LECTURE #18

FREE ELECTRON THEORY FAILED TO PREDICT THE T^3 DEPENDENCE OF C_V, THUS SUGGESTING THAT WE NEED TO ADD SOMETHING TO OUR THEORY OF SOLIDS.

IN PARTICULAR, CONSIDER ELASTIC VIBRATIONS OF A CRYSTAL WITH ONE ATOM IN THE PRIMITIVE CELL.

THESE ELASTIC VIBRATIONS COME IN TWO VARITIES:

(1) <u>LONGITUDINAL</u>: DISPLACEMENT OF ATOMS IS PARALLEL TO THE PROPAGATION DIRECTION (ONE POSSIBLE POLARIZATION)
↳ $\boxed{\text{SEE FIG. 2}}$

(2) <u>TRANSVERSE</u>: DISPLACEMENT OF ATOMS IS PERPENDICULAR TO THE PROPAGATION DIRECTION (TWO POSSIBLE POLARIZATIONS)
↳ $\boxed{\text{SEE FIG. 3}}$

<u>ASSUME</u>: (1) ENTIRE PLANES OF ATOMS MOVE IN PHASE
⇒ 1-D PROBLEM

(2) ELASTIC RESPONSE FOLLOWS HOOKE'S LAW
⇒ FORCE IS PROPORTIONAL TO DISPLACEMENT
⇒ QUANTUM THEORY OF ELASTIC WAVES (i.e., PHONONS) WILL HAVE SOLUTIONS ANALOGOUS TO THE HARMONIC OSCILLATOR

BEFORE DEVELOPING THE QUANTUM THEORY OF PHONONS, WE NEED TO DETERMINE THE DISPERSION RELATIONSHIP (i.e, ω VERSUS k RELATIONSHIP) FOR ELASTIC WAVES.

LABEL ATOMIC PLANES AS: $\ldots, s-2, s-1, s, s+1, s+2, \ldots$
WITH CORRESPONDING DISPLACEMENTS: $u_{s-1}, u_s, u_{s+1}, \ldots$

FURTHER ASSUME THAT NEAREST NEIGHBOR INTERACTIONS DOMINATE.

FORCE CONSTANT (SPRING CONSTANT)

$$\therefore \quad \underset{\substack{\uparrow \\ \text{FORCE ON PLANE } s}}{F_s} = C\underbrace{(u_{s+1} - u_s)} + C\underbrace{(u_{s-1} - u_s)}$$

RELATIVE DISPLACEMENT BETWEEN ADJACENT PLANES

ATOMIC MASS

$$\therefore \quad M \frac{d^2 u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s)$$

SEEK TRAVELING WAVE SOLUTIONS OF THE FORM:

SPACING BETWEEN ATOMIC PLANES

$$u_s = u\, e^{iska} e^{-i\omega t}$$

DISPLACEMENT AMPLITUDE

$$\therefore -\omega^2 M u e^{iska} e^{-i\omega t} = Cu\left[e^{i(s+1)ka} + e^{i(s-1)ka} - 2e^{iska}\right] e^{-i\omega t}$$

