Exercise set 3 (due Thursday Feb 5)

(Note: this will take much longer than your previous homeworks, so you need to start working on it as soon as you can)

- 1 Consider a square lattice of parameter a in which nearest neighbor atoms are connected with springs of constant k such that the potential energy of the lattice can be written as:

  $$V = \sum_{<ij>} \frac{1}{2} k(|\vec{r}_{ij}| - a)^2$$

  for **nearest neighbor** atoms i and j belonging to the lattice. $\vec{r}_i(t)$ is the dynamical variable showing the position of atom i at time t, and $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$.

  Note that this is NOT a harmonic potential, so you will have to Taylor expand it up to second order and then use the harmonic form in your equations of motion (in the expression for the force, keep only the terms linear in the displacements in the expansion of the force in powers of the displacements.)

  Write down Newton's equation of motion for an atom i, assuming it only moves in the plane of the lattice.

  Now use the normal mode coordinates $u_k = \sum_i u_i \frac{e^{ik.R_i}}{\sqrt{N}}$ and rewrite the linearized equations of motion in terms of u_k and show that now the modes are decoupled.

  Deduce the phonon dispersion relation of this lattice using the plane wave form as a solution.

  How many branches do we have? Plot the dispersion relation along the $\Gamma \to X$, $X \to M$ and $M \to \Gamma$ directions where $X(\pi/a, 0)$ and $M(\pi/a, \pi/a)$. Discuss your results.

  Use the Debye model to calculate the heat capacity of this system:

  First find DOS and the Debye frequency, then write down the expression for the heat capacity per mode and sum over all modes to get C_v versus T. How does it vary with the temperature? Was that expected according to what we saw in class? and why?

  Make a plot of C_v versus T.

- 2 Kittel Chapter 5, problem 1 (page 128)

- 3 Kittel Chapter 6, problem 1 (page 157). Do the same calculation in 2D.

- 4 Kittel Chapter 6, problem 2 (page 157)

- 5 Kittel Chapter 6, problem 3 (page 157)