Homework III

1. Consider a two dimensional crystal containing identical atoms of mass M, which occupy the sites of square lattice of side a in the absence of phonon excitations. Let the sides of the square unit cell be parallel to the x and y directions respectively, with an atom at the origin. Let the force constant for nearest neighbors (a distance a apart) be K_1, and the force constant for next-nearest neighbors (a distance $a\sqrt{2}$ apart) be K_2; assume that all other force constants vanish. Assume that only in-plane motions of the atoms are allowed.

   (a) Calculate the dynamical matrix
   $$D^{\alpha\beta}(\vec{k}) = \frac{1}{M}\sum_m A^{\alpha\beta}_{nm} e^{i\vec{k}\cdot(\vec{R}_{m0}-\vec{R}_{n0})}.$$

   (b) Calculate the frequencies and polarization vectors for phonons propagating in the x direction ($k_y = 0$) as a function of k_x.

   (c) Discuss the pathology that occurs in the previous part when $K_2 = 0$. Why does it occur?

2. In this problem you will be asked to fill in the missing steps in the presentation in class of lattice dynamics in three dimensions. For simplicity consider a structure with one atom of mass M per unit cell. Let the time dependent position of the n^{th} atom be $\vec{R}_n(t) = \vec{R}_{n0} + \delta\vec{R}_n(t)$, where R_{n0} are the equilibrium positions, assumed to be points on a Bravais lattice.

   (a) Assuming that the interaction between atoms is representable by a sum of pair potentials between each atom $U(|\vec{R}_n - \vec{R}_m|)$, show that to quadratic order in $\delta\vec{R}_n$, the lattice Hamiltonian may be written
   $$H = \sum_n \frac{P_n^2}{2M} + \frac{1}{2}\sum_{nm} \delta\overrightarrow{R}_n \cdot \overleftrightarrow{A}_{nm} \cdot \delta\overrightarrow{R}_m + \text{constant}.$$
   Derive expressions for $\overleftrightarrow{A}_{nm}$ for the cases $n \neq m$ and $n = m$. Do not hesitate to use component notation, if you prefer.

   (b) From the equation of motion for $\delta\overrightarrow{R}_n$, show that the three normal mode frequencies $\omega_{\vec{k}\mu}$ and the corresponding polarization vectors $\vec{u}_{\vec{k}\mu}$ ($\mu = 1, 2, 3$) are given by the solution to the eigenvalue problem
   $$\omega^2_{\vec{k}\mu}\vec{u}_{\vec{k}\mu} = \overleftrightarrow{D}(\vec{k}) \cdot \vec{u}_{\vec{k}\mu},$$
   where
   $$\overleftrightarrow{D}(\vec{k}) = \frac{1}{M}\sum_m \overleftrightarrow{A}_{nm} e^{i\vec{k}\cdot(\vec{R}_{n0}-\vec{R}_{m0})}.$$

3. Read Sander section 5.1.6, pp. 86–87, and then do Sander problem 4 on page 112. Begin by stating the relationship between $\overleftrightarrow{D}(\vec{k})$ above and Sander's $\mathbf{G}(\mathbf{k})$.

4. Read Marder pp. 326–336 and Sander pp. 107–110, 42–44.