


Condensed Matter Physics
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Lecture - 13
Debye Theory of Specific Heat, Lattice Vibrations – Worked Examples

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Problem 32

Given the Debye frequency of sodium as 3.3×10^{12} Hz, calculate its molar specific heat at 10 K assuming Debye's T^3 law.

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In the Debye theory of Debye frequency of sodium is given as 3.3 into 10 to the power 12 hertz.

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Debye freq. of Na = 3.3×10^{12} Hz.


Molar sp. heat at 10 K ?

$$C_V = \frac{12}{5} \pi^4 N k_B \left(\frac{T}{\Theta_D} \right)^3 = 494.5 \frac{\text{J}}{\text{kg mol} \cdot \text{K}}$$

$\nu_D = 3.3 \times 10^{12}$ Hz.

$$h \nu_D = 6.6 \times 10^{-34} \times 3.3 \times 10^{12} = k_B \Theta_D$$


$\Theta_D = 157 \text{ K}.$



So we are asked to calculate the molar specific heat at ten K using Debye theory, law at low temperature. So basically, we have the expression C_v according to Debye theory, $\frac{12}{5} \pi^4 \frac{N k_B T}{\theta_D^3}$. And to calculate θ_D , we are given ν_D as three point three into ten to the power 12, so $h \nu_D$ is 6.6×10^{-34} into Planck constant 3.3×10^{12} . And therefore, and this is equal to $k_B \theta_D$ where k_B is the Boltzmann constant. So with this θ_D works out to be 157 Kelvin, using this C_v can be straight away found out to using this expression as 494.5 joules per kg mol per degree K. (Refer Slide Time: 02:03)

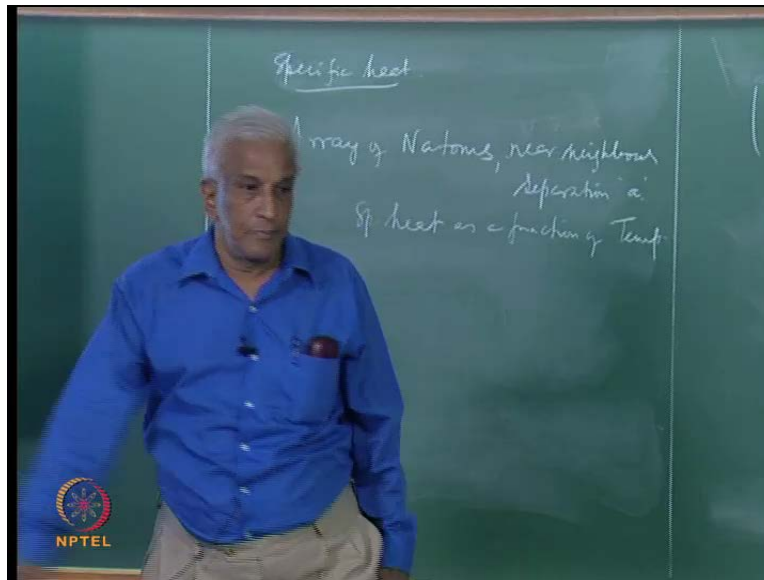
Problem 33

Consider an array of N similar atoms, the separation between nearest neighbours being a . Discuss the specific heat of the system on the basis of Debye approximation and show that at low temperature the specific heat is proportional to T .

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We next proceed to consider an array of N .

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Atoms near neighbor separation of a , so we are asked to discuss specific heat as a function of temperature.

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Solution:

In Debye's 'continuous medium' approximation,

$$\frac{\omega}{q} = c$$

where c is the velocity of the elastic wave.

The density of states in a one-dimensional medium can be obtained by: $d\omega = cdq$



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Now we have to do this, we go back to calculate the phonon dispersion relation, phonon in Debye's continuum, we can say this as dispersion relation for sound waves, $\omega = cq$, where or vq if you like where v is the speed of sound. So $d\omega = v dq$.

