Solid State Physics
Lecture 51
Phonons with Diatomic Basis

Hello, we have been discussing about vibration of crystals and the quantum of that that is phonon. (Refer Slide Time: 00:43)

Now, we will discuss if we have two atoms per primitive basis then how what are the properties of the lattice vibration and phonon. If we have two atoms in the basis, the phonon dispersion relation shows new features in the crystals. If we consider for example, sodium chloride or diamond structure sodium chloride is ionic, diamond is covalent. If we consider these kind of structures then we can understand what is 2 atom basis. These are compounds with 2 atom basis diamond is not a compound its still elemental carbon, but there are 2 atoms in the basis. So, if we have this kind of an arrangement in the crystal, then we will have longitudinal acoustic that is called LA mode, we will have transverse acoustic that is called TA mode. We will have longitudinal optical LO mode and transverse optical TO mode. Now longitudinal and transverse you know the meaning why are we calling some branches acoustic some phonon branches and some other phonon branches optical, this will be clear as we progress through our discussion. So, if we if we want to find out how many branches will be there we will see that the number of degree of freedom of the atoms, that plays an important role in determining the number. If we have 'p' number of atoms in the primitive basis here we are considering p = 2 and if we have N capital N number of primitive unit cells in the crystal. Then we will have 'pN' number of atoms in the crystal each atom has three degrees of freedom. So, total '3 pN' degrees of freedom. This is these are the number of degrees of freedom in the crystal. Now the number of allowed wave vectors that is k values in a single branch is n. If we consider just one Brillouin zone therefore, the longitudinal acoustic and transverse acoustic these two branches will have a total of 3N modes accounting for 3 N degrees of freedom and so, 3N modes is occupied by longitudinal acoustic plus transverse acoustic branches. So, now we are left with (3p - 3)N these many degrees of freedom we are left with and they correspond to optical branches. These many optical branches will be there. Now let us consider a cubic crystal and two different type of atoms for example, sodium chloride with masses M_1 and M_2. M_1 lie on one set of planes and M_2 lie on another set of planes. (Refer Slide Time: 06:07)

So, its not exactly like sodium chloride, but there are two different kind of atoms one I am drawing with empty circles and the other I am drawing with dots ok. So, the lattice constant is this much let us call this atom with M_1 mass and this atom with M_2 mass. And if we now consider the displacement of the atoms, this displacement we call u_s, this one is $u_(s+1)$, this ones displacement is u_{s-1}. So, this is the s^{th} layer, this is (s + 1), this is (s - 1). The other kind of atoms we call it the call the displacement v, v_s, $v_{(s+1)}$, $v_{(s-1)}$ this kind of nomenclature. So, we have M_1 lying on one plane, M_2 lying on another plane. Now if we want to write down the equations of motion, we will be able to write down for M_1 type of atoms $M_1 \frac{d^2 u_s}{dt^2} = C(v_s + v_{(s-1)} - 2u_s$ Similarly, for M_2 kind of atoms $M_2 \frac{d^2 v_s}{dt^2} = C(u_{(s+1)} + u_{(s)} - 2v_s$. Assuming only nearest neighbor planes they influence they exert this elastic force on one atom or one plane of atoms. With these equations of motion we look for a solution in the form of a traveling wave with different amplitude u and v for on alternating planes. So, u_s can be expressed in our trial solution as $u_s = u \exp{(isKa)} \exp{(-i\omega t)}$. Similarly, $v_s = v \exp{(isKa)} \exp{(-i\omega t)}$. Now putting these into the equations of motion we will be able to find $-\omega^2 M_1 u = Cv[1 + \exp{(iKa)}] - 2Cu$ and for the other one $-\omega^2 M_2 v = Cu[1 + \exp{(iKa)}] - 2Cv$. Now, these are homogeneous linear equations having a solution only if the determinant of the coefficients of u and v vanish. We can make a determinant using the coefficients of u and v and if that coefficient vanishes, then only we will have a nontrivial solution to these equations otherwise we can always find a trivial solution u = v = 0. But we are not interested in that kind of a solution; that means, there is no vibration at all. We are interested in a nontrivial solution where there exists phonons and that kind of solution exists only if the determinant of the coefficient goes to 0 that means let us write down the determinant $\begin{vmatrix} 2C - M_1\omega^2 & -C[1+\exp{(iKa)}] \\ -C[1+\exp{(iKa)}] & C - M_2\omega^2 \end{vmatrix}$ = 0 (Refer Slide Time: 12:30)

This determinant has to be 0 for a nontrivial solution to exist; that means, let us work out this determinant. $M_1M_2\omega^4 - 2C(M_1+M_2)\omega^2 + 2C^2(1-\cos Ka) = 0$. So, we can exactly solve this equation for omega square, but if we examine some limiting cases that would be easier. So, let us consider a limiting case that offers us a good understanding of the situation without working out too difficult algebra. So, in our limiting case we will consider $Ka \ll 1$. So, this is one limiting case and we will consider another limiting case $Ka = \pm\pi$ this is another limiting case. So, this one is near the center of the zone and this one is at the zone boundary. So, let us number this one as 1 and this one as 2 these two limiting cases we are going to consider. If we consider the case one that is small value of k we can write, $\cos Ka \simeq 1 - \frac{1}{2}K^2a^2$ we drop the higher order terms we ignore them because $Ka \ll 1$ and higher order terms will be much smaller in magnitude. So, the roots of the above equation can be given as $\omega^2 \simeq 2C(\frac{1}{M_1} + \frac{1}{M_2})$. This corresponds to the optical branch and $\omega^2 \simeq \frac{C/2}{M_1+M_2}K^2a^2$, corresponds to the acoustic branch. And if we now consider the first Brillouin zone that is limited by $-\frac{\pi}{a} \leq K \leq \frac{\pi}{a}$ this is the first Brillouin zone, where a is the lattice constant and if we consider at $K_{max} = \pm\frac{\pi}{a}$, these roots are $\omega^2 = \frac{2C}{M_1}$ and the other one is $\omega^2 = \frac{2C}{M_2}$ these are the simple roots at the zone boundary. So, if we now want to understand pictorially how the particles that is the atoms displace in the transverse acoustic and transverse optical branches. (Refer Slide Time: 18:29)

We can draw a picture like this in a transverse acoustic wave transverse acoustic mode of phonon, we can consider an atom here let us say its positively charged, this is negatively charged and this one is positively charged again, negatively charged here, positively charged, negatively charged, positively charged, negatively charged, positively charged like this. So, the wave goes somewhere somewhat like this, this is the transverse acoustic mode. On the other hand, if we have positively and negatively charged ions and if we have an optical branch, the optical mode makes the atoms displace like this, this one is a positively charged one let us say the negatively charged one comes here then the other positively charged one will move somewhere here. The next negatively charged one will come somewhere here, the next positively charged one will be located here, then this one is for the negatively charged one, here the positively charged one, negatively charged again and the final one is again positively charged. So, there are two waves basically one is that of positively charged ions, the drawing is not perfect forgive me for that and the other one is for the negatively charged ions like this. How does this kind of a wave get created? Consider an electromagnetic wave moving through a medium. So, if we apply an electric field in the material, we will have positively charged atoms moving along a certain direction and negatively charged ions moving along exactly the opposite direction. So, this kind of a situation can be created by an electric field; that means, the electric field of an electromagnetic wave can make this kind of a wave propagate into the medium. On the contrary, a sound wave that does not have any polarity it will make the positively charged ion and the negatively charged ions move along the same direction. Hence, this one is the left hand side one is an acoustic mode while the right hand side one is a transverse optical mode of phonon. This makes the idea the nomenclature of acoustic mode and optical mode clear. Now, if we consider the optical branch at K = 0, we will find $\frac{u}{v} = -\frac{M_2}{M_1}$. The atoms vibrate against each other, but their center of mass is fixed. If the two atoms carry opposite charges we may excite a motion of them motion under the electric field they will move in the opposite direction that will make the optical branch you can see. And in the optical branch case that is the reason that is what is signified by this minus sign electric field makes them move along two different directions. But in general the ratio of u and v will be complex number. Another solution for the amplitude ratio of small k may be obtained as u = v. If we have u = v the atoms and their centers of mass move together as it will have a long wavelength and these are called acoustic branches.