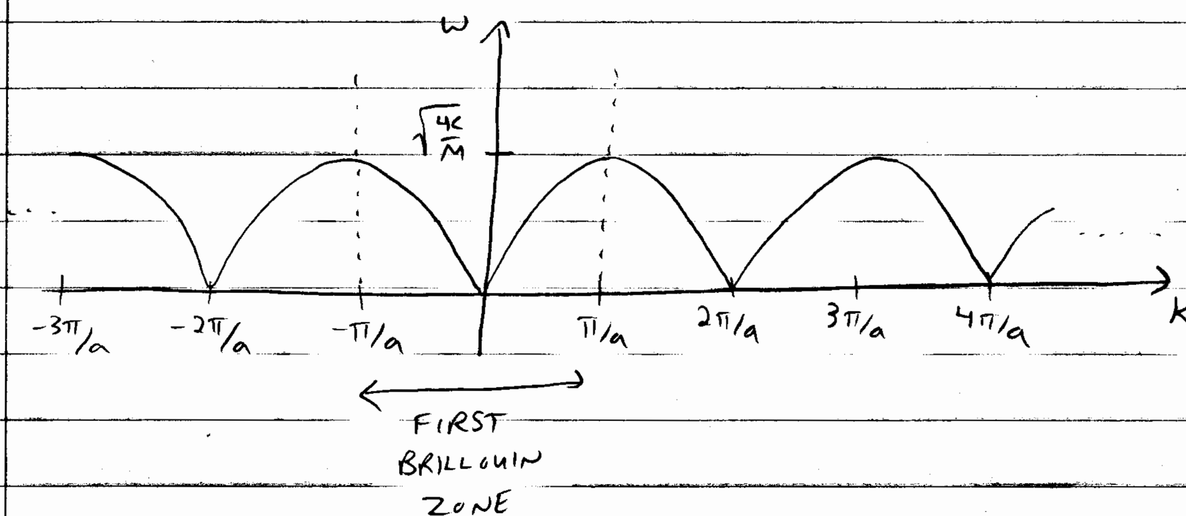
$$\Rightarrow \quad -\omega^2 M = C\left[\underbrace{e^{ika} + e^{-ika}}_{2\cos ka} - 2\right]$$

$$\therefore \quad \omega^2 = \frac{2C}{M}(1 - \cos ka)$$

Since $2\sin^2\frac{x}{2} = 1-\cos x$,

$$\omega^2 = \frac{4C}{M}\sin^2\frac{ka}{2}$$

$$\omega = \sqrt{\frac{4C}{M}}\left|\sin\frac{ka}{2}\right|$$



NOTE: (1) DISPERSION RELATION IS PERIODIC IN THE RECIPROCAL LATTICE ⇒ FIRST BRILLOUIN ZONE CONTAINS ALL UNIQUE INFORMATION ABOUT ω VERSUS k.

(2) GROUP VELOCITY: $V_g = \frac{d\omega}{dk} = \sqrt{\frac{Ca^2}{M}}\cos\frac{ka}{2}$

$\Rightarrow V_g = 0$ AT $k = \frac{\pi}{a}$

⇒ STANDING WAVE AT THE BRILLOUIN ZONE BOUNDARY

(3) $ka \ll 1 \Rightarrow \cos ka \simeq 1 - \frac{1}{2}(ka)^2$

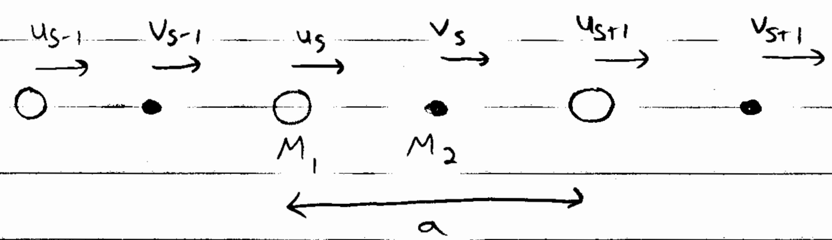
$$\Rightarrow \omega^2 = \frac{2C}{M}\left(\frac{1}{2}(ka)^2\right) = \frac{C}{M}k^2a^2$$

$$\therefore \quad \omega = \sqrt{\frac{Ca^2}{M}}\, K \Rightarrow \text{LINEAR DISPERSION RELATION}$$

$\Rightarrow$ THIS IS ANALOGOUS TO THE CONTINUUM THEORY OF ELASTIC WAVES WHERE $\omega = vk$

$\uparrow$ SOUND VELOCITY

REANALYZE THE DISPERSION RELATION FOR 2 ATOMS PER PRIMITIVE CELL (e.g., NaCl OR DIAMOND CRYSTAL STRUCTURES):



ASSUME ONE FORCE CONSTANT AND TWO DIFFERENT MASSES. (NOTE THE ANALYSIS YIELDS THE SAME QUALITATIVE FEATURES FOR TWO IDENTICAL ATOMS IN NONEQUIVALENT SITES IN THE PRIMITIVE CELL -- i.e, TWO DIFFERENT FORCE CONSTANTS AND ONE MASS)

