Werkgroep 10 Fysica van de Vaste Stof – 17 febr 2011 Oplossingen

Oefenopgaven over roostertrillingen en fononen (Kittel H4).

Problem 4.3 in Kittel. For the problem treated by (18) to (26), find the amplitude ratio u/v for the two branches at $K_{max} = \pi/a$. Show that at this value of K the two lattices act as if decoupled: one lattice remains at rest while the other lattice moves.

Solution:

From Eqn. (21) in Kittel, let $K = K_{max} = \pi/a$, we get:

$$\det \begin{pmatrix} 2C - M_1\omega^2 & 0 \\ o & 2C - M_2\omega^2 \end{pmatrix} = 0 \tag{15}$$

The solution to this equation gives the normal modes frequencies at this K value:

$$\omega^2 = 2C/M_1; \qquad \omega^2 = 2C/M_2 \tag{16}$$

Substitute this expression of ω^2 in to (20) in Kittel, we found:

- When $\omega^2 = 2C/M_1$, it follows that:

$$\frac{u}{v} \to \infty \tag{17}$$

  which gives a mode that u is finite, and v is zero.

- When $\omega^2 = 2C/M_2$, it follows that:

$$\frac{u}{v} = 0 \tag{18}$$

  which gives a mode that v is finite and u is zero. In any cases, the two lattices act as if decoupled: one lattice remains at rest while the other lattice moves.

Problem 4.5 in Kittel. To assist solving the following problem, solve this with coupling constants C_1 and C_2, then set $C_1 = C$, and $C_2 = 10C$. Consider the normal modes of a linear chain in which the force constants between nearest-neighbor atoms are alternately C and $10C$. Let the masses be equal, and let the nearest-neighbor separation be $a/2$. Find $\omega(k)$ at $k = 0$ and $k = \pi/a$. Sketch in the dispersion relation by eye. This problem simulates a crystal of diatomic such as H_2.

Solution:

Now as in Fig. 3, let the coupling constants be in general C_1, and C_2, then the equations of motions are:

$$\begin{aligned} M\ddot{u}_{n,1} &= C_1(u_{n,2} - u_{n,1}) - C_2(u_{n,1} - u_{n-1,2}) \\ &= C_1 u_{n,2} + C_2 u_{n-1,2} - (C_1 + C_2)u_{n,1} \\ M\ddot{u}_{n,2} &= C_2(u_{n+1,1} - u_{n,2}) - C_1(u_{n,2} - u_{n,1}) \\ &= C_2 u_{n+1,1} + C_1 u_{n,1} - (C_1 + C_2)u_{n,2} \end{aligned} \tag{19}$$

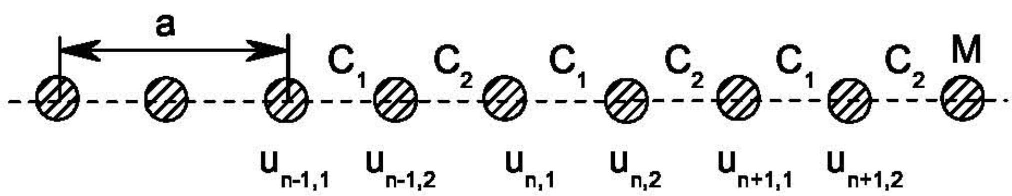

Figure 3: The diatomic linear chain with alternating coupling constants.

For the normal modes, they are in the form:

$$\begin{aligned} u_{n,1} &= A_1 \mathrm{e}^{\mathrm{i}(kna-\omega t)} \\ u_{n,2} &= A_2 \mathrm{e}^{\mathrm{i}(kna-\omega t)} \end{aligned} \tag{20}$$

substitute (20) in to (19), we have:

$$\begin{aligned} A_1[\omega^2 M - (C_1 + C_2)] + A_2(C_1 + C_2\mathrm{e}^{-\mathrm{i}ka}) &= 0 \\ A_1(C_1 + C_2\mathrm{e}^{\mathrm{i}ka}) + A_2[\omega^2 M - (C_1 + C_2)] &= 0 \end{aligned} \tag{21}$$

to have non trivial solutions, it requires:

$$\det \begin{pmatrix} \omega^2 M - (C_1 + C_2) & C_1 + C_2\mathrm{e}^{-\mathrm{i}ka} \\ C_1 + C_2\mathrm{e}^{-\mathrm{i}ka} & \omega^2 M - (C_1 + C_2) \end{pmatrix} = 0 \tag{22}$$

this gives the dispersion relations of:

$$\omega^2 = \frac{1}{M}\left(C_1 + C_2 \pm \sqrt{C_1^2 + C_2^2 + 2C_1C_2\cos ka}\right) \tag{23}$$

set $C_1 = C$, and $C_2 = 10C$, we found the dispersion relation is:

$$\omega^2 = \frac{C}{M}\left(11 \pm \sqrt{101 + 20\cos ka}\right) \tag{24}$$

and at $k = 0$, and $k = \pi/a$, the normal mode frequencies are:

