Introduction to Solid State Physics
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Lecture – 42
Derivation of wave equation for motion of atoms in a crystal

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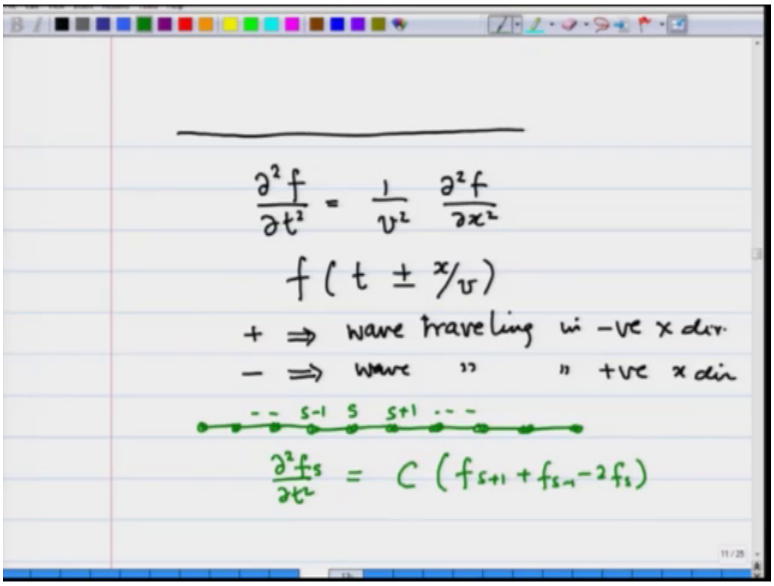

In the previous lecture, I motivated the wave motion and showed you that if I have a continuous medium right a string or air in a pipe or the sound travelling in free medium. The equation of motion satisfied was d 2 f by dt square equals 1 over v square d to f by dx square again emphasizing that I am actually doing a one-dimensional motion and the solution is f t plus or minus x over v wave plus sign means wave travelling and negative x-direction and minus sign means wave travelling in positive x-direction.

And then I showed at the end of the lecture that if instead I have discrete masses then I cannot write the second derivate with respect to x and wrote the equation as d 2 f by dt square and now f will be at s-th side. So, let us call this s-th side this is s minus 1, s plus 1 and so on; and so on is equal to constant f s plus 1 plus f s minus 1 minus 2 f s this is what I had just intuitively I said should be the equation. Now, I have actually I am going to show you that this is the equation when you have these discrete sides.

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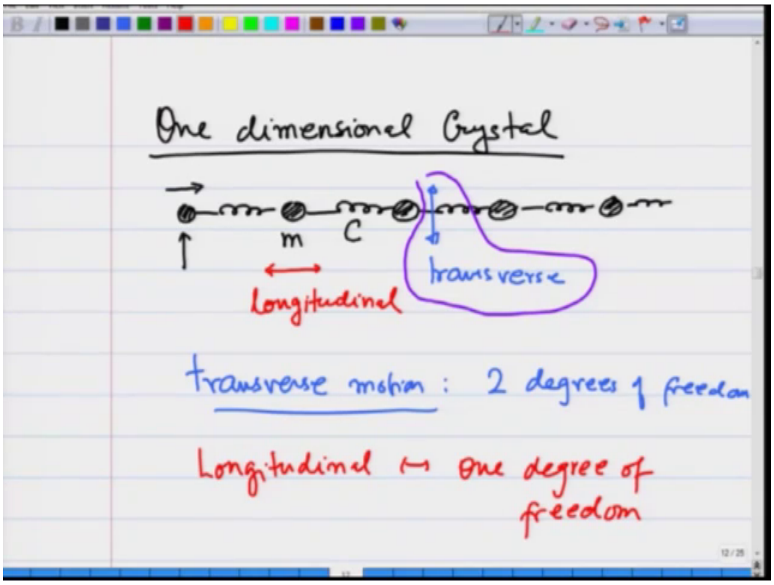

So, let us assume a one dimensional crystal where I have these atoms arranged along let us say the x-axis with connected by spring, right. So, with some spring constant C, mass of each atom is m, they are all identical atoms and I disturb one of the atoms either longitudinally or transverse.

So, I can have two kinds of motions for this if my atoms get displaced perpendicular to the length and the displacement obviously, then travels along the length is transverse or I could have a displacement of these atoms along the length. This will be called longitudinal and right away I will tell you that if I have a transverse motion it has 2 degrees of freedom why?

