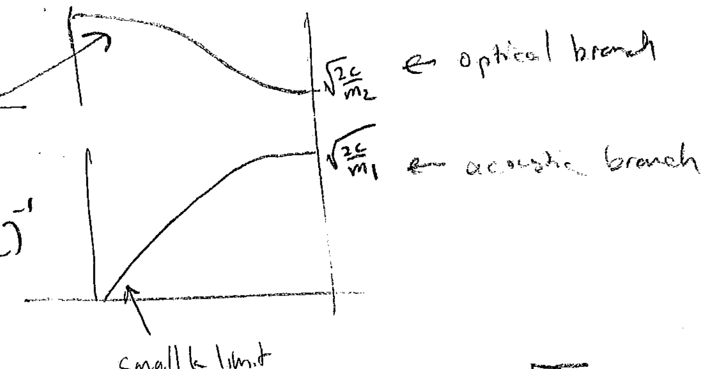
day 14 pg 1

$W = \sqrt{\frac{2c}{\mu}}$

$\mu = \left(\frac{1}{m_1}+\frac{1}{m_2}\right)^{-1}$



handout w/ Mathematica plot

$$W = a\sqrt{\frac{c}{2M_{tot}}}\,k = \left(\frac{a}{2}\right)\sqrt{\frac{c}{m_{ave}}}\,k$$

Forbidden Frequencies (bandgap)

Can skip these derivations:

upper branch

$$k=0 \rightarrow w^2 = \frac{c(m_1+m_2)+\sqrt{c^2(m_1+m_2)}}{m_1m_2}$$

$$= 2c\,\frac{(m_1+m_2)}{m_1m_2}$$

$$= \boxed{\frac{2c}{\mu}} \quad \text{with } \mu = \left(\frac{1}{m_1}+\frac{1}{m_2}\right)^{-1}$$

$k = \pi/a \quad (\cos ka = -1)$

$$\rightarrow w^2 = c\left[\frac{(m_1+m_2)+\sqrt{m_1^2+2m_1m_2+m_2^2-4m_1m_2}}{m_1m_2}\right]$$

$$= c\left[\frac{m_1+m_2+|(m_1-m_2)|}{m_1m_2}\right]$$

$$= \boxed{\frac{2c}{m_2}} \quad \text{if } m_1 > m_2$$

lower branch

$k = \pi/a \rightarrow$ same as ↑ except $-|m_1-m_2|$

so $w^2 = \boxed{\frac{2c}{m_1}}$

$k \approx 0 \quad (\cos ka \simeq 1 - \frac{1}{2}k^2a^2\ ;\ 1-\cos ka \simeq \frac{1}{2}k^2a^2$

$$\rightarrow w^2 = c\left[\frac{m_1+m_2-\sqrt{(m_1+m_2)^2 - m_1m_2k^2a^2}}{m_1m_2}\right]$$

$$= \frac{c(m_1+m_2)}{m_1m_2}\left[1 - \underbrace{\sqrt{1-\frac{m_1m_2k^2a^2}{(m_1+m_2)^2}}}_{1-\frac{1}{2}\frac{m_1m_2k^2a^2}{(m_1+m_2)^2}}\right]$$

$$= \boxed{\frac{c}{2M_{tot}}k^2a^2}$$

Optical vs Acoustic

To figure out what the difference is, plug in the two equations for ω back into the 2 equations of motion.

(Translation: what are the eigenvectors that correspond to the two eigenvalues?)

2 eqns
$$\begin{cases} \omega^2 m_1 u_s = 2C u_s - C(1+e^{-ika}) v_s \\ \omega^2 m_2 v_s = -C(1+e^{ika}) u_s + 2C v_s \end{cases}$$

For simplicity, I'll just consider where $k=0$

lower branch: $\omega = 0 \rightarrow$
$$\left.\begin{array}{l} 0 = 2C u_s - 2C v_s \\ 0 = -2C u_s + 2C v_s \end{array}\right\}$$
same result $\underline{u_s = v_s}$

2 atoms are in phase! $\overrightarrow{u}$ $\overrightarrow{v}$

upper branch: $\omega = \sqrt{\frac{2C}{\mu}} \rightarrow$ $2C \frac{m_1}{\mu} u_s = 2C u_s - 2C v_s$

$\frac{m_1}{\mu} = \frac{m_1}{m_1 m_2}(m_1+m_2) = \frac{m_1}{m_2} + 1$

$\cancel{2C u_s} + 2C \frac{m_1}{m_2} u_s = \cancel{2C u_s} - 2C v_s$

$\underline{v_s = -\frac{m_1}{m_2} u_s}$

2 atoms are out of phase!

