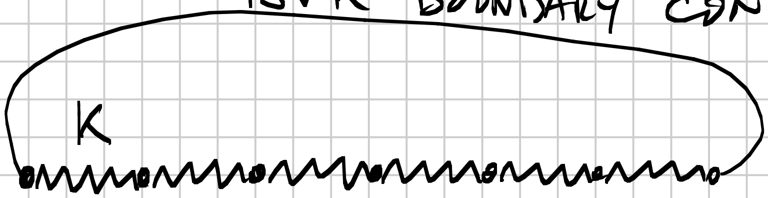
LECTURE # 21

Note Title 11/19/2008

BVK BOUNDARY CONDITIONS



N ATOMS

$$u_m(q) = e^{iqma}$$

q = NORMAL MODES OF OSCILLATIONS

NORMAL MODES = # ATOMS

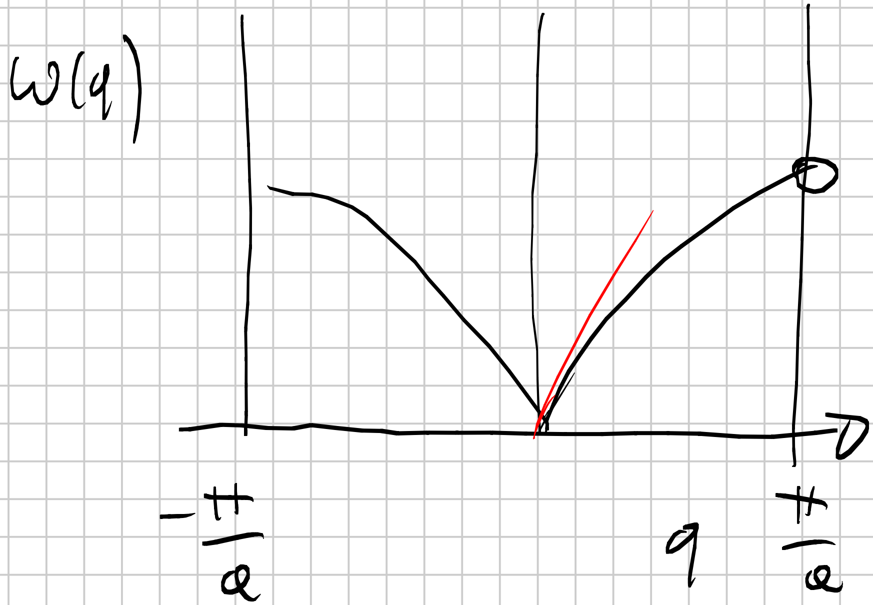
$\omega(q)$

DEC 3RD
KAIJIE XU
→ FINAL 2007 SOLUTION

DEC 11th FINAL
THU

$\boxed{\text{DEC 9 10} \quad \text{NOV 29}}$

$\boxed{\cancel{\text{DEC 2 – 8}}}$

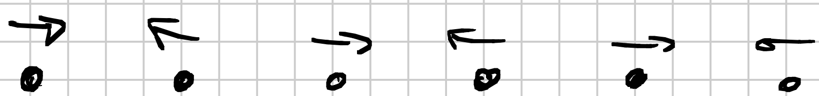


$$\omega(q) = \sqrt{\frac{4K}{M}}\left|\sin\frac{qa}{2}\right|$$

$$\omega(q) \sim \sqrt{\frac{K}{M}}\, a q \sim v_{\text{SOUND}} \cdot q$$

FOR SMALL q

$$q = \frac{\pi}{a} \qquad u\left(\frac{\pi}{a}\right) \sim e^{i\frac{\pi}{\cancel{a}} n \cancel{a}} \left\langle \begin{matrix} +1 \\ -1 \end{matrix} \right.$$

