

Answer Set 5

Physics 240B

A&M 22.2 a) Label displacements of the M_1 mass by u and displacements of the M_2 mass by v . I will define the mass indicated by u_n as being between those indicated by v_n and v_{n-1} . Equations of motion:

$$M_1 \ddot{u}_n = -K(2u_n - v_n - v_{n-1})$$

$$M_2 \ddot{v}_n = -K(2v_n - u_n - u_{n+1})$$

Now assume $u_n = u e^{i(kna - \omega t)}$ and $v_n = v e^{i(kna - \omega t)}$. Here a represents the spacing between consecutive M_1 masses. Substitute into the equations of motion, cancel an overall factor of $e^{i(kna - \omega t)}$, and divide by v to get

$$-\omega^2 M_1 \frac{u}{v} = -K \left(2 \frac{u}{v} - 1 - e^{-ika} \right)$$

$$-\omega^2 M_2 = -K \left(2 - \frac{u}{v} - e^{ika} \frac{u}{v} \right)$$

Next solve each equation for $\frac{u}{v}$ and equate the two expressions to get (ultimately) a quadratic equation in ω^2 :

$$M_1 M_2 (\omega^2)^2 - 2K(M_1 + M_2)(\omega^2) + K^2(2 - 2 \cos ka) = 0$$

Solving,

$$\begin{aligned} \omega^2 &= \frac{K(M_1 + M_2)}{M_1 M_2} \pm \frac{1}{M_1 M_2} \sqrt{4K^2(M_1 + M_2)^2 - 4K^2 M_1 M_2 (2 - 2 \cos ka)} \\ &= \frac{K}{M_1 M_2} (M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos ka}) \end{aligned}$$

- b) For $M_1 \gg M_2$, this chain should reduce to a monatomic chain with masses M_1 , springs $K/2$, and lattice constant a . (The alteration of the spring constant is because springs in series add exactly like resistors in parallel: a given total length change corresponds to smaller displacements in the individual springs, and hence a smaller force, compared to a single spring where the entire length change is taken up within the spring.) The dispersion relation becomes

$$\omega^2 = 2 \frac{K}{M_2}$$

or

$$\omega^2 = \frac{K}{M_1} (1 - \cos ka) = 2 \frac{K}{M_1} \sin^2 \frac{ka}{2}$$

The upper branch from part a) disappears, since now there are only half as many modes. The lower branch remains.

- c) This time the equivalent monatomic chain has masses M_1 , springs K , and lattice constant $a/2$. The dispersion relation becomes

$$\omega^2 = \frac{2K}{M_1} \left(1 \pm \cos \frac{ka}{2} \right) = \frac{4K}{M_1} \sin^2 \frac{ka}{2} \text{ or } \frac{4K}{M_1} \cos^2 \frac{ka}{2}$$

The sine branch gives exactly the original modes, for the inner half of the Brillouin zone. The cosine branch gives the modes originally in the outer half of the Brillouin zone.

A&M 22.3 a) Plug into equation (22.37) to get $\omega^2 = \frac{2K_o}{M} \pm \frac{1}{M} \sqrt{2K_o^2 + 2\Delta^2 + 2(K_o^2 - \Delta^2) \cos ka}$.

At $\Delta = 0$ this is $\omega^2 = \frac{2K_o}{M} \pm \frac{1}{M} \sqrt{2K_o^2 + 2K_o^2 \cos ka} = \frac{2K_o}{M} \pm \frac{1}{M} \sqrt{2K_o^2 (2 \cos^2 \frac{ka}{2})} = \frac{2K_o}{M} \pm \frac{2K_o}{M} \cos \frac{ka}{2} = \frac{4K_o}{M} \sin^2 \frac{ka}{4}$ or $\frac{4K_o}{M} \cos^2 \frac{ka}{4}$. The first of these is clearly (22.29), where the a from (22.29) is half of our a . For the second, let $k' = 2\pi/a - k$. The second (optical) branch becomes $\omega = 2\sqrt{K_o/M} |\cos(\pi/2 - \frac{k'a}{4})| = 2\sqrt{K_o/M} |\sin \frac{k'a}{4}|$; that is, each point on this branch in the reduced Brillouin zone of the diatomic lattice corresponds to a point in the larger Brillouin zone of the monatomic lattice, with the correct dispersion relation.

b) Generally the coefficient of Δ^2 and K_o^2 inside the square root are comparable, so we can expand and get a $(\Delta/K_o)^2$ term. The exception is if $\cos ka$ is so close to -1 that the Δ^2 and K_o^2 terms are comparable; that is, $\frac{1+\cos ka}{1-\cos ka} \approx \frac{\Delta^2}{K_o^2}$. Expanding the cosines, taking a square root, and dropping a factor of two (this is just order of magnitude anyway) gives the desired condition $|\pi - ka| \approx \Delta/K_o$. When the Δ^2 terms are comparable to the K_o^2 terms, the square root is of order Δ , as is the difference between the square root and what it would be with $\Delta = 0$. In relative terms, the correction is of order Δ/K_o (for both ω^2 and ω).

1. First, the energy is

$$U = \frac{1}{2} \sum_n [K_1(u_{n+1} - u_n)^2 + K_2(u_{n+2} - u_n)^2].$$

The equations of motion come from differentiating U :

$$M\ddot{u}_m = -\frac{\partial U}{\partial u_m} = -\frac{1}{2} [-2K_1(u_{m+1} - u_m) + 2K_1(u_m - u_{m-1}) + 2K_2(u_m - u_{m-2}) - 2K_2(u_{m+2} - u_m)]$$

To solve, guess the travelling wave $u_m = ue^{ikma - i\omega t}$. Plug this guess back into the equations of motion:

$$-\omega^2 M = K_1(e^{ika} - 1) - K_1(1 - e^{-ika}) - K_2(1 - e^{-2ika}) + K_2(e^{2ika} - 1) = 2K_1(\cos ka - 1) + 2K_2(\cos 2ka - 1).$$

Here I've already divided through by $ue^{ikma - i\omega t}$. So the dispersion relation is

$$\omega(k) = 2\sqrt{K_1/M} |\sin ka/2| \sqrt{1 + \frac{K_2 \sin^2 ka}{K_1 \sin^2 ka/2}}.$$

To lowest order in K_2/K_1 , this becomes

$$\omega(k) = 2\sqrt{K_1/M} |\sin ka/2| \left(1 + \frac{K_2 \sin^2 ka}{2K_1 \sin^2 ka/2}\right) = 2\sqrt{K_1/M} |\sin ka/2| + 4\sqrt{K_2^2/K_1 M} |\sin ka/2| \cos^2 ka/2.$$

The second term, a correction to the nearest-neighbor treatment, vanishes at the Brillouin zone center ($k=0$) and edges ($k = \pi/a$), and takes on its maximum (small) value near $k = \pm 0.4\pi/a$.