Solid State Physics
Lecture 53
Phonon Heat Capacity

Hello. We have been discussing about phonons and lattice vibrations. In the context of Drude model and Sommerfeld model we calculate the electronic contribution to heat capacity the thermal properties of matter, now we will discuss about the Phononic contribution to the thermal properties of matter that is heat capacity the phonons contribution to it. (Refer Slide Time: 00:50)

So, when we say heat capacity, we usually mean heat capacity at constant volume that is C_v, but. So, this is the more fundamental quantity which can be obtained using thermodynamics at the $C_v = (\frac{\partial U}{\partial T})_V$. And this one although its a fundamental quantity, its difficult to measure from experiment because keeping the volume constant when the temperature is changing its extremely difficult. So, its in experiment the way it is done or the easier way it is done is to measure C_p heat capacity at constant pressure which is nothing, but $C_p = (\frac{\partial U}{\partial T})_P$ at constant pressure and in thermodynamics you have learned the relationship between C_v and C_p. So, here we will be interested in C_v because we are doing the theory and in theory calculating C_v is easier from experiment one can measure C_p and with the relationship one can find out what is the corresponding C_v. We will here concentrate only on the phonons contribution to C_v and this quantity is called the phonons contribution to C_v is called the C_{lat} that comes from the lattice. Phonon waves just like photon waves that is electromagnetic waves can be polarized and if we consider a polarization index p then we can write the lattice contribution to the internal energy $U_{lat} = \Sigma_K \Sigma_p U_{Kp}$. So, what is U_{Kp}? So, let us write this one the summations remain as it is $\Sigma_K \Sigma_p$, $U_{lat} = \Sigma_K \Sigma_p \langle n_{Kp} \rangle \hbar\omega_{Kp}$. This gives us the lattice contribution to the energy where this quantity $\langle n_{Kp} \rangle$, this is the thermal equilibrium of phonons average number of phonons at thermal equilibrium for wave vector K and polarization p and this can be obtained from the Planck distribution function. What is Planck distribution? In Planck distribution you get the average number of bosons as $\langle n \rangle = \frac{1}{\exp{(\frac{\hbar\omega}{\tau})} - 1}$ where $\tau = k_B T$. So, how do we obtain this? Let us find that out. (Refer Slide Time: 06:11)

Let us work out the Planck distribution. Let us consider a set of identical harmonic oscillators in thermal equilibrium. If we consider this the ratio of the number of oscillators in $\frac{(n+1^{th})\ state}{n^{th}\ state}$ if this quantity is given as $\frac{N_{n+1}}{N_n}$, this can be written as $\exp \frac{-\hbar\omega}{\tau}$ where $\hbar\omega$ is the energy of one phonon or one boson and higher the excited state fewer is the number. So, if there is a negative sign, this is the ratio that this kind of a ratio will be obtained $N_{n+1} < N_n$. And τ as we have discussed earlier its just $k_B T$. Thus the fraction of the total number of oscillators in the n^{th} quantum state that can be written as. When we say fraction; that means, fraction of the total number of oscillators total number of phonons in this context equals $\frac{N_n}{\Sigma_{s=0}^{\infty} N_s}$. How do we obtain this? This we can obtain using exponential $\frac{N_n}{\Sigma_{s=0}^{\infty} N_s} = \frac{\exp{(-n\hbar\omega/\tau)}}{\Sigma_{s=0}^{\infty} \exp{(-s\hbar\omega/\tau)}}$. So, we see that the average oscillation quantum number of an oscillator that can be given as if we make an average over n using this distribution function, how do we make an average? We multiply this one with we multiply the numerator with s and sum over s we do not multiply anything here in the denominator, the denominator remains just like this. So, it will be given as $\langle n \rangle = \frac{\Sigma_s s \exp{(-s\hbar\omega/\tau)}}{\Sigma_s \exp{(-s\hbar\omega/\tau)}}$. We have to now calculate this quantity now let us find out two summations. (Refer Slide Time: 11:10)

If we get an infinite series $\Sigma_s x^s$ we can write this as, $\Sigma_s x^s = \frac{1}{1-x}$ provided $x < 1$. And if we have $\Sigma_s s x^s$ that is given as $\Sigma_s s x^s = x\frac{d}{dx}\Sigma_s x^s$ and this quantity is it sums to $\frac{x}{(1-x)^2}$ of course, this is also valid for $x < 1$. Now if we put $x = \exp{(\hbar\omega/\tau)}$, then get the relevance of these two series from with these two sums here and using this we can calculate the $\langle n \rangle = \frac{x}{1-x}$ which putting this value of x can be calculated to be $\frac{1}{\exp{(\hbar\omega/\tau)} - 1}$ this is the Planck distribution function. (Refer Slide Time: 13:41)

Now, let us find out let us count the normal modes. Normal modes of phonon that we are interested in. So, the energy of a collection of oscillators for frequency $\omega K p$ if it is in thermal equilibrium, then the total energy can be obtained the internal energy that is $U_{lat} = \Sigma_K \Sigma_p \frac{\hbar\omega_{Kp}}{\exp{(\hbar\omega/\tau)}-1}$. Its convenient to replace this summation by an integral how do we do that? If we suppose that the crystal has $D_p(\omega)d\omega$ number of modes for a given polarization p within the frequency range $\omega \rightarrow \omega + d\omega$. If we assume this then the total energy can be obtained using this integral form $\Sigma_p \int d\omega D_p(\omega) \frac{\hbar\omega}{\exp{(\hbar\omega/\tau)}-1}$. The heat capacity is found by differentiating with respect to the temperature. So, we have $x = \frac{\hbar\omega}{\tau}$ if we now put this, then this quantity is putting the value of $x = \frac{\hbar\omega}{k_B T}$ then we can calculate $\frac{\partial U}{\partial T} = C_{lat} = k_B \Sigma_p \int d\omega D_p(\omega) \frac{x^2 \exp x}{(\exp x - 1)^2}$ this quantity. So, this quantity can be evaluated the integral is difficult, but it can be performed and that gives us C_{lat} provided we know the expression for the density of states. So, now, it becomes important to learn the expression for the density of states.