ASSUME NEAREST NEIGHBOR INTERACTIONS DOMINATE:

$$M_1 \frac{d^2 u_s}{dt^2} = C\left(v_s + v_{s-1} - 2u_s\right)$$

$$M_2 \frac{d^2 v_s}{dt^2} = C\left(u_{s+1} + u_s - 2v_s\right)$$

SEE TRAVELING WAVE SOLUTIONS:

$$u_s = u e^{iska} e^{-i\omega t}, \quad v_s = v e^{iska} e^{-i\omega t}$$

$$\therefore \quad -\omega^2 M_1 u = Cv\left(1+e^{-ika}\right) - 2Cu$$
$$-\omega^2 M_2 v = Cu\left(e^{ika}+1\right) - 2Cv$$

THIS 2X2 SERIES OF EQUATIONS HAS A NONZERO SOLUTION ONLY IF THE DETERMINANT OF THE COEFFICIENTS OF THE UNKNOWNS (u AND v) VANISHES:

$$\begin{vmatrix} 2C - M_1\omega^2 & -C\left(1+e^{-ika}\right) \\ -C\left(1+e^{ika}\right) & 2C - M_2\omega^2 \end{vmatrix} = 0$$

$$(2C - M_1\omega^2)(2C - M_2\omega^2) - C^2\left(1+e^{-ika}\right)\left(1+e^{ika}\right) = 0$$

$$4C^2 + M_1 M_2 \omega^4 - 2C(M_1+M_2)\omega^2 - C^2\left(2 + e^{ika} + e^{-ika}\right) = 0$$

$$\therefore \quad M_1 M_2 \omega^4 - 2C(M_1+M_2)\omega^2 + 2C^2(1-\cos ka) = 0$$

USING THE QUADRATIC FORMULA, THE EXACT SOLUTION FOR ω^2 CAN BE DETERMINED.

HOWEVER, THE LIMITING BEHAVIOR IS MORE INSTRUCTIVE.

(1) $ka \ll 1 \Rightarrow \cos ka \simeq 1 - \frac{1}{2}k^2a^2$

$$M_1 M_2 \omega^4 - 2C(M_1+M_2)\omega^2 + C^2k^2a^2 = 0$$

$\Rightarrow \omega^2 \simeq 2C\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \rightarrow$ ~~CONSTANT DISPERSION RELATION~~

OR

$\omega^2 \simeq \dfrac{\frac{1}{2}C}{M_1+M_2} k^2a^2 \rightarrow$ LINEAR DISPERSION RELATION

(2) $Ka = \pm\pi$ (ZONE BOUNDARY)

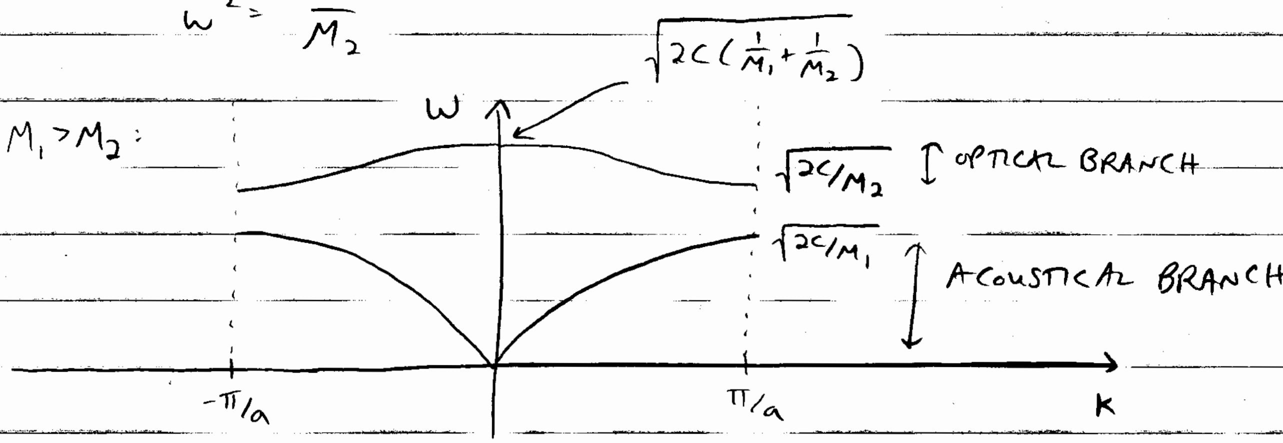
$$M_1 M_2 \omega^4 - 2C(M_1+M_2)\omega^2 + 4C^2 = 0$$

