Homework 3
289A Statistical mechanics of crystalline solids
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Question 1: Pick a nearest neighbor pair on a triangular lattice and determine a symmetry invariant form for its force constant. You can do this by first determining the point group that leaves the pair cluster unchanged. Then express the force constant matrix as a sum over a tensor basis:

$$\begin{pmatrix} \Phi_{xx} & \Phi_{xy} \\ \Phi_{yx} & \Phi_{yy} \end{pmatrix} = \Phi_{xx}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \Phi_{xy}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \Phi_{yx}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \Phi_{yy}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Apply the Reynolds operator to each of the tensor basis elements using the point group that leaves that cluster invariant (note that if you use symmetry operations that exchange the sites of the pair, you need to apply a transpose to your force constant matrix). This will yield a smaller set of symmetry invariant tensor basis elements.

Question 2: Determine the dynamical matrix for a triangular lattice assuming only nearest neighbor spring constants. As force constants, use your results from question 1. Leave the dynamical matrix in parametric form (i.e. in terms of the independent coefficients of the force constants).

Question 3: Determine the reciprocal lattice for a triangular lattice. Construct the Brillouin zone and trace out high symmetry directions in the Brillouin zone.

Question 4: Since the dynamical matrix has dimensions 2x2, you can come up with analytical expressions for its eigenvalues. The vibrational frequencies are the square root of these eigenvalues. Plot the dispersion curves along high symmetry directions for a particular set of numerical values for the force constants.

Question 5: Pick a non-zero k-point in the Brillouin zone (e.g. a high symmetry point) and on an ideal triangular grid, plot the displacement field corresponding to the different eigenvectors at that k-point.