As I showed in this blue thing out here right, let me use a different color for the transverse motion. The motion could be along the plane of this screen or perpendicular to it. So, there are 2 degrees of freedom; longitudinal, however, has one degree of freedom only that is along the length of the string. Let us see what is the equation of motion of this string is going to be.

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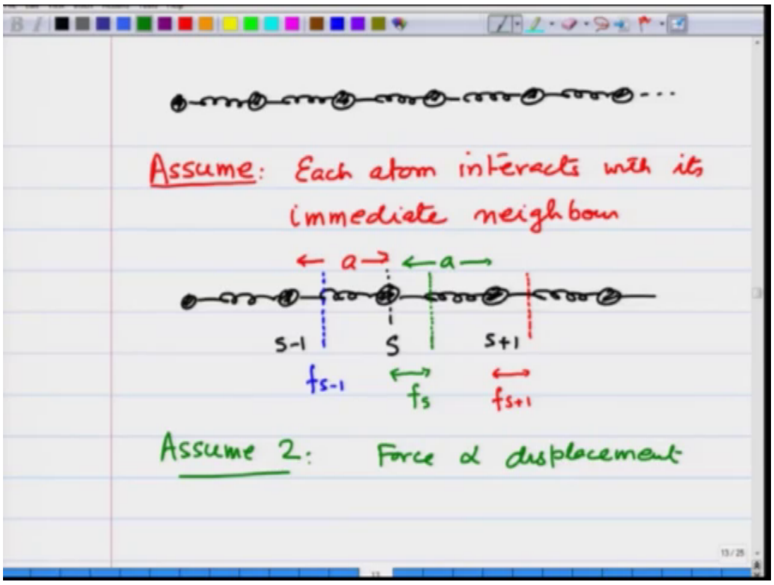

So, let me make this string again here is an atom and I am going to assume ok. We will generalize it later right now I will assume for simplicity each atom interacts with its immediate neighbour; that is if I have an atom at s. So, let me make this string again an atom at s side will interact only with s minus 1 and s plus 1 no others.

In general, there could be and there will be interaction with other atoms also, but right now for simplicity I am not taking that. You could also assume that the only force which is large enough to be taken into consideration is that with the neighbouring atoms others are very small. But, one can generalize it which we will do later right now just focus on the idea.

Now, let this atom be displaced by a distance f s ok. So, it has a new position f s. Let the next one be displaced by f s plus 1; this is displaced by f s plus 1 and let the previous one be displaced by f s minus 1 so that the distances between these atoms change they change from. The equilibrium distance which was a right, let me use a different color which was a two slightly different and I am assuming a force proportional to the displacement that is spring like force right.

So, that is assumption number one was that each atom interacts with its immediate neighbour assumption 2, force is proportional to displacement. In fact, I readied you for this because I was kept making these springs between the atoms. So, it is like a spring between these atoms and force is proportional to displacement let us see the directions of those these forces and how the force on s-th atom looks like.

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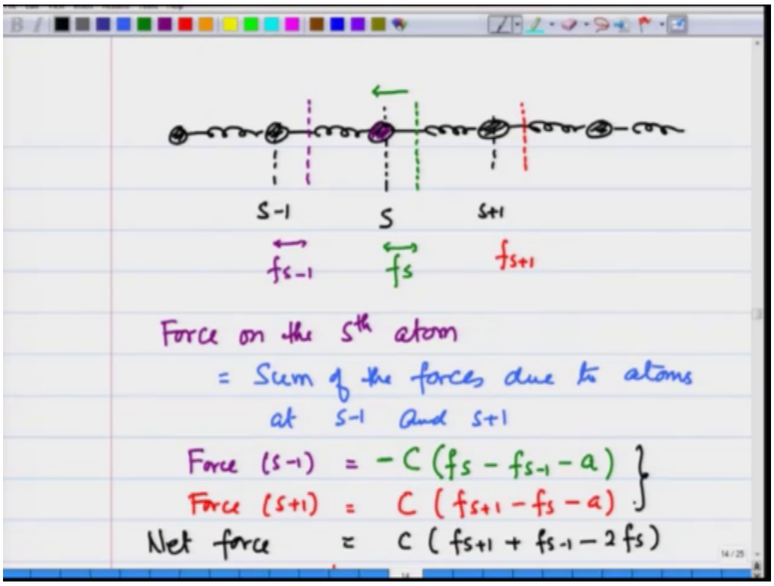

So, let me make this figure again here are these atoms connected by springs and only neighbouring atoms are applying forces on each other. This was the s-th atom, this is s plus 1 atom and the interaction is only with the neighbouring atoms this fellow has been displaced by f s, this fellow has been displaced by f s plus 1 and this fellow the last one the previous one has been displaced by f s minus 1.

