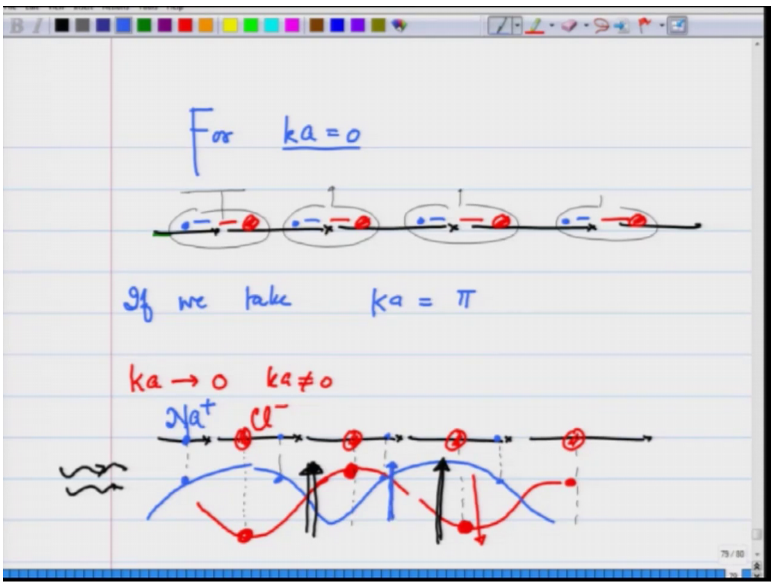

And when you calculate the displacements, what you are going to find is that in the acoustic mode for k a equals 0, all the atoms u is going to come out to be equal to v. And what you are going to see is that all atoms, I am leaving this as an exercise for you all atoms they are displaced together as one unit. So, I am going to have this whole thing move up as one unit, this whole thing moves up as one unit, this whole thing move up as one unit and they go back and forth. On the other hand, if you take k a equals pi, then only the heavy atom is going to go back and forth. This I will give you in an assignment to work out the ratio of u and v for the acoustic mode.

So, finally, I have taken the two extreme limits where k equals 0 and k equals pi, let me take mode where k a is nearly equal to 0, but not equal to 0. That means, I have a large wavelength, in that case the way these modes are going to look and you should work this out on the computer right, you are going to see that in the optical mode the orange one, the large one they are going to shift one way, and the blue ones are going to shift the other way.

So, let me make this here and then show how they are going to change. So, in the large wavelength limit the way they are going to look is like this. Let me make the line here. Let me make the other line also for the blue one. The way these are going to look is going to be the blue ones will be here here, here, here. And you are going to see wave like this. On the other hand, the orange ones are going to be displaced as we saw earlier exactly in the opposite direction.

So, these are going to be the orange ones, these are going to be the blue ones, and the orange ones are going to be in the opposite direction to the blue ones. So, now, we will understand the meaning of the optical mode. Suppose, I had an electromagnetic wave coming in; and at some point it had an electric field shown like this. So, at this point, it had (Refer Time: 22:12) shown like this. And as I said in the beginning of the previous lecture, suppose these atoms smaller ones are Na ions Na plus and the red ones are Cl minus.

You will see that because of this electric field of the electromagnetic wave the Cl ions are going to go down in the direction opposite to the electric field whereas, the blue ions are going to move up in the direction of the electric field. So, an electromagnetic wave can excite a long wavelength, electromagnetic wave can excite can create a motion which is like the optical mode motion, and therefore, these are known as optical modes. So, with this, I hope I have given you a good picture of what the displacements in optical and acoustic modes are. You learn little more when you do the assignment problems that I am going to give you.

Thank you.