Solutions

PHY 481/581 - HOMEWORK SET 3

Northern Arizona University — Due: 10/15/2018

1 1D Monatomic Solid

Problem 1. Derive the dispersion relation for the monatomic 1D solid. Utilize the equation of motion for the atom located at equilibrium position $x_n = na$, where a is the spacing between atoms at equilibrium (unit cell), given by

$$M\ddot{u}_n = -\alpha\big[2u_n - u_{n+1} - u_{n-1}\big] \tag{1}$$

where u_n is the displacement from equilibrium for atom n and α is the "spring constant." Hint: start with the solution $u_n = Ae^{i(kx_n - \omega t)}$ and note that $x_{n+1} = a(n+1)$, *etc.*

2 1D Diatomic Solid

Problem 2. Derive the dispersion relation for the longitudinal oscillations of a one-dimensional diatomic mass-and-spring crystal where the unit cell is of length a and each unit cell contains one atom of mass m_1 and one atom of mass m_2 connected together by springs with spring constant α.

Problem 3. Determine the frequencies of the acoustic and optical modes at $k = 0$ as well as at the Brillouin zone boundary.

Problem 4. Sketch the dispersion in both reduced and extended zone scheme.

① $u_n = Ae^{i(kx_n - \omega t)}$, $u_{n-1} = Ae^{i(kx_{n-1} - \omega t)}$

$x_n = na$

$$\underset{(1)}{M\ddot{u}_n} = -\alpha\left[\underset{(2)}{2u_n} - \underset{(3)}{u_{n+1}} - \underset{(4)}{u_{n-1}}\right]$$

$$u_n = Ae^{i(kna - \omega t)} \qquad u_{n-1} = Ae^{i(k(n-1)a - \omega t)}$$

$$\dot{u}_n = -i\omega Ae^{i(kx_n - \omega t)}$$

$$\ddot{u}_n = (-i\omega)(-i\omega)Ae^{i(kx_n - \omega t)}$$

$$+i^2\omega^2$$

$$= -\omega^2 Ae^{i(kna - \omega t)} \qquad (1)$$

$$2u_n = 2Ae^{i(kna - \omega t)} \qquad (2)$$

$$u_{n+1} = Ae^{i(k(n+1)a - \omega t)} \qquad (3)$$

$$u_{n-1} = Ae^{i(k(n-1)a - \omega t)} \qquad (4)$$

$$u_{n+1} = Ae^{i[kna + ka - \omega t]}$$

$$u_{n-1} = Ae^{i[kna - ka - \omega t]}$$

$$u_{n+1} = \cancel{A}\cancel{e^{ikna}} e^{ika} \cancel{e^{-i\omega t}}$$

$$u_{n-1} = \cancel{A}\cancel{e^{ikna}} e^{-ika} \cancel{e^{-i\omega t}}$$

$$2u_n = 2\cancel{A}\cancel{e^{ikna}} \cancel{e^{-i\omega t}}$$

Sum α

$$-\omega^2 \cancel{A}\cancel{e^{ikna}} \cancel{e^{-i\omega t}}$$

$$-M\omega^2 = +\alpha\left[\underbrace{e^{ika} + e^{-ika} + -2}\right]$$

$$\cos(ka) + i\cancel{\sin}(ka)$$

$$+ \cos(ka) - i\cancel{\sin}(ka) - 2$$

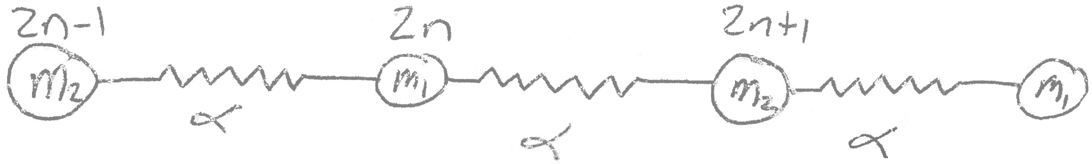
$$= [2\cos(ka) - 2]\alpha$$

$$-\omega^2 = \frac{2\alpha}{M}[\cos(ka) - 1]$$

half-ang. form.