$$\Rightarrow \omega^2 = \frac{2C}{M_1}$$

OR

$$\omega^2 = \frac{2C}{M_2}$$

$M_1 > M_2$:



NOTE: AT $k=0$, $-\omega^2 M_1 u = 2Cv - 2Cu$

$\therefore$ OPTICAL BRANCH: AT $k=0$, $\omega = \sqrt{2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right)}$

$$\therefore -2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right)M_1 u = 2Cv - 2Cu$$

$$-u - \frac{M_1}{M_2}u = v - u$$

$$\therefore \frac{u}{v} = -\frac{M_2}{M_1}$$

$\Rightarrow$ ATOMS VIBRATE AGAINST EACH OTHER (180° OUT OF PHASE); IF THE ATOMS POSSESS OPPOSITE CHARGES, THIS MOTION CAN BE EXCITED BY THE ELECTRIC FIELD OF A LIGHT WAVE $\Rightarrow$ "OPTICAL BRANCH"

ACOUSTICAL BRANCH: AT $K=0$, $\omega=0$ $\Rightarrow$ $u=v$

$\Rightarrow$ ATOMS MOVE TOGETHER ANALOGOUS TO LONG WAVELENGTH ACOUSTIC VIBRATIONS $\Rightarrow$ "ACOUSTICAL BRANCH"

$\rightarrow$ $\boxed{\text{SEE FIG. 10}}$

NOTE: WAVELIKE SOLUTIONS DO NOT EXIST FOR FREQUENCIES BETWEEN $\sqrt{\frac{2C}{M_1}}$ AND $\sqrt{\frac{2C}{M_2}}$

$\Rightarrow$ FREQUENCY GAP AT THE ZONE BOUNDARY

	Name	Field
	Electron	—
	Photon	Electromagnetic wave
	Phonon	Elastic wave
	Plasmon	Collective electron wave
	Magnon	Magnetization wave
—	Polaron	Electron + elastic deformation
—	Exciton	Polarization wave

Figure 1 Important elementary excitations in solids. The origins of the concepts and the names of the excitations are discussed by C. T. Walker and G. A. Slack, Am. J. Phys. 38, 1380 (1970).

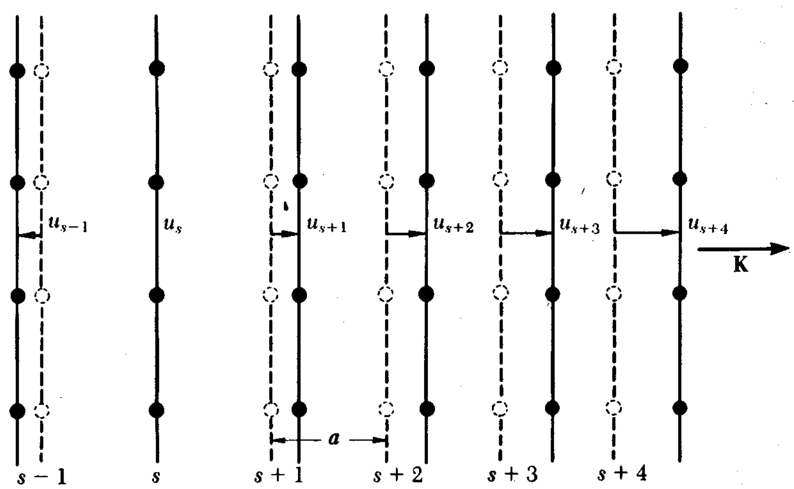


Figure 2 (Dashed lines) Planes of atoms when in equilibrium. (Solid lines) Planes of atoms when displaced as for a longitudinal wave. The coordinate u measures the displacement of the planes.