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For a one-dimensional lattice the number of modes in the range dq is given by:

$$dn = \frac{L}{\pi} dq$$
$$= \frac{L}{\pi c} d\omega$$

The energy of the system is evaluated by:

$$U = \int_0^{\omega_D} \left(\frac{h\omega}{e^{h\omega/k_B T} - 1} \right) \frac{L}{\pi c} d\omega$$


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We have an array of N atoms in a linear passions, so we have a one-dimensional lattice with lattice constant a .

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One dimensional lattice with lattice constant 'a'.

No. of modes in interval $dq = \frac{L}{\pi} dq = \frac{L}{\pi v} d\omega$

Internal energy $U = \int_0^{\omega_D} \frac{h\omega}{(e^{h\omega/k_B T} - 1)} \frac{L}{\pi v} d\omega$

$\chi = h\omega/k_B T \rightarrow \propto T^2$

$C_v = \left(\frac{\partial U}{\partial T} \right)_v \propto T$




We have already discussed the vibration such crystal lattice, and the modes are given by L by π dq that is the number of modes number of modes in an interval dq , so converting this into ω . And the energy internal energy is known to be say integral 0 to ω_D of h cross ω by e to the power h cross ω by $K B T$ minus one into L by π v $d\omega$.

So we make a change a variable by taking x equal to h cross ω by $K B T$, so that the integral goes as proportional to T square. And therefore, the specific heat, which is du by $d t$ constant v is proportional to T . So the specific heat of such a system is a linear function of temperature.

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Problem 34

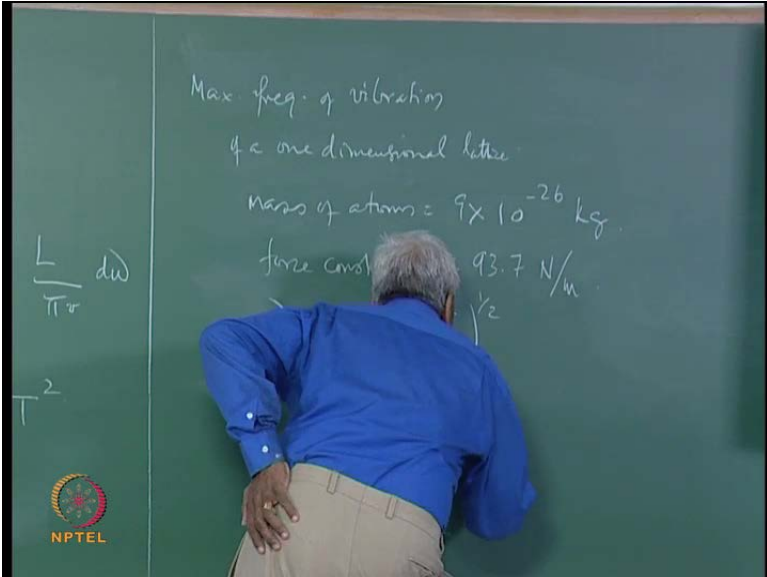
Calculate the maximum frequency of vibration in a one-dimensional lattice of identical atoms of mass 9.0×10^{-26} kg if the force constant of the nearest neighbour interaction is 93.7 N/m.



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Next we are ask to calculate the maximum frequency of vibration of one dimensional lattice again a problem on lattice vibration.

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Max freq. of vibration
for one dimensional lattice
mass of atoms = 9×10^{-26} kg
force const = 93.7 N/m
 $\frac{1}{2}$

$\frac{L}{\pi v}$
 T^2




Where the mass of atom is given as 9×10^{-26} kilograms. The force constant between near neighbor is given as 93.7 Newton per meter. So the maximum ν_{\max} is $1/\pi \sqrt{f/m}$, this is this. So substituting, we get 9.9×10^{12} hertz.

