Mon. Oct. 01

* Now that we have a better picture of bonds between atoms in solids, we are in a position to develop more accurate models of their properties (thermal, optical etc.)

- The Debye model showed us that the coupled behavior of oscillations alters heat capacity

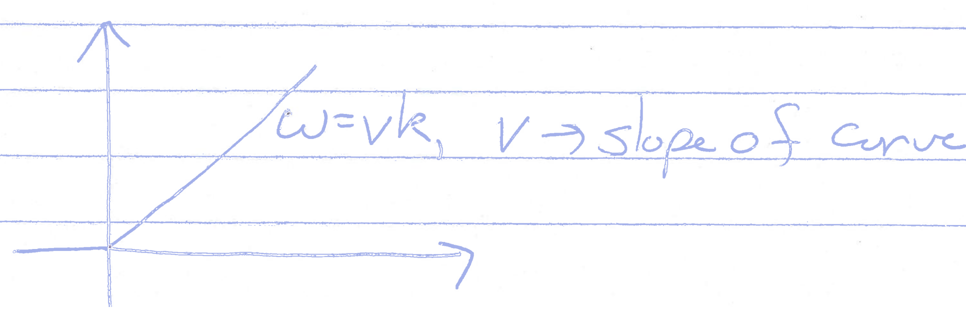
- That model assumed the following dispersion relation

$$\omega = vk$$

Where v = speed of sound. This result is directly analogous to

$$\omega = ck$$

for electromagnetic waves in vacuum where c = speed of light



- Recall that $\omega, k \to \infty$ are not physical solutions, and we discovered there is an upper limit to $\omega = \omega_D$, determining the Debye frequency

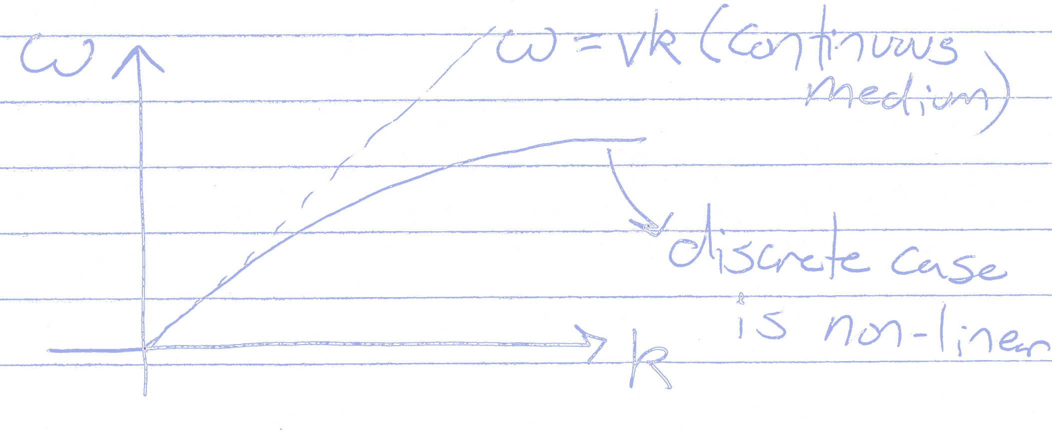
- given by $\omega_D = V_s (6\pi^2 n)^{1/3}$, V_s for "sound"

in other words, upper limit is determined by the density $n = N/Vol$ (atomic density)

- the material parameter is V_s (sound speed)

- although the Debye model gives us a correct answer, the discrete nature of a solid was not built into the model

- What does the discrete nature do to the dispersion relation?



- For the continuum, $V = \omega k$, and we see that the speed can be obtained by

$$\frac{d\omega}{dk} = V \text{ (constant)}$$

- For the discrete case, we have the same relation, but $V \neq$ constant

- we see that for low values of k, or long wavelengths, the two curves overlap

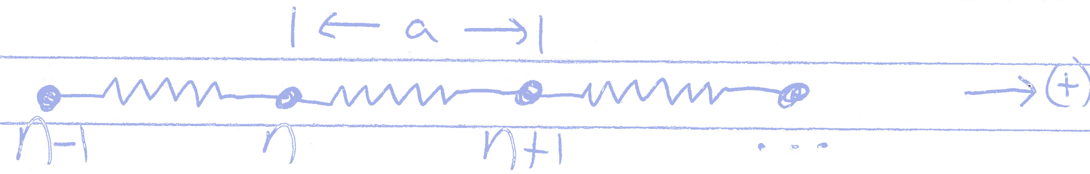
- in other words, when $\lambda >> a$, where 'a' is the spacing between atoms, the wave "sees" a continuum

- when $\lambda \sim a$, the wave "sees" a diffraction grating ($k \sim 2\pi/a$)

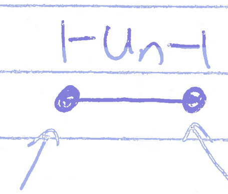
- the wave slows around this value due to increased scattering

→

- the modelling is straightforward, and we will start with a 1D model



- each spring has constant α
- separation between atoms is 'a'
- $u_n \equiv$ displacement for atom away from equilibrium



equilib.

displaced by (+) distance (to left would give (−) displacement)

- We solve for the equation of motion for atom 'n' which generalizes to any atom in the solid
- Newton's 2nd law

$$F = ma$$

→

Newton's law takes the form

$$F = M\ddot{u}_n$$

where M is the mass of the atom & F is the force on atom 'n'.

