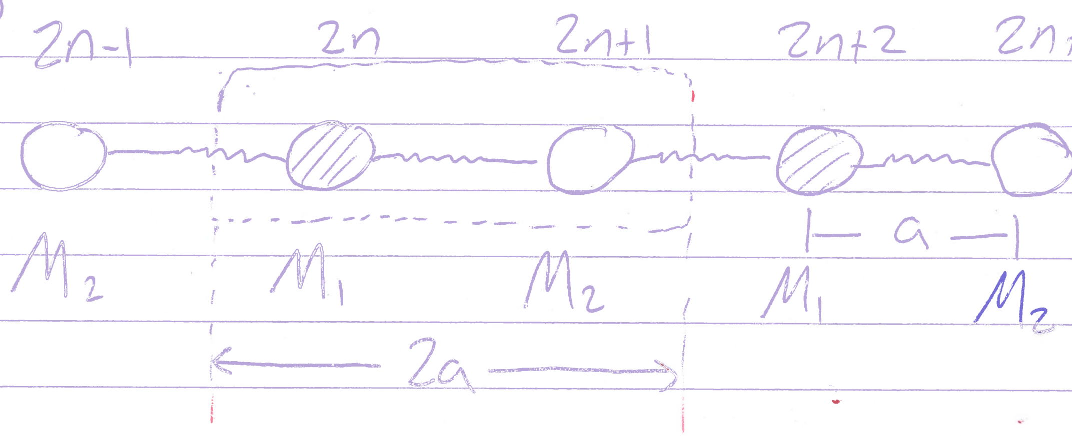
Mon. Oct. 08

- last time we began our discussion of a simple 1D model of a diatomic solid with alternating atoms of mass M_1 + M_2, e.g. NaCl

- image of model:



- unit cell of length '2a'

- Similar to the monatomic case, we set up our diff. eqs.

$$M_2 \ddot{u}_{2n+1} = -\alpha\left[2u_{2n+1} - u_{2n} - u_{2n+2}\right]$$

$$M_1 \ddot{u}_{2n+2} = -\alpha\left[2u_{2n+2} - u_{2n+1} - u_{2n+3}\right]$$

- we once again guess the solution as the wave equation

$\longrightarrow$

- let's use matrix form:

$$\begin{bmatrix} u_{2n+1} \\ u_{2n+2} \end{bmatrix} = \begin{bmatrix} A_1 e^{iX_{2n+1}} \\ A_2 e^{iX_{2n+2}} \end{bmatrix} e^{-i\omega t}$$

- plug these equations back into the diff. eqs. + obtain

$$\begin{bmatrix} 2\alpha - M_1\omega^2 & -2\alpha\cos(ka) \\ -2\alpha\cos(ka) & 2\alpha - M_2\omega^2 \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = 0$$

- from linear algebra, we know the determinant must vanish for a non-trivial solution

$$\begin{vmatrix} 2\alpha - M_1\omega^2 & -2\alpha\cos(ka) \\ -2\alpha\cos(ka) & 2\alpha - M_2\omega^2 \end{vmatrix} = 0$$

