CHAPTER 22

22.1

a) $$U^{harm} = \sum_n \sum_{m>0} \frac{1}{2} K_m \left[u(na) - u[(n+m)a] \right]^2$$

The equation of motion is

$$M\ddot{u}(na) = \frac{-\partial U^{harm}}{\partial u(na)}$$

where M is the mass. And at any instant, the ion whose equilibrium position is 'na' is diplaced from equilibrium by an amount $u(na)$.

$$M\ddot{u}(na) = \sum_{m>0} -K_m \left[2u(na) - u[(n-m)a] - u[(n+m)a] \right]$$

and we seek solutions to the above equation of the form,

$$u(na,t) \propto e^{i(kna - \omega t)}$$

where $k = \frac{2\pi}{a}\frac{n}{N}$, n is an integer.

a equilibrium length of the 'spring'

now we take the values lying between $-\pi/a$ and π/a.

$$-M\omega^2 e^{i(kna-\omega t)} = \sum_{m>0} -K_m \left[2 - e^{-ikma} - e^{ikma} \right] e^{i(kna-\omega t)}$$

$$= \sum_{m>0} -2K_m (1 - \cos mka)\, e^{i(kna-\omega t)}$$

$$\Rightarrow \quad \omega(k) = 2\sqrt{\sum_{m>0} \frac{K_m \left(\sin^2 \frac{mka}{2}\right)}{M}}$$

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b) When k is very small, ie at long wavelength limit, we can approximate $\sin \frac{nka}{2}$.

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} \cdots\cdots$$

Only the first term is valid since k is very small.

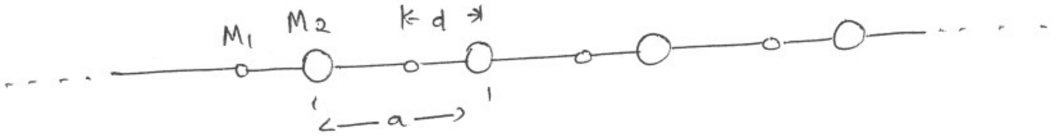
$$\omega = 2\sqrt{\sum_{n>0} \frac{K_n}{M} \frac{n^2 k^2 a^2}{4}}$$

$$= a\left(\sum_{n>0} \frac{K_n}{M} n^2\right) |k|$$

c)

Q2.2

a) Consider a diatomic linear chain of atoms of mass M_1 and M_2.



assuming only the nearest neighbours interact, the harmonic potential energy is,

$$U^{harm} = \frac{K}{2}\sum_n [u_1(na) - u_2(na)]^2 + \frac{K}{2}\sum_n [u_2(na) - u_1([n+1]a)]^2$$

'u_1' and 'u_2' are the displacemets of atoms.

The equations of motion are,

$$M_1\ddot{u}_1(na) = -\frac{\partial U^{harm}}{\partial u_1(na)} = -K[u_1(na) - u_2(na)] - K[u_1(na) - u_2([n-1]a)] \quad -①$$

$$M_2\ddot{u}_2(na) = -\frac{\partial U^{harm}}{\partial u_2(na)} = -K[u_2(na) - u_1(na) - u_2(na) + u_1([n+1]a)] \quad -②$$

we seek solutions of type,

$$u_1(na) = \epsilon_1 e^{i(kna - \omega t)}$$

$$u_2(na) = \epsilon_2 e^{i(kna - \omega t)}$$

where ϵ_1 and ϵ_2 are constants.

with Born-von karman boundary condition,

$$e^{ikNa} = 1$$

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

substituting

$$\left.\begin{aligned}(M_1\omega^2 - 2K)\varepsilon_1 + K(1+e^{-ika})\varepsilon_2 &= 0\\ K(1+e^{ika})\varepsilon_1 + (M_2\omega^2 - 2K)\varepsilon_2 &= 0\end{aligned}\right\}.$$

