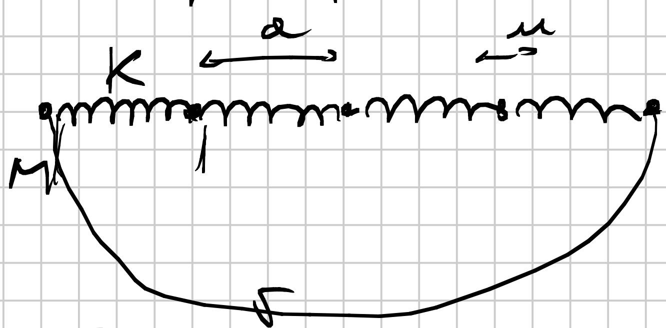
LECTURE # 18

Note Title 11/7/2007

Theory of harmonic crystal



Born von Karmann boundary conditions

$\boxed{N \text{ atoms}}$

K spring constant

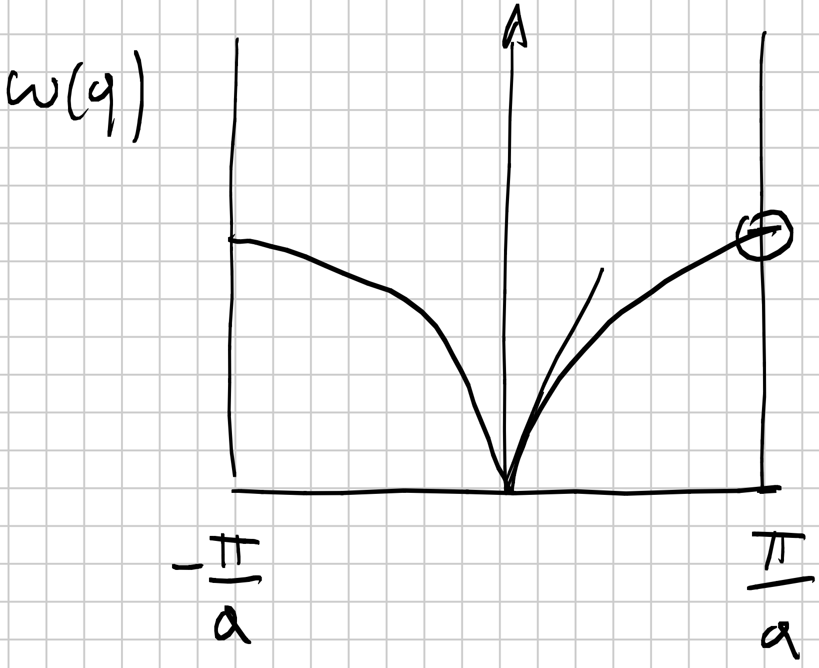
$$u_n(q) = e^{iqna}$$

$$q = \frac{2\pi}{N} n \qquad 0 < n < N-1$$

q = normal modes of oscillation

modes = N atoms

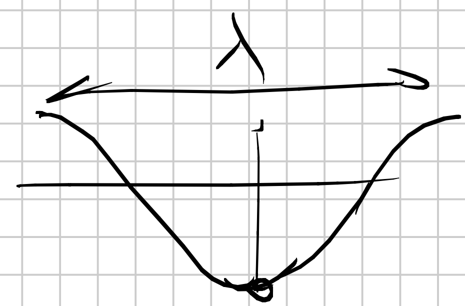
$$\omega(q)$$



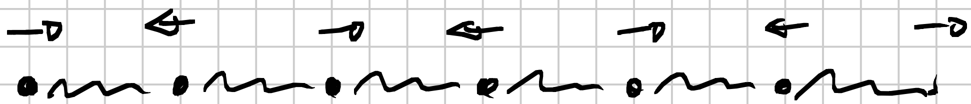
$$\omega(q) = \sqrt{\frac{4K}{M}}\left|\sin\frac{qa}{2}\right|$$