$\overrightarrow{u}$ $\overleftarrow{v}$

if ionic, get oscillating dipole moment which gives off radiation. That's why "optical". And also can be excited by external radiation

Review: 1D 1 atom/cell $\rightarrow$ 1 acoustic
2 atoms $\rightarrow$ 1 acoustic + 1 optical branch
guess? 3 $\rightarrow$ 1 + 2
N $\rightarrow$ 1 + N-1

(last chapter) 3D 1 atom/cell $\rightarrow$ 3 acoustic (1 long 2 transv) {guess 3D 2 atoms? $\rightarrow$ 3 acoustic + 3 optical}

HW 2D " $\rightarrow$ 2 acoustic (1 long, 1 transv.)

Phonon Dispersion

Si

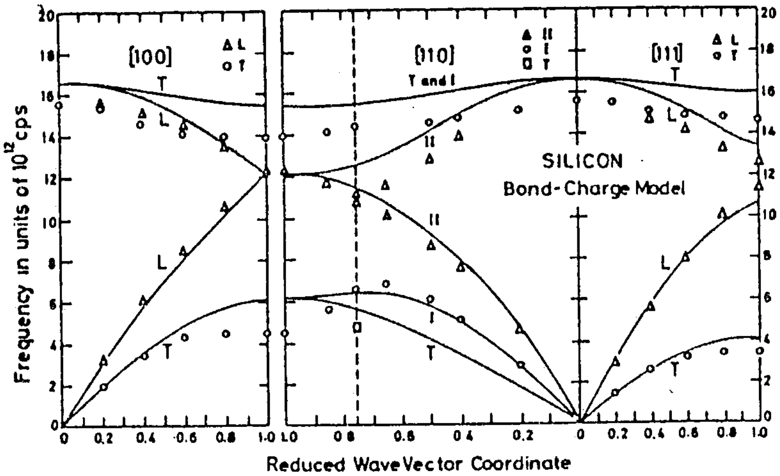
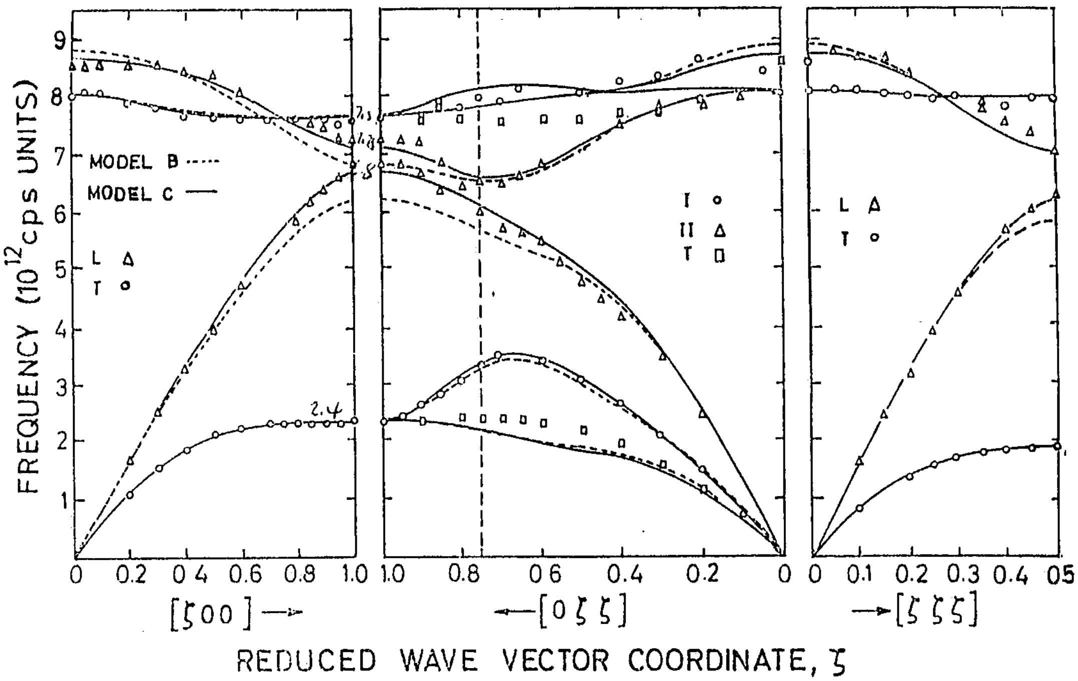


FIGURE 16. Comparison of Martin's bond charge model calculation with the experimental phonon frequencies in Si. (From Martin, R. M., *Phys. Rev.*, 186, 871, 1969. With permission.)

