Introduction to Solid State Physics
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Lecture – 43
Solution of the wave equation for a crystal and the relation between ω frequency and wavevector k

Let me start this lecture by quickly recalling what we had done so far.

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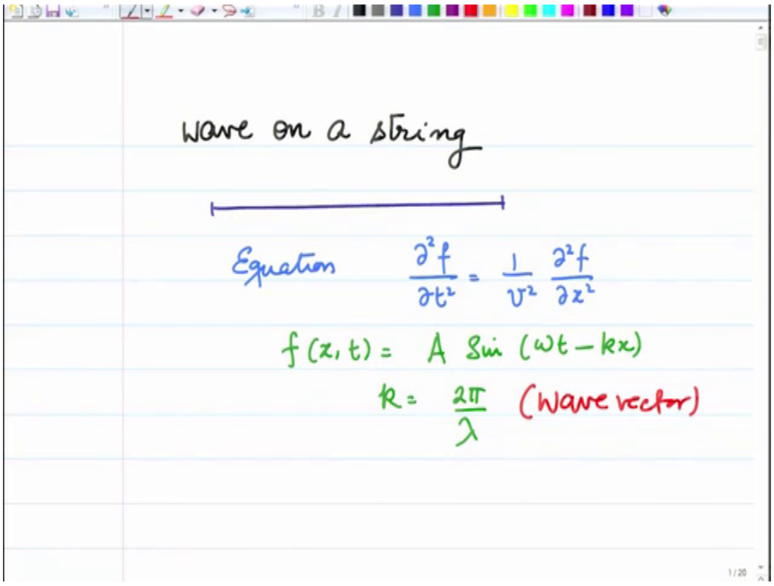

So, recall that I had started with wave on a string. So, I will make the string now and we had obtained the equation of the wave as d 2 f over dt square equals 1 over v square d 2 f by dx square; we have taken a one dimensional string. And, the solution with a given frequency and which I call the harmonic solutions were given as f x, t as some amplitude sin of omega t minus k x where k is 2 pi over lambda and I am going to give it a name now it is called the wave vector.

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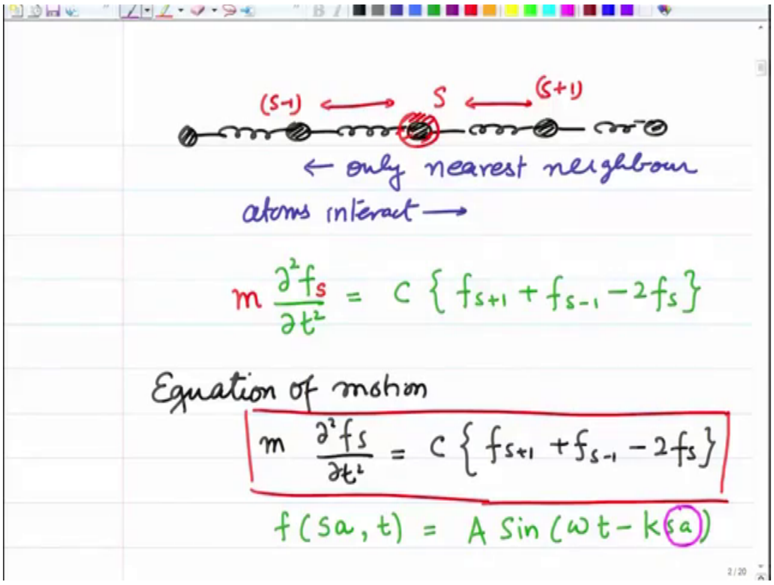

This is for a continuous string and then we generalize this to the case where I have these point particles of mass m connected by some spring of interacting with each other. And we made an approximation that only nearest neighbour atoms interact and under that assumption I will also give the equation for these atoms.

Now, they are discrete I motivated you how to come to a discrete equation and then we wrote the equation for the displacement of these atoms are as d 2 f over dt square is equal to the coefficient of the interaction times f s plus 1 plus f s minus 1 minus 2 f s and I am missing a few terms here. There should be a mass term with the displacement and this is displacement for the s-th atom and then that as follows.

So, what we are doing is we are writing the equation for this s-th atom out here I am showing you on top of the screen this is interacting with the next atom s plus one-th atom and s minus one-th atom only the next nearest atoms and then this becomes the equation. So, let me write it again in the same color the equation of motion for this atom at the s-th side is d 2 f s over dt square is equal to C, where C is the spring constant, so to speak is f s plus 1 plus f s minus 1 minus 2 f s this is the equation of motion.

All atoms are identical, they are interacting with only with nearest neighbours and then this becomes the equation and I had also arrived at this equation through finite difference formula for the second derivative. I would urge you to go back and look at the first lecture.

So, through all this what we have said is this is the equation of motion when these atoms are at discrete sides at distances a from each other and are connected through springs or equivalently they are interacting with forces only with the nearest neighbour and the force is proportional to the displacement spring like force.