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Problem 35

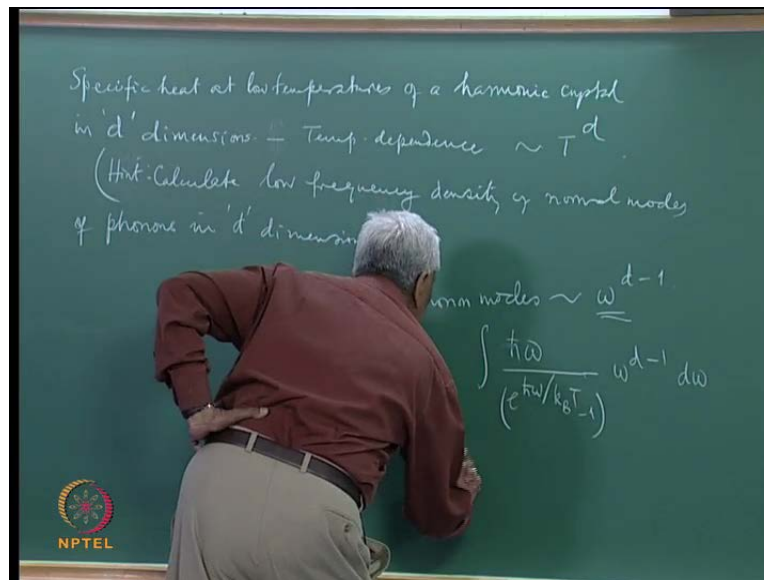
Show that the specific heat at low temperature of a harmonic crystal vanishes as T^d in d dimensions. (Hint: Calculate the low frequency density of normal modes of phonons in d dimensions).



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The next question is to show that the specific heat at low temperatures of a harmonic crystal in d dimensions.

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The dimensionality can be one dimension, two dimension, three dimension can be in general d dimensions. So we want to see what is its temperature dependence. We want to show that the specific heat goes as T to the power d, where T is the temperature. So we are given the hint that we had to calculate, this is the hint, the low frequency density of normal modes of phonons in d dimensions, that is the hint given.


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Solution

Density of phonon modes in d dimensions is proportional to $(\omega)^{d-1}$ and so the internal energy is

$$\int \frac{\hbar\omega}{(e^{\hbar\omega/k_B T} - 1)} (\omega)^{d-1} d\omega.$$

So the low temperature specific heat is when $\hbar\omega/k_B T$ tends to infinity and the integral goes as $(k_B T)^d$ times a constant.



So if we take phonons in say, in general we have the density of phonon modes goes as omega to the power d minus 1. If d is the dimensionality then for example, if d is 3, if it is 3 dimensional, we know the density of phonon modes goes as omega square. If it is one dimensional, it doesn't depend on omega at all, so it is omega depend 0 and so on. So this is something that we have already considered.

Therefore, the density of phonon modes goes to the omega d minus one, therefore the internal energy which is the average energy u is the integral of h cross omega by e to the power h cross omega by K B T minus 1. This is the weighting function the average energy times omega to the power d minus one d omega. This is the energy and then this is the phonon density of states, so this is the integral that has to be calculated, so the U goes as this, so this will be in general goes as integral something times omega to the power d by e to the power h cross omega by K B T minus one d omega times h cross.

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The chalkboard shows the following derivation:

$$U \sim \frac{\partial}{\partial T} \int_0^{\infty} \left(\frac{h\omega^d}{e^{h\omega/k_B T} - 1} \right) d\omega$$

$$\sim \frac{\partial}{\partial T} (k_B T)^{d+1} \int_0^{\infty} \frac{x^d}{(e^x - 1)} dx$$

$$\sim T^d$$

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And therefore the specific heat is just dU by dT at constant volume, and therefore, the specific heat and in particular we are talking about low temperature limit, so we are considering the limit h cross omega by K B T, where T tending to 0 is tends to infinity as T tends to 0. So the integral will become integral 0 to infinity of this quantity the derivative with respect to temperature of this. So this will go as constant into omega.

So here we have the function $h \propto \omega^3$ to the power d by e to the power $h \propto \omega$ by $k_B T$ minus 1 d by $d\omega$. And when I make a change in variable, this is going to give me d by dT of $k_B T$ to the power d times a definite integral x to the power d by e to the power x minus 1 dx ah into some constant. So this going to be a number because this is definite integral, this goes as T to the power d , this is going become d plus one and when I differentiate with respect to temperature, this is going to go as T to the power d in d dimensions is what we are required to prove.