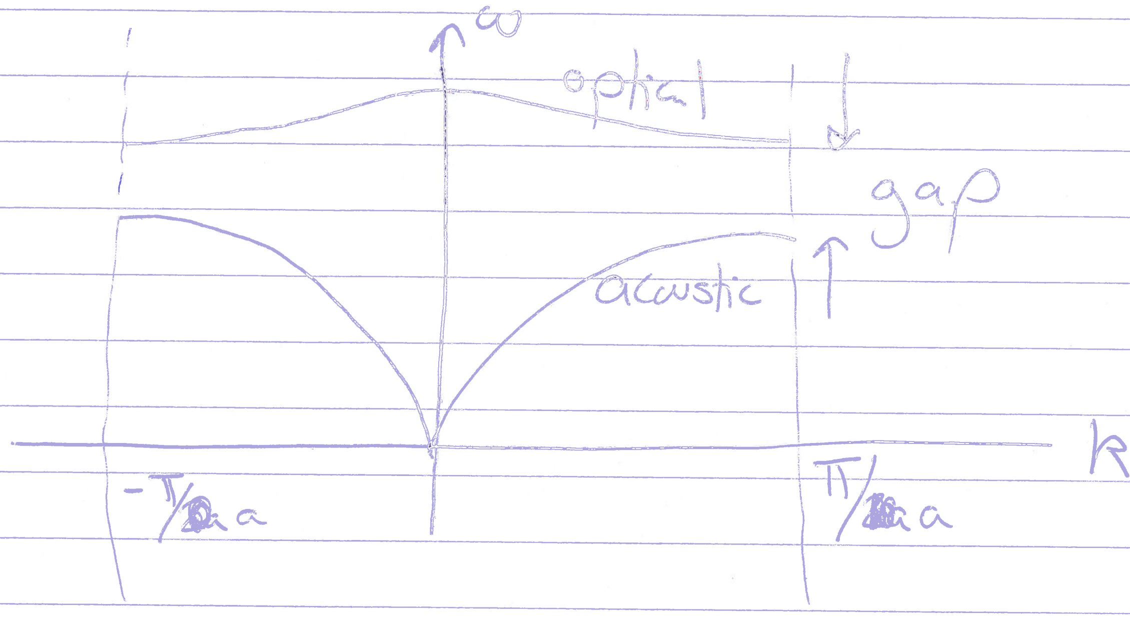
(homogeneous linear eqs.)

- Solving for ω^2 we get

$$\omega^2 = \alpha\left(\frac{1}{M_1} + \frac{1}{M_2}\right) \pm \alpha\sqrt{\left(\frac{1}{M_1} + \frac{1}{M_2}\right)^2 - \frac{4\sin^2(ka)}{M_1 M_2}}$$

- the (−) minus sign gives the "acoustic" branch + (+) sign gives "optical" branch

- check and see what happens when $M_1 = M_2$
- plot of dispersion relation



- the gap associtates the band of forbidden modes to the two branches
- the solid acts as a filter
- for the acoustic branch, $\omega_{max} = \sqrt{\frac{2\alpha}{M_2}}$ (boundary)
- for the optical branch, $\omega_{max} = \sqrt{\frac{2\alpha}{M_1}}$ (boundary)

for the case of $M_1 < M_2$

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- for the optical branch, the max. frequency occurs at $k=0$ ($\delta \to \infty$)

and take the value of

$$\omega = \left[2\alpha \left(\frac{1}{M_1} + \frac{1}{M_2} \right) \right]^{1/2}$$

- note that the optical branch does not change much (approx. constant)

- around $k=0$, we see that the entirety of the lattice shifts back and forth for acoustic branch

- for the optical branch, atoms vibrate approximately 180° out of phase //

*See slides

- recall that for the 1D monatomic solid, we obtained 1 mode per atom (or per unit cell)