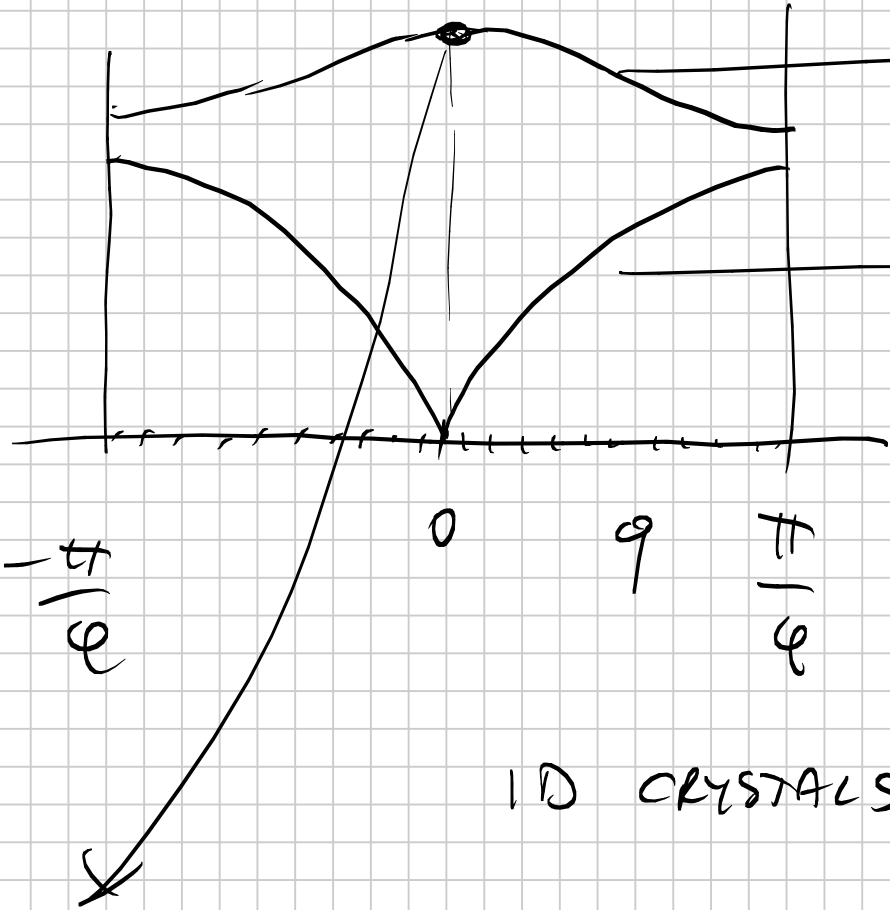


CRYSTAL WITH BASIS

N UNIT CELLS

2 ATOMS/CELL

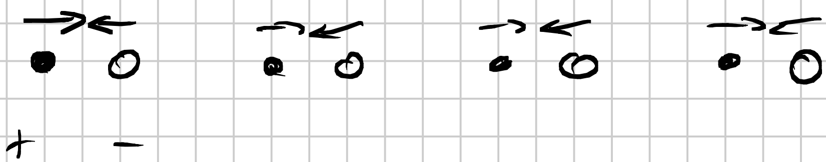
$2N$ DEGREES OF FREEDOM



OPTICAL BRANCH

ACOUSTIC BRANCH

1D CRYSTALS



FCC LATTICE

Pb NO BASIS

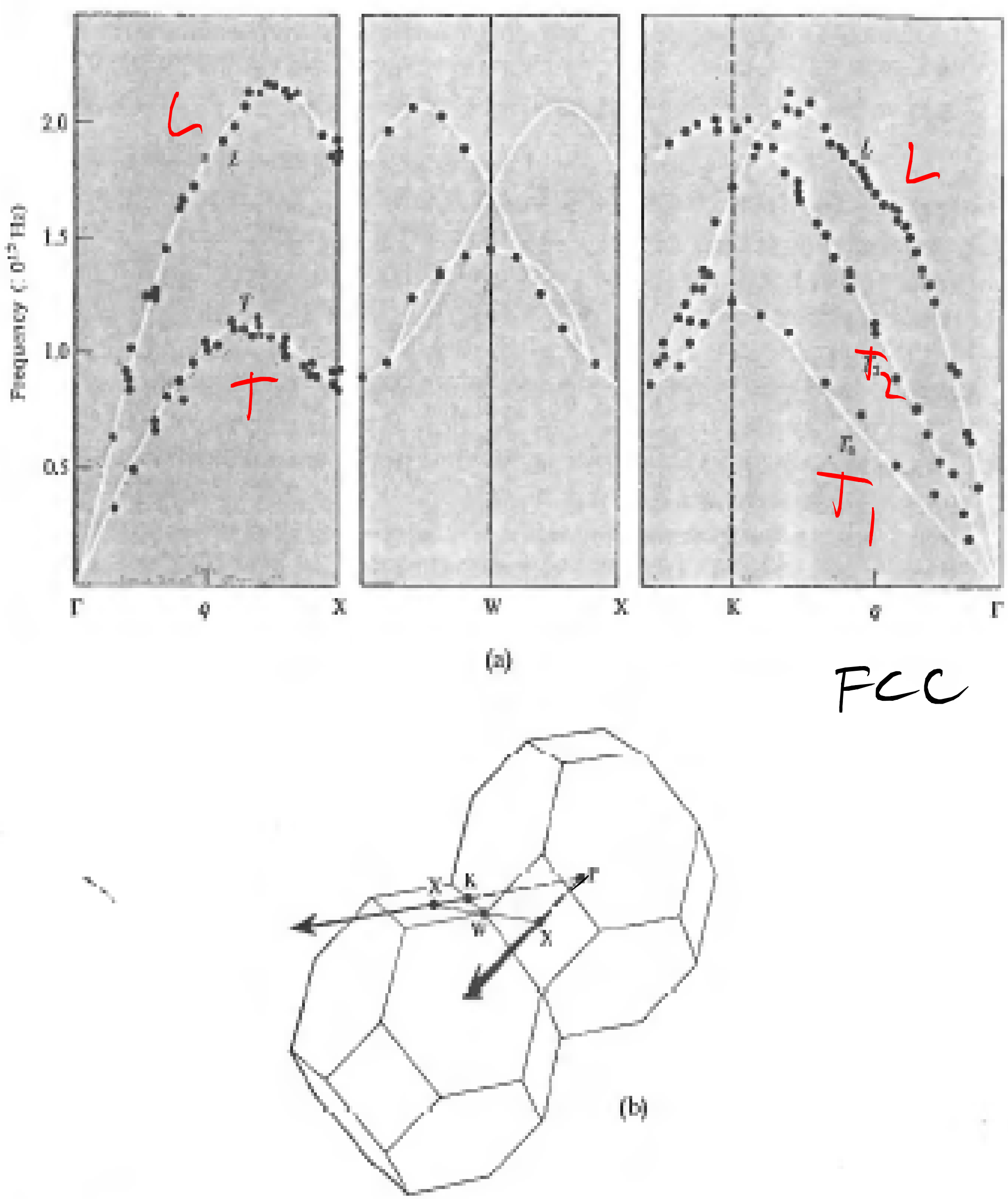