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

2



(1) $m_2 \ddot{u}_{2n+1} = -\alpha\left(2u_{2n+1} - u_{2n} - u_{2n+2}\right)$

(2) $m_1 \ddot{u}_{2n+2} = -\alpha\left(2u_{2n+2} - u_{2n+1} - u_{2n+3}\right)$

Ansatz: $$\begin{bmatrix} u_{2n+1} \\ u_{2n+2} \end{bmatrix} = \begin{bmatrix} A_1 e^{ik(2n+1)a} \\ A_2 e^{ik(2n+2)a} \end{bmatrix} e^{-i\omega t}$$

left:

(1) $$m_2\left(A_1 e^{ik(2n+1)a} \frac{d^2}{dt^2}\left(e^{-i\omega t}\right)\right)$$

$$= m_2 A_1 e^{i2kna} e^{ika} - \omega^2 \cancel{e^{-i\omega t}}$$

right: $$-\alpha\left(2A_1 e^{ik(2n+1)a} - A_2 e^{ik(2n)a} - A_2 e^{ik(2n+2)a}\right) \cancel{e^{-i\omega t}}$$

- the time-dependence cancels from both sides

$$\Rightarrow -m_2 A_1 \cancel{e^{i2kna}} e^{ika} \omega^2$$ $*\ e^{i2kna}$'s cancel

$$= -\alpha\left(2A_1 \cancel{e^{i2kna}} e^{ika} - A_2 \cancel{e^{i2kna}} - A_2 \cancel{e^{i2kna}} e^{i2ka}\right)$$

#~~1~~2 continued:

$$\Rightarrow -m_2 A_1 e^{ika} \omega^2$$

$$= -\alpha\left(2A_1 e^{ika} - A_2 - A_2 e^{i2ka}\right)$$

- divide through by e^{ika}

$$\Rightarrow -m_2 A_1 \omega^2$$

$$= -\alpha\Big(2A_1 \underbrace{- A_2 e^{-ika} - A_2 e^{ika}}_{-A_2\left(\cos(ka) - i\cancel{\sin(ka)} + \cos(ka) + i\cancel{\sin(ka)}\right)}\Big)$$

$$\Rightarrow -m_2 \omega^2 A_1$$

$$= -\alpha\left(2A_1 - A_2 \cdot 2\cos(ka)\right)$$

for eq.(1)

$$(1)\ -m_2 \omega^2 A_1 = -2\alpha A_1 + 2\alpha A_2 \cos(ka)$$

$$-m_2 \omega^2 A_1 + 2\alpha A_1 - 2\alpha A_2 \cos(ka) = 0^*$$

#2 continued:

left

(2): $m_1 \frac{d^2}{dt^2}\left(A_2 e^{ik(2n+2)a} e^{-i\omega t}\right)$

$= -m_1 \omega^2 A_2 e^{i2kna} e^{i2ka} \cancel{e^{-i\omega t}}$

right: $-\alpha\left(2A_2 e^{ik(2n+2)a} - A_1 e^{ik(2n+1)a} - A_1 e^{ik(2n+3)a}\right)\cancel{e^{-i\omega t}}$

* the time-dependence cancels from both sides & we have

$\Rightarrow -m_1 \omega^2 A_2 \cancel{e^{i2kna}} e^{i2ka}$

$= -\alpha\left(2A_2 \cancel{e^{i2kna}} e^{i2ka} - A_1 \cancel{e^{i2kna}} e^{ika} - A_1 \cancel{e^{i2kna}} e^{i3ka}\right)$

* the e^{i2kna}'s cancel

#2continued:

$$\rightarrow -m_1 \omega^2 A_2 e^{i2ka}$$

$$= -\alpha\left(2A_2 e^{i2ka} - A_1 e^{ika} - A_1 e^{i3ka}\right)$$

$*$ divide through by e^{i2ka}:

$$\Rightarrow -m_1 \omega^2 A_2$$

$$= -\alpha\left(2A_2 - A_1 \underbrace{\left[e^{-ika} + e^{ika}\right]}_{\substack{\cos(ka) - i\sin(ka) \\ + \cos(ka) + i\sin(ka) = 2\cos(ka)}}\right)$$

$$\Rightarrow -m_1 \omega^2 A_2$$

$$= -2\alpha A_2 + \alpha A_1 \cdot 2\cos(ka)$$

$$\Rightarrow -m_1 \omega^2 A_2 + 2\alpha A_2 - 2\alpha A_1 \cos(ka) = 0 \quad (2)^*$$

$*$ combine with $(1)^*$

$$-m_2 \omega^2 A_1 + 2\alpha A_1 - 2\alpha A_2 \cos(ka) = 0$$

#2 continued:

$$\Rightarrow \begin{bmatrix} -2\alpha\cos(ka) & 2\alpha - m_1\omega^2 \\ 2\alpha - m_2\omega^2 & -2\alpha\cos(ka) \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} = 0$$