GaAs



SnTe

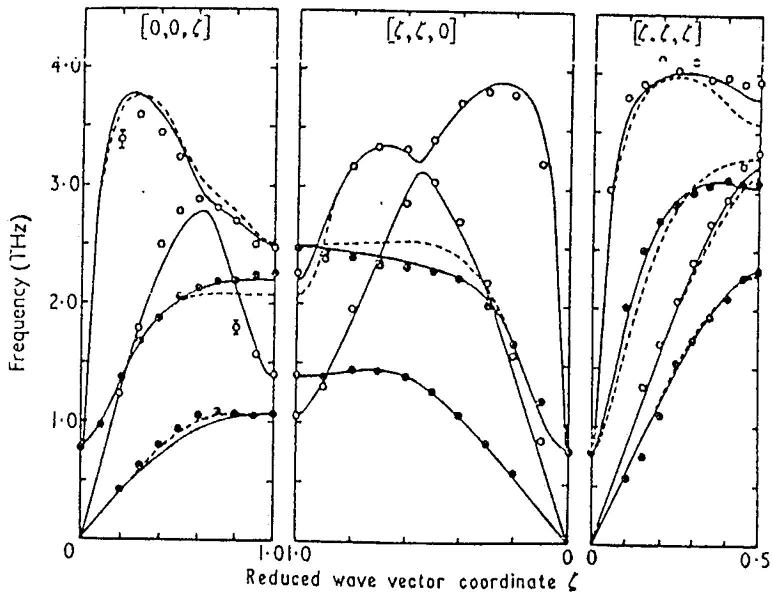


FIGURE 15. Dispersion curves for SnTe along the principal symmetry directions. The solid curve represents a 14-parameter shell model fit (modified to include free carrier screening effects). (From Cowley, E. R., *J. Phys. C. Solid State Phys.*, 2, 1916, 1969. With permission.)

guess at 2D 2 atoms/cell? → 2 acoustic + 2 optical
LA, TA LO, TO

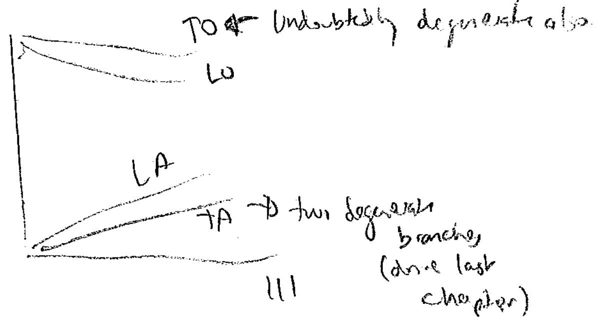
what does these look like?

~~Side note: effect of finite length → coupled eqn's → N×N matrix → N frequencies important~~