- for the diatomic solid, we have 2 atoms per cell – 2N atoms, N cells

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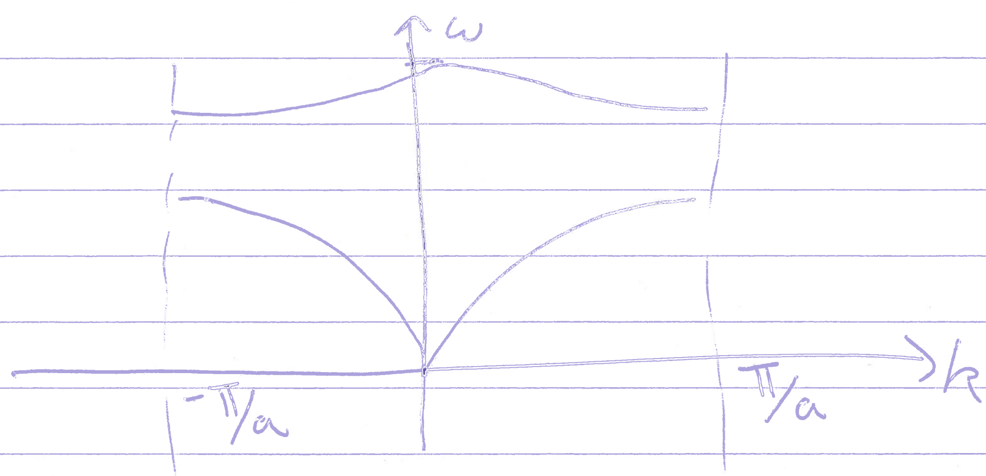
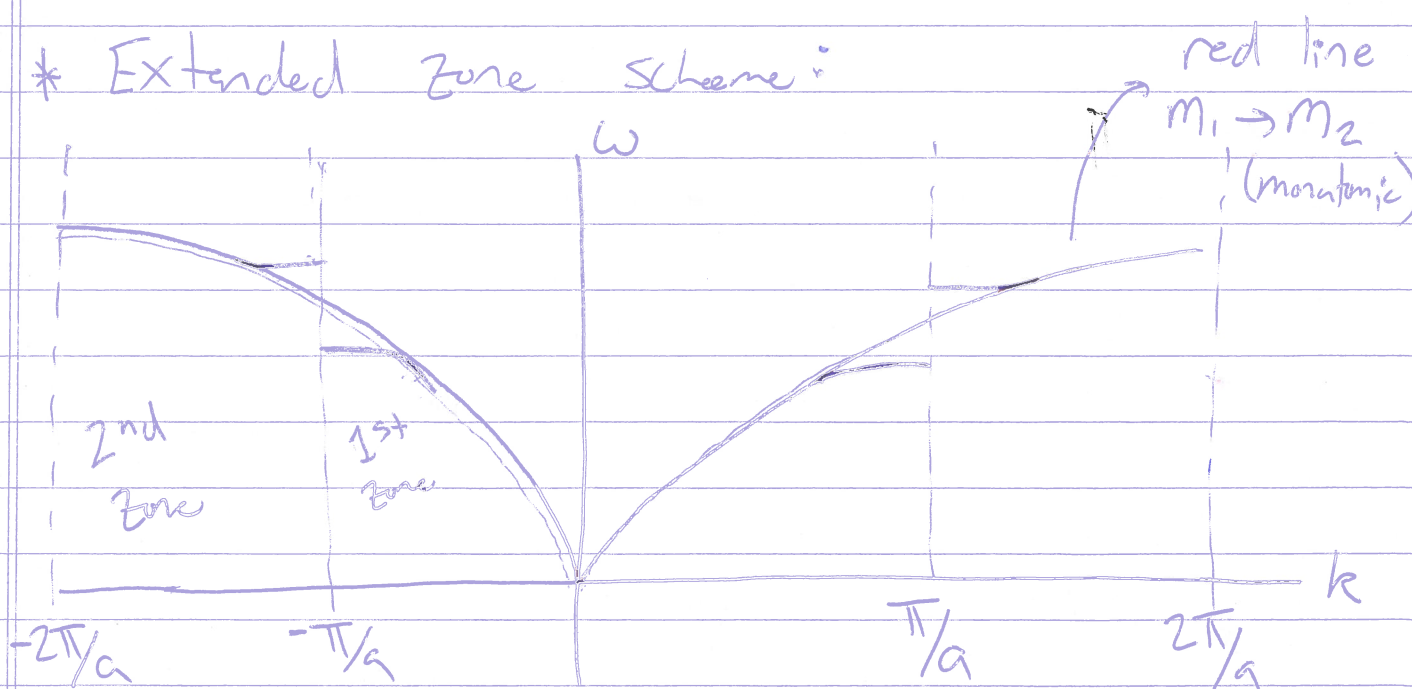
- the two atoms have different mass + different degrees of freedom, so we have $2N$ total modes

- in other words there are two modes for each wave number k + thus we have two branches



* Extended zone scheme:



- note for $m_1 = m_2$, cell $\to a \to a/2$
- thus mass diff responsible for freq. gap.