- at $k = 0$, we have:

$$\begin{aligned} \omega &= \sqrt{\frac{22C}{M}} &&: \text{for optical branch} \\ \omega &= 0 &&: \text{for acoustic branch} \end{aligned} \tag{25}$$

- at $k = \pi/a$, we have:

$$\begin{aligned} \omega &= \sqrt{\frac{20C}{M}} &&: \text{for optical branch} \\ \omega &= \sqrt{\frac{2C}{M}} &&: \text{for acoustic branch} \end{aligned} \tag{26}$$

The dispersion relation is drawn in Fig. 4.

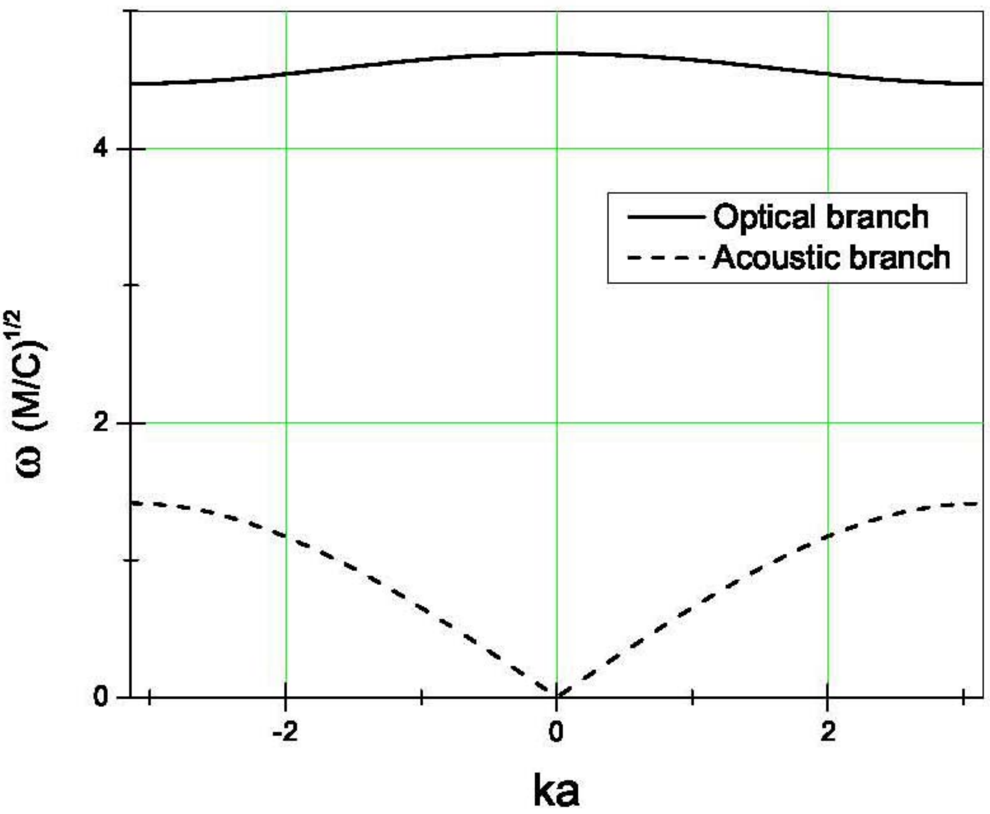

Figure 4: The dispersion relation for diatomic linear chain with alternating coupling constants $C_1 = C$, and $C_2 = 10C$.

Verder werd het volgende probleem genoemd:
Zeer veel inzicht kan ook verkregen worden door bij het probleem van twee verschillende atomen per primitieve cel (Kittel blz 95 – 99) in de oplossing van Eq (22) [zie de uitdrukking gegeven op college] het geval van M1 = M2 te beschouwen, en aan te tonen dat de situatie (de dispersierelatie) van het geval van één atoom per primitieve cel wordt herkregen. Dit is ook probleem 22.2 in Ashcroft en Mermin, en de uitwerking wordt hieronder gepresenteerd

Problem 22.2 in Ashcroft and Mermin: Diatomic Linear Chain. Consider a linear chain in which alternate ions have mass M_1 and M_2, and only nearest neighbors interact.

