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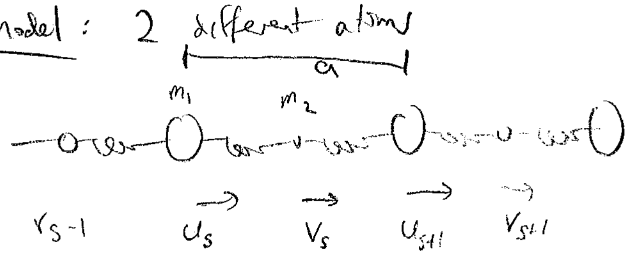
<u>Next model</u>: 2 different atoms



$$m_1 \frac{d^2 u_s}{dt^2} = C\left[(v_s - u_s) - (u_s - v_{s-1})\right]$$

$\frac{d^2 u_s}{dt^2} \to -w^2 u_s$, $\quad v_{s-1} \to v_s e^{-ika}$

$$\boxed{+w^2 m_1 u_s = +2C u_s + -C(1+e^{-ika})v_s}$$

Similarly $\quad \boxed{+w^2 m_2 v_s = -C(1+e^{+ika})u_s + 2C v_s}$ $\quad$ coupled equations!

typo in Eqn 21 pg 98!

Solve w/ Matrix:

$$0 = \begin{pmatrix} 2c - w^2 m_1 & -c(1+e^{-ika}) \\ -c(1+e^{+ika}) & 2C - w^2 m_2 \end{pmatrix}\begin{pmatrix} u_s \\ v_s \end{pmatrix}$$

$\to$ det = 0 for nontrivial soln

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$$(2c - w^2 m_1)(2c - w^2 m_2) - c^2 \underbrace{(1+e^{+ika})(1+e^{-ika})}_{1 + e^{ika} + e^{-ika} + 1} = 0$$

$= 2 + 2\cos ka$

$= 2c^2(1+\cos ka)$

$$m_1 m_2 w^4 - 2c(m_1 + m_2)w^2 + c^2\left(4 - 2(1+\cos ka)\right) = 0$$

$4 - 2 - 2\cos ka$

$2c^2(1-\cos ka) = 0$

quadratic eqn in w^2

$$w^2 = \frac{+\cancel{2}c(m_1+m_2) \pm \sqrt{\cancel{4}c^2(m_1+m_2)^2 - \cancel{4}(m_1 m_2)(2c^2(1-\cos ka))}}{\cancel{2}m_1 m_2}$$

$w = \sqrt{}$ $\to$ All that

plotted w/ mathematica for

$m_1 = 3$, $m_2 = 1$, $C = 1$, $a = 1$

$\boxed{\text{Hand out to Class}}$

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```
In[16]:= m1 = 3; m2 = 1; c = 1; a = 1;

In[17]:= w1[k_] = Sqrt[2 c (m1 + m2) + Sqrt[4 c^2 (m1 + m2)^2 - 4 (m1 m2) (2 c^2 (1 - Cos[k a]))]]
```

Out[17]= $\sqrt{8+\sqrt{64-24\,(1-\text{Cos}[k])}}$

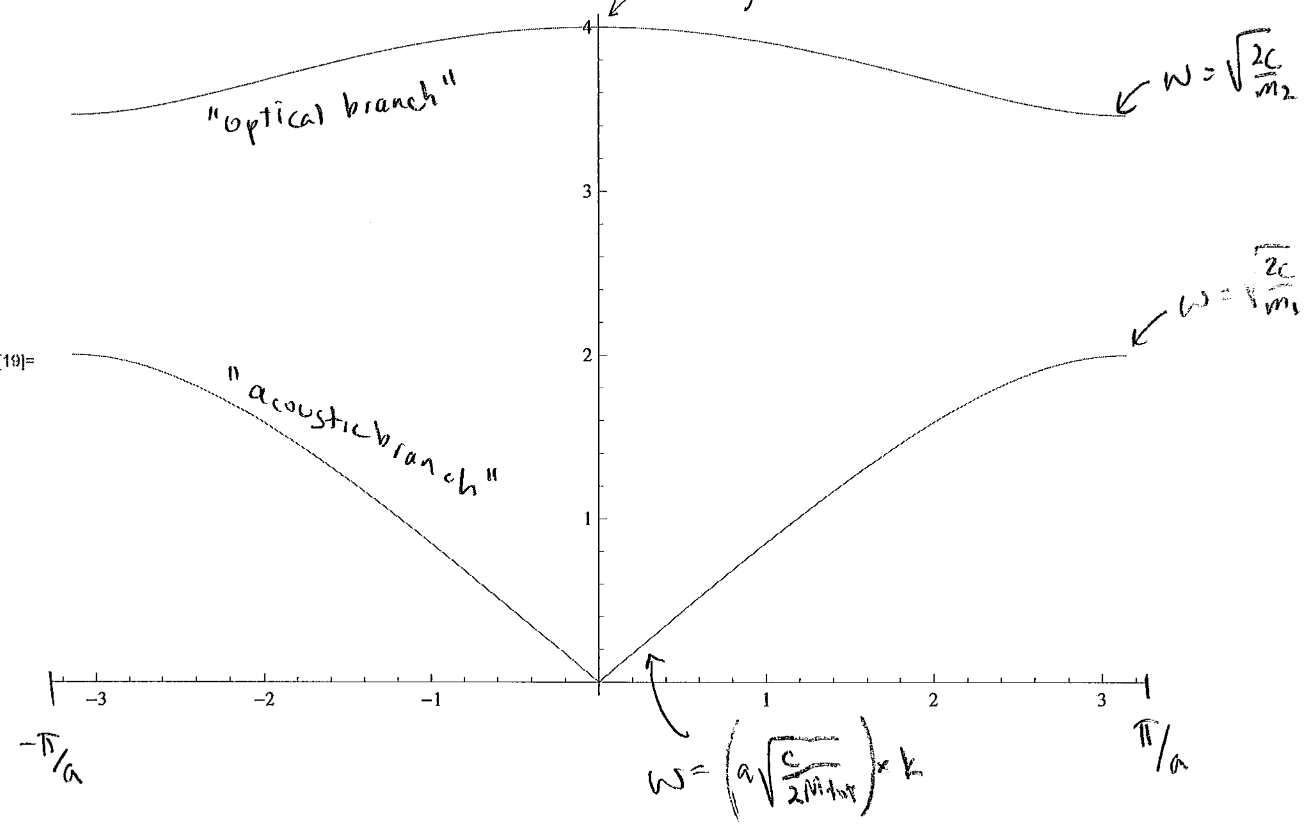
```
In[18]:= w2[k_] = Sqrt[2 c (m1 + m2) - Sqrt[4 c^2 (m1 + m2)^2 - 4 (m1 m2) (2 c^2 (1 - Cos[k a]))]]
```

Out[18]= $\sqrt{8-\sqrt{64-24\,(1-\text{Cos}[k])}}$

