LECTURE # 19

Note Title 11/9/2007

VIBRATIONS / PHONONS

Chapt 22 — 422 - 437 ←

437 - 443 Read only

Chapt 23 — All

Chemical model $(\hbar = 0)$

$$E(t) = E_0 + \langle K \rangle + \langle V \rangle$$

$\langle K \rangle$ ↓ Kinetic energy

$\langle V \rangle$ ↓ Potential energy springs

Solid with N atoms $\qquad$ $3N$ degrees of freedom

$$\left\langle \frac{p^2}{2m} \right\rangle = 3N \frac{K_B T}{2}$$

$$\langle V \rangle = 3N \frac{K_B T}{2}$$

VIRIAL THEOREM

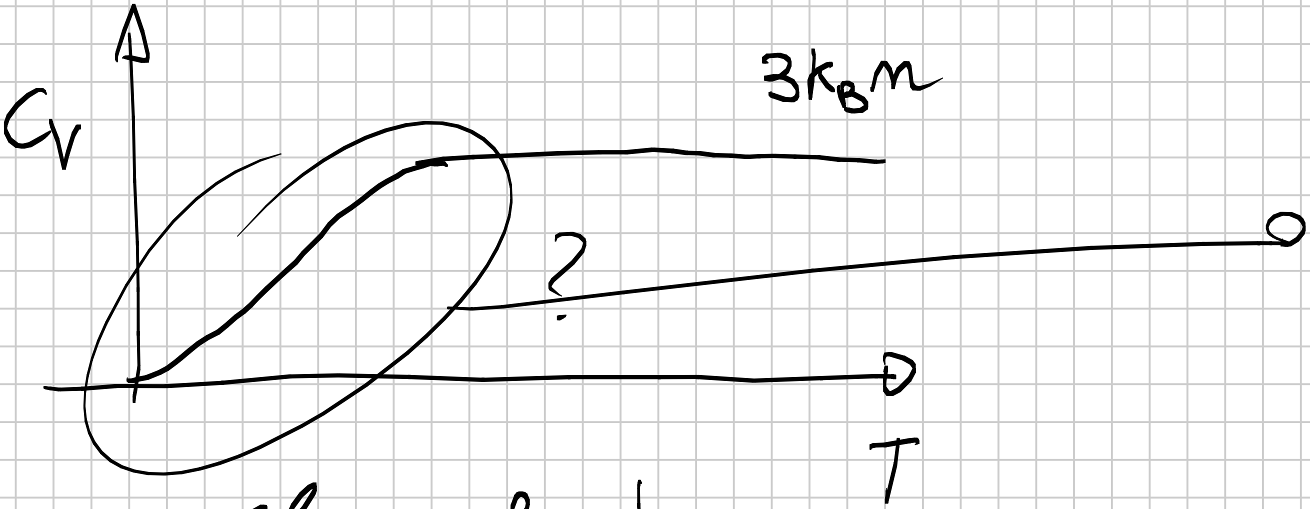
$V \sim \frac{1}{2} k x^2$

$\Rightarrow 2\langle K \rangle = 2 \langle V \rangle$

$$\boxed{E = 3 N K_B T}$$

$$C_V = \frac{1}{V} \left(\frac{\partial E(T)}{\partial T} \right)_V = 3 \frac{N}{V} k_B$$

DOULONG AND PETIT LAW



We need

$\hbar \neq 0$

Quantum case

classical harmonic O.

$\underline{\vec{q}} \to$ MODE

$$H = \sum_{q \in BZ} \hbar \omega_q \left(a_q^{\dagger} a_q + \frac{1}{2} \right)$$

EACH MODE IS HARMONIC OSCILLATOR $\omega(q)$ $\Longrightarrow$

$a_q^{\dagger}$ a_q create and destroy <u>quanta of oscillations</u>* for a given mode $\underline{q}$