N TOT # OF Pb ATOMS

3N NORMAL MODES OF OSCILLATION

$\vec{q} = (q_x, q_y, q_z)$

1 LONGITUDINAL $\quad \vec{u}_L \parallel \vec{q}$

2 TRANSVERSAL MODES $\vec{u}_T \perp \vec{q}$



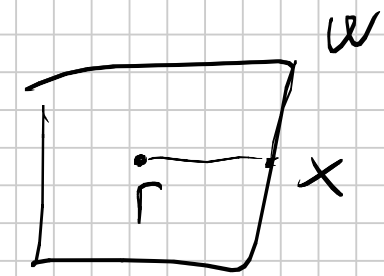
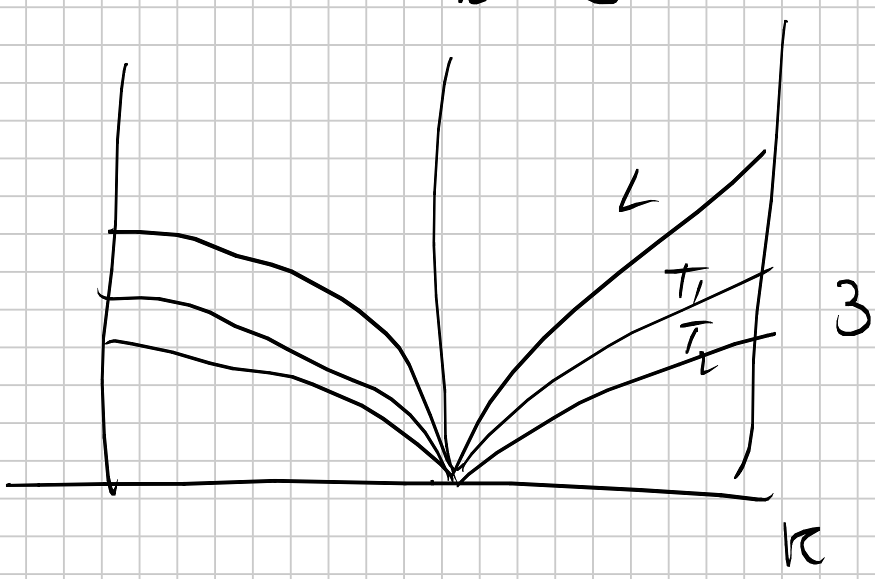


