LECTURE #36

Note Title 4/17/2009

$$\frac{\langle E\rangle}{N} = \langle T\rangle + \langle V\rangle = \frac{3}{2}k_B T + \frac{3}{2}k_B T = 3k_B T$$

$$C_V = \frac{1}{V}\frac{\partial\langle E\rangle}{\partial T} = 3k_B\frac{N}{V} = 3k_B n$$

$$H = \sum_n \frac{\hat{p}_n^2}{2m} + \frac{1}{2}K(\hat{u}_n - \hat{u}_{n+1})^2$$

FOR 1 OSCILLATOR

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}k\hat{x}^2 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

$$\hat{a} = \frac{\hat{x}}{x_0} + i\,\frac{\hat{p}}{p_0} \qquad x_0 = \sqrt{\frac{2\hbar}{M\omega}}$$

$$[\hat{x}\ \hat{p}] = i\hbar \qquad H = \hbar\omega\left(a^{+}a + \frac{1}{2}\right)$$

$$[\hat{a}\ \hat{a}^{+}] = 1$$

$$\hat{a}_q = \frac{1}{\sqrt{N}} \sum_n e^{i\vec{q}\cdot\vec{R}_n}\left(\frac{\hat{u}_n}{u_0} + i\,\frac{\hat{p}_n}{p_0}\right)$$

$$u_0 = \sqrt{\frac{2\hbar}{M\,\omega(q)}}$$

$$H^{tot} = \sum_q \hbar\omega(q)\left(\hat{a}_q^{+}a_q + \frac{1}{2}\right)$$

PHONON = QUANTUM OF EXCITATION IN A

GIVEN MODE

$$[a_q \;\; a_q^+] = 1$$

$$\langle a_q^+ a_q \rangle = \langle n_q \rangle = \frac{1}{e^{\frac{\hbar\omega(q)}{k_B T}} - 1}$$

BOSE - STAT

$\mu = 0$ BECAUSE THE # PHONONS IS NOT CONSERVED

$$\langle E \rangle = \sum_q \hbar\omega(q) \langle n_q \rangle = \sum_q \hbar\omega(q) \frac{1}{e^{\frac{\hbar\omega(q)}{k_B T}} - 1}$$

(1) EINSTEIN MODEL (INDEPENDENT OSCILLATORS)

$\hbar\omega(q) = \hbar\omega_E$ INDEPENDENT OF q

$$\langle E \rangle = \overbrace{3N}^{\#\text{ OF q STATES}} \cdot \frac{\hbar\omega_E}{e^{\frac{\hbar\omega_E}{K_B T}} - 1}$$

$$\frac{\hbar\omega_E}{K_B T} = x$$

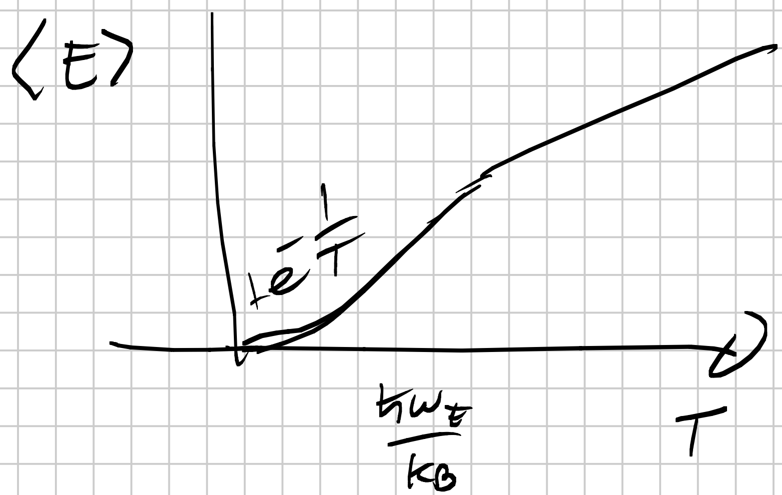
$$\langle E \rangle = 3N\ K_B T\ \frac{x}{e^x - 1}$$

$K_B T >> \hbar\omega_E \Rightarrow x << 1$

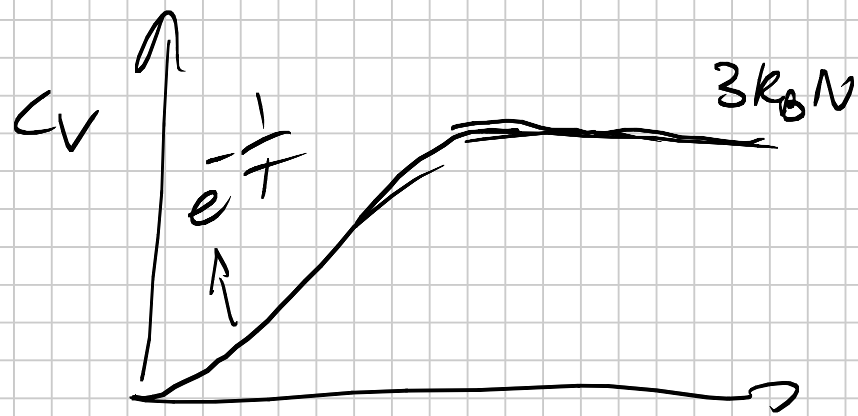
$\frac{x}{\cancel{1} + x \cancel{-1}} \to 1 \Rightarrow \langle E \rangle = 3N K_B T$

