1 Dynamical Matrix

The functions written to generate the tensor basis for homework 2 have been integrated into new routines to calculate the dynamical matrix for an arbitrary 2 dimensional structure as a function of force constants and k-vectors. The calculated dynamical matrix is implemented in the following questions to generate the required dispersion curves and displacement fields.

2 Reciprocal Lattice

The reciprocal lattice for the honeycomb structure is shown in fig. 1. The vectors for the reciprocal lattice are perpendicular to the realspace vectors and were computed in one step with

$$\mathbf{L}^{\star} = 2\pi \left(\mathbf{L}^{-1}\right)^{\intercal} \tag{1}$$

Because the honeycomb structure shares the same triangular lattice as the previous homework assignment, the result is identical.

3 Dispersion curves

The dynamical matrix and corresponding eigenvalues and eigenvectors were calculated numerically. A high symmetry path in reciprocal space was traced out to get the values of frequencies at various k-points using arbitrarily selected force constants.

4 Displacement fields

Using the eigenvectors at the high symmetry k-point $\mathbf{M}$, four displacement fields can be generated for the honeycomb structure. Each displacement field corresponds to the activation of a single frequency at $\mathbf{M}$, with each eigenvector describing the displacement of the two basis atoms.

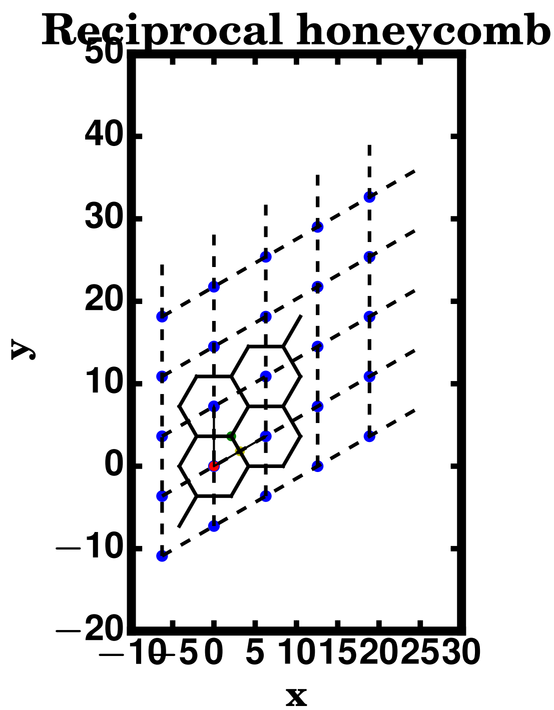

Figure 1: Reciprocal lattice of honeycomb structure

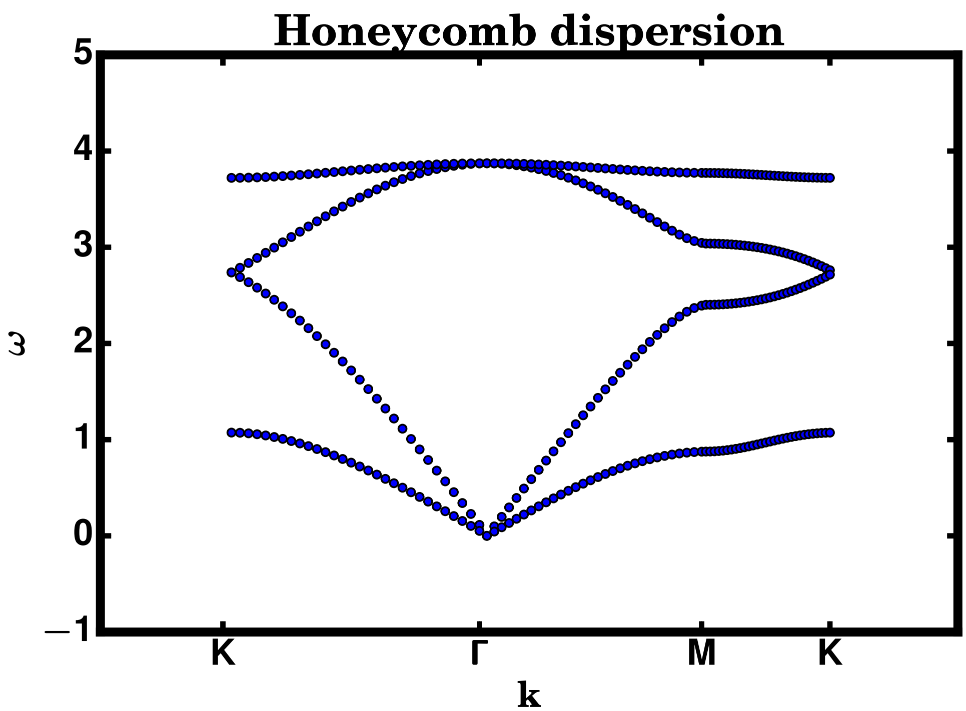

Figure 2: Dispersion curves for honeycomb structure following a high symmetry path in reciprocal space