And, then we said since this is a wave equation this is like the generalization of the wave equation for discrete masses a solution for a given frequency would also look like f. The difference from the wave equation is instead of x now I am going to have s a where is the distance between the atoms at time t is like A sin omega t minus k sa. This is the solution that I had proposed last time and we are going to explore this further this time.

So, the only difference between a continuous string and these discrete masses that now that x that was there in the continuous string has been replaced now by this case k sa and these are sitting at discrete points. Let us now look at the nature of the solution.

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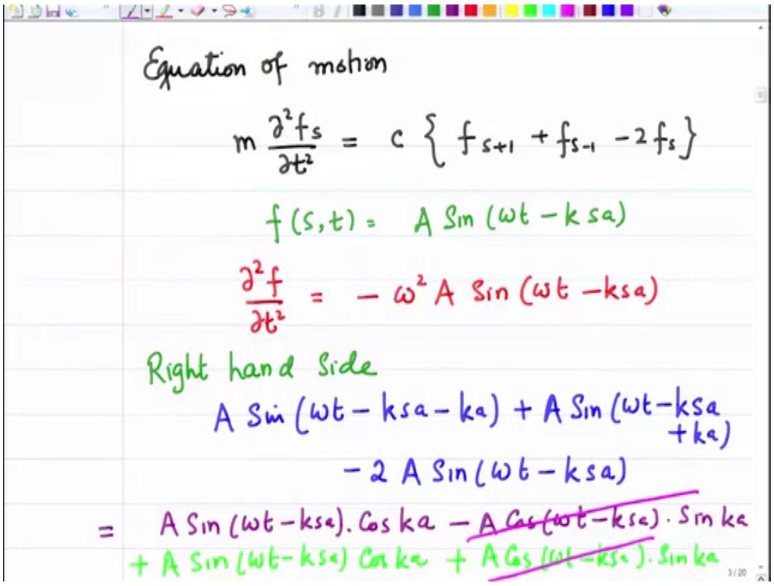

So, let me write the whole thing all over again. The equation of motion is d 2 f over dt square is equal to it is a mass term C times f s plus 1 and this is for the s-th atom plus f s minus 1 minus 2 f s and the solution I am looking for is of the form f at s a or s just s is fine t is equal to some amplitude A sin of omega t minus ksa.

Let us take the derivatives if I take the time derivative d 2 f over dt square would be equal to minus omega square A sin of omega t minus ksa. Let us also calculate the right hand side now; so, this is my left hand side the right hand side is going to be f s plus 1.

So, that is going to be a sin of omega t minus k sa minus k a plus f s minus 1. So, that is going to be A sin of omega t minus ksa plus ka minus 2 times f s which is going to be A sin of omega t minus ksa let us calculate this. So, this I am going to write as equal to first term is going to be A sin of omega t minus ksa times cosine of k a minus A cosine of omega t minus ksa times sin of ka.

The second term is going to be plus A sin of omega t minus ksa times cosine of ka plus A times cosine of omega t minus ksa times sin of ka and there is the third term which I am going to include in the next screen, but for the first two terms you can immediately see that this term cancels with the second term and I am left with 2 A sin omega t minus ksa cosine ka.

So, let us see how does it work out? I will go to the next page.

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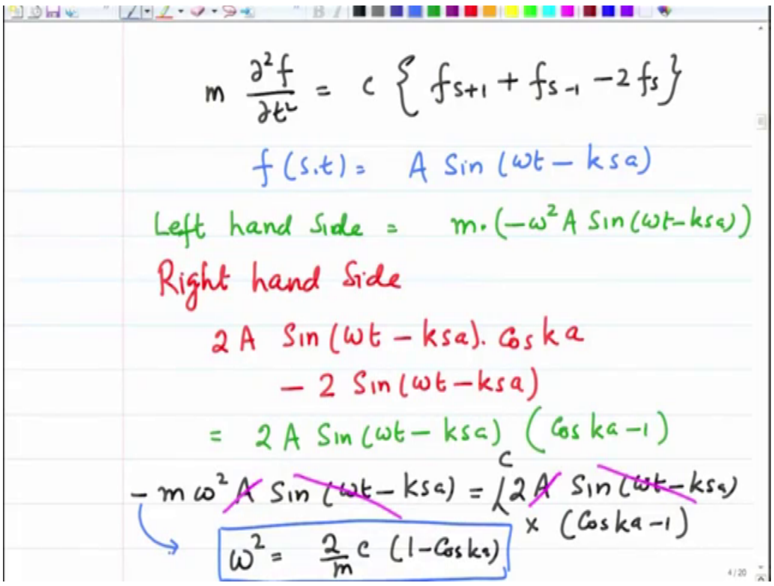

So, I am looking for the solution let me rewrite this looking for the solution of this equation d 2 f by dt square times m is equal to C f s plus 1 plus f s minus 1 minus 2 f s and I have taken the solution to be of the form f s t equals A sin of omega t minus ksa and then we have found by substituting at end that the left hand side is equal to mass times minus omega square A sin of omega t minus ksa this is times. And, the right hand side s which we calculated just now it is 2A sin of omega t minus ksa times cosine of ka and the last term was which I had not included in the previous slide is 2 times sin of omega t minus ksa.