The above pair of equations have solution provided the determinant of coefficients is zero.

$$(M_1\omega^2 - 2K)(M_2\omega^2 - 2K) = K^2(1+e^{-ika})(1+e^{ika})$$

$$M_1M_2\omega^4 - (2KM_1 + 2KM_2)\omega^2 + 4K^2 = 2K^2(1+\cos ka)$$

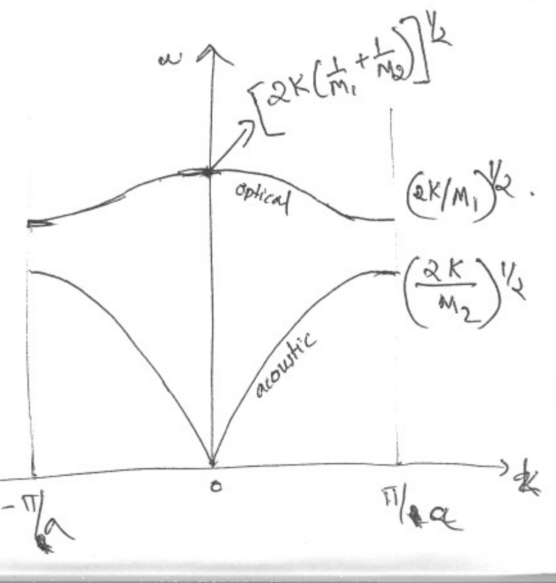
$$\omega^4 - \frac{2K(M_1+M_2)}{M_1M_2}\omega^2 + \frac{4K^2}{M_1M_2} - \frac{2K^2(1+\cos ka)}{M_1M_2} = 0.$$

$$\omega^2 = \frac{K(M_1+M_2)}{M_1M_2} \pm \frac{1}{2}\sqrt{\frac{4K^2(M_1+M_2)^2}{(M_1M_2)^2} - 4\,\frac{2K^2(1-\cos ka)}{M_1M_2}}$$

$$\omega^2 = \frac{K}{M_1M_2}\left[(M_1+M_2) \pm \sqrt{(M_1+M_2)^2 - 2M_1M_2(1-\cos ka)}\right]$$

$$\Rightarrow \quad \omega^2 = \frac{K}{M_1M_2}\left[(M_1+M_2) \pm \sqrt{M_1^2 + M_2^2 + 2M_1M_2\cos ka}\right]$$

$M_1 < M_2$.



22.2

b).

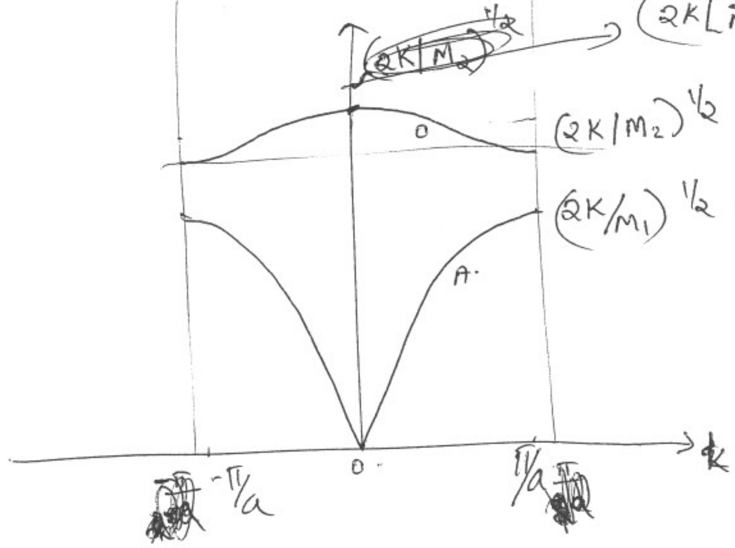
when $M_1 \gg M_2$,

$M_1 + M_2 \approx M_1$

$$\omega^2 = \frac{K}{M_1 M_2}\left(M_1 \pm \sqrt{M_1^2 + 2M_1M_2\cos ka}\right)$$