```
In[19]:= Plot[{w1[k], w2[k]}, {k, -Pi, Pi}]
```

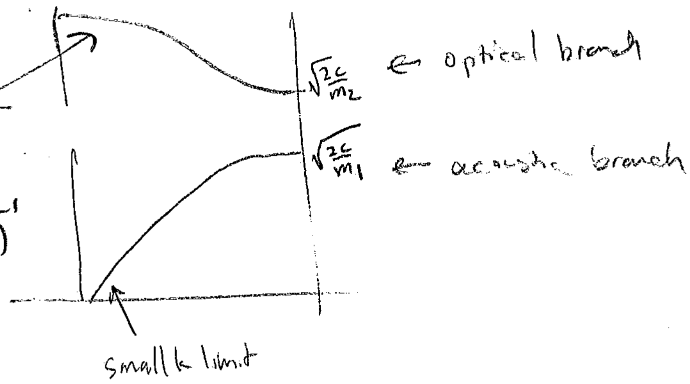
$\omega = \sqrt{\frac{2c}{\mu}}$; $\mu = \left(\frac{1}{m_1} + \frac{1}{m_2}\right)^{-1}$

Out[19]=



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

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



$$W = a\sqrt{\frac{c}{2}} \times k$$

Can skip these derivations:

upper branch

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

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

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

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

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

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

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

lower branch

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

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

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

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

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

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

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

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

<u>lower branch</u>: $\omega = 0 \rightarrow$
$$\left.\begin{aligned} 0 &= 2Cu_s - 2Cv_s \\ 0 &= -2Cu_s + 2Cv_s \end{aligned}\right\} \text{ same result } \boxed{u_s = v_s}$$

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

<u>upper branch</u>: $\omega = \sqrt{\frac{2C}{\mu}} \rightarrow 2C\frac{m_1}{\mu} u_s = 2Cu_s - 2Cv_s$

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

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

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

2 atoms are out of phase!

$\vec{u}\ \overleftarrow{v}$

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

Review: 1D 1 atom/cell → 1 acoustic
2 atoms/cell → 1 acoustic + 1 optical branch
guess? $\begin{cases} 3 \\ N \end{cases}$ → 1 + 2 ; 1 + N−1

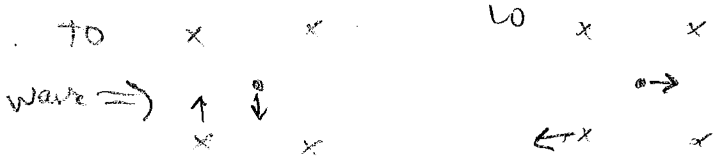
(last chapter) 3D 1 atom/cell → 3 acoustic (1 long 2 transv)

guess: 3D 2 atoms? → 3 acoustic + 3 optical?

HW 2D " → 2 acoustic (1 long, 1 transv.)

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

what does these look like?



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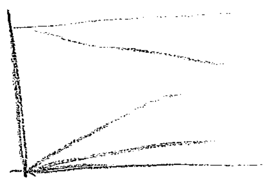
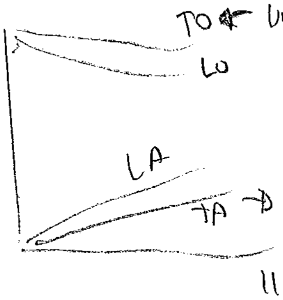


See Fig 8a pg 96

3D, 2 atoms/cell Germanium

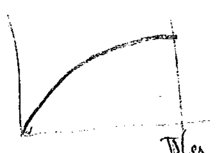


TO ← Undoubtedly degenerate also

TA → two degenerate branches (drive last chapter)

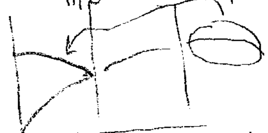
$ { handout w/ Si, GaAs, SnTe → why GaAs optical split at $k=0$?, see next page

Final note: Zone folding



1D, 1 atom/cell

vs



RLV translation, looks like folded

They are the same!

1D 2 atoms/cell lattice const 2a
→ but same atom!