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Problem 36

Specific heat data for a nonmagnetic metal at different temperatures is given below:

| Temperature T (K) | Specific heat, C ($\times 10^{-4}$ J / mol, K) |
|-------------------|---|
| 1 | 7.2 |
| 1.5 | 12.0 |
| 2 | 16.1 |
| 2.5 | 22.5 |
| 3 | 41.4 |

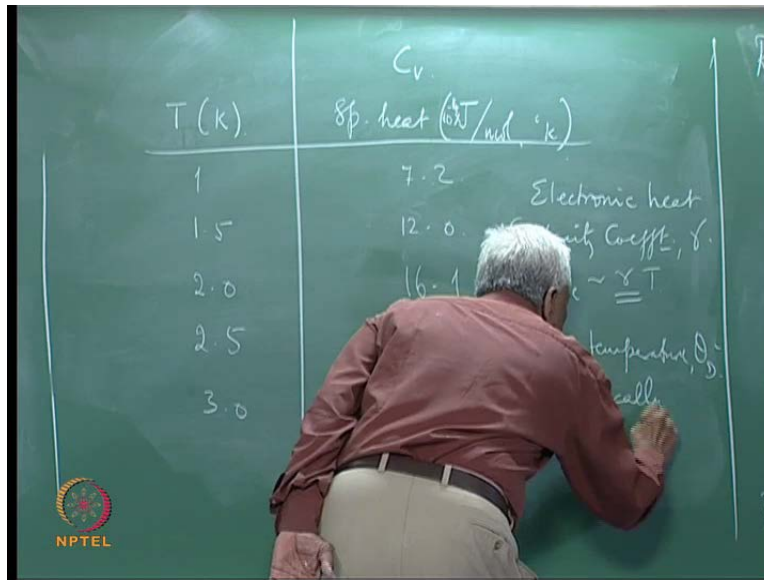
Determine the electronic heat capacity coefficient and the Debye temperature graphically.

Universal gas constant $R = 8.31$ J/mol, K.



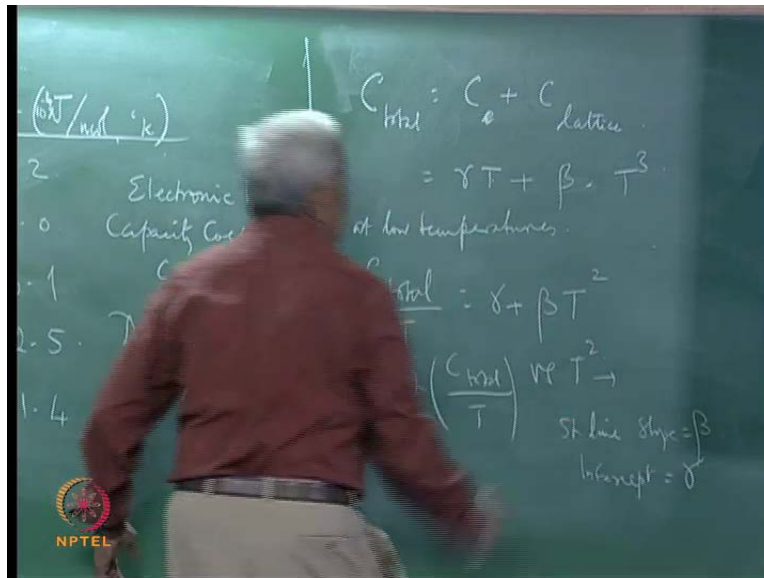
The next question we are given the set of specific heat values data, experimental measurements, the results of experimental measurements are tabulated specific heat versus temperature.

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So T temperature and specific heat in joules per mol degree Kelvin into 10 to power minus 4 . So at a temperature of 1 K the specific heat is seven point two into ten to the power minus four. At 1.5 K, this is 12 ; at 2 K, it turns out to have a value, 16.1 ; at 2.5 K, it is 22.5 ; and at 3 K, it is 41.4 into 10 to the power minus 4 joule per mol degree K. So this is the data that is given. So we are required to find the electronic heat capacity coefficient, remember we wrote this as $C_{\text{electronic}}$ goes as γT , so this is the γ and the Debye's temperature by a graphical method. How do we do this, we already have consider this problem in a metal the heat capacity generally is given as sum of two terms in total heat capacity is the electronic heat capacity plus the lattice heat capacity.