$\left(2K\left[\frac{1}{M_1}+\frac{1}{M_2}\right]\right)^{1/2} \approx \left(\frac{2K}{M_2}\right)^{1/2}$.

and the



c) $M_1 \approx M_2 = M$

$$\omega^2 = \frac{K}{M^2}\left(2M \pm \sqrt{2M^2 + 2M^2\cos ka}\right)$$

$$\omega^2 = \frac{K}{M}\left(2 \pm \sqrt{2}\cdot\sqrt{1+\cos ka}\right).$$

$$= \frac{K}{M}\left(2 \pm \sqrt{2}\sqrt{2\cos^2\frac{ka}{2}}\right)$$

$$\omega^2 = \frac{2K}{M}\left(1 \pm \cos\frac{ka}{2}\right)$$

$$\omega^2 = \frac{4K}{M}\sin^2\frac{ka}{4} \quad \text{or} \quad \frac{4K}{M}\cos^2\frac{ka}{4}$$

$\Rightarrow$

$$\left.\begin{aligned} \omega_1 &= \sqrt{\frac{K}{M}}\, 2\sin\frac{ka}{4} \\ \omega_2 &= \sqrt{\frac{K}{M}}\, 2\cos\frac{ka}{4} \end{aligned}\right\}$$

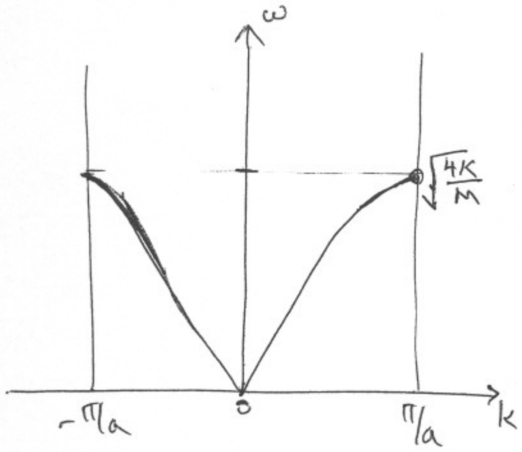
for monoatomic linear chain, there is only one frequency

$$\omega_{mono} = 2\sqrt{\frac{K}{M}}\,\sin\frac{ka}{2}.$$

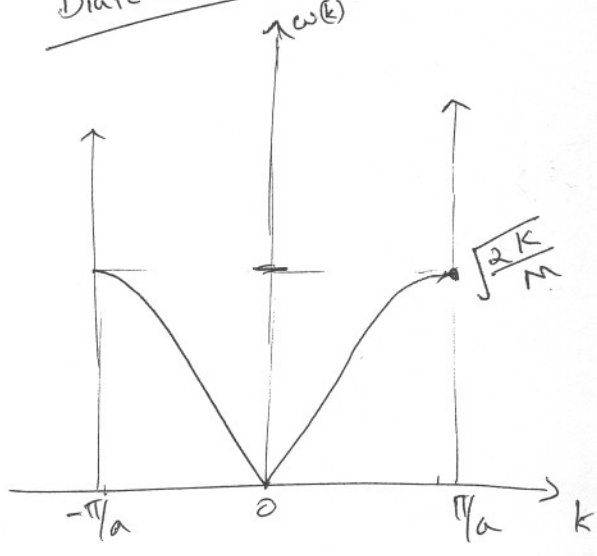
$$v_g^{mono}\ \frac{\partial \omega_{mono}}{\partial k} = 2\sqrt{\frac{K}{M}}\,\frac{a}{2}\cos\frac{ka}{2}. = \underline{\underline{a\sqrt{\frac{K}{M}}\,\cos\frac{ka}{2}.}}$$

$$v_g. = \frac{\partial \omega_1}{\partial k} = 2.\sqrt{\frac{K}{M}}\,\frac{a}{4}\cos\frac{ka}{4}. = \frac{a}{2}\sqrt{\frac{K}{M}}\cos\frac{ka}{4}$$

<u>monoatomic</u>



<u>Diatomic $M_1 = M_2 = M$</u>



Monoatomic : at $\omega = \sqrt{\frac{4K}{M}}$, the group velocity vanishes.