- We assume that the force is applied only by the two adjacent atoms @ $(n+1)$ & $(n-1)$
- and also assume the harmonic approx. i.e. Hooke's law $F \propto u$
- the force on atom n by atom $(n+1)$:

$$F_{n,n+1} = \alpha\left(u_{n+1} - u_n\right)$$

- while the force on atom n by atom $(n-1)$:

$$F_{n,n-1} = \alpha\left(u_{n-1} - u_n\right)$$

- combining the forces on each:

$$M\ddot{u}_n = \alpha\left(u_{n+1} - u_n\right) + \alpha\left(u_{n-1} - u_n\right)$$

$$= -\alpha\left[2u_n - u_{n+1} - u_{n-1}\right] \quad (1)$$

- We make an educated guess:

$$u_n = A e^{i(kx_n - \omega t)} \qquad (2)$$

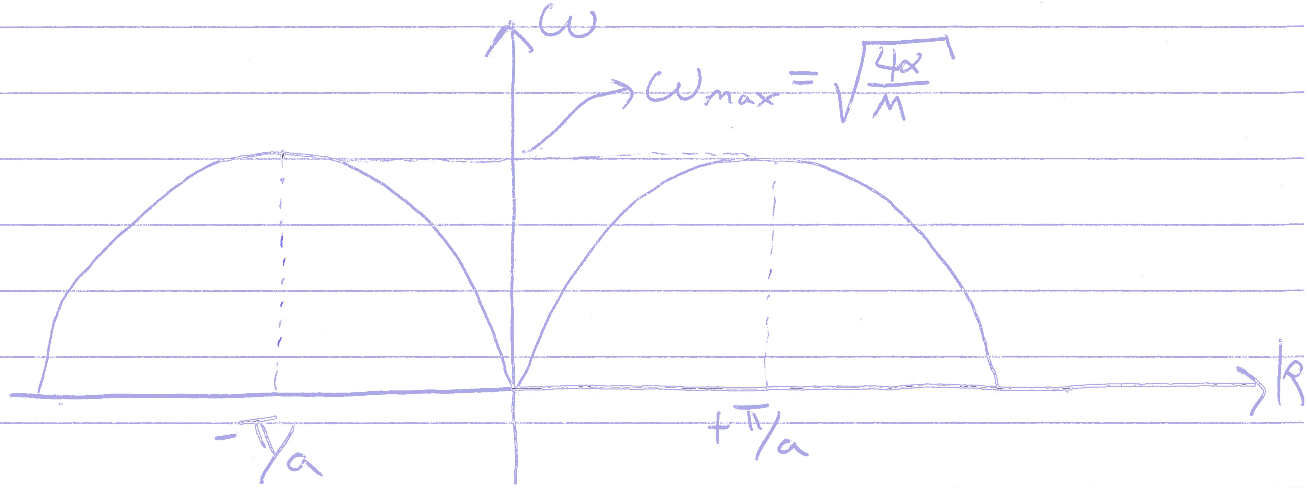
where $x_n = na$, the equilibrium position of atom 'n'

- this is a traveling wave with atoms oscillating at frequency ω
- plug solution [Eq. (2)] into wave equation [Eq. (1)]
- a HW assignment will be to show

$$\omega = \sqrt{\frac{4\alpha}{M}} \left| \sin\left(\frac{ka}{2}\right) \right| \qquad (3)$$

- this is the dispersion relation for discrete atoms (closer to reality than continuum case)
- Compare with continuum case $\omega = vk$

- plot of discrete case:



- maximum of $\sin\left[\frac{ka}{2}\right]$ occurs at

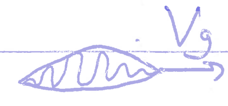
$$\frac{ka}{2} = \frac{\pm\pi}{2} \quad \text{or} \quad k = \pm\pi/a$$

- let's unpack this result a little

(1) only frequencies $0 < \omega \leq \omega_m$ can propogate through crystal

(2) for small k, $\sin(ka/2) \simeq ka/2$ (linear) & matches with continuum

(3) speed of the wave: group velocity $V_g = \frac{d\omega}{dk}$ is more accurate for high frequencies



- when $k = \pi/a$, we find $\frac{\partial \omega}{\partial k} = 0$

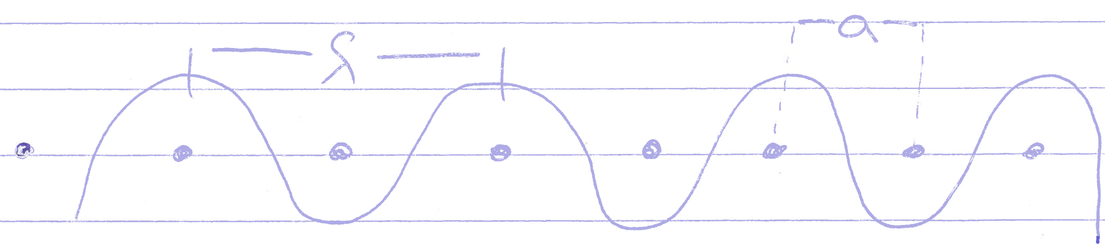
or speed of group velocity $\to 0$

- What is the physical interpretation?

$$k = \frac{2\pi}{\lambda} \quad \& \quad \lambda = \frac{2\pi}{k}$$

- for $\pi/a \Rightarrow \lambda = \frac{2\pi}{\pi/a} = 2a$

- when the wavelength is twice the spacing of atoms, we get a standing wave



- caused by interaction of lattice with high frequency mode