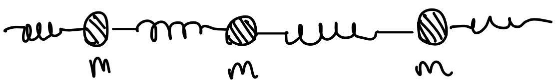
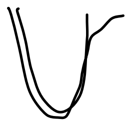
Last time:

<u>1D - Solid (monatomic)</u>

Phys 425
Lecture 12





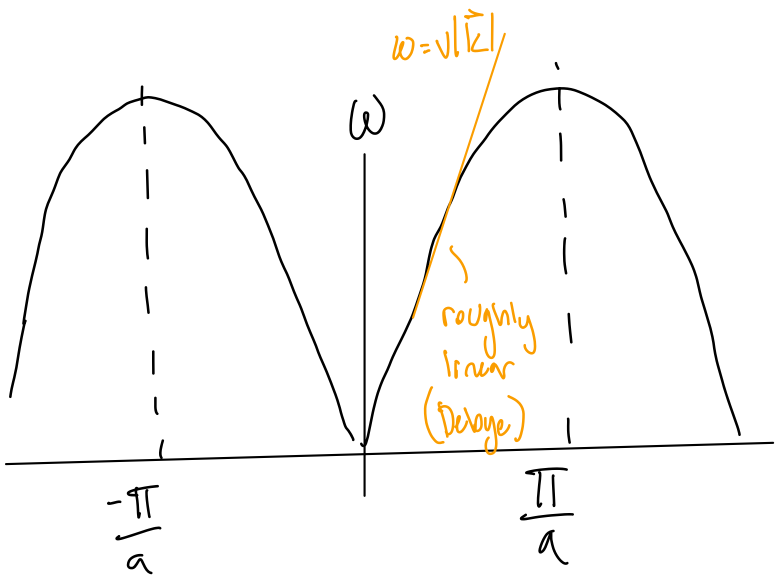
$$m\frac{d^2}{dt^2}u_n = \gamma\left[u_{n+1} + u_{n-1} - 2u_n\right]$$

assume wave solutions:

$$u_n = Ae^{i(kna - \omega t)}$$

$$\Rightarrow \quad m\omega^2 = 2\gamma\left[1 - \cos(ka)\right] = 4\gamma\sin^2\left(\frac{k}{a}\right)$$

This is a periodic dispersion



- Normal Modes: (solutions)

  are identical in every periodic copy beyond

  $$-\frac{\pi}{a} < k < \frac{\pi}{a}$$

Low k limit $\left(k \ll \frac{\pi}{a},\ \lambda \gg a\right)$

$\hookrightarrow$ atoms oscillate in phase

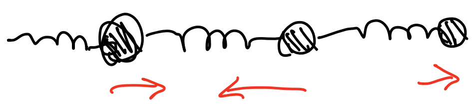
Debye model

$$\omega \approx \sqrt{\frac{\gamma}{m}}\,ka = vk \quad \sim \text{where } \boxed{v = \sqrt{\frac{\gamma}{m}}\cdot a}$$

For high K, $\left(K = \frac{\pi}{a}\right)$ – highest k we can have

$(\lambda = 2a)$ – lowest λ we can have

neighboring atoms will oscillate out of phase



2 velocities:

$V_{group} = \frac{\partial \omega}{\partial K}$

speed of the wave packet

$V =$ slope, at $\frac{\pi}{a}$, $V = 0$

$V_{phase} = \frac{\omega}{K}$

speed of individual particles in a medium

For large λ, low K, the phase velocity will be equal to the group (velocity)

For small λ, high K, $\underline{V_{group}} \neq V_{phase}$

↳ 0 @ boundaries

We call this region the first Brillouin zone.

The reciprocal lattice's Wigner-Seitz cell (smallest G cell)

If we can figure out the physics in the first Brillouin zone, we know it everywhere else. (1st BZ)

Aside: (BZ integrals)

$$\langle E \rangle = \sum_{|\vec{k}|} \hbar\omega(\vec{k}) \left(\frac{1}{e^{\beta\hbar\omega(k)}-1} + \frac{1}{2} \right)$$