Diatomic, ($M_1 = M_2$) : at $\omega = \sqrt{\frac{2K}{M}}$ the group velocity vanishes.

22·3

a)

(~~22.37~~)

equation 22·37 is

$$\omega^2 = \frac{K+G}{M} \pm \frac{1}{M}\sqrt{K^2+G^2+2KG\cos ka}$$

$$K = K_0 + \Delta$$

$$G = K_0 - \Delta \qquad , \Delta << K_0 .$$

when $\Delta = 0$,

$$\Rightarrow K = G = K_0$$

now the latice constant $a \to a/2$

$$\omega^2 = \frac{2K_0}{M} \pm \frac{1}{M}\sqrt{2K_0^2 + 2K_0^2\cos\frac{ka}{2}}$$

$$= 2\frac{K_0}{M} \pm \frac{\sqrt{2}K_0}{M}\sqrt{2}\cos\frac{ka}{4}$$

$$= \frac{2K_0}{M}\left(1 \pm \cos\frac{ka}{4}\right)$$

$$\omega^2 = \frac{4K_0}{M}\sin^2\frac{ka}{8} \quad \text{or} \quad \frac{4K_0}{M}\cos^2\frac{ka}{8} .$$

$$\left.\begin{aligned} \omega_1 &= 2\sqrt{\frac{K_0}{M}}\sin\frac{ka}{8} \\ \omega_2 &= 2\sqrt{\frac{K_0}{M}}\cos\frac{ka}{8} \end{aligned}\right\} .$$

The amplitude ratio,

?

$$\frac{\varepsilon_2}{\varepsilon_1} = \mp \frac{K_0(1+e^{ika})}{K_0|(1+e^{ika}|}$$

b) $\Delta \neq 0$

$$\omega^2 = \frac{2K_0}{M} \pm \frac{1}{M}\sqrt{(K_0+\Delta)^2 + (K_0-\Delta)^2 + 2(K_0+\Delta)(K_0-\Delta)\cos ka}$$

$$\omega^2 = \frac{2K_0}{M} \pm \frac{1}{M}\left[K_0^2 + \cancel{2K_0\Delta} + \Delta^2 + K_0^2 - \cancel{2K_0\Delta} + \Delta^2 + (2K_0^2 + 2\Delta^2)\cos ka\right]^{1/2}$$

$$\omega^2 = \frac{2K_0}{M} \pm \frac{1}{M}\left[2K_0^2 + 2\Delta^2 + 2(K_0^2+\Delta^2)\cos ka\right]^{1/2}$$

$$\omega^2 = \frac{2K_0}{M} \pm \frac{1}{M}\left[4K_0^2\cos^2\frac{ka}{2} + 4\Delta^2\cos^2\frac{ka}{2}\right]^{1/2}$$

$$\omega^2 = \frac{2K_0}{M} \pm \frac{1}{M}\, 2\cos\frac{ka}{2}\left[K_0^2+\Delta^2\right]^{1/2}.$$

$$= \cancel{\frac{2K_0 \pm 2K_0}{M}} \quad \cancel{\frac{2K_0}{M}\left[1 \pm \cos\frac{ka}{2}\right]}$$

$$\omega^2 = \frac{2K_0}{M}\left[1 \pm \left(1+\left(\frac{\Delta}{K_0}\right)^2\right)^{1/2}\cos\frac{ka}{2}\right]$$

~~It shows that the disper~~