HW #4 Solutions

Chp. 3 No 10: Transverse wave velocity

$$u = u_0\, e^{ik(x+y+z)/\sqrt{3}}\, e^{-i\omega t}$$

[111]

transverse : $u + v + w = 0$ e.g. $+u - v + 0 \cdot w = 0$ $\vec{u} = \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$

$$\rho \frac{\partial^2 u}{\partial t^2} = C_{11} \frac{\partial^2 u}{\partial x^2} + C_{44}\left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) + (C_{12} + C_{44})\left(\underbrace{\frac{\partial^2 v}{\partial x \partial y}}_{= -\frac{\partial^2 u}{\partial x \partial y}} + \underbrace{\frac{\partial^2 w}{\partial x \partial z}}_{= 0}\right)$$

$$= -\frac{k^2}{3}(C_{11} + 2C_{44} - C_{12} - C_{44})\, u$$

$$= -\frac{k^2}{3}(C_{11} - C_{12} + C_{44})\, u$$

$$\rho \frac{\partial^2 u}{\partial t^2} = -\rho \omega^2 u = -\frac{k^2}{3}(C_{11} - C_{12} + C_{44})\, u \Rightarrow \rho \omega^2 = \frac{k^2}{3}(C_{11} - C_{12} + C_{44})$$

$$V_s = \frac{\omega}{k}$$

$$\Rightarrow \quad V_s^2 = \frac{(C_{11} - C_{12} + C_{44})}{3\rho}$$

$$\Rightarrow \quad V_s = \left[\frac{1}{3}(C_{11} - C_{12} + C_{44})/\rho\right]^{\frac{1}{2}}$$

Chp. 3 No 13

$$\vec{R}(\vec{r}) = [u_0\hat{x} + v_0\hat{y} + w_0\hat{z}]\exp[i(\vec{K}\vec{r} - \omega t)]$$

ⓐ

$$\rho\frac{\partial^2 u}{\partial t^2} = -\omega^2\rho u = \{-K_x^2 C_{11} - C_{44}(K_y^2 + K_z^2)\}u - (C_{12}+C_{44})(K_xK_y v + K_xK_z w)$$

$$\rho\frac{\partial^2 v}{\partial t^2} = -\omega^2\rho v = \{-K_y^2 C_{11} - C_{44}(K_x^2 + K_z^2)\}v - (C_{12}+C_{44})(K_xK_y u + K_yK_z w)$$

$$\rho\frac{\partial^2 w}{\partial t^2} = -\omega^2\rho w = \{-K_z^2 C_{11} - C_{44}(K_x^2 + K_y^2)\}w - (C_{12}+C_{44})(K_xK_z u + K_yK_z v)$$

$$\vec{u} = \begin{pmatrix} u \\ v \\ w \end{pmatrix}$$

$$\Rightarrow \quad \omega^2\rho\,\vec{u} = \underbrace{\begin{pmatrix} K_x^2C_{11} + C_{44}(K_y^2+K_z^2) & (C_{12}+C_{44})(K_xK_y) & (C_{12}+C_{44})K_xK_z \\ (C_{12}+C_{44})K_xK_y & K_y^2C_{11} + C_{44}(K_x^2+K_z^2) & (C_{12}+C_{44})K_yK_z \\ (C_{12}+C_{44})K_xK_z & (C_{12}+C_{44})K_yK_z & K_z^2C_{11} + C_{44}(K_x^2+K_y^2) \end{pmatrix}}_{\hat{=}\,\hat{S}}\vec{u}$$

$$\Rightarrow \det|\hat{S} - \omega^2\rho\,\mathbb{1}| = 0 \qquad \Rightarrow \det|\tfrac{1}{K^2}\hat{S} - v^2\rho\,\mathbb{1}| = 0$$

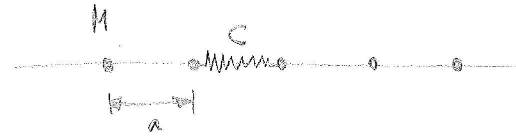
ⓑ $\sum_i r_i$ $\qquad r_i$ = Roots of determinantal eq.