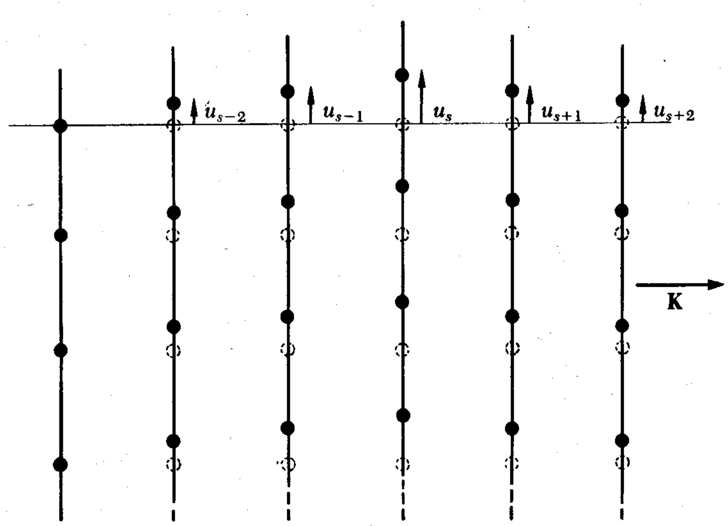


Figure 3 Planes of atoms as displaced during passage of a transverse wave.

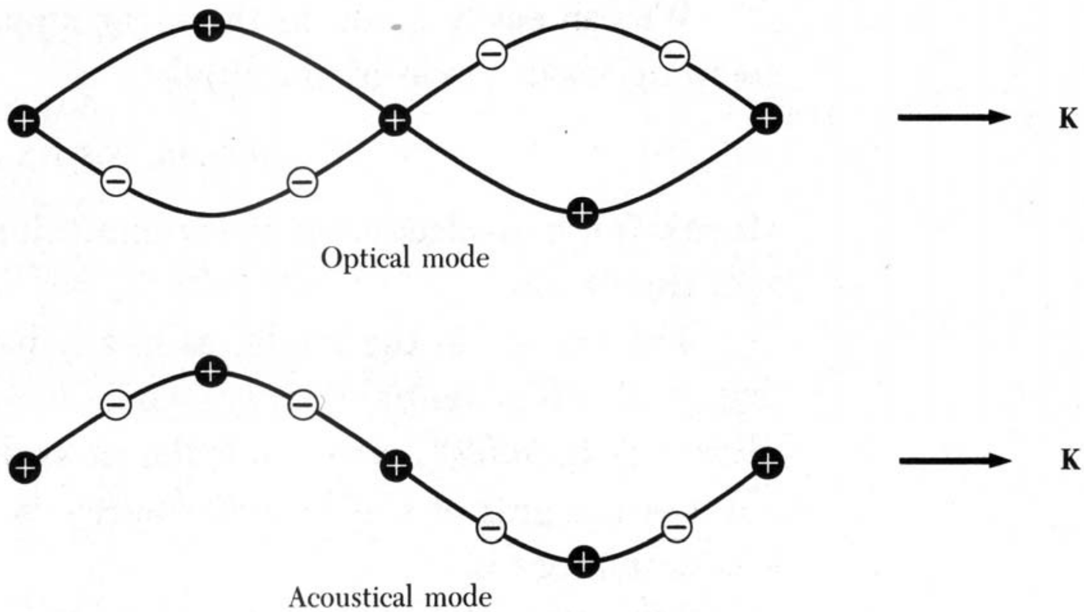


Figure 10 Transverse optical and transverse acoustical waves in a diatomic linear lattice, illustrated by the particle displacements for the two modes at the same wavelength.