SMALL q

$$\omega(q) \sim \sqrt{\frac{K}{M}}\, a q \sim v_s q$$



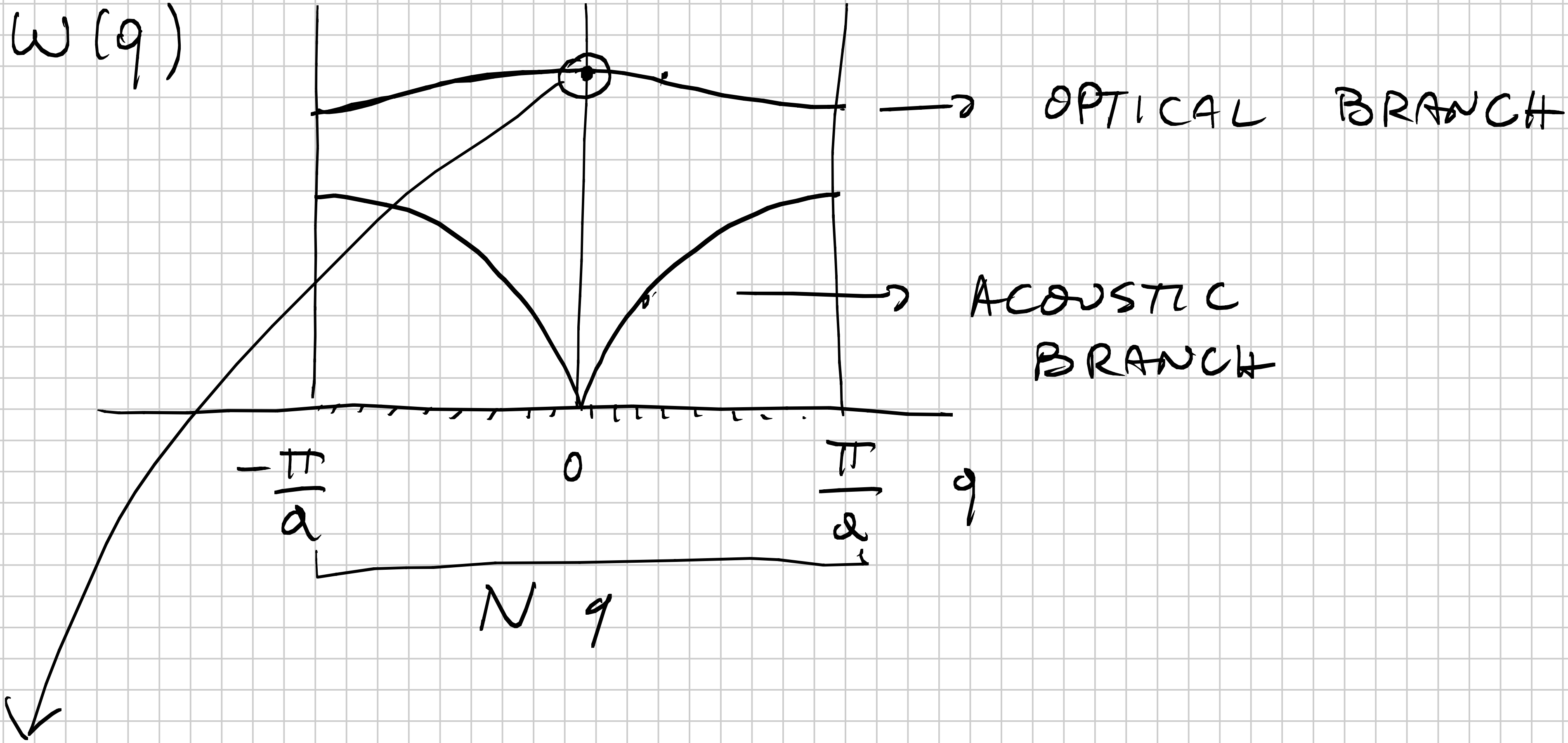
$$q = \frac{\pi}{a} \Rightarrow \lambda = \frac{2\pi}{q} = \underline{\underline{2a}}$$