$$\frac{1}{K^2}\sum_i S_{ii} = \frac{1}{K^2}\left(C_{11}(K_x^2+K_y^2+K_z^2) + 2C_{44}(K_x^2+K_y^2+K_z^2)\right) = C_{11} + 2C_{44} \hat{=} v^2\rho$$

$$v^2 = \frac{C_{11} + 2C_{44}}{\rho}$$

Chp. 4 No 1: Monoatomic linear lattice

$$u_s = u\cos(\omega t - sKa)$$



a) $$E = E_{kin} + E_{pot} = \sum_s E_{kin}^{(s)} + \sum_s E_{pot}^{(s)} = \sum_s \frac{1}{2} M v_s^2 + \sum_s \frac{1}{2} C (d_{s,s+1})^2$$

$$= \sum_s \frac{1}{2} M \left(\frac{du_s}{dt}\right)^2 + \sum_s \frac{1}{2} C (u_s - u_{s+1})^2$$

s runs over all atoms

b) dispersion-relation $\omega = \sqrt{\frac{4C}{M}}\,\left|\sin \frac{1}{2} Ka\right|$

$$E_s = \frac{1}{2} M\left(\frac{du_s}{dt}\right)^2 + \frac{1}{2} C (u_s - u_{s+1})^2$$

$$\frac{d}{dt} u_s = -u\sin(\omega t - sKa)\,\omega$$

$$= \frac{1}{2} M\left(-u\omega \sin(\omega t - sKa)\right)^2 + \frac{1}{2} C u^2 \left(\cos(\omega t - sKa) - \cos(\omega t - sKa - Ka)\right)^2$$

$$= \frac{1}{2} M u^2\omega^2 \sin^2(\omega t - sKa) + \frac{1}{2} C u^2 \left(\cos^2(\omega t - sKa) + \cos^2(\omega t - sKa - Ka) - 2\cos(\omega t - sKa)\cos(\omega t - sKa - Ka)\right)$$

$$\langle E_s\rangle = \frac{1}{2} M u^2\omega^2 \overbrace{\langle \sin^2(\omega t - sKa)\rangle}^{=\frac{1}{2}} + \frac{1}{2} C u^2 \Big(\overbrace{\langle \cos^2(\omega t - sKa)\rangle}^{=\frac{1}{2}} + \overbrace{\langle \cos^2(\omega t - sKa - Ka)\rangle}^{=\frac{1}{2}} - 2\langle \cos(\omega t - sKa)\cos(\omega t - sKa - Ka)\rangle\Big)$$

$$= \frac{1}{4} M u^2\omega^2 + \frac{1}{2} C u^2 \Big(1 - 2\underbrace{\langle \cos(\omega t - sKa)\cos(\omega t - sKa - Ka)\rangle}_{\stackrel{!}{=} \frac{1}{2}\cos(Ka)}\Big)$$

$$= \frac{1}{4} M u^2\omega^2 + \frac{1}{2} C u^2 (1 - \cos(Ka))$$

$$\langle \cos(\omega t - sKa)\cos(\omega t - sKa - Ka)\rangle = \frac{\omega}{2\pi}\int_0^{\frac{2\pi}{\omega}} dt\, \cos(\omega t - sKa)\cos(\omega t - sKa - Ka)$$

$z = \omega t - sKa$

$$= \frac{1}{2\pi}\int_0^{2\pi} dz\, \cos(z)\cos(z - Ka) = \frac{1}{2\pi}\int_0^{2\pi} dz\, \cos(z - z + Ka)$$

$$- \frac{1}{2\pi}\int_0^{2\pi} dz\, \sin(z)\sin(z - Ka)$$

$\cos(\alpha - \beta) = \cos\alpha\cos\beta + \sin\alpha\sin\beta$

$$= \cos(Ka) - \frac{1}{2\pi}\int_0^{2\pi} dx\, \cos(x)\cos(x - Ka)$$

$\sin(z + \pi) = \cos(z)$

$z = x + \pi$

$$\Rightarrow \quad 2\cdot\frac{1}{2\pi}\int_0^{2\pi} dx\, \cos(x)\cos(x - Ka) = \cos(Ka)$$

