Physics 140A Winter 2011

Homework 5 due Thursday February 23 at 5pm

1. 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 interactions C.

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

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

where s runs over all atoms.

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

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

where in the last step we have used the dispersion relation for this problem.

2. In class and in the text we discussed the case of crystal vibrations in the presence of a basis of two unlike atoms. For this problem (see Eqs. 18-26 in Kittel), find the amplitude ratio 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.

3. 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 the dispersion relation based on your results. This problem simulates a crystal of diatomic molecules such as H_2.

4. Consider point ions of mass M and charge e immersed in a uniform sea of conduction electrons - this is a model for metallic systems. The ions are imagined to be in stable equilibrium when at regular lattice points. If one ion is displaced a small distance r from its equilibrium position, the restoring force is largely due to the electric charge within the sphere of radius r centered at the equilibrium position. Take the number density of ions (or of conduction electrons) as $3/4\pi R^3$, which defines R. (a) Show that the frequency of a single ion set into oscillation is $\omega = \sqrt{e^2/MR^3}$. (b) Estimate the value of this frequency for sodium, roughly. (c) Based on your results, estimate the order of magnitude of the velocity of sound in the metal.

Homework Solutions – HW5

Note Title 2/19/2010

1 (a) wave $u_s = u\cos(\omega t - ksa)$

$$\text{Energy} = \sum_s \underbrace{(KE)_s}_{\text{Kinetic energy of mass \# s}} + \underbrace{(PE)_{s,s+1}}_{\text{potential energy of spring between s, s+1}}$$

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

(b) substituting, ..

$$E = \frac{1}{2}M\sum_s\left[-\omega u\sin(\omega t - ksa)\right]^2$$

$$+ \frac{1}{2}C\sum_s u^2\Big[\cos(\underbrace{\omega t - ksa}_{\equiv\alpha}) - \cos(\underbrace{\omega t - k(s+1)a}_{\equiv\alpha - ka})\Big]^2$$

$\Rightarrow$

$$E = \frac{1}{2}M\omega^2u^2\sum_s \sin^2(\omega t - ksa)$$

$$+ \frac{1}{2}Cu^2\sum_s\left[-2\sin\left(\frac{2\alpha - ka}{2}\right)\sin\left(\frac{ka}{2}\right)\right]^2$$

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

time average of $\sin^2\alpha = \frac{1}{2}$, $\sin^2\left(\alpha - \frac{Ka}{2}\right) = \frac{1}{2}$

the time average per atom is:

$$E_0 = \frac{1}{4} M\omega^2 u^2 + C u^2 \frac{1}{2} (1 - \cos Ka))$$

$$\left\{ \begin{array}{l} \cos 2t = 1 - 2\sin^2 t \\ \sin^2 t = \frac{1 - \cos 2t}{2} \end{array} \right\}$$ use this identity here

now, the dispersion relation is:

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

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

and hence $$E_0 = \frac{1}{4} M\omega^2 u^2 + \frac{1}{2} C u^2 \left(\frac{M\omega^2}{2C}\right)$$

$$\boxed{E_0 = \frac{1}{2} M\omega^2 u^2}$$

(2) coupled eqns: $$-\omega^2 M_1 u = Cv(1+e^{-ika}) - 2Cu$$
$$-\omega^2 M_2 v = Cu(1+e^{+ika}) - 2Cv$$

for $K = \frac{\pi}{a}$, $e^{\pm i\pi} = -1$, so eqns become:

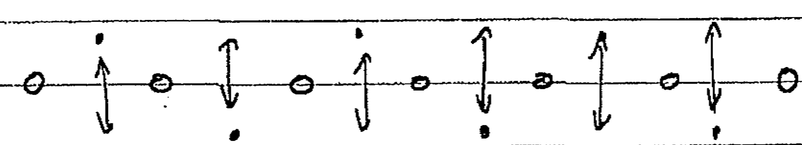
$$-\omega^2 M_1 u = -2Cu$$
$$-\omega^2 M_2 v = -2Cv$$

these eqns are decoupled. In other words, if

both $\begin{cases} u = 0 \\ v = v_0 e^{i(\omega t - Kas)} \end{cases}$ and $\begin{cases} u = u_0 e^{i(\omega t - Kas)} \\ v = 0 \end{cases}$

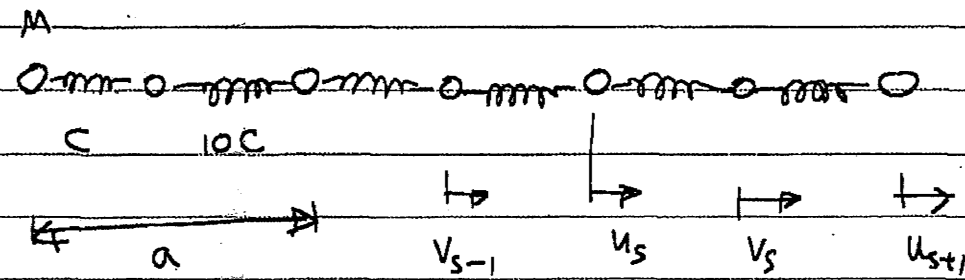
are solutions. So one sublattice can move while the other remains at rest.