* PHONONS

$$H_{osc} = \sum_{\substack{q \in BZ \\ \lambda}} \hbar\omega_\lambda(q) \left(a^\dagger_{q\lambda} a_{q\lambda} + \frac{1}{2} \right)$$

$$\text{Tot } E = E_0 + \langle H_{\text{Oscillation}} \rangle \qquad \langle\ \rangle \text{ thermal average}$$

$$= E = E_0 + \sum_{\substack{q \in BZ \\ \lambda}} \frac{\hbar\omega_\lambda(q)}{2} + \sum_{\substack{q \in BZ \\ \lambda}} \langle a^\dagger_{q\lambda} a_{q\lambda} \rangle \hbar\omega_\lambda(q)$$

$$\langle a^\dagger_{q\lambda} a_{q\lambda} \rangle = \langle n_{q\lambda} \rangle = \frac{1}{e^{\frac{\hbar\omega_\lambda(q)}{k_B T}} - 1}$$

$$\boxed{E(T) = \sum_{\substack{q \in BZ \\ \lambda}} \frac{\hbar \omega_\lambda(q)}{e^{\frac{\hbar \omega_\lambda(q)}{k_B T}} - 1}}$$

Einstein (1905) $\longrightarrow$

(1907)

Solid with

N atoms

$$\hbar \omega(q) \sim \hbar \omega_E$$

$$E(T) = \boxed{\sum_{\substack{q \in BZ \\ \lambda}}} \frac{\hbar \omega_E}{e^{\frac{\hbar \omega_E}{k_B T}} - 1} = 3N \frac{\hbar \omega_E}{e^{\frac{\hbar \omega_E}{k_B T}} - 1}$$

(1) Limit $\quad k_B T >> \hbar\omega_E$

$$e^{\frac{\hbar\omega_E}{k_B T}} \sim 1 + \frac{\hbar\omega_E}{k_B T} \qquad \frac{\hbar\omega_E}{k_B T} \to << 1$$

$$e^x \sim 1 + x$$

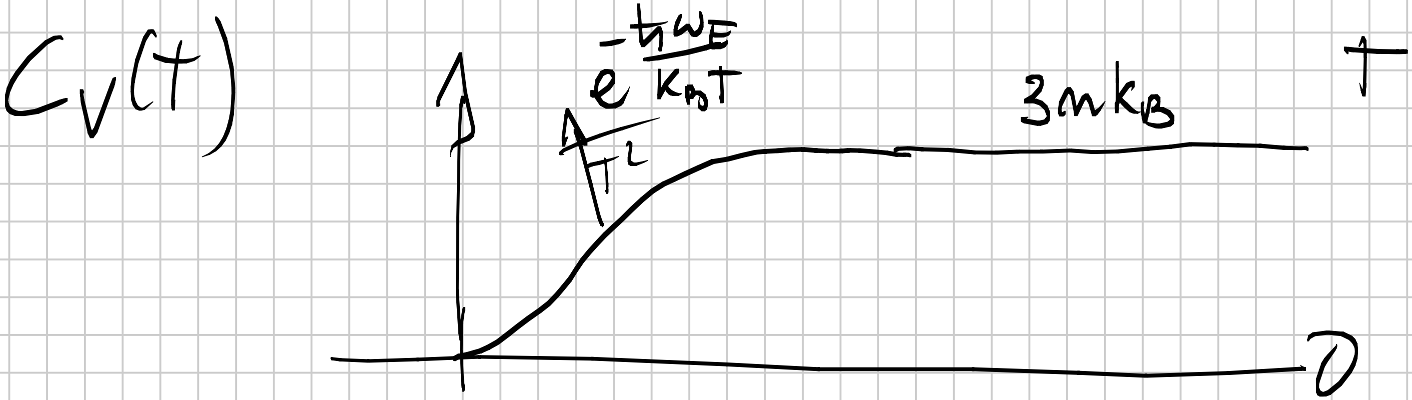
$$E(T) = 3N \frac{\cancel{\hbar\omega_E}}{\cancel{\hbar\omega_E}} k_B T = 3N k_B T$$