This simplifies to 2A sin of omega 2 omega t minus ksa times cosine ka minus 1. Equating the two sides of the equation we now get minus m omega square A sin of omega t minus ksa is equal to 2A sin of omega t minus ksa times cosine of ka minus 1 and this would give me a relationship between omega and k.

So, let us now quickly cancel the terms on two sides I can cancel A on the two sides I can cancel sin omega t minus ksa on the two sides and I am left with omega square is equal to 2 over m, I am sorry there was C also out here C 1 minus cosine of ka. Notice that the sin because of this minus sign out here the right hand side now has become 1 minus cosine ka.

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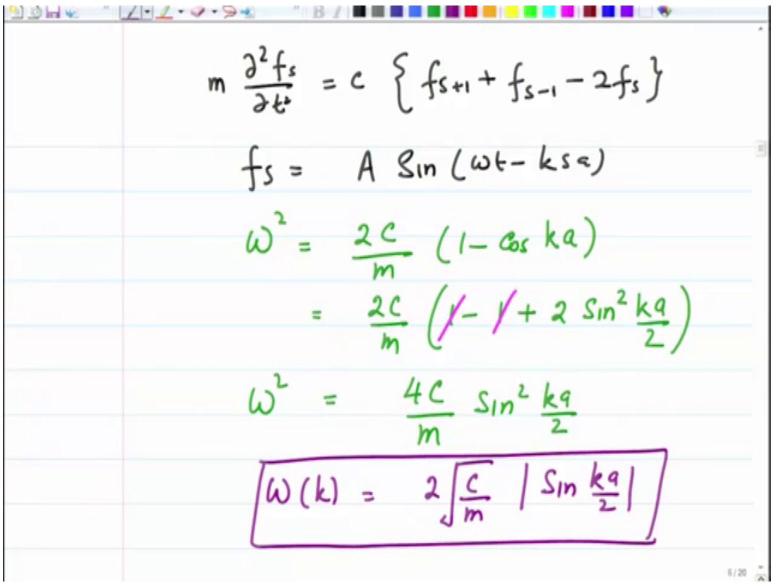

So, let us write this what we got we got for the solution of this equation equal C f s plus 1 minus f plus f s minus 1 minus 2 f s. Assuming a solution f s equals A sin of omega t minus ksa we got the relationship omega square is equal to 2 C over m 1 minus cosine of ka which I can explain I am write as 2C over m 1 minus 1 plus 2 sin square ka by 2. This 1 cancels and I end up getting that omega square is equal to 4C over m sin square ka by 2 and therefore, omega as the function of k is given as 2 square root of C over m modulus of sin ka by 2 modulus because omega is always positive; this is my answer.

So, what have we learnt?

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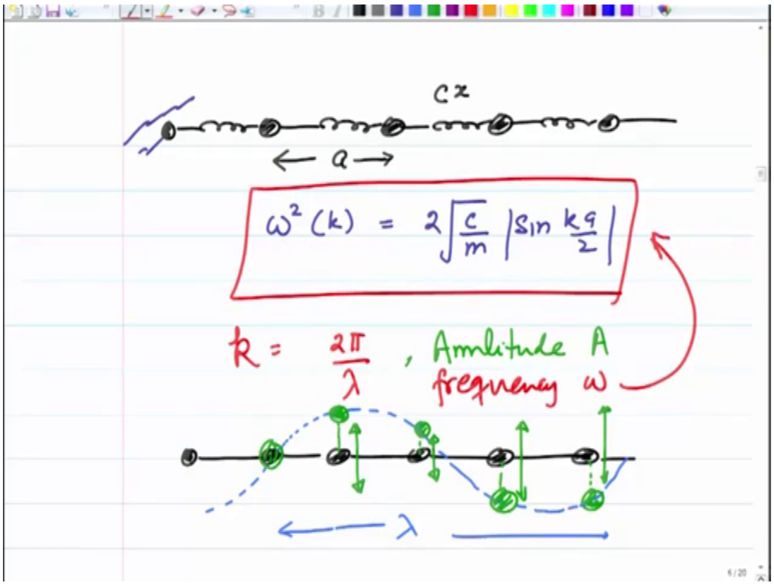

Let us understand that what we have learnt is that given a one-dimensional chain it is an infinitely long chain of atoms which are at a distance a from each other and interact with each other through a force proportional to the distance or the elongation of this spring C x, then if I disturb one of the atoms right, I just disturb it if I give it a push if I do it properly I can have harmonic waves here travelling with frequency omega square related to the k as sin ka by 2 modulus because it is positive. Let me again put it in a box. Recall, what is k? k is 2 pi over lambda.