Now, force on the s-th atom; this atom, right, the s-th a force on the s-th atom. There will be force due to the atom on the right and the force due to atom on the left. So, this will be equal to sum of the forces due to atoms at s minus 1 and s plus 1 assuming only neighbouring atoms apply the forces. Now, what about the force due to s minus 1? So, let us calculate force, s minus 1. I am just labelling it s minus 1. It is going to be proportional to f s minus f s minus 1 and you may you want to subtract a alright and there is some constant.

Let us see if the direction is right if f s minus f s minus 1 minus a s positive; that means, the spring is stretched then the force on the s-th atom if the spring is stressed will be to the left a string stress a spring will pull it in. So, I should put a minus sign here. Now, let us write the force due to s plus 1. This would be equal to f s plus 1 minus f s minus a time C. Let us see again what the direction would be if f s minus 1 minus f s minus a is positive; that means, this is stretched right. Then again the spring will try to go back to its original position and therefore, it will pull this s-th atom to the right. So, this direction is correct.

Now, let us add the two and see what the net forces. So, net force will be the sum of these two and what do you get? You get C f s plus 1 plus f s minus 1 minus 2 f s net force is the sum of these two. I have added these two and this is the force we get.

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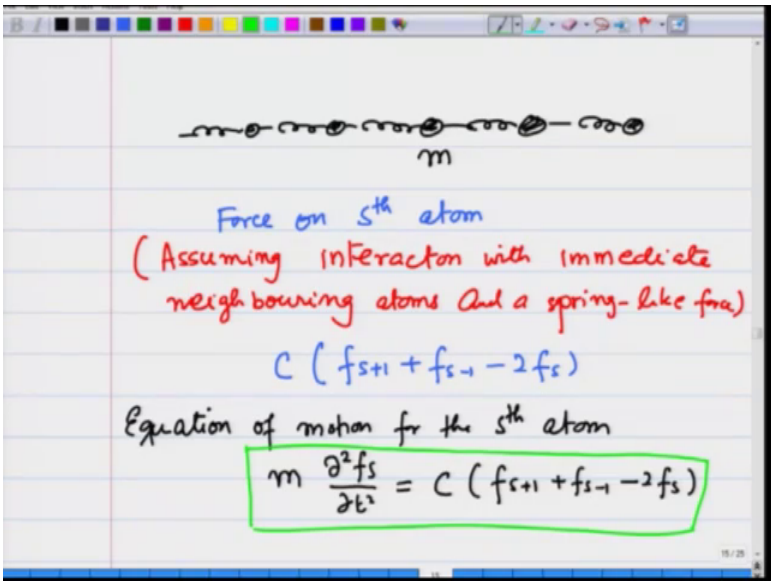

So, let us see what we have got. We have this one dimensional crystal with each atom with mass m and we have found that the force on s-th atom and let me write it again assuming interaction with immediate neighbouring atoms and a spring like force this is the assumption and then the force on the s-th atom came out to be some constant spring constant C times f s plus 1 plus f s minus 1 minus 2 f s.

And therefore, the equation of motion for the s-th atom will be mass of the atom d 2 f s by dt square is equal to C times f s plus 1 plus f s minus 1 minus 2 f s. Let me box it and pause for a moment to give you time to go back to the previous lecture and see that when we took the wave equation for the continuous medium for a string or air or whatever and discretized it this intuitively it gave us exactly the same equation. So, the equation of motion for this s-th atom is this which is discretized form of the wave equation, right.

