

1-4-2 The Density of states in three dimension:

In three dimension the wave equation (standing wave) is

$$u = Ae^{ik \cdot r} = Ae^{i(k_x x + k_y y + k_z z)} \quad (16)$$

The periodic boundary conditions:

$$u(r) = u(r + L) \quad (17)$$

So, using the boundary conditions:

$$Ae^{i(k_x x + k_y y + k_z z)} = Ae^{i(k_x x + k_y y + k_z z)} \cdot e^{i(k_x L + k_y L + k_z L)}$$

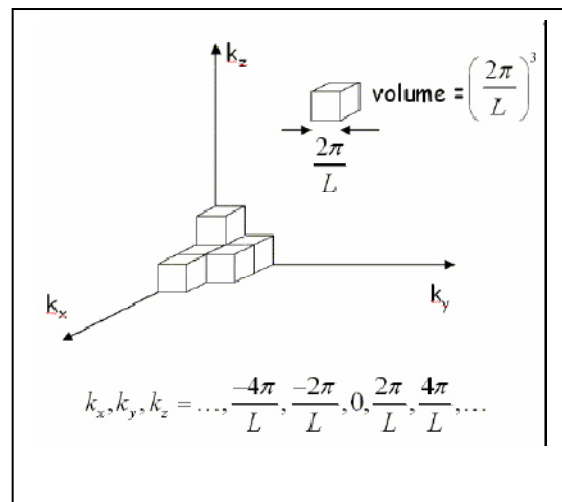
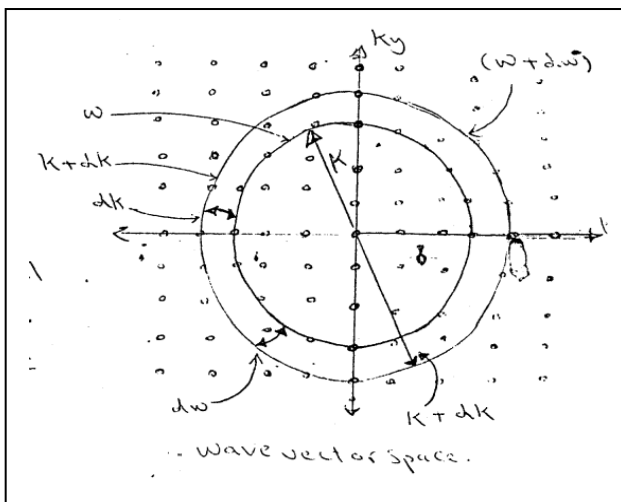
That is:
$$e^{i(k_x L + k_y L + k_z L)} = 1 \quad (18)$$

So that :
$$k_x, k_y, k_z = \left(n \frac{2\pi}{L}, m \frac{2\pi}{L}, l \frac{2\pi}{L}\right) \quad (19)$$

Therefore, for each point in the lattice space, there is one allowed value of $\vec{k}$ per volume

$\left(\frac{2\pi}{L}\right)^3$ where each lattice point represent a mode of vibration in the k space which

represents a sphere in the wave vector space with radius equal $(k + dk)$



The number of state is given by:

$N = (\text{the volume of a sphere with radius } k) / (\text{the volume of point})$

$$N = \frac{4\pi k^3 / 3}{(2\pi / L)^3} = \frac{V}{(2\pi)^3} \cdot \frac{4\pi}{3} k^3 \quad (20)$$

The density of state is

$$D(\omega) = \frac{dN}{dk} \frac{dk}{d\omega} = \frac{V}{(2\pi)^3} \cdot 4\pi \frac{\omega^2}{v_0^2} \frac{dk}{d\omega}$$

$$D(\omega) = \frac{V}{2\pi^2} \frac{\omega^2}{v_0^3} \quad (21)$$

For long wavelengths, there are two transverse, one longitudinal acoustic modes. So the total density of state is

$$D(\omega) = \frac{3V}{2\pi^2} \frac{\omega^2}{v_0^3} \quad (22)$$

1-5 Debye Theory for Specific Heat:

Debye suppose in his theory for specific heat of the solid materials that the solid material atoms vibrate as group vibration where the idea of independently vibration of atoms is not practical idea because the atoms interaction with each other and the motion of any atom effect on all other atoms, thus it produce a vibration of all atoms.

The wave shape which produced by the group oscillators is an acoustical wave which is flood of phonon. When a sound wave (acoustical wave) propagate in solid material, the atoms do not vibrate independently but it ordered its motion where all atoms moves in the same amplitude and in constant phase relation obeys to propagation relation ($\omega = v_0 k$), that is mean the angular frequency of vibration mode is a dependent quantity on the wave vector and not constant quantity, the lattice vibration angular frequency cover a large range values of k . The angular frequency spectrum is cut off in a certain value of angular frequency, this frequency is called cut off frequency or Debye frequency (ω_D) and it is

the maximum of angular frequency. The Debye frequency (ω_D) is constant value for all atoms which is longitudinal or transverse.

To calculate the heat capacity we must know the total number of the vibration modes and the total energy. The total number of vibration modes for crystal with volume V and consist of N atoms is:

$$3N = \int D(\omega) d\omega \quad (22)$$

Where $D(\omega)$ is the density of state which equal to

$$D(\omega) = \frac{3V}{2\pi^2} \frac{\omega^2}{v_o^3} = \frac{V}{2\pi^2} \left(\frac{2}{v_T^3} + \frac{1}{v_L^3} \right) \omega^2 \quad (23)$$

Where v_T represent the transversal wave velocity and v_L represent the longitudinal wave velocity and $\left(\frac{1}{v_T^3}\right)$ multiply by 2 because the transversal wave is two polarizer wave.

