Phys 4050 Assignment 3

1. Vibrations of square lattice. Consider transverse vibrations of a planar square lattice of rows and columns of identical atoms and let u_{lm} denote the displacement normal to the plane of the lattice of the atom in the lth column and mth row (See figure below). The mass of each atom is M. Assume force constants such that the equation of motion is

$$M(d^2u_{lm}/dt^2) = C[(u_{l+1,m} + u_{l-1,m} - 2u_{lm}) + (u_{l,m+1} + u_{l,m-1} - 2u_{lm})] \ .$$

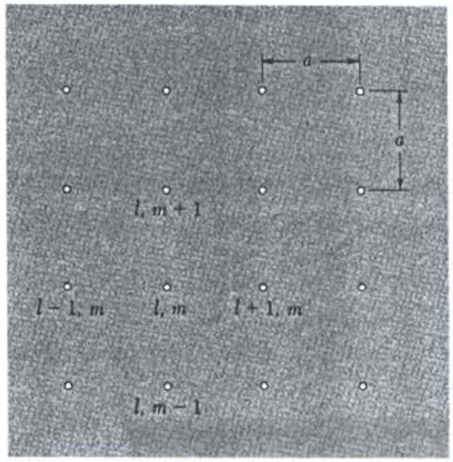

Figure 13 Square array of lattice constant a. The displacements considered are normal to the plane of the lattice.

a) Assume solutions of the form

$$u_{lm} = u(0)\exp[i(lK_x a + mK_y a - \omega t)]$$

where a is the spacing between nearest neighbour atoms. Show that the equation of motion is satisfied if

$$\omega^2 M = 2C(2 - \cos K_x a - \cos K_y a)$$

b) Show that the region of K space for which independent solutions exist may be taken as a square of side $2\pi/a$. This is the first Brillouin zone of the square lattice. Sketch ω vs. K for $K = K_x$ with $K_y = 0$ and for $K_x = K_y$.

2. 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 neighbour interaction c.

a) Show that the total energy of the wave is

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

where s runs over all atoms.

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

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

3. Atomic vibrations in a metal. Consider point ions of mass M and charge e immersed in a uniform sea of conduction electrons. 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

b) Estimate the value of this frequency for sodium.

c) Using the above results, estimate the order of magnitude of the velocity of sound in the metal.

4. Density of modes for a monatomic linear lattice.

a) From the dispersion relation derived for a monatomic linear lattice of N atoms with nearest neighbour interactions, show that the density of modes is

$$D(\omega) = \frac{2N}{\pi} \frac{1}{(\omega_m^2 - \omega^2)^{1/2}}$$

where ω_m is the maximum frequency.

b) Suppose that an optical phonon branch has the form $\omega(K) = \omega_o - AK^2$ near $K = 0$ in three dimensions. Show that

$$D(\omega) = \left(\frac{L}{2\pi}\right)^3 \frac{2\pi}{A^{3/2}} (\omega_o - \omega)^{1/2} \quad \text{for } \omega < \omega_o$$

$$D(\omega) = 0 \quad \text{for } \omega > \omega_o$$

5. Heat Capacity of layer lattice. Consider a dielectric crystal made up of layers of atoms, with rigid coupling between layers so that the motion of the atoms is restricted to the plane of the layer. Show that the phonon heat capacity in the Debye approximation in the low temperature limit is proportional to T^2.