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The electronic heat capacity goes as γT and the lattice heat capacity goes as constant times T^3 at low temperature. Therefore, C_{total} by T is $\gamma + \beta T^2$; constant γ can be written as γ . So this means if we plot the total specific heat divided by the temperature versus T^2 , this will be a straight line, whose slope is β and the intercept on the y-axis gives you the electronic heat capacity coefficient.

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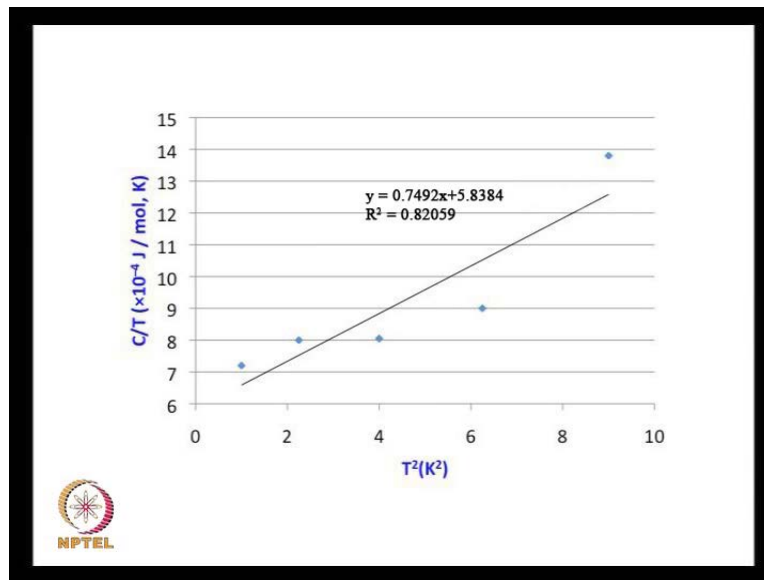
Solution

| $C/T (\times 10^{-4} \text{ J / mol, K})$ | $T^2 (\text{K}^2)$ |
|---|--------------------|
| 7.2 | 1 |
| 8 | 2.25 |
| 8.05 | 4 |
| 9 | 6.25 |
| 13.8 | 9 |

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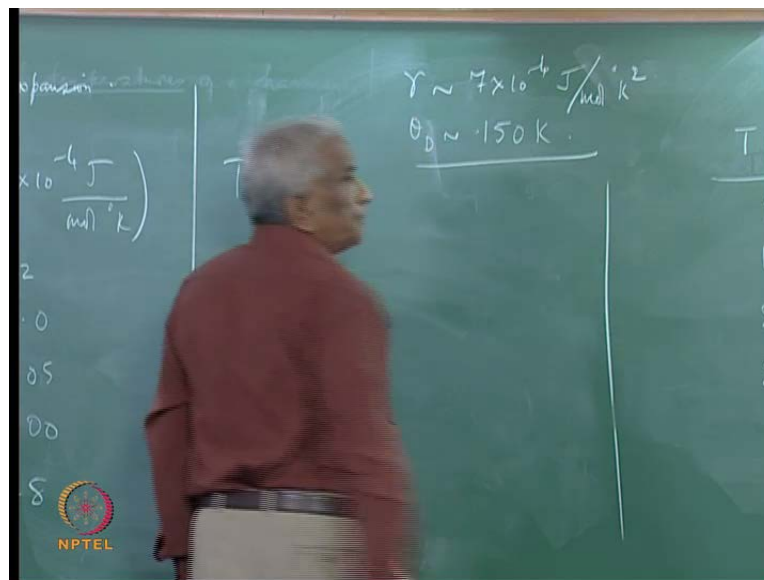
So using the given data, we arrive at the following table.

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So these are the values, which are plotted graphically, and we find the plot of C by T versus T square turns out to be an approximate straight line at low temperature which diverges later.

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So passing a straight line, through these points, we get the slope and intercept which give the heat capacity coefficient gamma as approximately 7 into 10 to the power minus 4 joule mol K square. And Debye's temperature is approximately 150 Kelvin.