

Introduction to Solid State Physics
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Lecture – 45
Waves in a crystal considering interaction among atoms beyond their nearest neighbours

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$$F_s = c [f_{s+1} - f_s] + c [f_{s-1} - f_s]$$
 Nearest neighbour interaction

$$F_s = c [f_{s+1} + f_{s-1} - 2f_s]$$

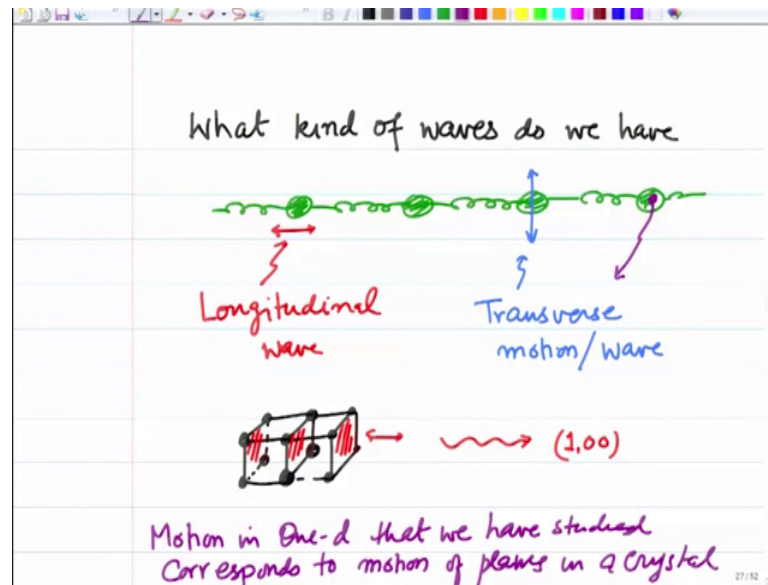
$$m \ddot{f}_s = m \frac{\partial^2 f_s}{\partial t^2} = c [f_{s+1} + f_{s-1} - 2f_s]$$

$$\omega^2 = \frac{4c}{m} \sin^2 \frac{ka}{2}$$

So, far what we have considered is chain of atoms or a one dimensional crystal with the atoms interacting through a force, which is proportional to the stretch of the assumed spring between them. So, we assume that the force on the atom at F site is proportional to $c f_{s+1} - c f_s + c f_s - c f_{s-1}$; that is the only thing that we assumed was the nearest neighbor interaction and we derived from this, that the force F_s is $c f_{s+1} + c f_{s-1} - 2c f_s$.

And therefore, the equation of motion that we obtained was $m \ddot{f}_s = c [f_{s+1} + f_{s-1} - 2f_s]$, where double dot is the second derivative of the displacement with respect to time and this was equal to $c f_{s+1} + c f_{s-1} - 2c f_s$. And assuming a wave like solution we obtained $\omega^2 = \frac{4c}{m} \sin^2 \frac{ka}{2}$ where a is the distance between the atoms I am showing in the top this is. What we have done so, far and then we of course, defined the Brillouin zone and showed you how k is defined only within the Brillouin zone we want to address certain general aspects now.

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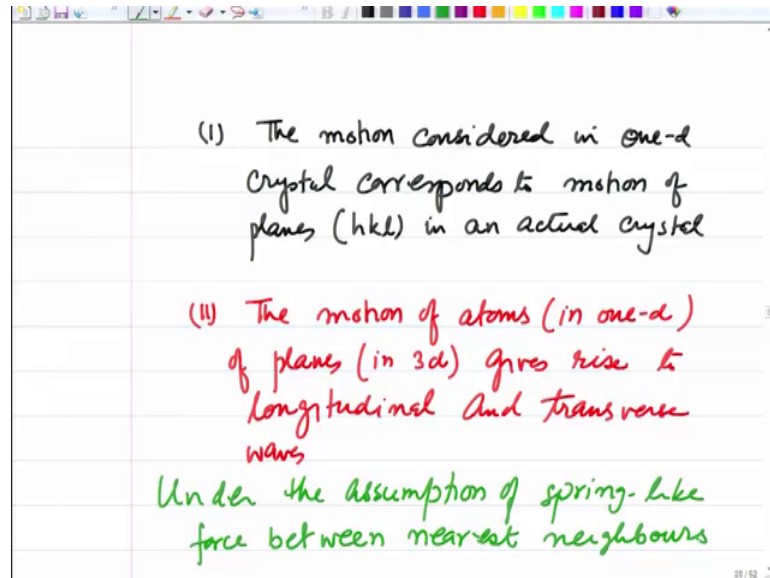
So, what kind of waves do we have? That is the first question I am going to answer. So, again looking back at this chain of atoms, I can have these atoms displaced in the direction of wave propagation and this will be a longitudinal wave. I can also have the atoms oscillating perpendicular to the direction of the chain, and this would be transverse motion or transverse wave. Transverse direction it can be in 2 directions; one is what I have shown in the plane of the screen the other displacement could be perpendicular to the screen. So, this is also transverse.

So, I could have transverse or longitudinal waves. You may also be wondering so, far as to how this one dimensional chain is related to what happens in a crystal. So, in a crystal what I am going to have? Suppose for simplicity I have a cubic crystal that is the atoms are sitting at these corners. What this one dimensional motion represents is the displacement of these planes. So, I could have for example, this plane oscillating like this and the wave propagating like this. This would be a longitudinal wave in the direction of $1\ 0\ 0$. Similarly I could have waves propagating along the diagonal I could have wave propagating along the body diagonal or phase diagonal.