(a). Show that the dispersion relation for the normal modes is:

$$\omega^2 = \frac{C}{M_1 M_2}\left(M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos ka}\right) \tag{1}$$

(b). Discuss the form of the dipersion relation and the nature of the normal modes when $M_1 \gg M_2$.

(c). Compare the dispersion relation with that of the monatomic linear chain when $M_1 = M_2$.

Solution:

(a). As in Fig. 1, let the coordinates of two atoms in the n^{th} unit cell be $u_{n,1}$ and u_{n_2}, then the equation of motions are:

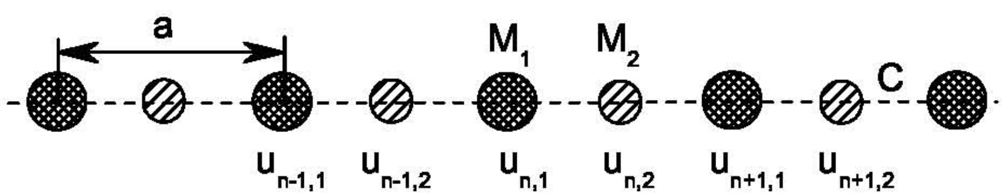

Figure 1: The diatomic linear chain with alternating masses.

$$\begin{aligned} M_1\ddot{u}_{n,1} &= C(u_{n,2} - u_{n,1}) - C(u_{n,1} - u_{n-1,2}) = C(u_{n,2} + u_{n-1,2} - 2u_{n,1}) \\ M_2\ddot{u}_{n,2} &= C(u_{n+1,1} - u_{n,2}) - C(u_{n,2} - u_{n,1}) = C(u_{n+1,1} + u_{n,1} - 2u_{n,2}) \end{aligned} \tag{2}$$

For the normal modes, they are in the form:

$$\begin{aligned} u_{n,1} &= A_1 \mathrm{e}^{\mathrm{i}(kna - \omega t)} \\ u_{n,2} &= A_2 \mathrm{e}^{\mathrm{i}(kna - \omega t)} \end{aligned} \tag{3}$$

substitute (3) in to (2), we have:

$$\begin{aligned} A_1(\omega^2 M_1 - 2C) + A_2 C(1 + \mathrm{e}^{-ika}) &= 0 \\ A_1 C(1 + \mathrm{e}^{ika}) + A_2(\omega^2 M_2 - 2C) &= 0 \end{aligned} \tag{4}$$

to have non trivial solutions, it requires:

$$\det \begin{pmatrix} \omega^2 M_1 - 2C & C(1+\mathrm{e}^{-\mathrm{i}ka}) \\ C(1+\mathrm{e}^{\mathrm{i}ka}) & \omega^2 M_2 - 2C \end{pmatrix} = 0 \tag{5}$$

this gives the dispersion relations of:

$$\omega^2 = \frac{C}{M_1 M_2}\left(M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos ka}\right) \tag{6}$$

(b). when $M_1 \gg M_2$, then $M_2/M_1 \ll 1$, expand (6):

$$\begin{aligned} \omega^2 &= \frac{C}{M_2}\left[\left(1+\frac{M_2}{M_1}\right) \pm \sqrt{1+\left(\frac{M_2}{M_1}\right)^2 + 2\frac{M_2}{M_1}\cos ka}\right] \\ &= \frac{C}{M_2}\left[\left(1+\frac{M_2}{M_1}\right) \pm \left(1+\frac{M_2}{M_1}\cos ka\right) + o(\left(\frac{M_2}{M_1}\right)^2)\right] \end{aligned} \tag{7}$$

- For "+" in (7), it follows that:

  $$\omega = \sqrt{\frac{2C}{M_2}}\left[1 + o(\frac{M_2}{M_1})\right] \tag{8}$$

  plug in to (4), we get:

  $$\frac{A_1}{A_2} \to 0 \tag{9}$$

  this gives a normal mode in which the atom with mass M_1 does not oscillate, while the atom with mass M_2 oscillate with frequency given in (9).

- For "-" in (7), it follows that:

  $$\omega = \sqrt{\frac{2C}{M_1}}\left|\sin\frac{ka}{2}\right|\left[1 + o(\frac{M_2}{M_1})\right] \tag{10}$$

  plug in to (4), we get:

  $$\frac{A_1}{A_2} \to 1 \tag{11}$$

  this gives a normal mode in which the two atoms within a same primitive cell move in phase, just a whole unit, since $M_1 \gg M_2$, the frequency is determined by the lager one, say M_1.