So, the picture that is coming to our mind now is that if I have this chain I am not bothering to make spring again and again, right and if I give it a displacement let me give something a displacement and the displacement is such that it has a wavelength lambda. That means, the displacement would go something like let us say right this distance being lambda then these atoms let me now show it in a different color, the atoms would be displaced at each point, right by I am show it in green. This atom remains where it is, this atom would be displaced here, this atom would be displaced here, this atom would be displaced down here, this atom would be displaced here and so on.

In the whole chain these atoms will be displaced like this and they would be oscillating just like in a wave they would be oscillating back and forth. With the amplitude omega, let me write this no sorry with the amplitude a and frequency omega right frequency omega given by this formula, ok. So, we have found a relationship like we have for waves in a medium like the sound waves or you may have studied electromagnetic waves there is a relationship between the frequency and the lambda. Similar relationship exists between omega and k for harmonic waves and this is the picture that we make and they will be oscillating back and forth and this wave travels.

The difference is that now the systems or the atoms that are oscillating back and forth and that are propagating the wave are at discrete points, it is not a continuous medium

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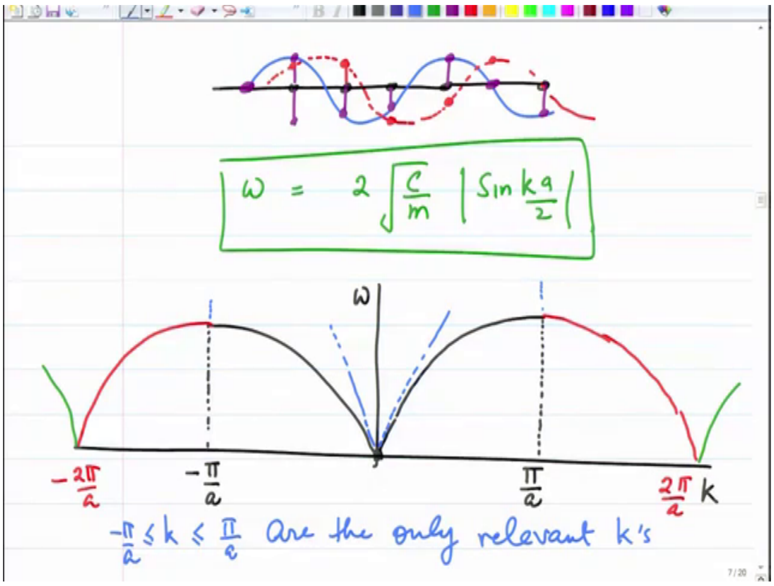

So, let me recap now the whole thing again. In this discrete system I have a wave where the atoms now get displaced like this at a given time and as the wave propagates next time the wave would have shifted further out. And these displacement of the atoms would be different, right according to where the position of the wave is. So, this wave is propagating and these atoms are going back and forth with a frequency given by 2 square root of C by m modulus sin ka by 2 ok.

Now, let us look at how this plot looks. If I would to plot omega versus k; at k equals 0, everything is 0. As you increase k it will go up like a sin wave and then it flattens out; same thing on the other side it flattens out and it hits a maximum at pi over a hits a maximum at minus pi over a. Remember there is a mod in the formula. So, minus pi over a on pi over it does not matter and if you increase k further it goes down. Again becoming 0 at 2 pi over a minus 2 pi over a and if I increase k further it repeats itself this is the picture of omega k versus k.

So, what you see is that omega has a periodic behaviour it is linear near the origin, like the sin curves for a small magnitude are linear near the origin then flattens out and then repeats itself. So, omega actually can be determined by all case only up to pi over a from minus pi over a 2 pi over a after that it repeats itself. So, I am just going to make a statement and then justify it further that only k in the range pi over a and minus pi over a are the only relevant k's to describe the behaviour of vibration of this discrete lattice. Let me justify it further omega does not change, but does it mean anything more.

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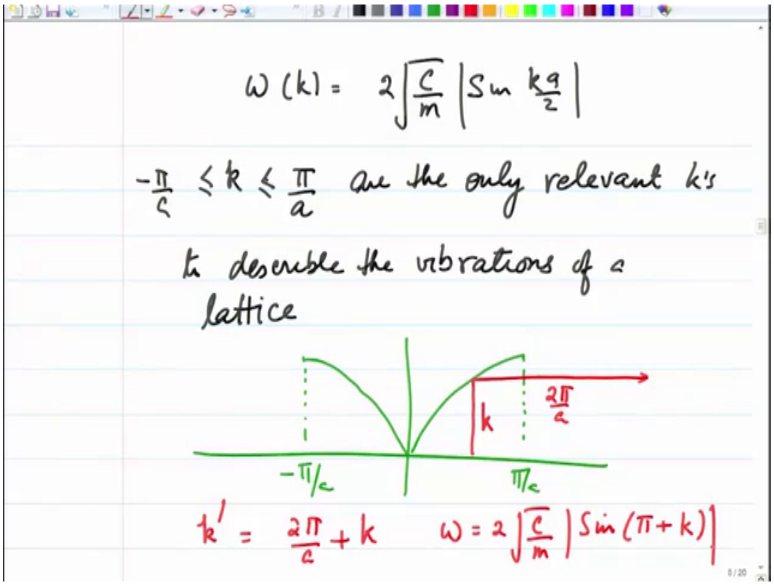

So, if we say let me write the formula again omega k is equal to 2 square root of C over m sin of ka by 2 modulus; if we say this notice that k we are saying is minus pi by a to pi by a are the only relevant k's to describe the vibrations of a lattice.