$$C_V \sim 3n k_B = \qquad \left(n = \frac{N}{V}, \text{density}\right)$$

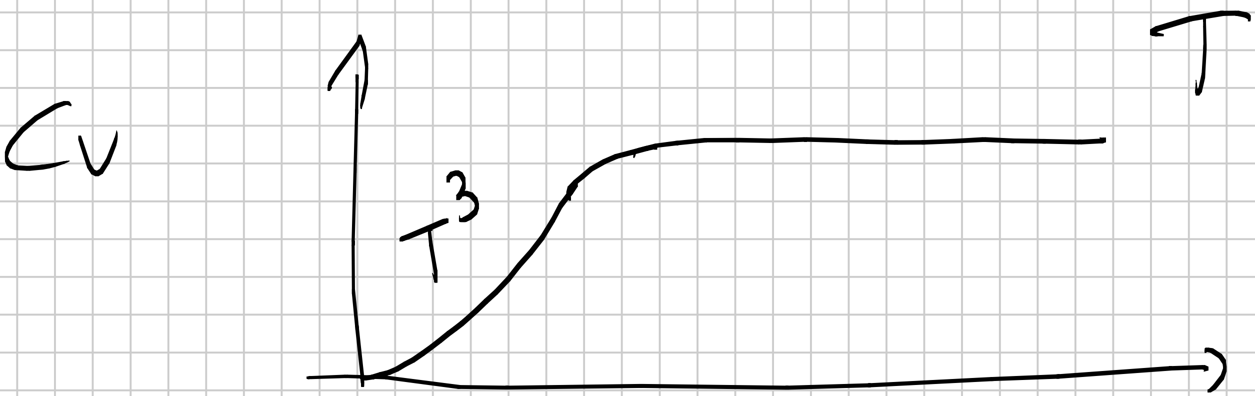
(2) Limit $\quad k_B T << \hbar\omega_E$

$$\underbrace{e^{\frac{\hbar\omega_E}{k_B T}}}_{} - 1 \sim e^{\frac{\hbar\omega_E}{k_B T}} \qquad \frac{\hbar\omega_E}{k_B T} >> 1$$

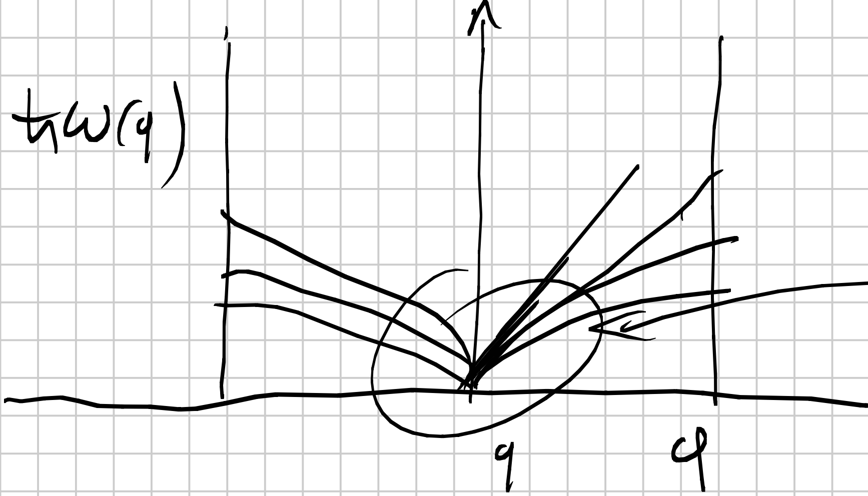
$$E = 3N\hbar\omega_E \, e^{-\frac{\hbar\omega_E}{k_BT}}$$