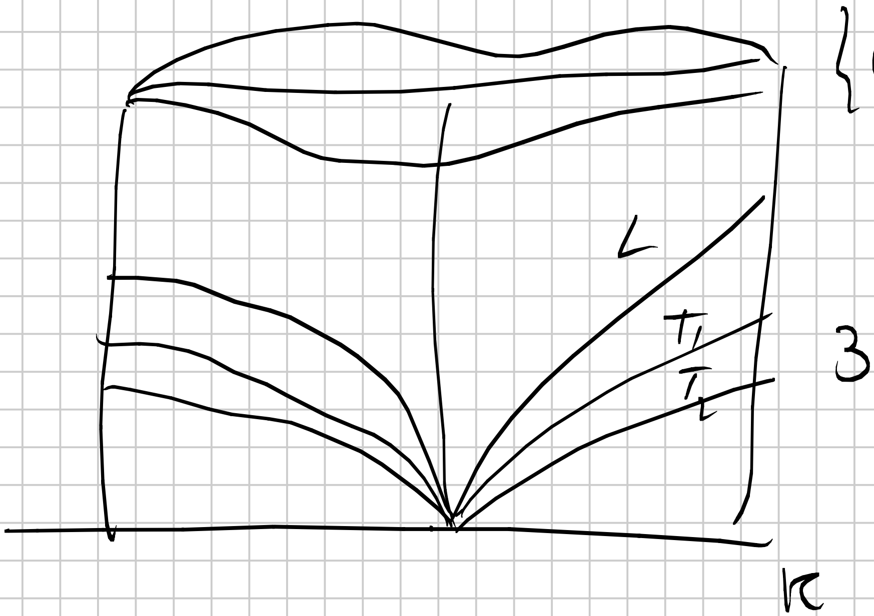
Figure 22.13
(a) Typical dispersion curves for the normal-mode frequencies in a monatomic Bravais lattice. The curves are for lead (face-centered cubic) and are plotted in a repeated-zone scheme along the edges of the shaded triangle shown in (b). Note that the two transverse branches are degenerate in the [100] direction. (After Brockhouse et al., *Phys. Rev.* 128, 1099 (1962).)

3D CRYSTAL WITH P ATOMS IN THE BASIS

N TOTAL # OF UNIT CELLS

$$\underbrace{3N}_{\#\text{ ACOUSTIC MODES}} + \underbrace{3(P-1)N}_{\#\text{ OPTICAL MODES}} = \boxed{\underbrace{3NP}_{\text{TOT \# ATOMS}}}$$





INTERACTING ATOMS WITH HARMONIC POTENTIAL

THERMAL EQUILIBRIUM

$$\langle E \rangle = \langle K \rangle + \langle V \rangle$$

CLASSICAL SYSTEM

$$\langle K \rangle = \frac{1}{2} k_B T \overbrace{3N}^{\text{\# DEGREES OF FREEDOM}}$$

$\langle V \rangle =$ VIRIAL THEOREM

HARMONIC POTENTIAL : $V(x) = \frac{1}{2} k x^2$

$$\langle K \rangle = \langle V \rangle$$

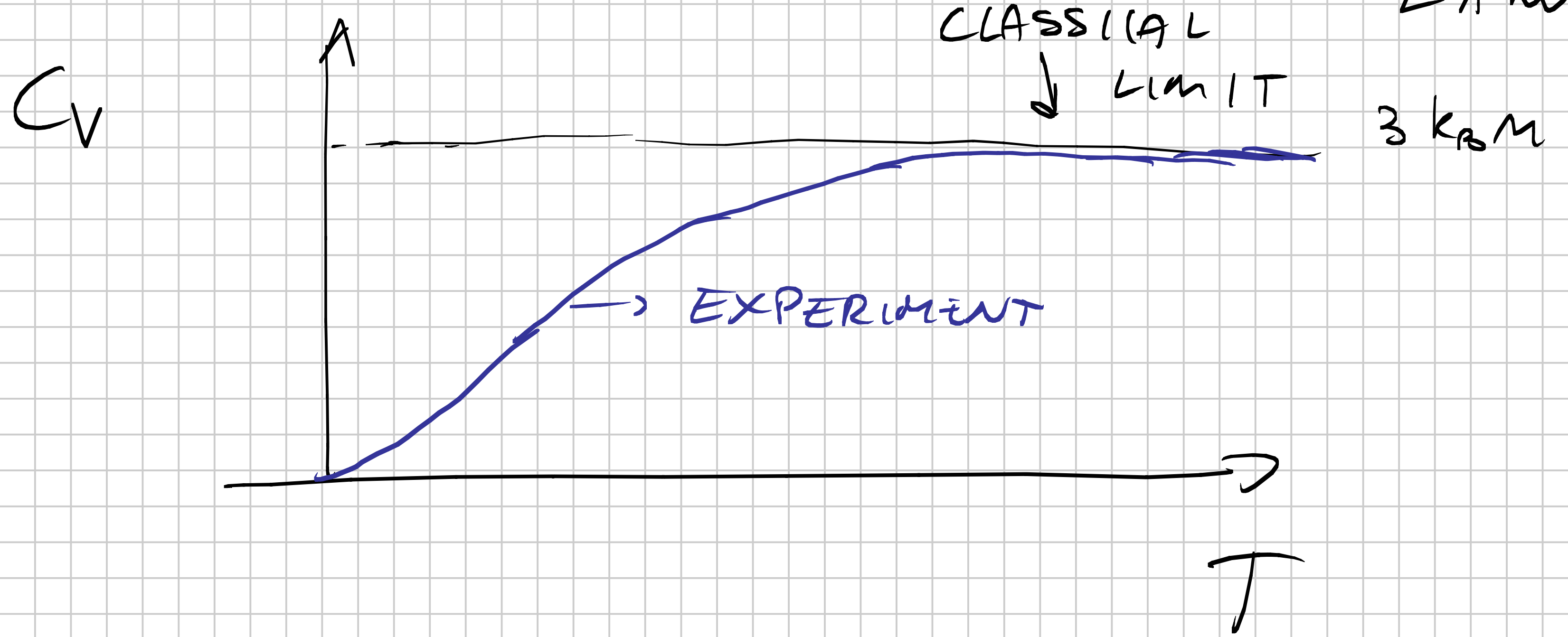
THEOREM: $V(x) \propto x^\lambda \Rightarrow 2\langle K \rangle = \lambda \langle V \rangle$