To determine or to procedure the integral in equation () we must know the maximum and the minimum boundaries of the frequency spectrum.

The minimum value is equal zero $\omega = 0$ and the maximum value of the frequency is ω_D (Debye frequency) or the cut off frequency which is defined by Debye .

Substitution of equation () in equation () and procedure the integral we will get ω_D

$$3N = \frac{V}{2\pi^2} \left(\frac{2}{v_T^3} + \frac{1}{v_L^3} \right) \int_0^{\omega_D} \omega^2 d\omega \quad (24)$$

$$\omega_D^3 = \frac{18 \pi^2 N}{V \left(\frac{2}{v_T^3} + \frac{1}{v_L^3} \right)} \quad (25)$$

$$\text{Or} \quad \left(\frac{2}{v_T^3} + \frac{1}{v_L^3} \right) = \frac{18 \pi^2 N}{V \omega_D^3} \quad (26)$$

The total vibration energy of all harmonic oscillators in the thermal equilibrium from $\omega = 0$ to ω_D is

$$U = \int_0^{\omega_D} \langle E \rangle D(\omega) d\omega \quad (27)$$

$$\text{Where } \langle E \rangle = \frac{\hbar \omega}{e^{\hbar \omega / k_B T} - 1} \quad (28)$$

So

$$\begin{aligned} U &= \int_0^{\omega_D} \frac{\hbar \omega}{e^{\hbar \omega / k_B T} - 1} \left[\frac{V}{2\pi^2} \left(\frac{2}{v_T^3} + \frac{1}{v_L^3} \right) \omega^2 \right] d\omega \\ &= \frac{9N}{\omega_D^3} \int_0^{\omega_D} \frac{\hbar \omega^3 d\omega}{e^{\hbar \omega / k_B T} - 1} \end{aligned} \quad (29)$$

We can simplify equation above by introduce the Debye temperature θ_D which is in the average of total thermal energy of the oscillator equal to a constant value to $\hbar \omega_D$

$$k_B \theta_D = \hbar \omega_D \Rightarrow \Rightarrow \omega_D = \frac{k_B}{\hbar} \theta_D = \frac{\theta_D}{T} \quad (30)$$

For simplicity suppose that

$$x = \frac{\hbar \omega}{k_B T} \Rightarrow \Rightarrow \omega = \frac{k_B T}{\hbar} x \Rightarrow \Rightarrow \therefore d\omega = \frac{k_B T}{\hbar} dx \quad (31)$$

$$x_m = \omega_D = \frac{\theta_D}{T}$$

By substitute equations (30, 31) in equation (30) we get

$$U = \frac{9Nk_B T^4}{\theta_D^3} \int_0^{x_m} \frac{x^3}{e^x - 1} dx \quad (32)$$

To answer this equation , there are two states

(1): when the temperature is high, where the temperature T is larger than Debye temperature θ_D ($T \gg \theta_D$), therefore x value is very small, and thus

$$e^x = 1 + x + \frac{x^2}{2} + \frac{x^3}{3} + \dots \quad (33)$$

Substitute equation () in equation () with neglect the high exponents, we get

$$U = \frac{9 N k_B T^4}{\theta_D^3} \int_0^{x_m} x^2 dx$$

$$U = \frac{3 N k_B T^4}{\theta_D^3} x_m^3 = \frac{3 N k_B T^4}{\theta_D^3} \left(\frac{\theta_D^3}{T^3} \right) = 3 N k_B T \quad (34)$$

The heat capacity at a constant volume is

$$c_v = \left(\frac{dU}{dT} \right)_v = 3 N k_B = 3 R \quad (35)$$

This result is completely equal to the heat capacity result in classical and Einstein theory.

(2) when the temperature is low, the temperature T is more less than the Debye temperature ($T \ll \theta_D$), therefore we can simplify the term $\left(\int_0^{x_m} \frac{x^3}{e^x - 1} \right)$ by using Zeta

Function as the equation below:

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \int_0^\infty x^3 \cdot \frac{e^{-x}}{1 - e^{-x}} dx = \int_0^\infty x^3 \cdot e^{-x} dx \sum_{n=0}^{n=\infty} e^{-nx}$$

$$= \int_0^\infty x^3 dx \sum_{n=0}^\infty e^{-x(n+1)} = \sum_{n=1}^\infty \int_0^\infty x^3 e^{-nx} dx = \sum_{n=1}^\infty \frac{6}{n^4} = \frac{\pi^4}{15}$$

Substitute this value in equation (32) we get

$$U = \frac{9 N k_B T^4}{\theta_D^3} \frac{\pi^4}{15} \quad (36)$$

So the heat capacity is

$$c_v = \left(\frac{dU}{dT}\right)_v = \frac{12}{5} \pi^4 R \left(\frac{T}{\theta_D}\right)^3 \quad (37)$$

That is means the specific heat vary with cubic T when the temperature is very small, equation (37) known as Debye law for cubic absolute temperature.

They found that the values of specific heat in Debye theory is in good agreement with the experimental result at low and high temperature , while at moderate temperature the result are not in good agreement with experimental result, therefore we can use Debye or Einstein theory to calculate the specific heat because the error ratio between this two theories is small.