What happens if I go beyond pi over a, right? So, suppose I take let me make this picture again this was my picture or omega versus k up to pi over a and minus pi over a and suppose I take a particular k point here and move it by 2 pi over a; that means, I take a new k prime which is equal to 2 pi over a plus k, what happens omega? Omega will become 2 root C over m mod sin of pi plus k mod which is same as sin k. So, omega does not change, what about the displacements?

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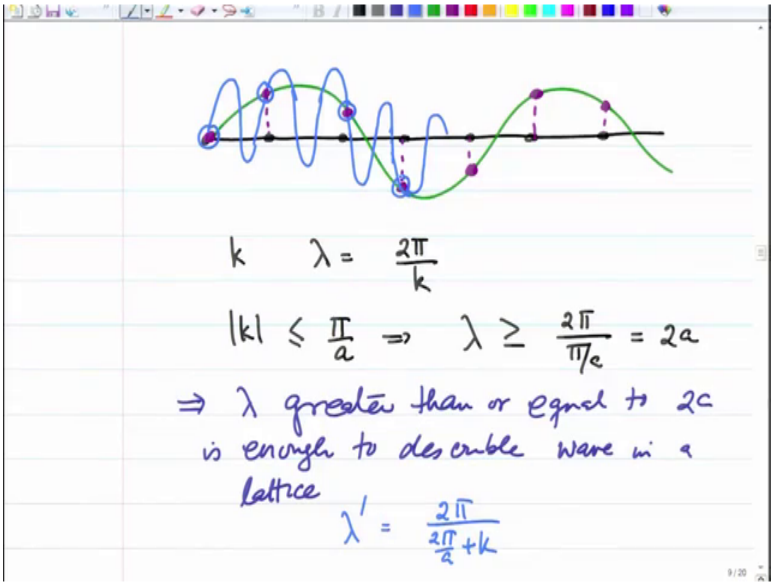

Let us look at the displacements. What would happen is that when I take these points and I take a particular k or a lambda. So, let me make a lambda these points are displaced at a given time like this which I am showing in purple. What will happen if I take k prime which is 2 pi over a. So, let us analyze it little.

So, when I is take a k the relevant lambda is 2 pi over k; when I say mod k is less than equal to pi over a this implies that lambda is greater than or equal to 2 pi over pi over a that is equal to 2a. So, what we are saying essentially by saying that k confined between minus pi over m a is the only relevant quantity also implies that lambda greater than or equal to 2a is enough to describe wave in a lattice.

What happens if I take shorter lambda? So, suppose I take a shorter lambda what you would find if I take a shorter lambda which corresponds to, right; so, let me take a shorter lambda, lambda prime which corresponds to some k prime which is 2 pi over 2 pi over a plus k and you can calculate this and what you would find is that the motion if I plot this curve right, suppose I take a shorter lambda you would find that each point is given the same displacement by the shorter lambda and also is motion direction is the same.

So, it does not matter whether I take lambda to be shorter corresponding to k prime or that lambda larger than 2a. Let me now show this mathematically.

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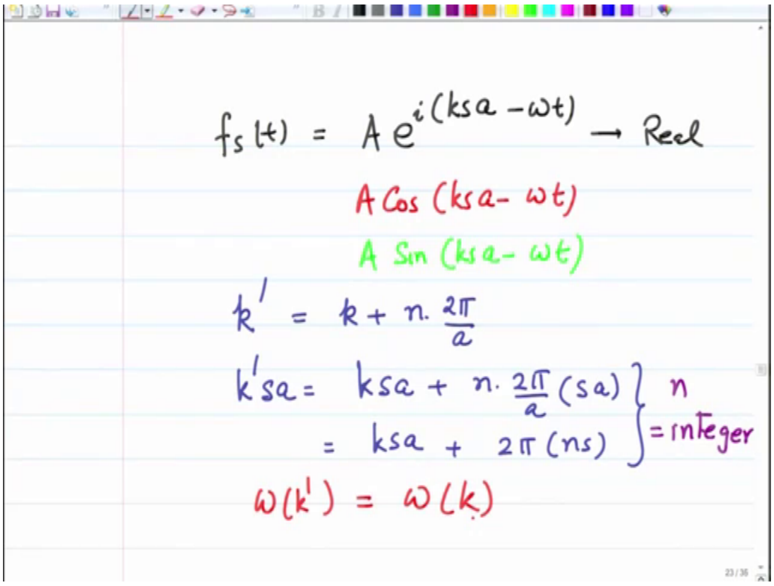

Recall that we have f s t written as an amplitude e raise to i k sa minus omega t or equivalently as cosine of ksa minus omega t or A sin ksa minus omega t. They are all the same thing, the only thing is that here we take the real part and a could be complex this I explain further and in my note that I will give to you.