$$E(T) = \langle K \rangle + \langle V \rangle = 3 k_B T N$$

SPECIFIC HEAT

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

DOULONG - PETIT LAW



WE NEED

QUANTUM HARMONIC CRYSTAL

$\vec{q} \longrightarrow$ HARMONIC OSCILLATOR

$$H = \frac{p^2}{2M} + \frac{1}{2} M \omega^2 x^2 \longrightarrow \frac{\hat{p}^2}{2M} + \frac{1}{2} M \omega^2 \hat{x} = H$$

$$[\hat{x}\ \hat{p}] = i\hbar$$

$$\hat{a} = \left(\frac{\hat{x}}{x_0}\right) + i\left(\frac{\hat{p}}{p_0}\right)$$

$$x_0 = 2M\hbar\omega$$

$$p_0 = \frac{2\hbar}{M\omega}$$

$$\hat{a}^+ = \left(\frac{\hat{x}}{x_0}\right) - i\left(\frac{\hat{p}}{p_0}\right)$$

$$H = \hbar\omega\left(a^+ a + \frac{1}{2}\right)$$

CRYSTAL : MANY MODES q

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

$a_q^{+} a_q \rightarrow$ # OF QUANTA OF OSCILLATION FOR MODE q

$\Rightarrow$ PHONONS

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

$[a_q \; a_{q'}^{+}] = \delta_{qq'}$

BOSONS

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

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

BOSE EINSTEIN STATISTICS

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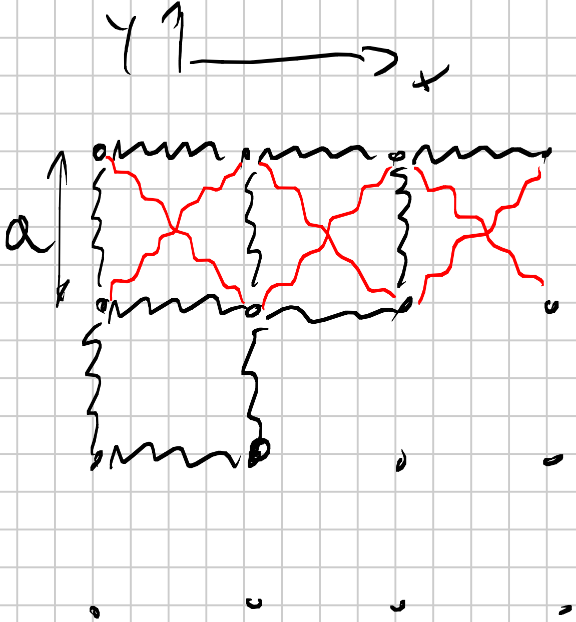
① EINSTEIN METHOD

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

② DEBYE METHOD $\longrightarrow$ C_V



$$\vec{q} = \left(\frac{\pi}{a}, 0\right)$$

2D SYSTEM

$\omega(q)$

2 MODES

① LONGITUDINAL MODE

$u \parallel \hat{x}$

① TRANSVERSAL MODE

$u \parallel \hat{y}$