(c). When $M_1 = M_2 = M$, (6) gives:

$$\omega^2 = \frac{C}{M}(2 \pm \sqrt{2 + 2\cos ka}) \tag{12}$$

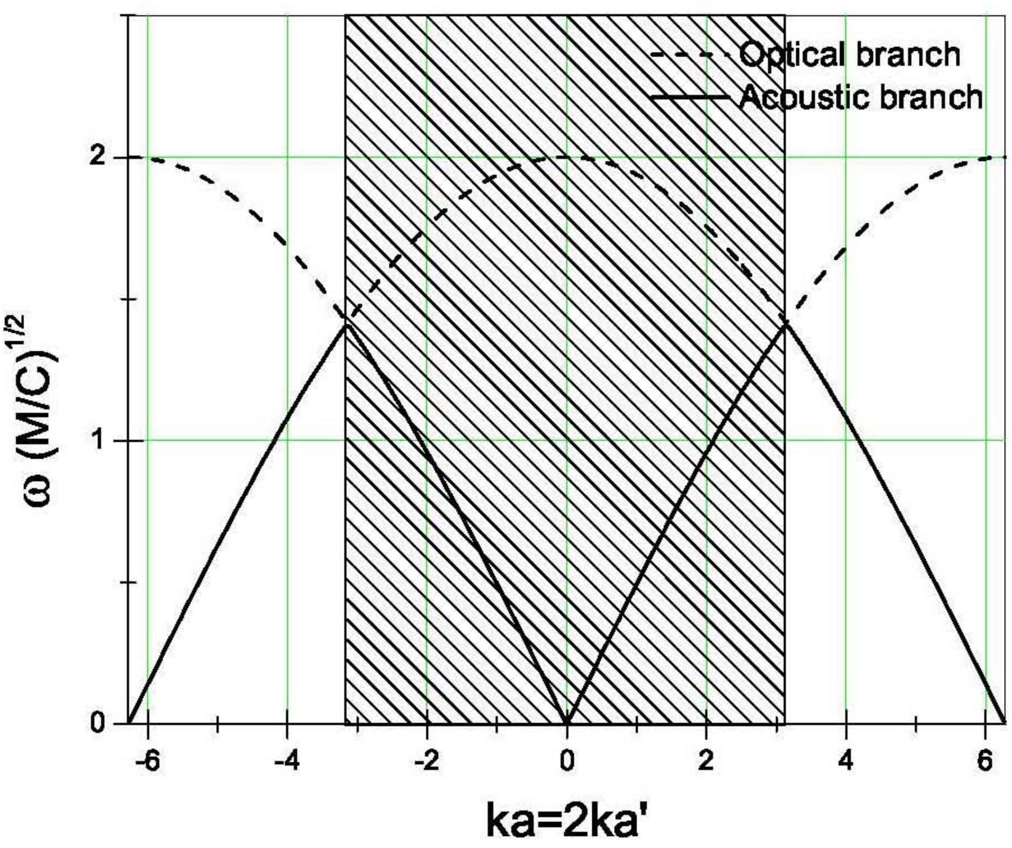

Figure 2: The dispersion relation for the diatomic linear chain when $M_1 = M_2 = M$. Shaded area gives the Brillouin zone for the diatomic chain.

this dispersion relation is shown as in Fig. 2, where for the first Brillouin zone for the diatomic chain is $ka \in [-\pi, \pi]$. In terms of the new lattice constant $a' = a/2$, the dispersion relation is then:

$$\omega^2 = \frac{2C}{M}(1 \pm \cos ka'), \qquad ka' \in [-\frac{\pi}{2}, \frac{\pi}{2}] \tag{13}$$

For the optical branch, consider the part with $ka' \in [-\frac{\pi}{2}, 0]$, then:

$$\omega^2 = \frac{2C}{M}(1 + \cos ka') = \frac{2C}{M}[1 - \cos(ka' + \pi)] \tag{14}$$

notice that $ka' + \pi \in [\frac{\pi}{2}, \pi]$, above expression indicates that the optical branch in dispersion relation for the diatomic chain in $[-\frac{\pi}{2}, 0]$ is equivalent to the acoustic branch in $[\frac{\pi}{2}, \pi]$. Similarly, the optical branch in dispersion relation for the diatomic chain in $[0, \frac{\pi}{2}]$ is equivalent to the acoustic branch in $[-\pi, -\frac{\pi}{2}]$. Thus, instead of describing the dispersion relation with both optical and acoustic branch in $ka' \in [-\frac{\pi}{2}, \frac{\pi}{2}]$, it is equivalent to just consider the acoustic branch in $ka' \in [-\pi, \pi]$, which is just the dispersion relation for the monatomic chain. Therefore, when setting $M_1 = M_2 = M$, the dispersion relation for monatomic chain is recovered.