Now, if I take k prime is equal to k plus some integer n 2 pi by a then k prime sa is going to be equal to k sa plus n points 2 pi by a times sa. So, this becomes k sa plus 2 pi times ns , where n is an integer. So, I can add 2 pi by a or any integer multiple of it and at the same time I have omega k prime is equal to omega k, that we have already discussed quite in detail.

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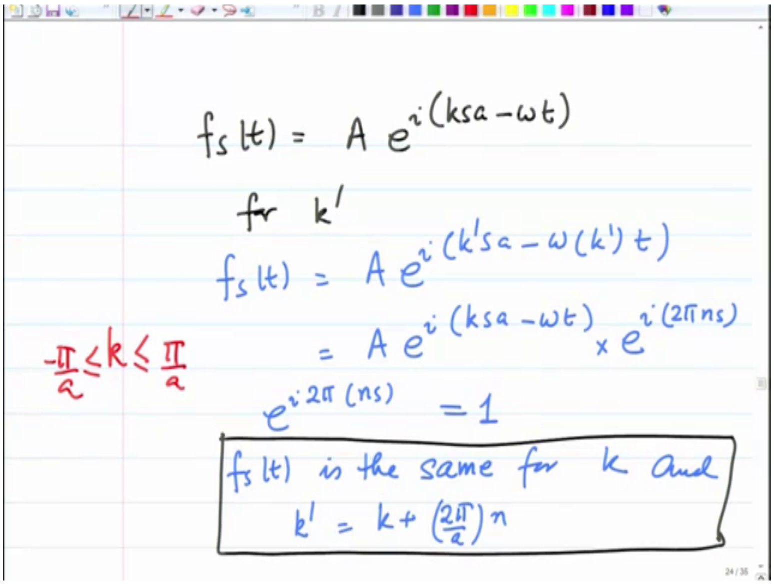

And therefore, the displacement f s t which was given as some amplitude e raise to i ksa minus omega t for k prime it is going to be f s t is equal to A e raise to i k prime s a minus omega k prime t which is equal to A e raise to i from whatever we did in the previous slide ksa minus omega t times e raised to i 2 pi ns.

Now, n and s both are integers therefore, e raise to i 2 pi ns is equal to 1. And, we find that f s t is the same for k and k prime is equal to k plus 2 pi over a times an integer n. So, again we see that if I take k confined to range between pi by a and minus pi by a, it describes all the motion of this discrete lattice because adding 2 pi by a to it does not really make any difference in the frequency or the displacement.

One more point you may ask is fine, the displacement is the same; what about the velocity?

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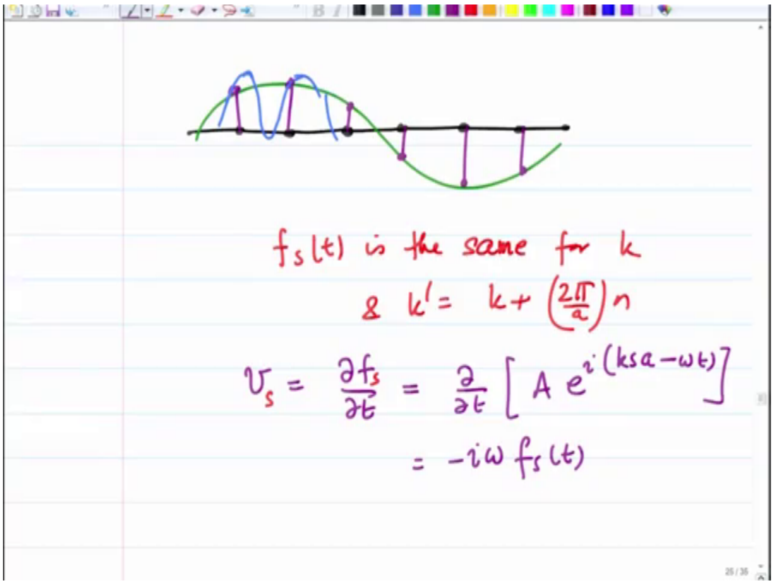

So, when I have this wave and I am claiming that with a lambda like this where the particles are displaced like this and another lambda which is shorter like this gives the same vibrations then we have found that f s t is the same for k and k prime equals k plus 2 pi by a times n and the velocity v is nothing, but d f by dt; let me put a subscript s here just to show for the s-th position. And, this is d by dt of A e raise to i ksa minus omega t which is nothing, but minus i omega f s t. So, if the displacement f s remains the same, so, does the velocity.

So, all these atoms have the same displacement same velocity and you can also show same acceleration. So, it does not really matter whether I take k and find in the Brillouin zone or k outside it the motion is the same and therefore, everything can be described ks within the Brillouin zone.

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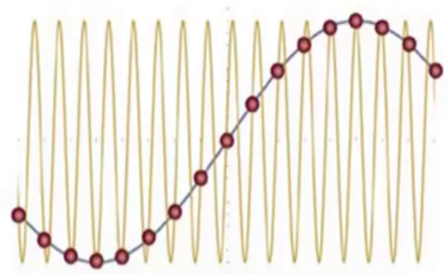

What I will do is I will make a nice picture and give a supplement to this to convince you that it is k between pi by a and minus pi by a that really is enough to describe the motion because omega anyway is the same and lambda therefore, I take 2a or greater any shorter lambda also gives you the same motion.

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Note on the displacement of atoms in a one-dimensional crystal lattice and equivalence of the wavevector k and $k + n(2\pi/a)$, where n is an integer and a is the lattice spacing

In the lecture we have solved the equation of motion for atoms in a one-dimensional crystal. Assuming nearest neighbor interaction and a spring-like force, the equation of motion is

$$m\frac{\partial^2 f_s}{\partial t^2} = C\{f_{s+1} + f_{s-1} - 2f_s\}$$

Here m is the mass of one atoms and C is the spring-coefficient. Its harmonic solution is (It is understood that in this solution $A = |A|e^{i\varphi}$ is complex and the real part of the solution above represents the displacement of the atoms)

$$f_s(t) = Ae^{i(ksa-\omega t)}$$

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and leads to the dispersion relation

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

Taking the real part of the solution above given the general displacement to be

$$f_s(t) = |A|\cos(ksa - \omega t + \varphi)$$

Now $|A|$ represents the amplitude of the wave and φ the phase. With different values of φ, solutions like $f_s(t) = |A|\cos(ksa - \omega t)$ or $f_s(t) = |A|\sin(ksa - \omega t)$ that are given in the lecture are obtained. Thus these are all equivalent solutions with only difference between them being the phase.

As pointed out in the lecture, $\omega(k)$ is the same for wavevector k and $k \pm n(2\pi/a)$ and therefore it is sufficient to consider k values confined to $-(\pi/a) \leq k \leq (\pi/a)$ i.e. in the first Brillouin zone.

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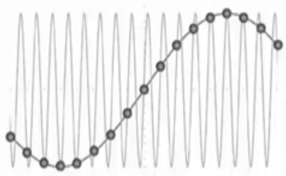
This is because in the factor $(ksa - \omega t + \varphi)$, replacing k by $k \pm n(2\pi/a)$ gives $(2\pi + ksa - \omega t + \varphi)$ with the same ω and $e^{2\pi i} = 1$. Furthermore, the velocity of the atoms is $-i\omega f_s(t)$ and therefore that is also the same. In other words, the wavevectors k and $k \pm n(2\pi/a)$ describe exactly the same motion. In the following figure we show this for the following parameters: $a = 1.$ $k = 0.1\pi$ $n = 1$



You notice that both the waves with different wavelengths corresponding to k and $k + (2\pi/a)$ give exactly the same displacement, and therefore the same velocity and the same acceleration for each of the atoms.

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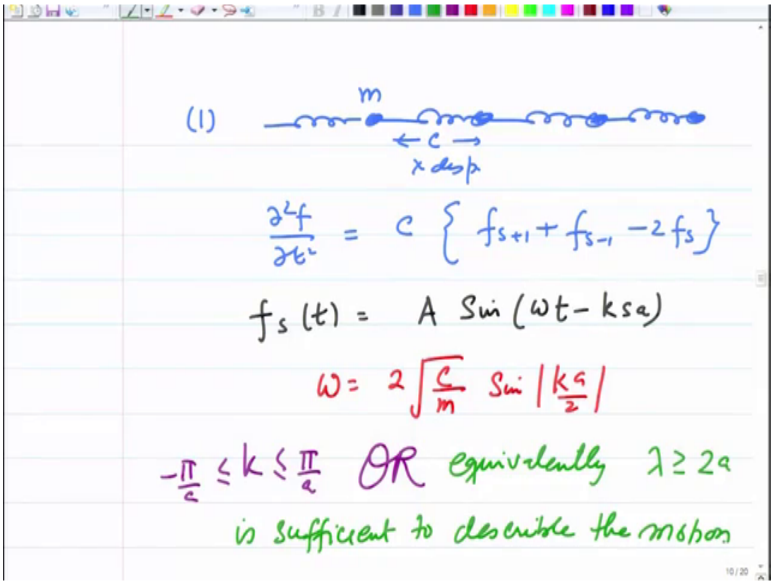

So, with this I will conclude this lecture is by saying that 1, in a discrete lattice with I keep making this spring again because I want to show that this force is proportional to C times displacement mass is m then the equation of motion is d 2 f by dt square is equal to C f s plus 1 plus f s minus 1 minus 2 f s and the solution f s t is wave like with an amplitude A and frequency sin omega t minus ksa and the relationship between omega and k is 2 root C over m sin mod ka over 2 and k between pi by a and minus pi by a or equivalently lambda greater than or equal to 2a is sufficient to describe the motion in this discrete lattice.