* take the determinant

$$-\left(2\alpha\cos(ka)\right)^2 + \left(2\alpha - m_2\omega^2\right)\left(2\alpha - m_1\omega^2\right) = 0$$

$$= -4\alpha^2\cos^2(ka) + 4\alpha^2 - 2\alpha m_1\omega^2 - 2\alpha m_2\omega^2$$
$$+ m_1 m_2 \omega^4 = 0$$

$$= 4\alpha^2\left(1 + -\cos^2(ka)\right)$$

$$+ \omega^2\left(-2\alpha(m_1+m_2)\right)$$

$$+ \omega^4(m_1 m_2)$$

$$= 0$$

#2 continued :

$$\Rightarrow \quad 4\alpha^2\sin^2(ka) + \omega^2\left(-2\alpha(m_1+m_2)\right) + \omega^4(m_1m_2) = 0$$

$$\frac{-b \pm \sqrt{b^2-4ac}}{2a}$$ → quad. formula

$a = m_1m_2$

$b = -2\alpha(m_1+m_2)$

$c = 4\alpha^2\sin^2(ka)$

$\omega^2 =$

$$-\frac{1}{(2m_1m_2)}\left(-2\alpha(m_1+m_2)\right) \pm \sqrt{\frac{\left(-2\alpha(m_1+m_2)\right)^2}{(m_1m_2)^2} - \frac{4m_1m_2\left(4\alpha^2\sin^2(ka)\right)}{(m_1m_2)^2}}$$

$$= \frac{\alpha(m_1+m_2)}{m_1m_2} \pm \sqrt{\frac{4\alpha^2(m_1+m_2)^2}{(m_1m_2)^2} - \frac{16\cancel{m_1m_2}\alpha^2\sin^2(ka)}{(m_1m_2)^{\cancel{2}}}}$$

$$= \alpha\left(\frac{m_1}{m_1m_2} + \frac{m_2}{m_1m_2}\right) \pm \frac{2\alpha}{2}\sqrt{\frac{m_1^2+m_2^2+2m_1m_2}{(m_1m_2)^2} - \frac{4\sin(ka)}{m_1m_2}}$$

#2 continued:

$$= \alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm \frac{2\alpha}{2}\sqrt{\frac{m_1^2}{m_1^2 m_2^2}+\frac{m_2^2}{m_1^2 m_2^2}+\frac{2m_1 m_2}{m_1^2 m_2^2}-\frac{4\sin(ka)}{m_1 m_2}}$$

$$= \alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm \frac{2\alpha}{2}\sqrt{\frac{1}{m_2^2}+\frac{1}{m_1^2}+\frac{2}{m_1 m_2}-\frac{4\sin(ka)}{m_1 m_2}}$$

$$\boxed{\omega = \alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm \alpha\sqrt{\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2-\frac{4\sin^2(ka)}{m_1 m_2}}}$$

$\longrightarrow$

Over

3

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

for $k \rightarrow 0$

$$\omega^2 = \alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm \alpha \sqrt{\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - 0}$$

$$= \alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm \alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right)$$

$$\Rightarrow \quad 2\alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \longrightarrow \text{optical}$$

$$\boxed{\omega = \sqrt{2\alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right)}}$$

$$\boxed{\omega = 0, \text{ for acoustic}}$$

- Zone boundaries: $k = \pm\pi/a$

$$\omega^2 = \alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm \alpha \sqrt{\left(\frac{1}{m_1}+\frac{1}{m_2}\right)^2 - \frac{4\sin(\pi/2)}{m_1 m_2}}$$

#3 Cont.

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

$$= \alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm \alpha\sqrt{\frac{1}{m_1^2}+\frac{1}{m_2^2}+\underbrace{\frac{2}{m_1 m_2}-\frac{4}{m_1 m_2}}_{-\frac{2}{m_1 m_2}}}$$

$$= \alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm \alpha\sqrt{\underbrace{\frac{1}{m_1^2}+\frac{1}{m_2^2}-\frac{2}{m_1 m_2}}_{\left(\frac{1}{m_1}-\frac{1}{m_2}\right)^2}}$$

$$= \alpha\left(\frac{1}{m_1}+\frac{1}{m_2}\right) \pm \alpha\left(\frac{1}{m_1}-\frac{1}{m_2}\right)$$

$(+) \rightarrow$ optical

$$\omega = \sqrt{\frac{2\alpha}{m_1}}$$

$(-) \rightarrow$ acoustic

$$\omega = \sqrt{\frac{2\alpha}{m_2}}$$

$m_1 < m_2$

(4)