Solid State Physics
Lecture 50
Analyzing the Dispersion Relation

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Now, let us discuss about the first Brillouin zone; the behavior of phonon dispersion inside the first Brillouin zone. We have already discussed that the range of K that is physically significant is within the first Brillouin zone that is $-\frac{\pi}{a} \rightarrow \frac{\pi}{a}$, this is the significant range. And, if we take the ratio of displacement of two successive planes that is if we take $\frac{u_{s+1}}{u_s}$, if we calculate this quantity we will find $\frac{u \exp{[i(s+1)Ka]}}{u \exp{(isKa)}}$ this is nothing but you can clearly see $\frac{u \exp{[i(s+1)Ka]}}{u \exp{(isKa)}} = \exp{(iKa)}$. So, the range $-\pi \rightarrow \pi$ covers all independent values of this quantity, of this exponential. The range of independent values of K is specified by $-\pi \leq Ka \leq \pi$ this is the range of independent K; that means, $-\frac{\pi}{a} \leq K \leq \frac{\pi}{a}$. This is the significant range and this is the first Brillouin zone for the linear lattice. That is that means, the Brillouin zone for the lattice that we have is the same as the Brillouin zone for the lattice vibration. (Refer Slide Time: 02:57)

Now, let us discuss the group velocity. You know that group velocity is the velocity at which energy propagates in a wave and energy is one of the most important physical quantities that in every context of physics we need to be we need to understand. So, the transmission of the transmission velocity of a wave packet is the group velocity and the group velocity is given as $\frac{d\omega}{dK}$. v_g denotes the group velocity, this is $v_g = \frac{d\omega}{dK}$. In three-dimension group velocity is given as the gradient in K-space of $\omega(K)$. This is the velocity of energy propagation in the medium. (Refer Slide Time: 04:12)

With the dispersion relation that we found here, this dispersion relation or this dispersion relation the same thing actually the group velocity we have according to the dispersion relation $\omega = \sqrt{\frac{4C}{M}} |\sin\frac{1}{2}Ka|$ absolute value of this because frequency cannot be negative. So, the group velocity becomes $v_g = \sqrt{\frac{Ca^2}{M}} |\cos\frac{1}{2}Ka|$. Remember group velocity can have negative sign; there is no restriction, although the frequency could not be negative. So, the group velocity is 0 at the zone boundary where $K = \pm a$, that you can readily see. The wave is a standing wave and we cannot expect any net transmission because when the wave hits the zone boundary there is no group velocity; the group velocity becomes 0. So, energy cannot flow out of it. So, the energy is confined within the Brillouin zone that we can clearly see from our calculation and therefore, it has to be a standing wave. The energy is not propagating beyond a Brillouin zone. That is something very important that we can see from our calculations. Now, let us see the long wavelength limit. The long wavelength limit is given as $Ka \ll 1$. If we have this limit working we can expand $\cos Ka \simeq 1 - \frac{1}{2}(Ka)^2$. We truncate the series right here. We do not write the next terms because $Ka \ll 1$. And, if we have this then the dispersion relation becomes $\omega^2 = \frac{C}{M}K^2a^2$ that is all because it is $1 - \cos(Ka)$. So, this is it. If we have this the result that the frequency is directly proportional to the wave vector as we can see here $\omega^2 \propto K^2$ in the long wavelength limit is equivalent to the statement that the velocity of sound is independent of frequency within this limit. Why are we talking about velocity of sound? Velocity of sound moves through a medium by making waves into the medium; that means, its it makes the lattice vibrate and in the case of lattice vibrant vibration with long wavelength we can see that ω and K these two are linear within this approximation being valid. And, therefore, we can say that the velocity of sound is independent of the frequency of that sound in the long wavelength limit therefore, the velocity can be given as $\frac{\omega}{K}$. This is the velocity of sound. This is the phase velocity of any wave and this remains a constant independent of frequency within a certain range of frequency that is large wavelength low frequency limit. This is exactly the result obtained from the continuum theory in elastic waves continuum theory of elastic waves. (Refer Slide Time: 09:07)

Now, let us find the force constant and see how it is let us see how the force constant is found from experiment. In metals the effective force may be quite long range and carried from iron to iron through the conduction electron C. Interactions have been found between planes of atoms separated by as many as 20 planes while in our assumption we have considered only the nearest plane interaction, nothing beyond. The generation of the dispersion relation to if we consider p number of nearest neighbor planes it is found from empirical observation to be $\omega^2 = \frac{2}{M}\Sigma_{p>0}C_p(1-\cos{(pKa)})$. So, what are we talking about? We are talking about more than nearest plane interaction, more than nearest neighbor interaction and empirically this has been found to be the dispersion relation provided p is the number that is index of the plane that we are considering here. Now, if we solve for the interplanar force constant C_p by multiplying both sides with $\cos{(rKa)}$, where r is an integer and then we integrate over the range of dependent values of K we can do that by in the following way. We multiply it with $\cos{(rKa)}$ and integrate over the range of K that is the first Brillouin zone. $M\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dK\omega_K^2\cos{(rKa)}$; r is an integer. $M\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dK\omega_K^2\cos{(rKa)} = 2\Sigma_{p>0}C_p\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dK(1-\cos{(pKa)}\cos{(rKa)}$ this is what we get. And, this is $\frac{2\pi C_r}{a}$. The integral vanishes except for p = r. This integral vanishes if $p \neq r$. So, the only term that survives is $\frac{2\pi C_r}{a}$. This is the only term that survives. With this we can write $C_p = -\frac{Ma}{2\pi}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} dK\omega_K^2\cos{(rKa)}$. So, this C_p gives us the force constant at range pa for a structure of monoatomic basis. This is the situation valid for metals for nonmetals whatever we have considered earlier that is nearest plane interaction is fine, for metals it is not fine. So, for metals this kind of a form of the interaction constant the force constant is observed empirically.