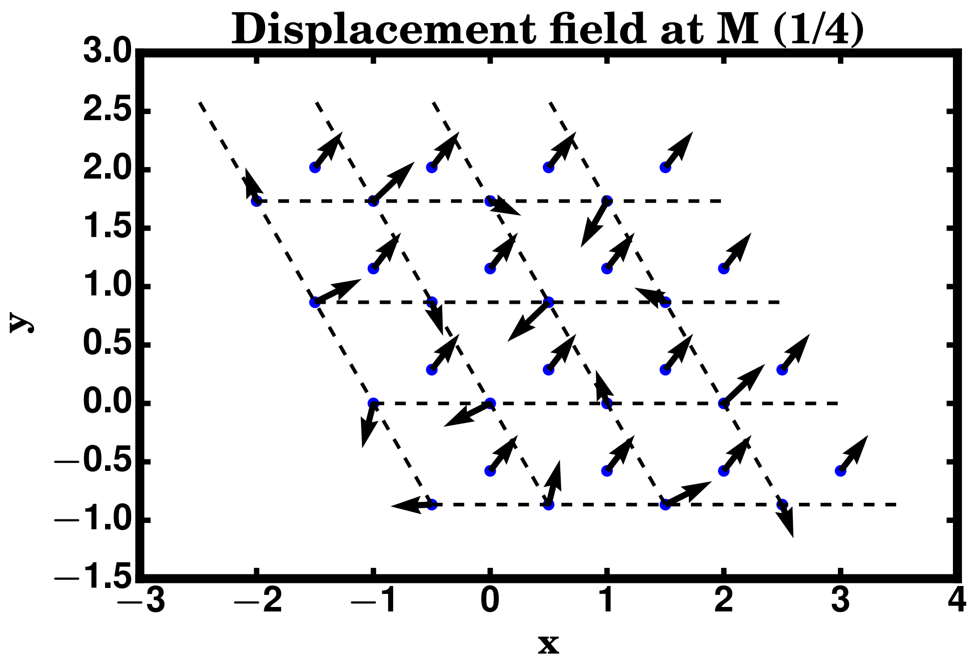

Figure 3: First displacement field at **M**

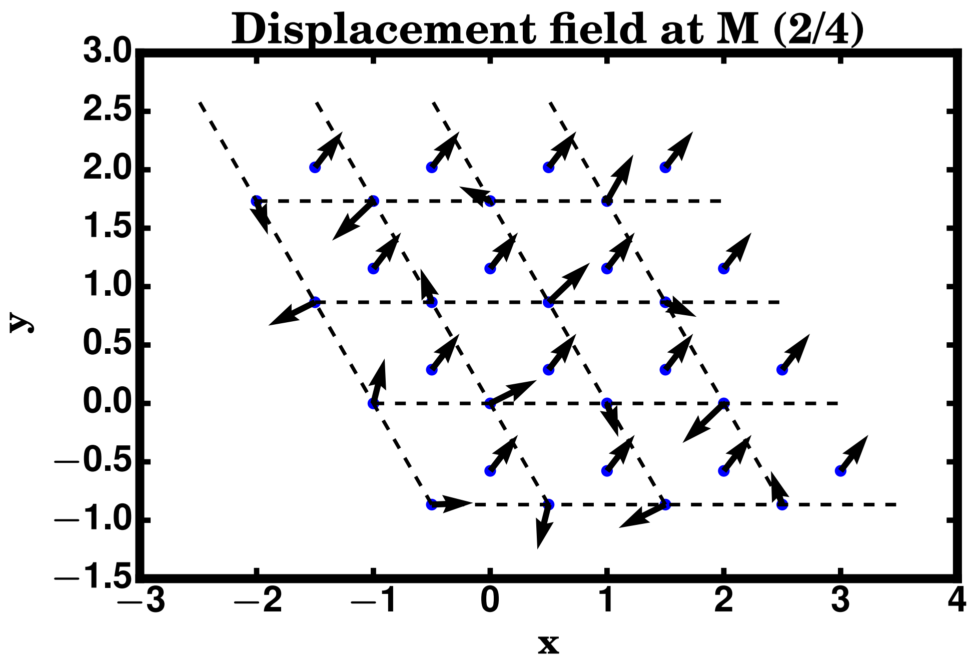

Figure 4: Second displacement field at $\mathbf{M}$

