489 Spring 2004 Homework 4

Due Monday, Feb. 23, 2004

1. BCC Lennard-Jones solid. This problem is analogous to FCC, covered in class.
   (a) Write down the energy for a BCC solid of interatomic spacing r in terms of the usual LJ parameters σ and ϵ. Show that for a BCC Bravais lattice, $\sum_j r^{-6} = 12.25$ and $\sum_j r^{-12} = 9.11$.
   (b) Derive the interatomic spacing of the equilibrium solid, R_0.
   (c) Derive the cohesive energy. Is it greater or less than FCC?
   (d) Derive the bulk modulus, B.

2. Work the first part of A&M 20.3. That is, derive the formulas for the relative cohesive energies of different structures. With this form, evaluate the relative cohesive energies of NaCl, CsCl and ZnS for m = 6, 8 and 10 (typical values according to table 20.6). When is NaCl the stable structure?

3. Madelung sum in 2D. For the square lattice in 2D (composed of + and - charges as shown below), find the Madelung constant by summing over neutral shells. You will need to break the ion charges into fractional charges (0.25 for inside corner, 0.75 for outside corner etc). Carry the sums far enough to show that of the series appears to converge to a number between 1.55 and 1.65. (The exact result is $\alpha = 1.6155$.)

$$\begin{array}{cccccccc} + & - & + & - & + & - & + & - \\ - & + & - & + & - & + & - & + \\ + & - & + & - & + & - & + & - \\ - & + & - & + & - & + & - & + \\ + & - & + & - & + & - & + & - \\ - & + & - & + & - & + & - & + \end{array}$$

4. A&M problem 22.2 (a), (b) and (c).
   (d) explain why the $M_1 = M_2$ case is identical to the monatomic linear chain, and what happens to the optic and acoustic branches.

5. Consider a monatomic square lattice with nearest neighbor distance a. The motion of the atoms is also restricted to be in the two-dimensional plane. Let the mass of each atom be M and assume there are interactions between first neighbors $\phi_1(r)$ and between second neighbors $\phi_2(r)$, where r is the distance between any pair of atoms.
   (a) Find explicit expressions for the dispersion curves $\omega(\mathbf{k})$ for $\mathbf{k}$ in the $(1, 0)$ direction. Do the motions of the atoms decouple into strictly longitudinal or transverse for k in this direction? Support your answer.
   (b) Give expressions for the velocities of sound in the (1,0) direction.
   Hint: Convince yourself that for this direction the problem is similar to a linear chain.