EINSTEIN



EXPERIMENT



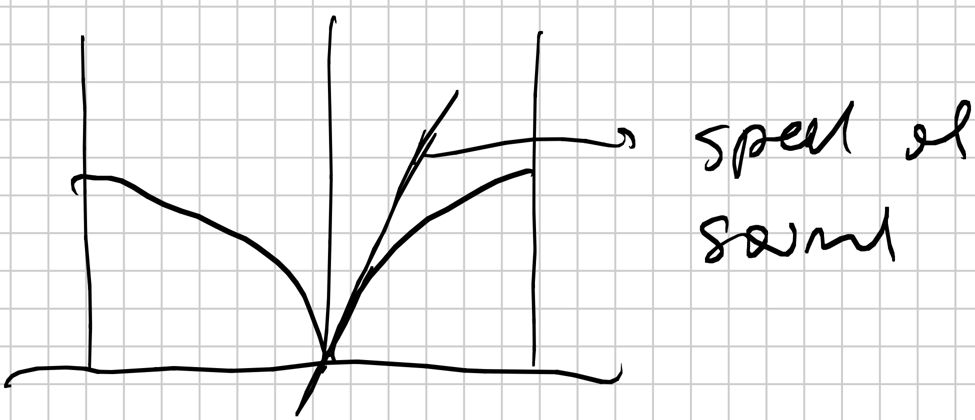
REASON:
AT LOW T ACOUSTIC MODES ARE IMPORTANT

$\hbar\omega(q)$ HAS STRONG q DEPENDENCE

DEBYE MODEL (1912)

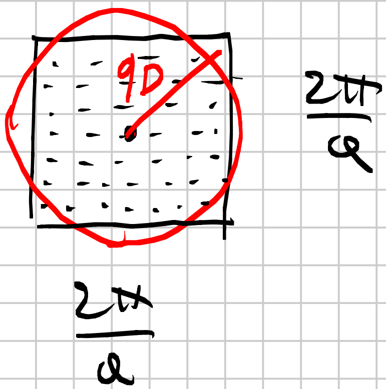
① $\hbar\omega(q) = \hbar v|\vec{q}|$

v speed of sound in the solid



② Spherical approx for the Brillouin Zone

$$\sum_{\vec{q} \in BZ}$$



$\boxed{\text{2D Case}}$

$$q_D \pi^2 = \left(\frac{2\pi}{a}\right)^2$$

q DEBYE

$$\frac{4}{3}\pi q_D^3 = \left(\frac{2\pi}{a}\right)^3$$

$$q_D^3 = 6\pi^2 \frac{1}{a^3} = 6\pi^2 n$$

DEBYE MODEL

$$\sum_q \to \frac{V}{(2\pi)^3}\int d\vec{q}$$

$$E = \overset{L+2T}{\downarrow}\!3 \sum_{q\in BZ} \frac{\hbar v|\vec{q}|}{e^{\frac{\hbar v|\vec{q}|}{k_BT}}-1} \longrightarrow$$

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

$$\frac{\hbar v q}{k_BT} = x$$

DEBYE TEMPERATURE

$$\hbar v q_D = k_B T_D$$

$$E = 3 \frac{4\pi}{(\hbar v)^3} \frac{(k_B T)^4}{(2\pi)^3} \int_0^{T_D/T} \frac{x^3}{e^x - 1} dx \cdot \frac{q_D^3}{q_D^3}$$

$$q_D^3 = 6\pi^2 n$$

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

Limit ① High T $\quad T \gg T_D$

$$\frac{T_D}{T} \ll 1 \qquad \int_0^{\varepsilon} \Rightarrow x \text{ is small}$$