So, different planes which you have studied earlier can oscillate and propagate a wave and this one dimensional motion that we have studied so far or the motion in 1 dimensional crystal that we have studied so far would be actually the motion of these planes and that is precisely what happens in a crystal. So, let me write this the motion in

one d that we have studied corresponds to motion of planes in a crystal. So, this is how we connect. So, what we have done is not a futile exercise is actually related to the motion of planes in a crystal and later, I will show you towards the end of this week's lectures that this is precisely what we study experimentally. So, that is one point I wanted to make.

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So, 2 points I have made is one that the motion considered in one d crystal corresponds to motion of planes, which are given by hkl you have studied that in an actual crystal. And point number 2 is that the motion of atoms in one d and of planes in 3 d gives rise to longitudinal and transverse waves. In a longitudinal wave the motion of planes is along the direction of the wave and in a transverse wave is perpendicular to the direction of the wave. And all this that we have studied is under the assumption of spring like force between nearest neighbors that is the simplification we take.

So, I want to take 1 step beyond it and see what happens, if all the planes or all the atoms were interacting how this dispersion relation be modified that is now the exercise I am going to take up. So, now, what we are going to see is let me make these planes right.

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$$F_s = \sum_{p>0} C_p (f_{s+p} - f_s) + C_p (f_s - f_{s-p})$$

Equation of motion for the s^{th} plane

$$m \frac{\partial^2 f_s}{\partial t^2} = \sum_{p>0} C_p (f_{s+p} - f_s) + C_p (f_s - f_{s-p})$$

This is a plane of atoms let me make these atoms in a crystal is to make the point that these are real calculations that we are doing and so on. And what I am going to assume now is that, suppose I have the s plane is going to interact with $s+1$ plane $s+2$ plane and so on.

And similarly $s-1$ plane $s-2$ plane and so on and the force on the s plane is going to F_s equals C_p due to the $s+p$ plane minus f_s plus C_p f_s minus f_{s-p} minus f_s . This is force due to the plane on the negative side plane on the positive side I have assumed that for the force by the $s+p$ plane, the coefficient of force is C_p it changes with each plane and then I have to sum over p .

Since I have taken p on the negative side also so, I will sum over p greater than 0 only. So, you can check all the direction of the force and everything is correct. Now the equation of motion for the s th plane is going to be $m \frac{d^2 f_s}{dt^2}$ is equal to summation p greater than 0 $C_p f_{s+p}$ plus f_s minus f_s plus $C_p f_s$ minus f_{s-p} minus f_s .

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$$m \frac{d^2 f_s}{dt^2} = \sum_{p>0} C_p (f_{s+p} + f_{s-p} - 2f_s)$$

Wave like solution for s^{th} plane

$$f_s(t) = A e^{i(k s a - \omega t)}$$
$$f_{s+p}(t) = A e^{i(k s a + k p a - \omega t)}$$
$$-m \omega^2 = \sum_{p>0} C_p (e^{i k p a} + e^{-i k p a} - 2)$$
$$= \sum_{p>0} 2 C_p (\cos k p a - 1)$$

So, the equation of motion that I have is $m \frac{d^2 f_s}{dt^2}$ is equal to summation over p greater than 0 C_p and now I can take all the terms together I can write this $f_{s+p} + f_{s-p} - 2f_s$ this is the equation of motion. Again I am going to assume a solution which is wave like. So, wave like solution for s^{th} plane is going to be f_s as a function of t is equal to some amplitude $A e^{i(k s a - \omega t)}$.

And therefore, for $s+p$ plane is going to be $A e^{i(k s a + k p a - \omega t)}$. And when I substitute this in the equation above what I am going to get is $m \omega^2$ is equal to summation p greater than 0 $C_p e^{i k p a} + e^{-i k p a} - 2$ and this leads to summation over p greater than 0 $2 C_p \cos$ of $k p a - 1$ there is a minus sign in front.

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$$m\omega^2 = \sum_{p>0} 2C_p (1 - \cos kpa)$$
$$= \sum_{p>0} 4C_p \sin^2 \frac{kpa}{2}$$
$$\omega^2 = \sum_{p>0} \left(\frac{4C_p}{m}\right) \sin^2 \frac{kpa}{2}$$

when $C_p \neq 0$ only for $p=1$

$$\omega^2 = \frac{4C}{m} \sin^2 \frac{kpa}{2}$$

And therefore, the equation of motion gives me $m\omega^2$. I take the minus sign to the other side summation $p > 0$ to $C_p (1 - \cos kpa)$, which is nothing, but summation $p > 0$ $4C_p \sin^2 \frac{kpa}{2}$. And therefore, in this case ω^2 becomes summation $p > 0$ $\frac{4C_p}{m} \sin^2 \frac{kpa}{2}$. This is the relationship that we get if we assume still spring like force between different planes but all the planes included.

In a special case when C_p is not equal to 0 only for $p=1$, you get $\omega^2 = \frac{4C}{m} \sin^2 \frac{kpa}{2}$, we get the previous relationship that we had obtained assuming only nearest interaction. So, we can do things in general and write the frequency of the travelling waves or the disturbances when other planes are also interacting, notice that I am still assuming a spring like interaction between the planes. So, this is a generalization of what we did earlier.

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(1) One-d motion considered so far is equivalent to motion of planes in an actual crystal

(2) Waves in a crystal could be longitudinal or transverse

(3) When we consider all crystal planes interacting then

$$\omega^2 = \sum_p \frac{4C_p}{m} \sin^2 \frac{kp_a}{2}$$

Assuming springlike force between planes

So, I end this lecture by noting again three things one that one d motion considered so far is equivalent to motion of planes in an actual crystal. Point number 2 that waves in a crystal could be longitudinal or transverse and point number 3 when we consider all crystal planes interacting then ω^2 equals summation p $\frac{4C_p}{m} \sin^2 \frac{kp_a}{2}$ assuming spring like force between planes.