Triangular lattice summary

March 28, 2021

Minor intro

A triangular lattice is defined by two primitive vectors, denoted a_1, a_2, and a lattice constant labled a. Here we will use

$$a_1 = a\hat{x}, a_2 = \frac{a}{2}\left(\hat{x} + \sqrt{3}\hat{y}\right)$$

By definition one gets the reciprocal lattice with primitive vectors

$$b_1 = \frac{2\pi}{a}\left(\hat{x} - \frac{1}{\sqrt{3}}\hat{y}\right), b_2 = \frac{4\pi}{\sqrt{3}}\hat{y}$$

Using these the first Brillouin zone is defined by a hexagon with vertices at:

$$\pm\frac{4\pi}{\sqrt{3}}\hat{y}, \pm\frac{2\pi}{a}\left(\hat{x} \pm \frac{1}{\sqrt{3}}\hat{y}\right)$$

Disperssion relation

Assuming every lattice vertex contains an atom with mass m, and a z axis NN interaction of strength D. Denote the displacement from equilibrium by u, one gets the following force equation:

$$m\ddot{u} = \sum_{i=1}^{6} D(u_i - u)$$

where u_i is the displacement of the nearest neighbour, substituting $u = Ae^{i(\omega t - kr)}$ we get a disperssion relation:

$$\omega^2(k_x, k_y) = \left(\frac{D}{m}\right)\left(6 - 2cosk_x a - 4cos\frac{k_x a}{2}cos\frac{\sqrt{3}k_y a}{2}\right)$$

knowing D, m one can calculate the phonon frequency at every point in BZ1.

Finding eigen-frequencies numerically

First we create a linear system of equations that is true for each vertex, similiar to the dispersion relation

$$m\ddot{u} = \sum_{i=1}^{6} D(u_i - u)$$

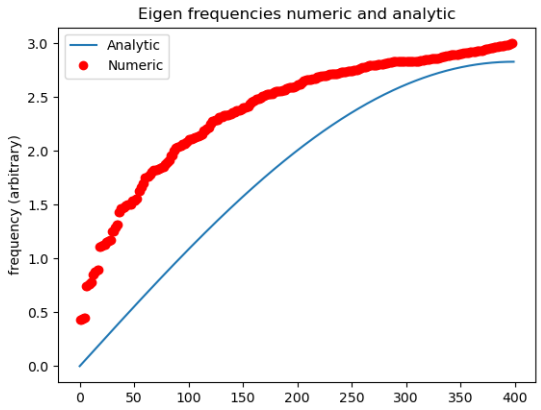
Next we assume a solution of the form $u = Ae^{i\omega_j t}$, substituting we get the following eigenvalue problem

$$(A - \omega^2 I)U = 0$$

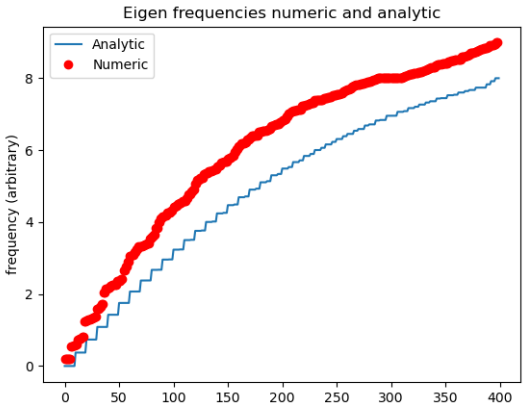
where U is a vector where each index corresponds to a node and A is the interaction matrix, by solving this eigenvalue problem numerically we get the lattice eigenfrequencies

This is where things go wrong

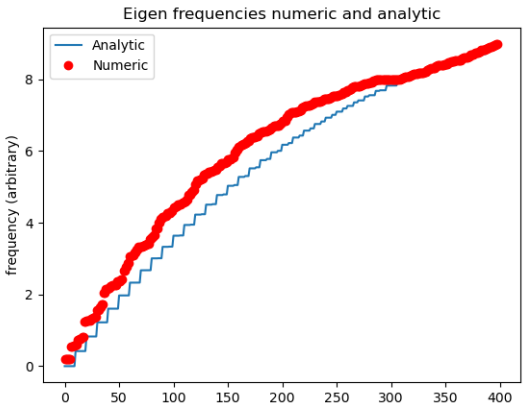
Once we try to calculate the frequncies in both ways things don't go as planned, for the numeric part it is a matter of simply finding eigen values, easy enough, the analytical solution is where things get weird, first one must choose the coordinates to calculate in BZ1, I tried two ways both do not produce similiar results to the numerical version:
1. calculate the frequencies along a line in BZ1, for example take the line $\lambda(0, \frac{2\pi}{\sqrt{3}a})$ from Γ to the edge of BZ produces the following plot:



2. calculating all points enclosed in the largest circle contained in BZ1 yields the following plot



this is better, once we mess around with interaction strength for the analytic one we get



while the last plot is really close, we are still not getting exactly the same values, and we had to cheat and slightly scale the plots differently to get the line shapes.