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

$$\int_0^{T_D/T} x^2\, dx = \frac{x^3}{3}\Big|_0^{T_D/T}$$

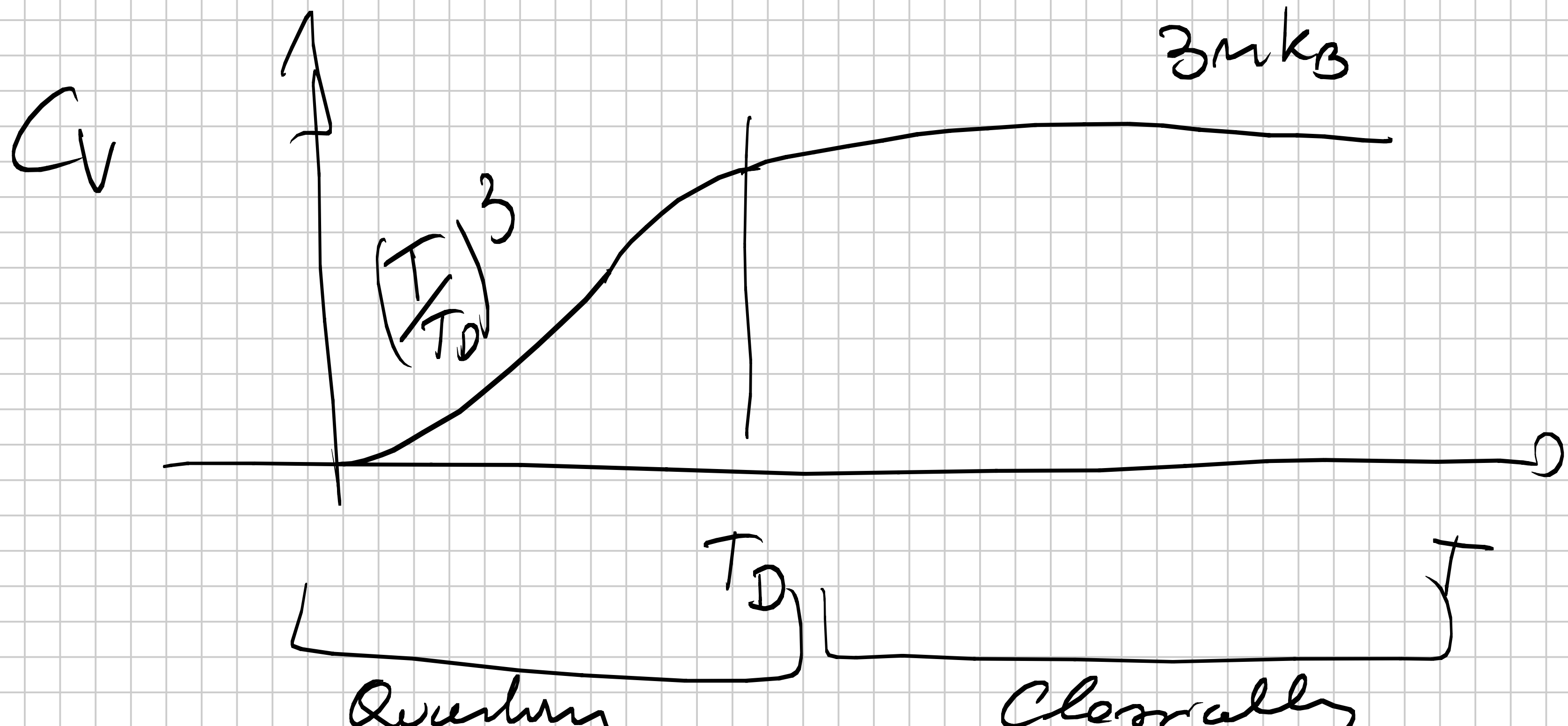
$$E = 9 N K_B T \cancel{\left(\frac{T}{T_D}\right)^3} \cdot \cancel{\left(\frac{T_D}{T}\right)^3} \cdot \frac{1}{3} \rightarrow 3 N K_B T$$

(2) $T << T_{DEBYE}$

$$\frac{T_D}{T} \longrightarrow \infty \qquad \int_0^{T_D/T} \frac{x^3}{e^x - 1}\, dx \sim \overbrace{\int_0^{\infty} \frac{x^3}{e^x - 1}\, dx}^{\frac{\pi^4}{15}}$$

$$E = 9 N k_B T \left(\frac{T}{T_D}\right)^3 \cdot \frac{\pi^4}{15} \quad \propto \quad T^4$$

$$C_V = \frac{1}{V}\frac{\partial E}{\partial T} = \frac{12}{5}\pi^4 n \, k_B \left(\frac{T}{T_D}\right)^3$$



ε_F

$T \gg \frac{\varepsilon_F}{k_B}$

$T < \frac{\varepsilon_F}{k_B}$

$k_B T_D \sim$ Energy of acoustic phonon at zone boundary $\sim$

$.1\ eV$ $\quad T_D \sim 10^2 \sim 10^3\ K$

$k_B T_F \sim$ Energy of e^- on FERMI SPHERE FOR METALS

$10 \sim eV$ $\quad T_F \sim 10^4 \sim 10^5\ K$