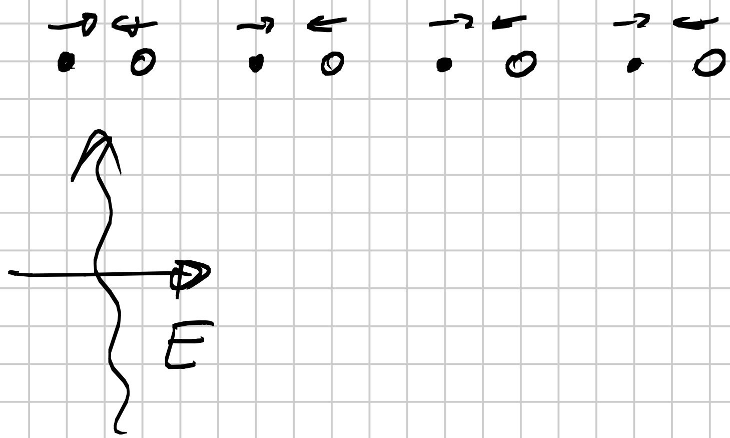
Crystal with basis

N unit cells
2 atoms on each cell

2N DEGREES OF FREEDOM



q = 0
OPTICAL BRANCH



1D Crystals

$\boxed{1D \to 3D}$ No basis FCC Pb

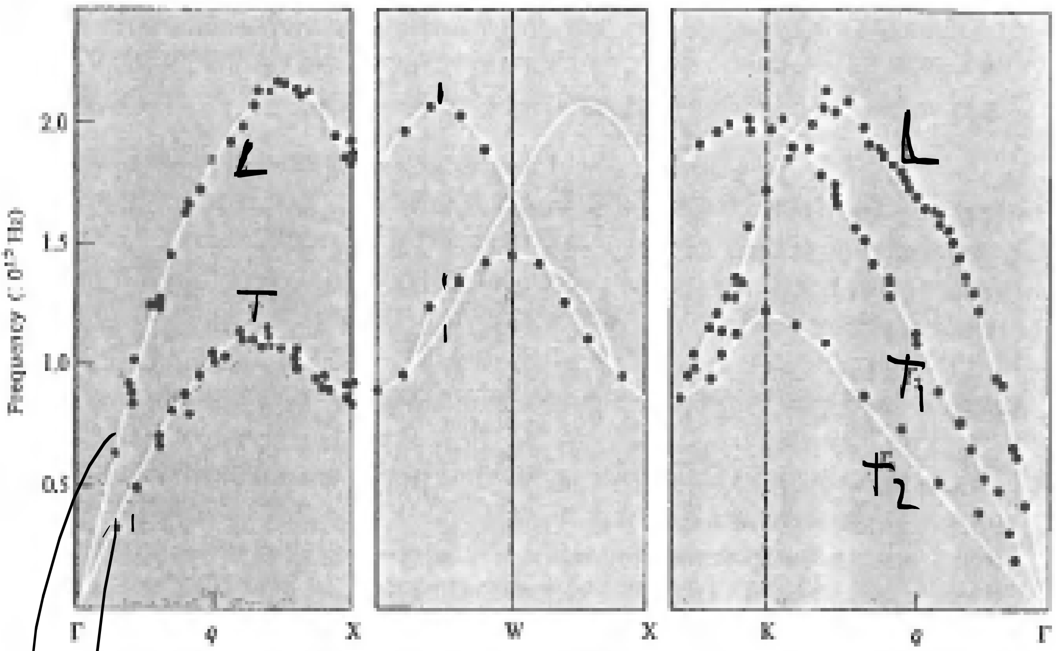
N TOT # UNIT CELLS = TOT # OF Pb IONS

- 3 $\quad 3N$ NORMAL MODES

N q WAVES $\Rightarrow$ $\forall q \to 3$ MODES

$\to$ 1 LONGITUDINAL MODE $\vec{u} \parallel \vec{q}$

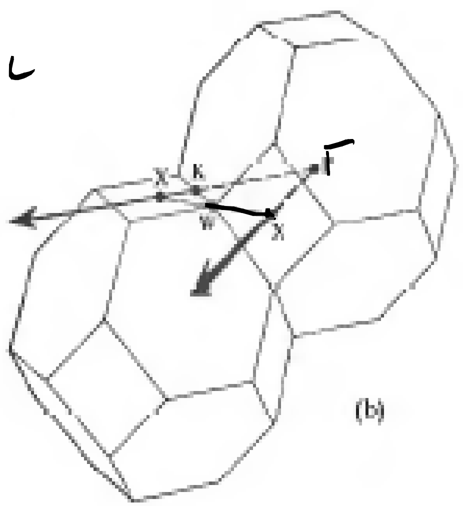
$\to$ 2 TRANSVERSAL MODES $\vec{u} \perp \vec{q}$



(a)