$$\Rightarrow \quad \frac{1}{2\pi}\int_0^{2\pi} dx\, \cos(x)\cos(x - Ka) = \frac{1}{2}\cos(Ka)$$

$$\langle E_s\rangle = \frac{1}{4}Mu^2\omega^2 + \frac{1}{2}Cu^2(1 - \cos(Ka))$$

$$= \frac{1}{4}Mu^2\omega^2 + \frac{1}{2}Cu^2\, 2\sin^2\frac{Ka}{2}$$

$$= \frac{1}{4}Mu^2\omega^2 + Cu^2\frac{\omega^2 M}{4C} = \underline{\underline{\frac{1}{2}Mu^2\omega^2}}$$

$\sin\frac{\alpha}{2} = \sqrt{\frac{1 - \cos\alpha}{2}}$

$1 - \cos\alpha = 2\sin^2\frac{\alpha}{2}$

dispersion relation

$\omega = \sqrt{\frac{4C}{M}}\,|\sin\frac{1}{2}Ka|$

$\sin^2\frac{1}{2}Ka = \frac{\omega^2 M}{4C}$

Chp 4 No 3: Basis of two unlike atoms

analog to page 87 in Kittel

$$M_1 \frac{d^2 u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s)$$

$$M_2 \frac{d^2 v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s)$$

$$u_s = u_0 e^{-i(\omega t - ska)} \qquad v_s = v_0 e^{-i(\omega t - ska)}$$

$$\Rightarrow \quad -\omega^2 M_1 u = Cv[1 + \exp(-ika)] - 2Cu$$

$$-\omega^2 M_2 v = Cu[1 + \exp(-ika)] - 2Cv$$

$$K_{max} = \frac{\pi}{2}$$

$$\Rightarrow \quad -\omega^2 M_1 u = -2Cu$$

$$-\omega^2 M_2 v = -2Cv$$

decoupled → if $u = 0$ $v \neq 0$
(movement independent)

M_1 atoms rest
M_2 atoms move

$$\frac{M_1 u}{M_2 v} = 1 \qquad \frac{u}{v} = \frac{M_2}{M_1}$$

Chp 4 No 5: Diatomic chain

calculation analog to the problem in Kittel on page 97

$$M \frac{d^2 u_s}{dt^2} = 10C(v_s - u_s) - C(u_s - v_{s-1}) = C(10v_s + v_{s-1} - 11u_s)$$

$$M \frac{d^2 v_s}{dt^2} = 10C(u_s - v_s) - C(v_s - u_{s+1}) = C(10u_s + u_{s+1} - 11v_s)$$

looking for plane-wave solutions

$$u_s = u_0 e^{-i(\omega t - sKa)} \qquad v_s = v_0 e^{-i(\omega t - sKa)}$$

eq. of motion

$$\Rightarrow \quad -M\omega^2 u = C(10v_0 + v_0 e^{-iKa} - 11u_0)$$

$$-M\omega^2 v = C(10u_0 + u_0 e^{-iKa} - 11v_0) \qquad \vec{u} = \begin{pmatrix} u \\ v \end{pmatrix}$$

$$-M\omega^2 \vec{u} = \begin{pmatrix} -11C & 10C + Ce^{-iKa} \\ 10C + Ce^{-iKa} & -11C \end{pmatrix} \vec{u}$$

$$\Rightarrow \quad \det \begin{vmatrix} 11C - M\omega^2 & -10C - Ce^{-iKa} \\ -10C - Ce^{-iKa} & 11C - M\omega^2 \end{vmatrix} = 0$$

$$\Rightarrow \quad \omega^2 = \frac{11C}{M} \pm \frac{\sqrt{101C^2 + 20C^2 \cos Ka}}{M}$$

$K = 0$: $\quad \omega = 0 \quad$ and $\quad \omega = \sqrt{\frac{22C}{M}}$

$K = \frac{\pi}{a}$ $\quad \omega = \sqrt{\frac{20C}{M}} \quad$ and $\quad \omega = \sqrt{\frac{2C}{M}}$

dispersion relation: