day 13 pg. 1

phase vs group velocity

Fresh metal: For now all identical items

$s-2 \quad s-1 \quad s \quad s+1 \quad s+2$

$\vdash a \dashv$ $\to u_s$ = displacement of atom s

(or could be planes of atoms)

"Harmonic Approximation"

Newton 2: $\sum_i F_s = m a_s$

$$\underbrace{\underset{\text{spring constant}}{C}(u_{s+1}-u_s)}_{\text{force from right-hand spring}} - \underbrace{C(u_s - u_{s-1})}_{\text{left hand}} = m \frac{d^2 u_s}{dt^2}$$

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

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

Going from $u_s$ to $u_{s+1} \to \Delta x = a \to$ phase factor of $e^{ika}$

$$\underline{u_{s+1} = e^{ika} u_s}$$

Plug in to eqn:

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

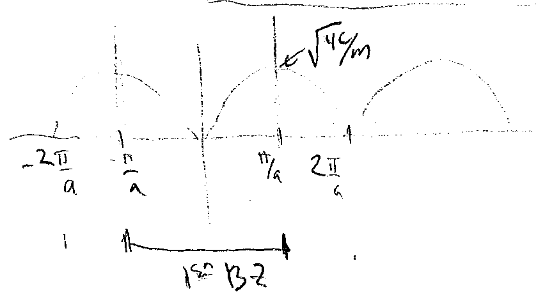
$$e^{ika} + e^{-ika} = 2\cos ka$$

$$m(+\omega^2) = 2C\left[1 - \cos ka\right]$$

$$\boxed{\omega = \left[\frac{2C}{m}\left(1-\cos ka\right)\right]^{1/2}}$$

dispersion relation

$$\boxed{\omega = \sqrt{\frac{4C}{m}}\left|\sin\frac{ka}{2}\right|}$$ because $\sin^2\frac{x}{2} = \frac{1}{2} - \frac{1}{2}\cos x$

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initial slope?

$$\frac{d\omega}{dk} = \sqrt{\frac{4c}{m}}\ \cos\frac{ka}{2}\left(\frac{a}{2}\right)\Bigg|_{\text{small } k}$$

$$v = \frac{a}{2}\sqrt{\frac{4c}{m}} = a\sqrt{\frac{c}{m}}$$

informative? Starts out linear, at least.

Periodicity? repeats over $\frac{ka}{2} = n\pi$ ($|\sin x|$ has period $\pi$, not $2\pi$)

$$k = \frac{2\pi}{a} n$$

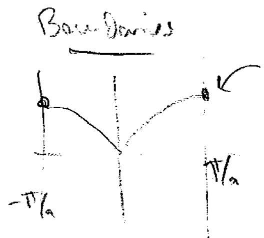
So $k' = k + \frac{2\pi n}{a}$ will have same value as $k$

What's special about $\frac{2\pi}{a}, \frac{4\pi}{a}, \frac{6\pi}{a}$ etc?

Reciprocal Lattice Vectors!

Summary: by subtracting an appropriate RLV from $k$, we always obtain an equivalent wavevector in 1st BZ

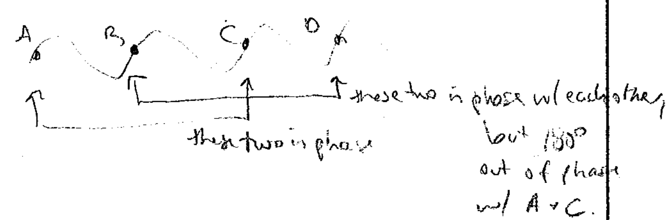
Boundaries




flat slope $\to v = 0$

Does that make sense?

Yes: $k = \pm\frac{\pi}{a} \to \frac{2\pi}{\lambda} = \frac{\pi}{a} \to \lambda = 2a$



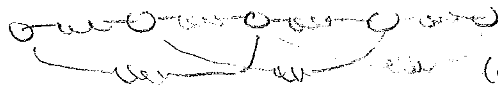

↑ ↓ ↑ ↓

later time

↓ ↑ ↓ ↑

This is a standing wave! Of course no velocity.

Possible extension: forces between next nearest neighbors



(diff spring constants)

or between 3rd nearest neighbors --- or 4th, etc.

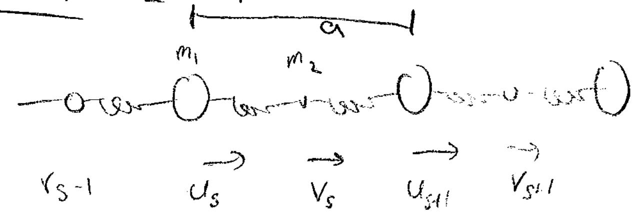
result: $C_p$ = spring constant between $p^{th}$ nearest neighbors

$$\omega = \left[\frac{2}{M}\sum_{p=1}^{\infty} C_p\left(1-\cos pka\right)\right]^{1/2}$$

book shows inverse relationship is

$$C_p = -\frac{Ma}{2\pi}\int_{-\pi/a}^{\pi/a} \omega^2 \cos pka \, dk$$

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




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

$$\boxed{+\omega^2 m_1 u_s = +2C\, u_s - C\left(1+e^{-ika}\right) v_s}$$

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

typo in Eqn 21 pg 98!

Solve w/ Matrix:
$$0 = \begin{pmatrix} 2C - \omega^2 m_1 & -C\left(1+e^{-ika}\right) \\ -C\left(1+e^{+ika}\right) & 2C - \omega^2 m_2 \end{pmatrix} \begin{pmatrix} u_s \\ v_s \end{pmatrix}$$

$\to$ det = 0 for nontrivial soln

$$\left(2C - \omega^2 m_1\right)\left(2C - \omega^2 m_2\right) - C^2 \underbrace{\left(1+e^{+ika}\right)\left(1+e^{-ika}\right)}_{1+e^{ika}+e^{-ika}+1} = 0$$

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

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

quadratic eqn in $\omega^2$

$$\omega^2 = \frac{+\cancel{2}C(m_1+m_2) \pm \sqrt{\cancel{4}C^2(m_1+m_2)^2 - \cancel{4}(m_1 m_2)\left(2C^2(1-\cos ka)\right)}}{\cancel{2}m_1 m_2}$$

$\omega = \sqrt{\phantom{x}}$ All that

plot w/ mathematica for

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

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

Linear chain of balls + springs, 2 different atoms

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]= $\sqrt{8 + \sqrt{64 - 24\ (1 - \mathrm{Cos}[k])}}$

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]= $\sqrt{8 - \sqrt{64 - 24\ (1 - \mathrm{Cos}[k])}}$

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]=