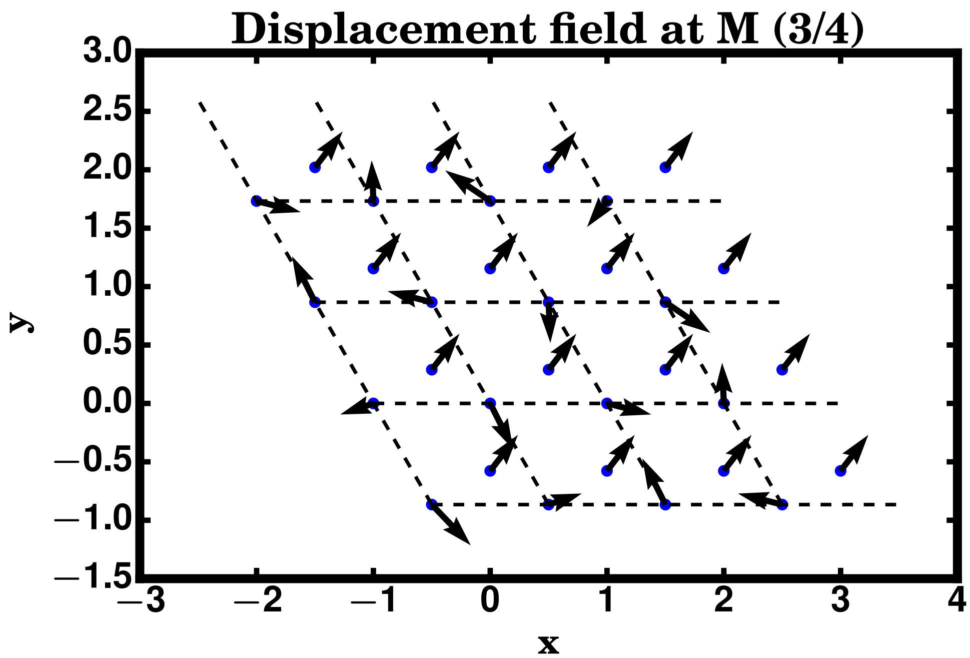

Figure 5: Third displacement field at **M**

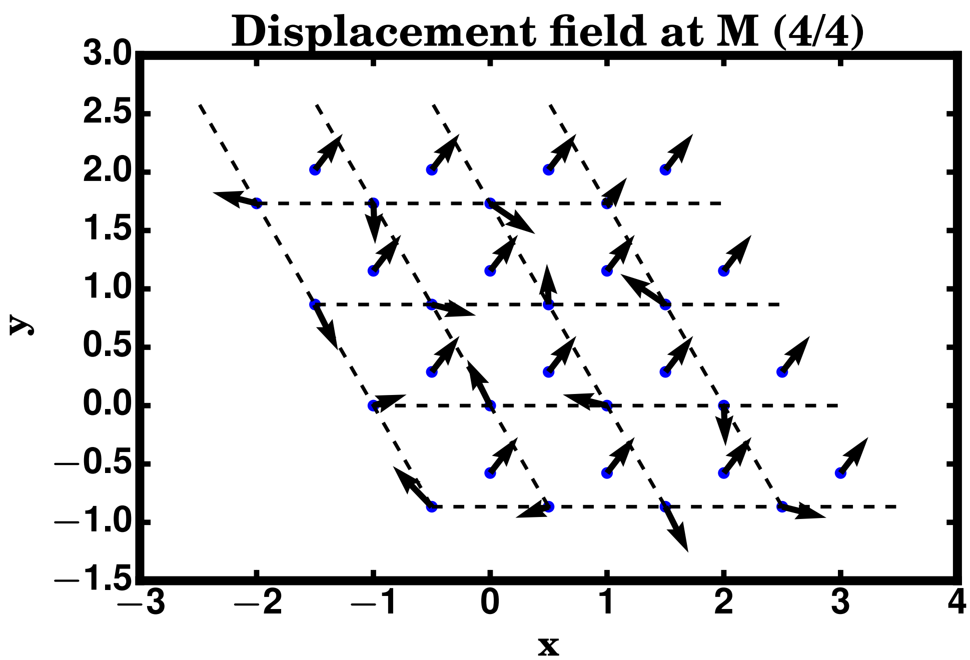

Figure 6: Fourth displacement field at **M**