LONGITUDINAL BRANCH

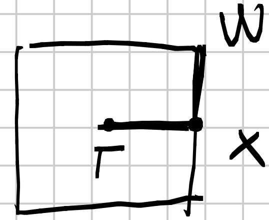
TRANSVERSAL BRANCH

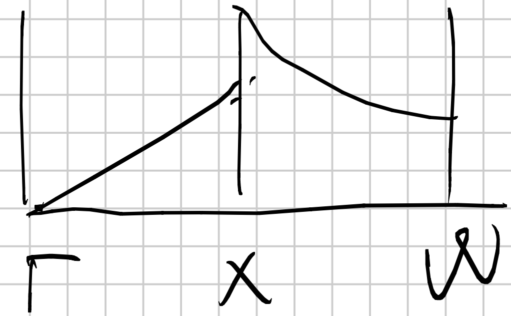


3D

(b)

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 FCC LATTICE

BRILLOUIN ZONE

↓

TRUNCATED OCTAHEDRON

$$\Gamma = (0,0,0)$$

$$X = \left(\frac{2\pi}{a},0,0\right)$$

$$W = \left(\frac{2\pi}{a}, \frac{\pi}{a}, 0\right)$$

Calculate the total E of crystal

3D crystal

N atoms

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

$$\langle T \rangle = \frac{k_B T}{2} \times 3N = \frac{3}{2} k_B T N$$

\# degrees of freedom

$\langle V \rangle$ VIRIAL THEOREM

$$V = \frac{1}{2} k x^2 \qquad V(x) = x^{\lambda}$$

THEOREM $\Rightarrow 2\langle T \rangle = \lambda \langle V \rangle$

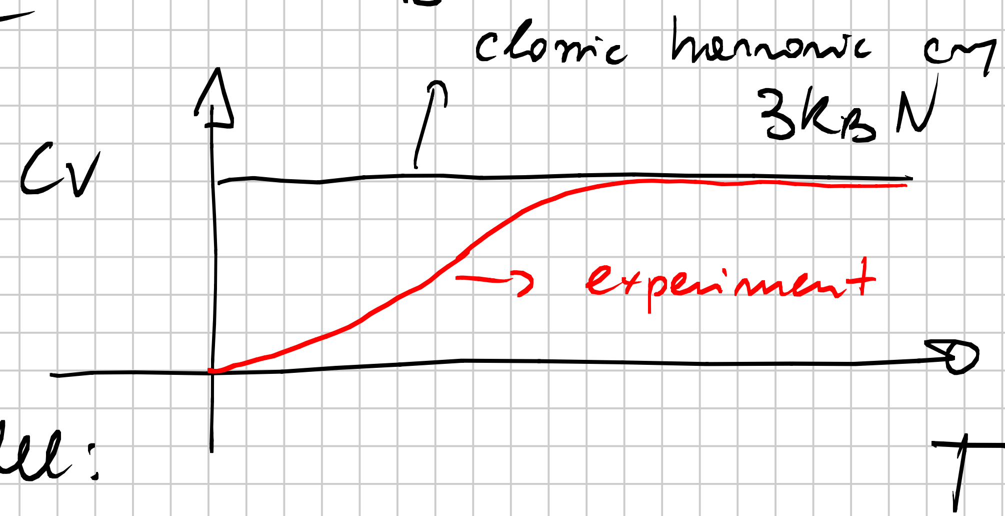
HARMONIC POTENTIAL

$$\langle T \rangle = \langle V \rangle$$

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

SPECIFIC ~~HEAT~~

$$C_V = \frac{d\langle E \rangle}{dT} = 3k_B N \rightarrow \text{CONSTANT}$$



We need new model:

Quantum Harmonic Crystal

Each $q \rightarrow 1$ Harmonic Oscillator

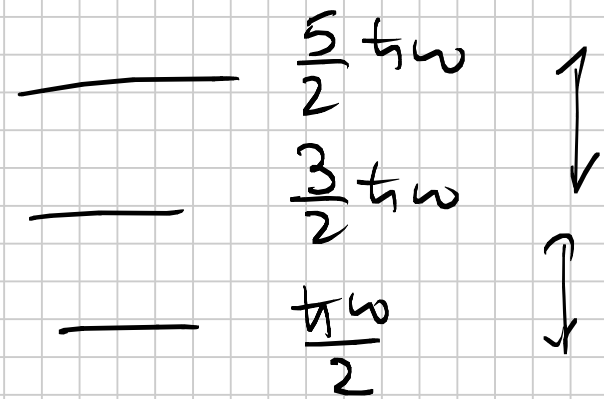
$$H = \frac{p^2}{2M} + \frac{1}{2} M \omega^2 x^2 \longrightarrow \frac{\hat{p}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2$$