~~Side note before DM on next page!~~

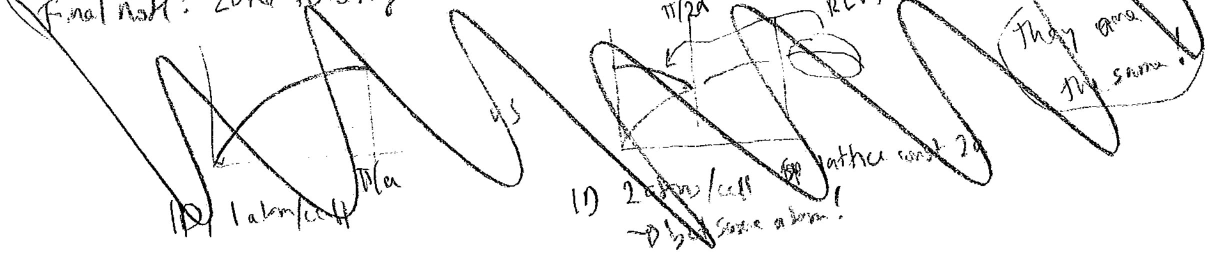
See Fig 8a pg 96

3D, 2 atoms/cell Germanium

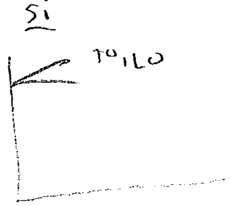


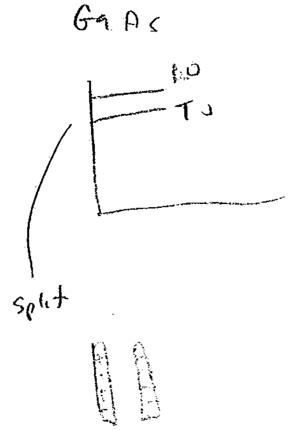
handout w/ Si, GaAs, SnTe → why GaAs optical split at k=0? see next page

~~Final note: zone folding~~



Physical insight:

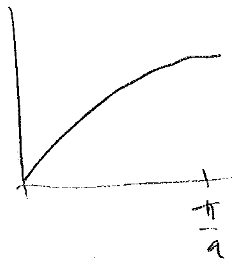




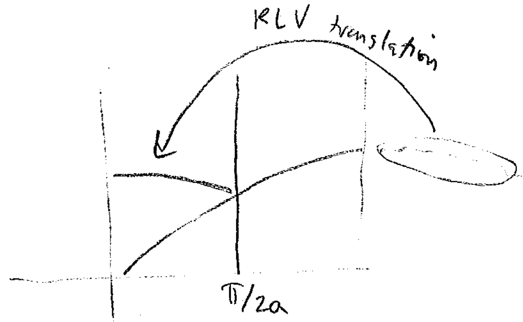
For LO, additional contribution to energy from Coulomb

Final Note

"Zone Folding"



1D, 1 atom/cell



1D, 2 atoms/cell lattice constant 2a
but same atom

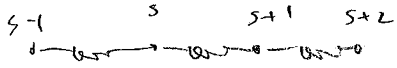
They must be the same!

The RLV translation makes it look like the curve has been "folded"

Day 14 pg 6

HW Problem 6 Set up

Finite length chain. Back to 1 mass only



before $$m\frac{d^2u_s}{dt^2} = C\left[u_{s+1} - 2u_s + u_{s-1}\right]$$

plane waves $u \sim e^{i(kx - \omega t)}$

$$m(-\omega^2 u_s) = C\left(+e^{ika}u_s + 2u_s + e^{-ika}u_s\right)$$

If finite, then not perfect plane waves! Can't use $e^{ika}u_s$ trick
(Still look for harmonic dependence in time, though)

For eg $s = 32$

$$\frac{m}{C}(+\omega^2)u_{32} = \cancel{C}\left(-u_{31} + 2u_{32} - u_{33}\right).$$

For $s = 33$ $$\frac{m}{C}(+\omega^2)u_{33} = -u_{32} + 2u_{33} - u_{34}$$

$s = 34$ $$\frac{m}{C}(+\omega^2)u_{34} = -u_{33} + 2u_{34} - u_{35}$$

Let $\frac{m\omega^2}{C} = \lambda$

$$\lambda\begin{pmatrix} u_1 \\ \vdots \\ \vdots \\ u_{100}\end{pmatrix} = \begin{pmatrix} \ddots & & & & & \\ -1 & 2 & 1 & & & \\ & -1 & 2 & 1 & & \\ & & -1 & 2 & 1 & \\ & & & -1 & 2 & 1 \\ & & & & & \ddots \end{pmatrix}\begin{pmatrix} u_1 \\ \vdots \\ \vdots \\ u_{100}\end{pmatrix}$$

λ = eigenvalues of $\mathfrak{D}$

→ There will be 100 different frequencies

→ each freq corresponds to a different oscillation

general true principle: one frequency per atom (or maybe 3, if in 3D).
But 10^{23} atoms!
Frequency spacing = miniscule

But what about first row and last row?

Need to make assumptions about bndy conds.

Examples: "wrap around" (periodic)

"fixed" $u_1 = 0$

etc.

what do the matrix rows look like?