Solid State Physics
Lecture 54
Phonon Density of States

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How do we find out the density of states? Let us do it in 1 dimension for simplicity of course. Let us consider a boundary value problem for vibration. We consider 1 dimensional line of (N + 1) particles and it has a length L. So, it looks like this and the end atoms are fixed. So, this one is fixed, this one is also fixed because we are interested in stationary modes. The lattice constant is 'a' that is the separation between two such atoms. Here s = 0, here s = N, sorry that makes it (N + 1) atoms. And the displacement of this atom is marked as u_s. So, we suppose that the particles at s = 0 and at s = N, this particle here and this particle here these two are fixed. Therefore, each normal vibration mode of polarization p has the form of a standing wave where u_s is the displacement of particles u_s is the displacement of particle 's'. How do we express u s then? We have done it earlier $u_s = u(0) \exp(-i\omega_{Kp}t) \sin(sKa)$. So, ω_{Kp} this quantity is related to the wave vector by the dispersion relation. Wave vector is K and the dispersion relation is something we did not determine yet. The wave vector K is restricted by the fixed N boundary condition. So, we will have the values of K allowed values of $K = \frac{\pi}{L}, \frac{2\pi}{L}, \frac{3\pi}{L}, \ldots\ldots, \frac{(N-1)\pi}{L}$ And if we now solve for $K = \frac{\pi}{L}$, we will get $u_s \propto \sin\left(\frac{s\pi a}{L}\right)$ from here. And it will vanish at s = 0 and s = N as we require from the boundary condition. The solution for $K = \frac{N\pi}{L}$ that is the maximum value there we will have for $K = \frac{N\pi}{L} = \frac{\pi}{a} = K_{max}$, we will have $u_s \propto \sin s\pi$. This permits no motion of any atom because $\sin s\pi$ vanishes at each atom. Therefore, there are (N - 1) allowed independent values of K as we have written down here. This number is equal to the number of particles allowed to move. Each allowed value of K is associated with a standing wave and for 1 dimensional line there is one mode for each interval. (Refer Slide Time: 06:41)

Interval means $\Delta K = \frac{\pi}{L}$, this part is an interval and for each interval there is one phonon mode. Therefore, the number of modes per unit range it is given as $\frac{L}{\pi}$ for $K \leq \frac{\pi}{a}$ in this range. And if we go beyond this that means, that will take us outside the first Brillouin zone, it will become 0 for $K \geq \frac{\pi}{a}$. There is no point in going beyond the Brillouin zone that does not represent anything physical. There are 3 polarizations; that means, there would be 3 different p indices for a 1 dimensional for each value of K in 1-dimension, 2 of these would be transverse and 1 would be longitudinal. In 3 dimension the polarization is not this simple, only for wave vectors in certain spatial crystal directions there would be 3 normal modes and otherwise it could be complicated. Now, we need to find out the density of states. $D(\omega)$ is our density of states, the number of modes per unit frequency range for a given polarization that is the density of states that we are interested in. So, $D_1(\omega)d\omega = \frac{L}{\pi}\frac{dK}{d\omega}d\omega$, which is $\frac{L}{\pi}\frac{d\omega}{\frac{d\omega}{dK}}$ the dispersion the group velocity the dispersion this can be obtained from dispersion relation. So, we can obtain the group velocity that is this quantity here $\frac{d\omega}{dK}$ from the dispersion relation and there is a singularity if this quantity if the dispersion relation becomes horizontal. If $\omega(K)$ is flat if the first order derivative goes to 0 then there is a singularity in the density of states ok. Now, we will discuss the density of states in 3 dimension. (Refer Slide Time: 10:27)

We apply periodic boundary condition over N^3 primitive cells. If we consider a cube with side 'L' and with these this arrangement $\overrightarrow{K}$ can be determined using the condition $\exp[i(K_x x + K_y y + K_z z)]$. This according to the periodic boundary condition would be $\exp[i(K_x(x + l) + K_y(y + l) + K_z(z + l))]$. If we have $K_x = K_y = K_z = 0$ or $\pm\frac{2\pi}{L}$ or $\pm\frac{4\pi}{L}$ up to $\pm\frac{2\pi}{L}$, this condition has to be satisfied. And so, with K these values of K_x, K_y and K_L these are the boundary conditions and from here we would find that there is one allowed value of K per $\left(\frac{2\pi}{L}\right)^3$ of volume in K space. this shows us there is one allowed value of K per $\left(\frac{2\pi}{L}\right)^3$ volume in the K space and this is for each polarization branch. If the volume of our specimen is $V = L^3$ because it is cubic the total number of modes with wave vector less than

K equals $(\frac{L}{2\pi})^3$ times the volume of the sphere of radius K that can be given as $N = (\frac{L}{2\pi})^3(\frac{4}{3}\pi K^3)$. This is the total number of modes with wave vector less than K and this is for each polarization type. (Refer Slide Time: 16:32)

