Solid State Physics
Lecture 49

Vibration of Crystals with Monatomic Basis

Hello. After discussing the Electronic Structure in Solids, we will move on to the Vibration of Solids that is the vibration of lattice a quantum of which is called Phonon. (Refer Slide Time: 00:39)

You have already learnt in the classical and quantum mechanics, the linear harmonic oscillator. Here, not that one oscillator oscillates, but the entire lattice vibrates and it causes a stationary wave in the solid as a result of that and we will understand how that occurs in solid and what are the consequences of that in solid; what would be what is the phonon that is the quantum of that vibration; what kind of energy momentum dispersion relation the phonons have, all these things we will study now and we will also try to understand its contribution to the properties of the material that is the solid under question ok. So, we will start with the vibration of crystals with monatomic basis that is there is a lattice plus only 1 atom in the basis. That kind of a crystal, we will consider first. So, if we consider an elastic vibration of a crystal with 1 atom in the primitive cell, there we want to find out the frequency of an elastic wave in terms of the wave vector that describes the wave in terms of the elastic constant. Here, we assume that the elastic response of the crystal is a linear function of the force. We make this assumption because this is valid for small vibrations and this makes the mathematics a lot easier. That is the reason, we make this assumption and if this assumption holds good, then the elastic energy would be quadratic in the relative displacement. If we consider a set of crystal planes, so one plane is given like this, these are the atoms that I am drawing. Another plane is say here, I am drawing the atoms. These are the positions of instantaneous positions of the planes. We call this plane, we mark this plane with s, this is (s + 1), this is (s + 2) and so on. This would be (s - 1) and so on, on this side as well. So, these are instantaneous positions of the plane. Let us assume that the planes would have been elsewhere, provided there was no displacement of the planes; that means, there was if there was no vibration, let us say the planes would be somewhere else and we can mark those planes with a different color say like this. This is one plane, say this is another plane without a displacement and this is another plane without a displacement. In this kind of a situation, we consider only nearest neighbor interaction; we do not consider that this plane feels the interaction from this one as well. We assume that s^{th} plane feels the interaction only from (s + 1) plane and (s -) 1 plane that is all. This is for simplicity. So, we would denote the displacement with u. This is not the coordinate. This is the displacement and if that is the case and if we consider the elastic constant relevant for this case like spring constant as C, we can write the force on the s^{th} layer as $F_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s)$. So, it is the displacement of $(s+1)^{th}$ plane and s^{th} plane that matters. So, the relative displacement comes in here gets multiplied with the elastic constant, likewise the relative displacement of (s - 1) and s^{th} plane that comes in here, gets multiplied with the same elastic constant because we are talking about the same material here, we are considering the same material here. That gives us the elastic force that this layer sth layer feels. This expression is linear in displacement and it looks like that of Hooke's law; C is the force constant and the value of C for a given material would be different for transverse and longitudinal waves. (Refer Slide Time: 08:25)

Now, if we want to write down the equation of motion of an atom in the s^{th} plane, then we can write it as $M\frac{d^2u_s}{dt^2} = C(u_{s+1}+u_{s-1}-2u_s)$. This is what we see from this equation of force here and force is just written as mass times the acceleration $M\frac{d^2u}{dt^2}$. So, what is capital M? Capital M is the mass of an atom and we look for solutions with all displacement having exponential time dependence that is periodic. So, we look for solutions with this kind of a time dependence. If this is the time dependence of u, then $\frac{d^2u_s}{dt^2}$, s subscript should be there . This quantity can be written as $\frac{d^2u_s}{dt^2} = -\omega^2 u_s$ and this equation that is the equation of motion can be re-casted into $-M\omega^2 u_s = C(u_{s+1}+u_{s-1}-2u_s)$. This is a difference equation in the displacement that is u and it has a traveling wave solution. What kind of a traveling wave solution?. The traveling wave solution would be of the form $u_{s\pm1} = u\exp{(isKa)}\exp{(\pm iKa)}$.

K is the wave vector for lattice vibration, we did not write small k to distinguish from the electronic wave vector. These are phononic wave vectors because these are the waves of the lattice vibration. a is the spacing between the planes in equilibrium. So, a is the difference between this plane and this plane something like that. K is the wave vector. So, a is something similar to the lattice constant, which is very similar to what we have done earlier for electrons. (Refer Slide Time: 13:11)

Now, we can write using this understanding so far $-\omega^2 Mu\exp{(isKa)} = Cu[\exp{[i(s+1)Ka]} + \exp{[i(s-1)Ka]} - 2\exp{(isKa)}]$. This is what we can write and now, we can cancel $u\exp{(isKa)}$ from both sides; this part from here as well as within this and here. So, this part gets cancelled from both sides. If we do that, we get $\omega^2 M = -C[\exp{(iKa)} + \exp{(-iKa)} - 2]$. This is what we obtain. And now, if we make use of the identity $2\cos{(Ka)} = \exp{(iKa)} + \exp{(-iKa)}$. All of you know this. If we make use of this on the above equation, we will obtain $\omega^2(K) = \frac{2C}{M}(1-\cos{(Ka)}$. This is what we obtain and cosine function is the periodic function. So, this will have unique values within a certain region which we call the first Brillouin zone. The boundary of the first Brillouin zone lies at $K = \pm\frac{\pi}{a}$. Now, $\frac{d\omega^2}{dK} = \frac{2C}{M}\sin{(Ka)} = 0$. Now, if we look at the zone boundaries, this quantity is 0; $\sin\pi = 0$, $\sin -\pi = 0$. The spatial significance of phonon wave vector that lies on the zone boundary, we will look at that. (Refer Slide Time: 17:56)

Now, using trigonometric identity, we can write that $\omega^2 = \frac{4C}{M}\sin^2\frac{1}{2}Ka$ and if that is true, then we can take the square root of this to find $\omega = \sqrt{\frac{4C}{M}}|\sin\frac{1}{2}Ka|$. If we now plot this quantity as a function of K, what do we obtain? Let us say K = 0 here, $K = -\frac{\pi}{a}$ here, $K = \frac{\pi}{a}$ here and $K = 2\frac{\pi}{a}$. This is the K-axis and in this axis, we plot $\frac{\omega}{\sqrt{\frac{4C}{M}}}$. Just for convenience, we take this one here. So, this part would be just a sine function; $\sin\frac{1}{2}Ka$. we will have the absolute value because we are taking the positive square root of sine function. So, we can plot it this way. This would be the kind of a plot that we have. So, you can see that at the zone boundary the dispersion becomes maximum. Therefore, at a maximum, its first order derivative should go to 0.