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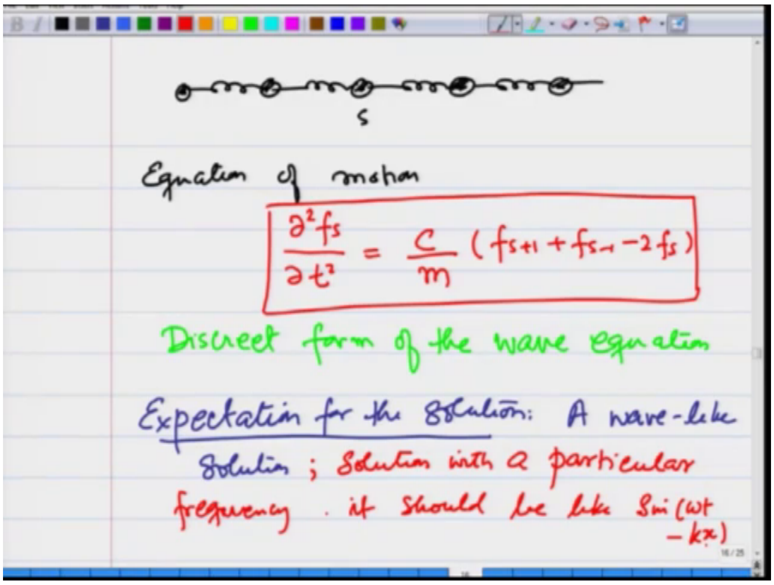

So, let us write this again I will keep making this to emphasize that what we are considering. So, the s-th atom satisfies the equation is d 2 f s by dt square is equal to C over m I have brought the m to the other side f s plus 1 plus f s minus 1 minus 2 f s and let me just to make the point again it is discrete form of the wave equation. This is the equation of motion.

If this is a discrete form of the wave equation I should expect similar solution for a given frequency omega, right. So, we now try that. So, this is assuming that atoms interact with only the neighbouring atoms and the force is spring like with C being the spring constant we found the equation of motion for the s-th particle which is of the form given here which is the discrete form of the wave equation.

So, expectation is for the solution will be a wave like solution. In particular, if I am looking for solution with a particular frequency it should be like sin omega t minus k x, except that x is not continuous anymore, right.

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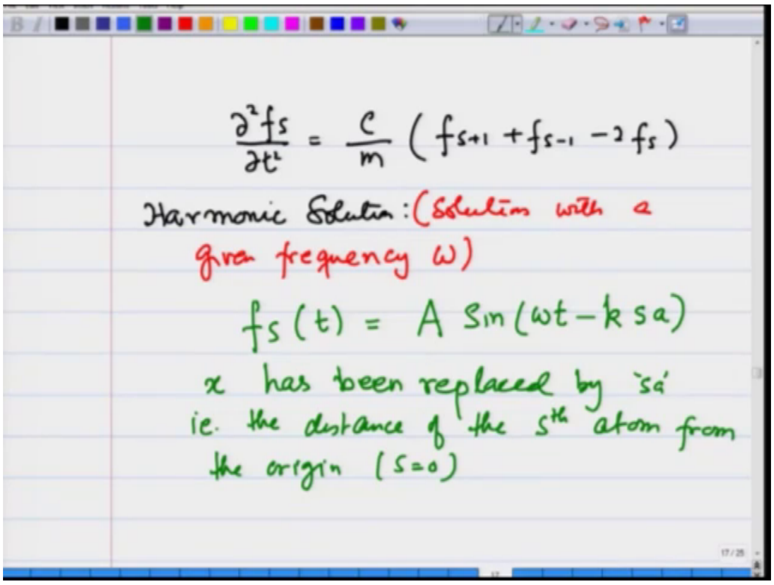

So, let me write this again. I will just focus on the wave equation now. So, I am looking for d 2 f s by dt square is equal to C over m I am looking for the solution f s plus 1 plus f s minus 1 minus 2 f s and I am looking for harmonic solution that is solution with a given frequency and let me also specify that frequency to be omega. Then the solution f s t this is at the s-th side should be some amplitude right some amplitude let us call it A sin of omega t minus k and instead of x now I have to put that discreet variable s times a, right. So, x has been replaced by s a that is the distance of the s-th atom from the origin which I will call s equal to 0.

So, hopefully by now I have brought you to a point where you understand that in a discrete lattice in a discreet crystal where atoms are a distance a away from each other and connected by springs and are interacting only with the nearest neighbours the equation of motion for an atom at s-th side is exactly like the wave equation; except that now we are writing that second derivate in discrete form. And therefore, the solution will also be wave like. In particular, if I am looking for solution with a particular frequency omega that is a harmonic solution it will have the form sin omega t minus k sa. And with this now I can find the relationship between omega and k. We will find the solution in the next lecture and discuss its properties.