Problem Set 4

PHYSICS 463
February 28, 2021

Kevin Evans
ID: 11571810

---

1. ***Monatomic linear lattice.*** Consider a longitudinal wave

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

which propagates in a monatomic linear lattice of atoms of mass M, spacing a, and nearest-neighbor interaction C.

(a) Show that the total energy of the wave is

$$E = \frac{1}{2}M\sum_s \left(\frac{\mathrm{d}u_s}{\mathrm{d}t}\right)^2 + \frac{1}{2}C\sum_s (u_s - u_{s+1})^2,$$

where s runs over all atoms.

Solution. For an atom, the classical kinetic energy is given by

$$T_s = \frac{1}{2}M\dot{u}_s^2.$$

Then for all atoms s, all the kinetic energies contribute to the total

$$T = \frac{1}{2}M\sum_s \left(\frac{\mathrm{d}u_s}{\mathrm{d}t}\right)^2.$$

The potential energy for a spring is

$$\begin{aligned} U_s &= \frac{1}{2}C(\Delta u)^2 \\ &= \frac{1}{2}C\left(u_s - u_{s+1}\right)^2. \end{aligned}$$

(I don't really understand why Δu is the difference between neighboring atoms, instead of the displacement from $u_s - 0 = u_s$. Isn't it normally the total displacement from equilibrium of the specific spring?)
Combining these, the total energy is

$$\begin{aligned} E &= T + U \\ &= \frac{1}{2}M\sum_s \left(\frac{\mathrm{d}u_s}{\mathrm{d}t}\right)^2 + \frac{1}{2}C\sum_s (u_s - u_{s+1})^2 \end{aligned}$$

(b) By substitution of u_s in this expression, show that the time-average total per atom is

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

where in the last step, we have used the dispersion relation (9) for this problem.

Solution. For the kinetic term,

$$\dot{u}_s = -\omega \sin(\ldots),$$

As $\left\langle \sin^2(\ldots) \right\rangle = 1/2$,

$$\implies \left\langle (\dot{u}_s)^2 \right\rangle = \frac{\omega^2 u^2}{2}.$$
$$\implies \langle T \rangle = \frac{1}{4} M \omega^2 u^2.$$

Next, for the potential term,

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

I'm not sure how to simplify the difference of cosines, so I'll just assume it'll simplify to the answer given in the question...

$$\langle U_s \rangle = \frac{1}{2} C \left(1 - \cos Ka\right) u^2.$$

Removing the sums (since it's per atom), the time-average total energy per atom is

$$\begin{aligned} \langle E \rangle &= \langle T \rangle + \langle U \rangle \\ &= \frac{1}{4} M \omega^2 u^2 + \frac{1}{2} C \left(1 - \cos Ka\right) u^2. \quad \square \end{aligned}$$

2. ***Basis of two unlike atoms.*** For the problem treated by (18) to (26), find the amplitude of the ratios u/v for the two branches at $K_{\text{max}} = \pi/a$. 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. At $Ka = \pi$ and using (20), the coupled equations become

$$-\omega^2 M_1 u = Cv \left[1 + \underbrace{\exp(-i\pi)}_{-1} \right] - 2Cu = -2Cu;$$
$$-\omega^2 M_2 v = Cu \left[\underbrace{\exp(i\pi)}_{-1} + 1 \right] - 2Cv = -2Cv.$$

These coupled equations now become decoupled, as there is no v-dependence in u, and vice-versa. So, the equations of motion will now look something like

$$u(t) \approx u \exp\left(\sqrt{2C/M_1 t} \right);$$
$$v(t) \approx v \exp\left(\sqrt{2C/M_2 t} \right).$$

3. ***Diatomic chain.*** Consider the normal modes of a linear chain in which the force constants between nearest-neighbor atoms are alternatively 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 molecules such as H_2.

   Solution. With reference to Figure 9 of Kittel, we can let u_s's spring constant be C and v_s's spring constant be $10C$. Then we can rewrite (18) as

$$M\ddot{u}_s = C(v_s + 10v_{s-1} - u_s - 10u_s);$$
$$M\ddot{v}_s = C(u_{s+1} + 10u_s - v_s - 10v_s).$$

   Using the ansatz (19),

$$\ddot{u}_s = -\omega^2 u(s);$$
$$\ddot{v}_s = -\omega^2 v(s).$$

   Substituting this in, we find

$$-\omega^2 M u_s = C\left(v_s + 10v_{s-1} - u_s - 10u_s\right);$$
$$-\omega^2 M v_s = C\left(u_{s+1} + 10u_s - v_s - 10v_s\right).$$

   Adding in the phase difference of Ka on the $s \pm 1$ terms,

$$-\omega^2 M u_s = C\left(v_s + 10\exp(-iKa)v_s - u_s - 10u_s\right);$$
$$-\omega^2 M v_s = C\left(\exp(iKa)u_s + 10u_s - v_s - 10v_s\right).$$

   In matrix form, we can equate the determinate of the system to zero,

$$\begin{vmatrix} 11C - M\omega^2 & -C\left[1 + 10\exp(-iKa)\right] \\ -C\left(10 + \exp(iKa)\right) & 11C - M\omega^2 \end{vmatrix} = 0,$$

   or

$$\left(11C - M\omega^2\right)^2 - C^2(1 + 10\exp(-iKa))(10 + \exp(iKa)) = 0.$$

   For $Ka = 0$,

$$(11C - M\omega^2)^2 = C^2(1 + 10)(10 + 1)$$
$$\omega^2(Ka = 0) \approxeq \frac{1}{M}\left(\sqrt{11^2C^2} + 11C\right)$$
$$\approxeq \frac{1}{M}\left(22C\right).$$

   For the zone boundary $Ka = \pi$,

$$(11C - M\omega^2)^2 = C^2(1 - 10)(10 - 1)$$
$$(11C - M\omega^2) = \pm 9C$$
$$\omega^2(Ka = \pm\pi) \approxeq \begin{cases} \frac{1}{M}\left(20C\right) \\ \frac{1}{M}\left(2C\right). \end{cases}$$

Sketching this out,