$$\omega = \sqrt{\frac{k}{M}} \qquad [\hat{x} \; \hat{p}] = i\hbar$$

$$\hat{a} = \left(\frac{\hat{x}}{x_0}\right) + i\left(\frac{\hat{p}}{p_0}\right) \qquad x_0 = 2m\hbar\omega$$

$$\hat{a}^{+} = \left(\frac{\hat{x}}{x_0}\right) - i\left(\frac{\hat{p}}{p_0}\right) \qquad p_0 = \frac{2\hbar}{M\omega}$$

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



$\hbar \omega(q)$ FOR EACH q

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

$\hat{a}^{+}_{q} \hat{a}_{q} \rightarrow$ # of quanta of the harmonic oscillator at q

$\Downarrow$

$\boxed{\text{PHONONS}}$

$[a_q \; a^{+}_{q}] = 1$ $\qquad$ $[a_q \; a^{+}_{q'}] = \delta_{qq'}$

BOSONS

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

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

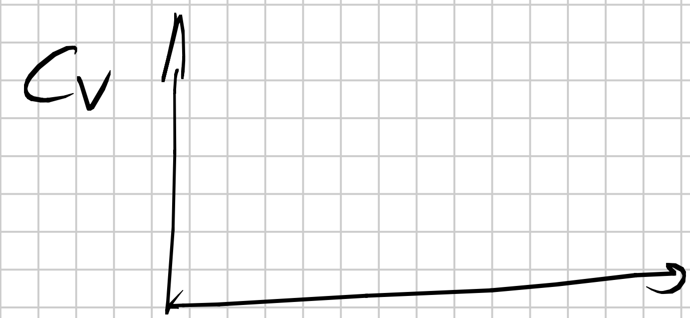
Bose statistics

$$\langle E\rangle = \sum_{q\in BZ} \frac{\hbar\omega(q)}{e^{\frac{\hbar\omega(q)}{k_BT}}-1} \longrightarrow E(T)$$

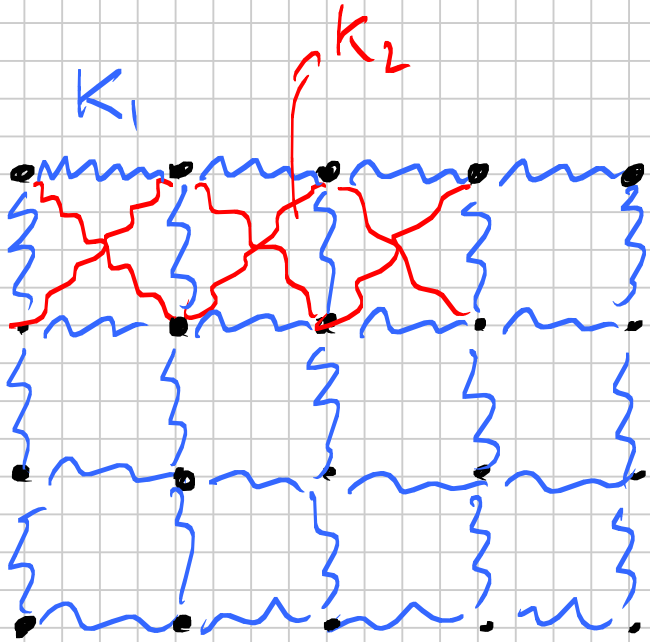
EINSTEIN METHOD

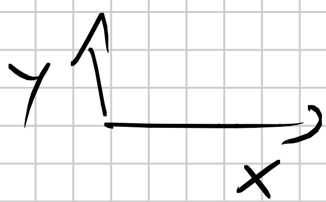
DEBYE METHOD

$\longrightarrow$



$\boxed{\text{FRI}}$





ω of normal mode of oscillation

for

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

→ LONGITUDINAL ω_L

→ TRANSVERSAL ω_T