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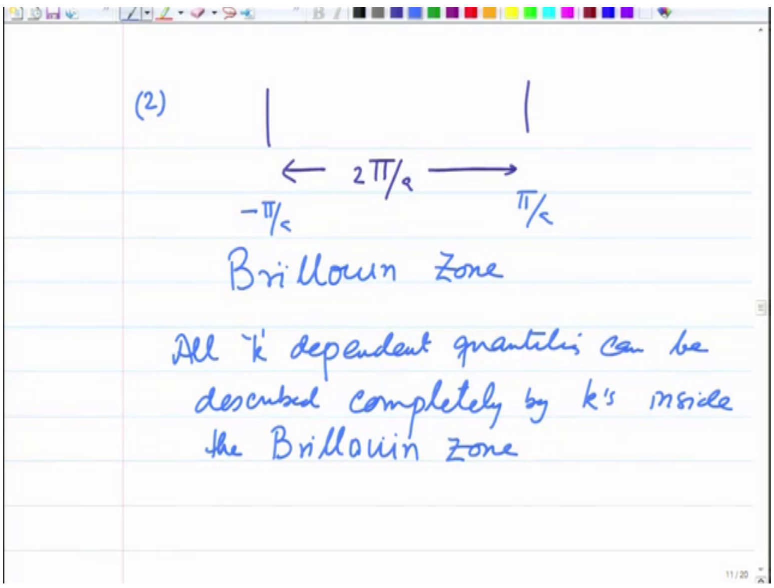

So, now some terminology this extent of k from minus pi by a 2 pi by a is known as Brillouin zone and you will find in all the crystal properties is the Brillouin zone whatever happens inside this keeps repeating itself. So, this is a very important concept. It is known as Brillouin zone, alright. And, all k dependent quantities can be described completely by k's inside the Brillouin zone. So, this is the conclusion.

So, this is the point number 2 and I have taken a particular kind of solution.

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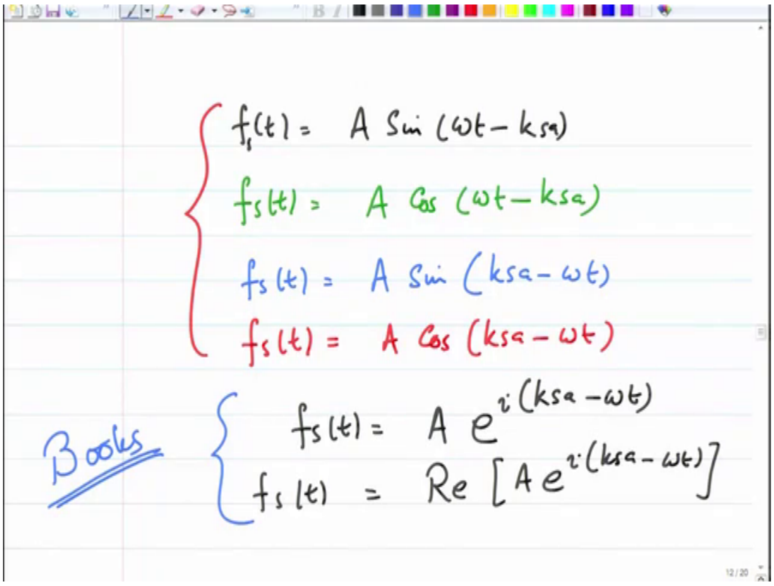

In describing solution I took f s t to be A sin omega t minus k s times a you could have taken equally well f s t as A cosine of omega t minus ksa equally well you could have taken f s t as A sin of ksa minus omega t or f s t is equal to A cosine ksa minus omega t; does not matter you change the sin and phase changes.

And, generally make maths easy what you do is you combine all this and write your f s t some amplitude e raised to i ksa minus omega t, because when you do this adding, subtracting, multiplying taking differentiation that becomes easy and finally, it is understood when you do this finally, when you are going to show the displacement is going to be real of this A e raised to I ksa minus omega t or imaginary part of this.

So, in the books this is what is followed. If you read the reference books that we have prescribed you will see that the solution is given as e raise to i ksa minus omega t and sometimes it is confusing because a lot of students asked if this is a complex quantity how is the displacement given. Displacement is given as it is real part and that is precisely when I did the exercise I showed you that I can do the same calculations with displacement taken as real. But, to facilitate the mathematics one does it with exponential and this is what you will find in most of the books.