Now we know, we can focus only on those k-values on $-\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$

$$\sum_{k} \rightarrow \sum' \rightarrow \frac{\overbrace{Na}^{\text{L of 1D solid}}}{2\pi} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}}$$

narrowing down to just BZ, not $-\infty \leftrightarrow \infty$

So: $$\langle E \rangle = \frac{Na}{2\pi} \int \hbar\omega(k) \left(\frac{1}{e^{\beta\hbar\omega(k)}-1} + \frac{1}{2} \right) dk$$

$$C = \frac{d\langle E \rangle}{dt}$$

Count # of modes: $$\frac{Na}{2\pi} \int_{-\frac{\pi}{a}}^{\pi/a} dk = N = \int g(\omega)\, d\omega$$

$$\Rightarrow \quad g(\omega) = \frac{d}{d\omega}\left(\frac{Na}{2\pi}\int_{-\pi/a}^{\pi/a} dk\right)$$

$$= \underbrace{2}_{\text{from symmetry of } \omega(k)} \frac{Na}{2\pi}\left|\frac{dk}{d\omega}\right|$$

unit conversion

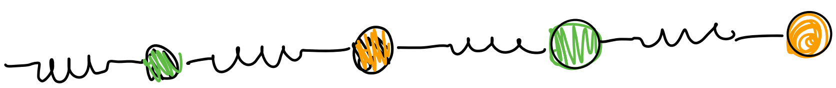
Phonon Density of States

$$\boxed{g(\omega) = D\left(\frac{L}{2\pi}\right)^{D}\frac{dk}{d\omega}\times 2}$$

D= dimension

Diatomic Model

$\dot{x} = \frac{dx}{dt}$



We can calculate $C = \frac{d\langle E\rangle}{dt}$

$$m\ddot{u}_n = \gamma_1(v_{n-1} - u_n) + \gamma_2(v_n - u_n)$$

displacement of the n^{th} one

$$m\ddot{v}_n = \gamma_1(u_{n+1} - v_n) + \gamma_2(u_n - v_n)$$

Assume wave solutions: you end up with some dispersion relation that looks like this:

For $m_1 = m_2 = m_n$

$$\omega_{\pm} = \sqrt{\frac{\gamma_1+\gamma_2}{2} \pm \frac{1}{m}(\gamma_1+\gamma_2)^2 - 4\gamma_1\gamma_2\sin^2\left(\frac{ka}{2}\right)}$$

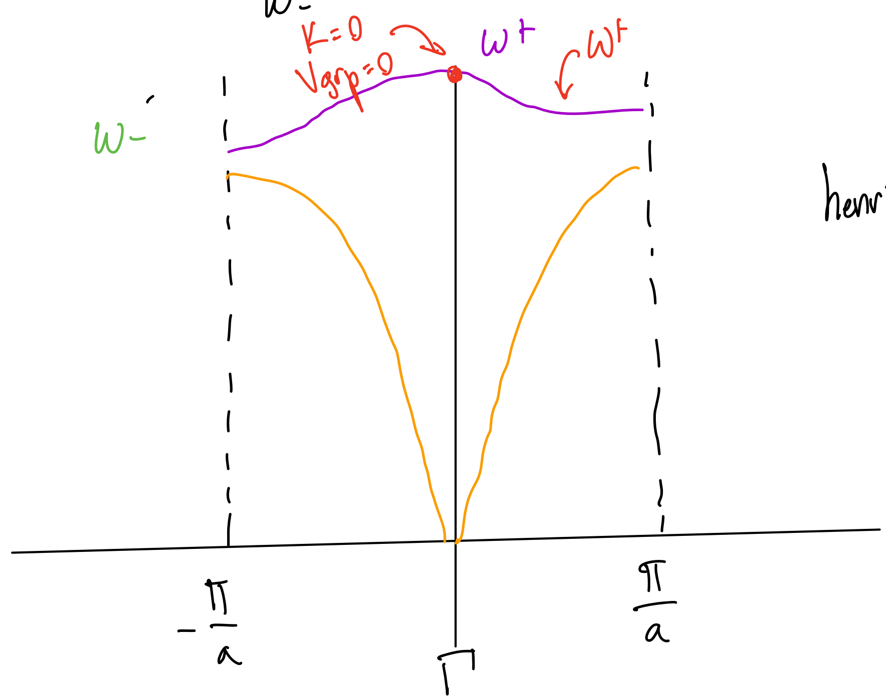
Now, we have 2 modes per k - state

every k state = 2 possible ω solns. (branches)

↳ total 2N

$\omega_+ \longrightarrow$ optical mode

$\omega_- \longrightarrow$ acoustic mode



henrique miranda phonon github

<u>Acoustic mode:</u> lower k linear limit where $\omega(k)$ looks like $v_{sound} \cdot \vec{k}$.

<u>Optical mode:</u>

modes are allowed to couple with EM waves

↓

Phonons

$$\omega_{optical} \approx ck$$

if k is anything besides close to zero, ω grows unbounded

(Need k close to zero)