Then the density of state for each polarization type becomes $D(\omega) = \frac{dN}{d\omega} = \frac{VK^2}{2\pi^2}\frac{dK}{d\omega}$. Now, we need to find out C_v and the density of states is available with us, but we do not know the value of this. We do not know the dispersion relation yet. So, we do not know how ω depends on K. So, we cannot calculate this quantity yet and for that we take the help of Debye, where he developed a model for density of states and that will help us find out this dispersion relation and then calculate the heat capacity. So, let us focus on the Debye model for the density of states. In the Debye approximation, the velocity of sound is taken as constant for each polarization type as it would be in the classical continuum limit elastic continuum limit. So, the dispersion relation would be given as $\omega = vK$, V is a constant the velocity of sound is a constant in this case that is what Debye assumed. And if we put this kind of an expression the density of states as we have calculated here in this expression would become $D(\omega) = \frac{V\omega^2}{2\pi^2v^3}$. Just put the relation this relationship here and you will get this quantity. So, this is the density of states that Debye model gives us. And if there are N primitive cells in the sample, the total number of acoustic phonon modes would also be N as we have discussed earlier. Therefore, we can put a cutoff frequency by integrating this equation we would be exhausted with the number of acoustic phonons by that cut off frequency. We can write ω_D, which is the Debye frequency or the cutoff frequency; cubed of this $\omega_D^3\frac{6\pi^2v^3N}{V}$. This expression is obtained by integrating this one here. If you integrate this density of states with respect to ω then you will get $\omega^3/3$ here that is what you will get from here and 3 times 2 is 6 and this part the left hand side of this equation will give you the number of acoustic phonons that is N. Therefore, ω_D^3 would have this kind of an expression. To this frequency they corresponds a cutoff wave vector in K space. The corresponding cutoff wave vector K_D is according to this dispersion relation $K_D = \frac{\omega_D}{v}$, which is $(\frac{6\pi^2N}{V})^{(1/3)}$. In the Debye model we do not allow modes of wave vector longer than K_D. Longer than K_D is not allowed its cutoff there the number of modes within $K \leq K_D$ has to be considered and this exhaust the number of degrees of freedom that is available with us that is that comes from the acoustic modes of phonon available with us. (Refer Slide Time: 22:29)

So, the internal that is thermal energy is given by $U = \int d\omega D(\omega)\langle n(\omega)\rangle\hbar\omega$. This would give us the internal energy and the range of this integral would be from 0 to ω_D because beyond that we do not have phonons available, we are exhausted up to ω_D. $D(\omega)$ the density of states $\frac{V\omega^2}{2\pi^2v^3}$ assuming constant velocity of sound within a certain range of ω of course times $(\frac{\hbar\omega}{e^{\hbar\omega/\tau}-1})$, the Planck function. This is the energy for each polarization type. For simplicity we assume that the phonon velocity is independent of polarization and if we assume that we can multiply this expression by 3 to obtain the internal energy. So, by multiplying with 3, we obtain $U = \frac{3V\hbar}{2\pi^2v^3}\int_0^{\omega_D}d\omega\frac{\omega^3}{e^{\hbar\omega/\tau}-1}$. Now, we substitute $x = \frac{\hbar\omega}{\tau} = \frac{\hbar\omega}{k_Bt}$. If we do this we obtain $U = \frac{3Vk_B^4T^4}{2\pi^2v^3\hbar^3}\int_0^{x_D}dx\frac{x^3}{e^x-1}$. x_D the upper limit of the integral is $\frac{\hbar\omega_D}{k_BT}$ which we write as $\frac{\theta}{T}$. Theta has the dimension of temperature. So, we call it Debye temperature. This can be expressed as $\theta = \frac{\hbar v}{k_B}(\frac{6pi^2N}{V})^{1/3}$. (Refer Slide Time: 27:10)

So, the total phonon energy U can be written after doing all these mathematics as $U = 9Nk_BT(\frac{T}{\theta})^{1/3}\int_0^{x_D}\frac{x^3}{e^x-1}$, where N is the number of atoms in the sample and $x_D = \frac{\theta}{T}$ as we have found out earlier. Now, comes the heat capacity. We have found out the internal energy. So, the heat capacity is $(\frac{\partial U}{\partial T})_V = C_v = \frac{3V\hbar^2}{2\pi^2v^3k_BT^2}\int_0^{\omega_D}d\omega\frac{\omega^4e^{\hbar\omega/\tau}}{(e^{\hbar\omega/\tau}-1)^2}$, which is $= 9Nk_B(\frac{T}{\theta})^3\int_0^{x_D}dx\frac{x^4e^x}{(e^x-1)^2}$. If we have $T \gg \theta$ the heat capacity approaches the classical value $C_v = 3Nk_B$. How about the opposite limit? At very low temperature we may approximate U by letting the upper limit go to infinity. So, we do not restrict it at x_D, we make it infinity because that does not matter the temperature is very low. (Refer Slide Time: 30:43)

So, we have $\int_0^\infty dx \frac{x^3}{e^x-1} = \int_0^\infty dx \ x^3 \Sigma_{s=1}^\infty \exp(-sx)$. This quantity becomes $6\Sigma_{s=1}^\infty \frac{1}{s^4}$ which is $\frac{\pi^4}{15}$, this is a standard sum. So, the internal energy can be approximately written as $U \simeq \frac{3\pi^4 N k_B T^4}{5\theta^3}$ for very low temperature, $T \ll \theta$. And if that is the case then C_v can be approximately written as $C_v = \frac{12\pi^4}{5} N k_B (\frac{T}{\theta})^3$, which is by putting these values we can write $234 N k_B (\frac{T}{\theta})^3$. So, the C_v goes as T^3 if the temperature is pretty low. This is known as the Debye T^3 law. So, we have evaluated two limits. In one limit temperature was much larger than the Debye temperature, where the C_v became a constant and approach the classical value and when the temperature is very low the C_v goes as T^3. For intermediate temperature we will have to explicitly evaluate this integral here to find out U and then take the temperature derivative of U to find out C_v, which is a more difficult task, but that gives a reasonable value of C_v that matches quite well with experiment. So, this is all about phonons that we wanted to discuss.