Qu. Einstein model to determine sp. Heat of solid at high and low temperature.

Ans. Einstein introduce the quantum theory to modify the classical results by incorporating the Planck's quantum concept that a harmonic oscillator can take energy in integral multiple of $h\upsilon$, where is the natural frequency of the oscillator. The solid consist of assembly of large number of monoatomic atoms situated at lattice point vibrates three degree of freedom have the energy of the Harmonic oscillator. Einstein independently calculated the energy of the oscillator as atoms and then determine sp. heat of the solid.

The wave mechanical treatment of the harmonic oscillator shows that its total energy ε_V is given by

$$\varepsilon_V = (n + \frac{1}{2})h\upsilon \qquad (1)$$

Einstein introduce the Equipartition Theorem, since the energy level be continuous of the Harmonic oscillator. The mean energy of Harmonic Oscillator with three degrees of freedom $(n_f = 6)$ is given as

$$\bar{\varepsilon}_V = \frac{\sum_0^\infty \varepsilon_V\, e^{-\varepsilon_V/kT}}{\sum_0^\infty e^{-\varepsilon_V/kT}} \qquad (2)$$

$$= \frac{\sum_0^\infty (n+\frac{1}{2})h\upsilon\, e^{-(n+\frac{1}{2})h\upsilon/kT}}{\sum_0^\infty e^{-(n+\frac{1}{2})h\upsilon/kT}}$$

$$= [\frac{\sum_0^\infty nh\upsilon\, e^{-(n+\frac{1}{2})h\upsilon/kT}}{\sum_0^\infty e^{-(n+\frac{1}{2})h\upsilon/kT}} + \frac{\frac{1}{2}h\upsilon\, e^{-(n+\frac{1}{2})h\upsilon/kT}}{e^{-(n+\frac{1}{2})h\upsilon/kT}}]$$

$$= [\frac{\sum_0^\infty nh\upsilon\, e^{-(n+\frac{1}{2})h\upsilon/kT}}{\sum_0^\infty e^{-(n+\frac{1}{2})h\upsilon/kT}} + \frac{1}{2}h\upsilon]$$

$$= [\frac{\sum_0^\infty nh\upsilon\, [e^{-(nh\upsilon/kT)} . e^{-(\frac{1}{2})h\upsilon/kT}}{\sum_0^\infty e^{-(nh\upsilon/kT)} . e^{-(\frac{1}{2})h\upsilon/kT}} + \frac{1}{2}h\upsilon]$$

$$= \left[\frac{\sum_{0}^{\infty} nh\upsilon\, [e^{-(nh\upsilon/kT)}}{\sum_{0}^{\infty} e^{-(nh\upsilon/kT)}.} + \frac{1}{2}h\upsilon\right]$$

Let, $e^{-h\upsilon/kT} = x$, then

$$\bar{\varepsilon}_V = \frac{\sum_{0}^{\infty} h\upsilon\, nx^n}{\sum_{0}^{\infty} x^n} + \frac{1}{2}h\upsilon$$

$$= \frac{\sum_{0}^{\infty} h\upsilon\,(0+1x^1+2x^2+3x^3+,\ldots,+)}{\sum_{0}^{\infty}(1+x+x^2+x^3+,\ldots,+)} + \frac{1}{2}h\upsilon$$

$$= \frac{h\upsilon\,\frac{x}{(1-x)^2}}{\frac{1}{(1-x)}} + \frac{1}{2}h\upsilon$$

$$= \frac{h\upsilon\ x}{(1-x)} + \frac{1}{2}h\upsilon$$

Putting the value of x, we get

$$\bar{\varepsilon}_V = \frac{h\upsilon\, e^{-\frac{h\upsilon}{kT}}}{1-e^{-\frac{h\upsilon}{kT}}} + \frac{h\upsilon}{2}$$

$$\bar{\varepsilon}_V = \frac{h\upsilon\, e^{-\frac{h\upsilon}{kT}}}{e^{-\frac{h\upsilon}{kT}}(e^{\frac{h\upsilon}{kT}}-1)} + \frac{h\upsilon}{2}$$

The exponential term cancelled and the equation is written as

$$\bar{\varepsilon}_V = \frac{h\upsilon}{(e^{\frac{h\upsilon}{kT}}-1)} + \frac{h\upsilon}{2} \quad (3)$$

Eq. (3) shows the mean energy equation for harmonic oscillator. The second term of left side of equation free from temperature which is known as zero point energy. The 1st term have temperature and depend upon in exponential form which is evaluated at high and low temperature.

At high temperature:

In Eq.(3), at high temperature

$kT >> h\upsilon$, then expansion of exponential term

$$e^{\frac{h\upsilon}{kT}} = 1 + \frac{h\upsilon}{kT} + (\frac{h\upsilon}{kT})^2 + ,..., +$$

Neglecting higher order terms,

$$\overline{\varepsilon}_V = \frac{h\upsilon}{(\frac{h\upsilon}{kT})} + \frac{h\upsilon}{2}$$

$$\overline{\varepsilon}_V = kT + \frac{h\upsilon}{2}$$

According to Equipartition theorem of energy, each atom have three degrees of freedom is equal to 3N. The energy of the Solid is expressed as

$$\overline{\varepsilon} = 3NkT + \frac{3N\,h\upsilon}{2} \qquad (4)$$

The sp. heat at high temperature

$$C_V = (\frac{d\overline{\varepsilon}}{dT})_V$$

Differentiating Eq.(4) with respect to T, we get

$$C_V = 3Nk \qquad (5)$$

Einstein calculated the sp. heat of solid with respect to temperature, the calculated value of sp. heat at high temperature is the same as experimental value. The Einstein theoretical approach is appreciable at high temperature for determining sp. heat of solid.

At low temperature:

At low temperature, in Eq. (3)

$kT << h\upsilon$,

then expansion of exponential term $e^{\frac{h\upsilon}{kT}}$ becomes very large hence, 1 is neglected and mean energy written as

$$\overline{\varepsilon} = 3Nh\upsilon\, e^{-\frac{h\upsilon}{kT}} + \frac{3N\,h\upsilon}{2} \qquad (6)$$

The sp. heat

$$C_V = \left(\frac{d\bar{\varepsilon}}{dT}\right)_V$$

The Eq. (6) is differentiated with respect to temperature as

$$C_V = 3Nk \left(\frac{h\upsilon}{kT}\right)^2 e^{-\frac{h\upsilon}{kT}}$$

$$C_V = 3Nk \left(\frac{E_T}{T}\right)^2 e^{-\frac{E_T}{T}} \tag{7}$$

The exponential term of Eq. (7) decrease rapidly with decreases of temperature , the calculated value of sp. heat is not agree with experimental results. This is the drawback of the Einstein theory and further theoretical prediction suggested by Debye which gives the good results throughout of temperature.

Discussion with graph

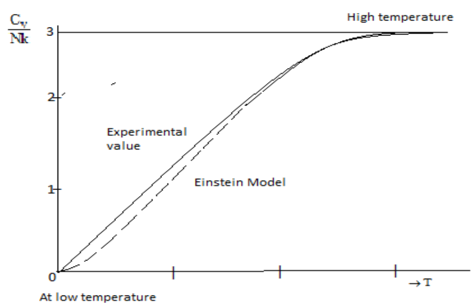

Fig.(1) Comparison of Einstein calculated Sp. heat with experimental results.

The calculated value of sp. heat by Einstein at high temperature and low temperature is shown in Fig.(1) with experimental results. Which is agree with high temperature and low temperature not agree an rapidly decrease with temperature.

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