note that for $K = \frac{\pi}{a}$, we have $e^{i(\omega t - \pi s)} = (-1)^s e^{i\omega t}$ so:



or vice versa

(3) We have the following:



eqns of motion are:

$$\begin{cases} M\ddot{u}_s = +C(V_s - u_s) + 10C(V_{s-1} - u_s) \\ M\ddot{V}_s = 10C(u_{s+1} - V_s) + C(u_s - V_s) \end{cases}$$

or

$$\begin{cases} M\ddot{u}_s = C(V_s + 10V_{s-1} - 11u_s) \\ M\ddot{V}_s = C(u_s + 10u_{s+1} - 11V_s) \end{cases}$$

now, look for solutions of form: $u_s = u\,e^{-i\omega t + isKa}$

$V_s = V\,e^{-i\omega t + isKa}$

then substituting,

$$\begin{cases} -M\omega^2 u = Cv(1 + 10e^{-iKa}) - 11Cu \\ -M\omega^2 v = Cu(1 + 10e^{+iKa}) - 11Cv \end{cases}$$

Solutions of ω are given by:

$$\begin{vmatrix} 11C - M\omega^2 & -C(1+10e^{-iKa}) \\ -C(1+10e^{+iKa}) & 11C - M\omega^2 \end{vmatrix} = 0$$

or

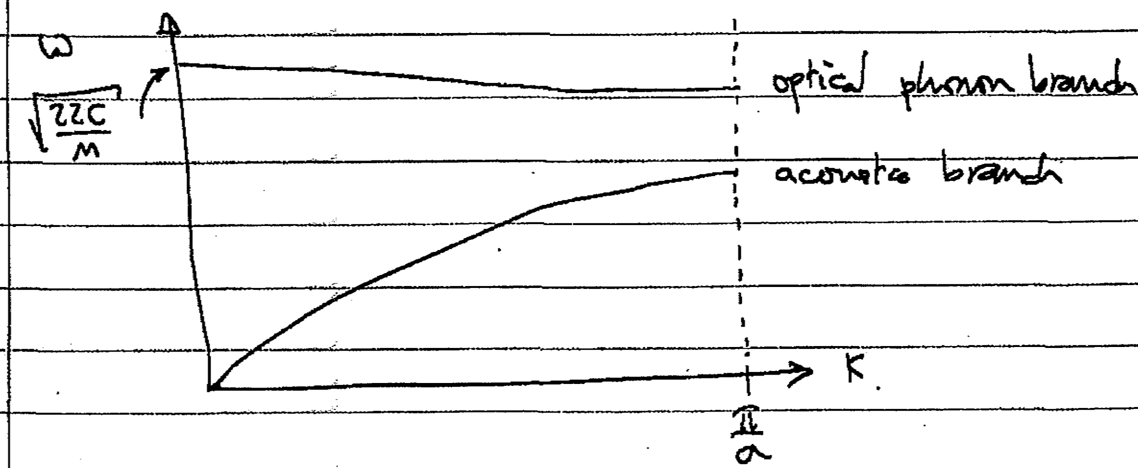
$$(11C - M\omega^2)^2 - C^2\left(1 + 10\left(e^{iKa} + e^{-iKa}\right) + 100\right) = 0$$

$$121C^2 - 22MC\omega^2 + M^2\omega^4 - 101C^2 - 20C^2\cos Ka = 0$$

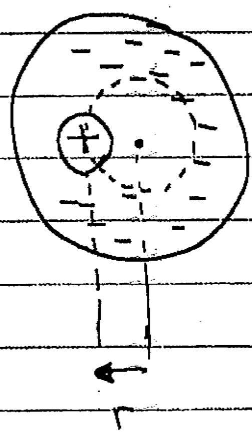
$$\Rightarrow M^2\omega^4 - 22MC\omega^2 + 20C^2(1 - \cos Ka) = 0$$

$$\omega^2 = \frac{22MC \pm \sqrt{(22MC)^2 - 400M^2C^2(1-\cos Ka)^2}}{2M^2}$$

$$\boxed{\omega^2 = 11\frac{C}{M} \pm \sqrt{\left(11\frac{C}{M}\right)^2 - 2\left(10\frac{C}{M}\right)^2 \sin^2\left(\frac{Ka}{2}\right)}}$$



(4)



electric field at ⊕ nucleus is equivalent to that of a single point ⊖ charge at distance r where charge is

$$Q = \rho \, \tfrac{4}{3}\pi r^3 = \frac{-3e}{4\pi R^3}\left(\tfrac{4}{3}\pi r^3\right) = -e\left(\frac{r}{R}\right)^3$$

so force is $F = +eE = +\frac{eQ}{r^2} = \frac{-e^2 r}{R^3}$

and eqn of motion is: $M\ddot{r} + \frac{e^2}{R^3} r = 0$

(a) so $\boxed{\omega = \sqrt{\frac{e^2}{MR^3}}}$

(b) for Na metal, density of conduction electrons is:

$$\rho = 2.65 \times 10^{22}\ \text{cm}^{-3} = \frac{1}{\frac{4}{3}\pi R^3}$$

$$\Rightarrow R = 2.08\ \text{Å}$$

$$\omega^2 = \frac{e^2}{MR^3} = \frac{(4.8 \times 10^{-10}\ \text{esu})^2}{\left(\frac{23\,g}{mol}\right)(6.022 \times 10^{+23}\ \text{mol}^{-1})^{-1}(2.08 \times 10^{-8}\ \text{cm})^3}$$

$$\Rightarrow \boxed{\omega = 2.6 \times 10^{13}\ \text{sec}^{-1}}$$

(c) $\omega = vK$

roughly, we can assume the above corresponds to a single atom or to $K = \frac{\pi}{a}$ in a linear chain

Then $v = \frac{\omega}{K} = \frac{\omega a}{\pi}$

where $a \simeq 3.6\ \text{Å}$

so $v \approx (2.6 \times 10^{13}\ \text{sec}^{-1})(3.6 \times 10^{-8}\ \text{cm})/\pi$

$$\boxed{\approx 3 \times 10^{5}\ \text{cm/sec}}$$