$K_B T << \hbar\omega_E \Rightarrow x >> 1$

$3N\ K_B T\ x\ e^{-x}$



$\Rightarrow$

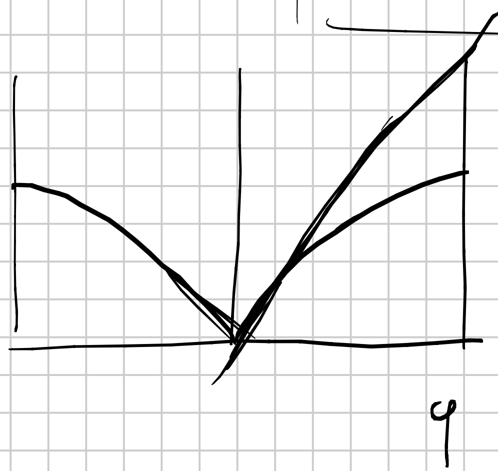


② DEBYE MODEL

$$\langle E \rangle = \sum_q \hbar\omega(q) \frac{1}{e^{\frac{\hbar\omega(q)}{k_B T}} - 1}$$

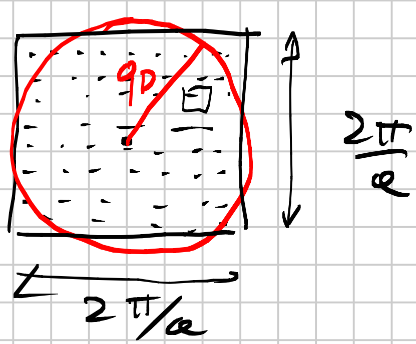
Ⓐ $\hbar\omega(q) = \boxed{\hbar v |q|}$

LINEAR APPROX FOR $\hbar\omega(q) \sim \hbar v |\vec{q}|$



Ⓑ $\sum_{q \in BZ} \rightarrow$ SPHERICAL APPROX FOR THE BZ INTEGRATION

2D



$$\sum_{q \in BZ} = N = \frac{\left(\frac{2\pi}{a}\right)^2}{\left(\frac{2\pi}{L}\right)^2}$$

$$\pi q_D^2 = \left(\frac{2\pi}{a}\right)^2 \Rightarrow \text{DEFINITION OF } q_D$$

$$q_D^2 \sim \frac{1}{a^2} \sim n$$

$$\hbar v q_D = \hbar \omega_D = \text{DEBYE ENERGY}$$

$$\frac{\hbar \omega_D}{k_B} = T_D = \text{'' TEMPERATURE}$$

3D

$$q_D^3 = 6\pi^2 \frac{N}{V}$$

$$\langle E \rangle = \sum_q \hbar \omega(q)\, n \Rightarrow \underbrace{\int \frac{d^3q}{(2\pi)^3}}_{\text{DEBYE SPHERE}} \frac{\hbar v |\vec{q}|}{e^{\frac{\hbar v |\vec{q}|}{k_B T}} - 1} =$$

$$\frac{4\pi}{(2\pi)^3} \int_0^{q_D} q^2 dq \frac{\hbar v q}{e^{\frac{\hbar v q}{k_B T}} - 1}$$

$$\hbar v q = \hbar \omega$$

$$\langle E \rangle = \int_0^{\omega_D} \frac{\omega^2}{2\pi^2 v^3} \frac{\hbar\omega}{e^{\frac{\hbar\omega}{k_B T}} - 1} \qquad \frac{\hbar\omega}{k_B T} = x$$

$$\langle E \rangle = 9 N k_B T \left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} \frac{x^3}{e^x - 1}\, dx$$

LARGE T $\quad T >> T_D \Rightarrow x << 1$

$$\frac{x^3}{e^x - 1} \sim \frac{x^3}{1 + x - 1} \sim x^2 \Rightarrow \int_0^{T_D/T} x^2\, dx$$

$$\Rightarrow \frac{1}{3}\left(\frac{T_D}{T}\right)^3 \Rightarrow \langle E \rangle = \overset{3}{\cancel{9}} N k_B T \cancel{\left(\frac{T}{T_D}\right)^3} \cdot \frac{1}{\cancel{3}} \cancel{\left(\frac{T_D}{T}\right)^3}$$

SMALL T $\quad T \ll T_D \Rightarrow \int_0^{T_D/T} \xrightarrow{\sim} \int_0^{\infty}$

$$\langle E \rangle = 3NK_BT\left(\frac{T}{T_D}\right)^3 \boxed{\int_0^{\infty} \frac{x^3}{e^x-1}\,dx} \rightarrow \frac{\pi^4}{15}$$

$$\langle E \rangle \propto T^4 \Rightarrow C_V \propto T^3$$