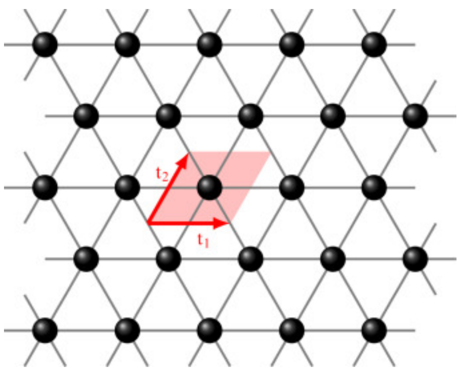
Triangular lattice summary

April 9, 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

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

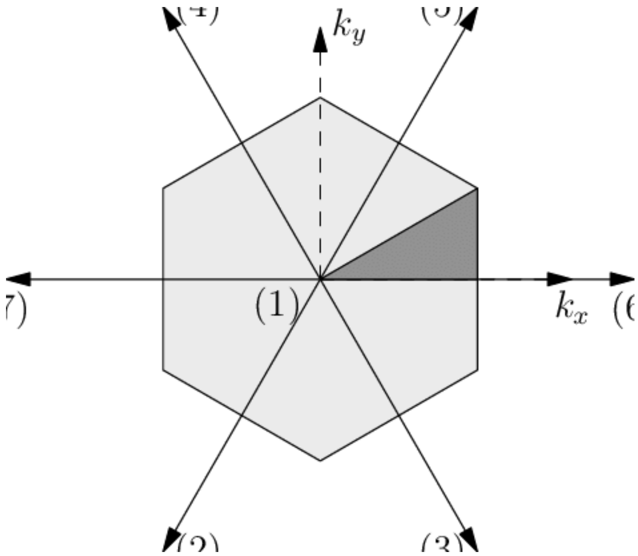


By definition one gets the reciprocal lattice with primitive vectors

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

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.
We impose periodic boundary conditions here, meaning every lattice point indeed has 6 neighbours.
for example for a 4*4 lattice the matrix A with $m = D = 1$ has the following form:

```
[[ 6. -1.  0.  0. -1. -1.  0.  0.  0.  0.  0. -1. -1.  0.  0. -1.]
 [-1.  6. -1.  0.  0. -1. -1.  0.  0.  0.  0.  0. -1. -1.  0.  0.]
 [ 0. -1.  6. -1.  0.  0. -1. -1.  0.  0.  0.  0.  0. -1. -1.  0.]
 [ 0.  0. -1.  6. -1.  0.  0. -1. -1.  0.  0.  0.  0.  0. -1. -1.]
 [-1.  0.  0. -1.  6. -1.  0.  0. -1. -1.  0.  0.  0.  0.  0. -1.]
 [-1. -1.  0.  0. -1.  6. -1.  0.  0. -1. -1.  0.  0.  0.  0.  0.]
 [ 0. -1. -1.  0.  0. -1.  6. -1.  0.  0. -1. -1.  0.  0.  0.  0.]
 [ 0.  0. -1. -1.  0.  0. -1.  6. -1.  0.  0. -1. -1.  0.  0.  0.]
 [ 0.  0.  0. -1. -1.  0.  0. -1.  6. -1.  0.  0. -1. -1.  0.  0.]
 [ 0.  0.  0.  0. -1. -1.  0.  0. -1.  6. -1.  0.  0. -1. -1.  0.]
 [ 0.  0.  0.  0.  0. -1. -1.  0.  0. -1.  6. -1.  0.  0. -1. -1.]
 [-1.  0.  0.  0.  0.  0. -1. -1.  0.  0. -1.  6. -1.  0.  0. -1.]
 [-1. -1.  0.  0.  0.  0.  0. -1. -1.  0.  0. -1.  6. -1.  0.  0.]
 [ 0. -1. -1.  0.  0.  0.  0.  0. -1. -1.  0.  0. -1.  6. -1.  0.]
 [ 0.  0. -1. -1.  0.  0.  0.  0.  0. -1. -1.  0.  0. -1.  6. -1.]
 [-1.  0.  0. -1. -1.  0.  0.  0.  0.  0. -1. -1.  0.  0. -1.  6.]]
```

Quantization

Consider a 20 by 20 lattice (400 vertices overall) with periodic boundary conditions, k value quantization is given by Bloch theorem

$$f(r + Na_1) = e^{ikNa_1} f(r) = f(r) \to kNa_1 = 2\pi m \to k = \frac{m}{N} b_1$$

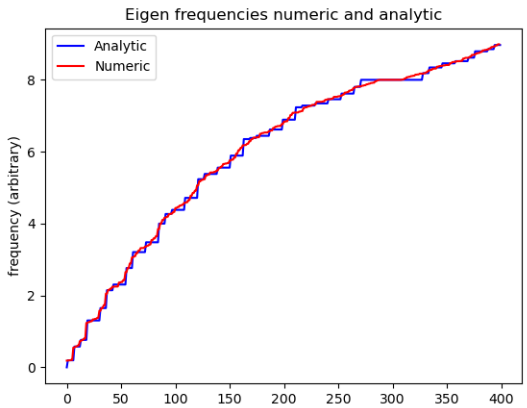
meaning in BZ1 of our lattice

$$k = \frac{p_1}{20} b_1 + \frac{p_2}{20} b_2$$

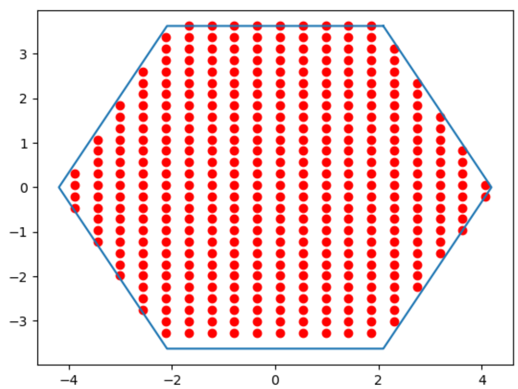
where $p_1, p_2 \in \pm\{0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10\}$
using these k vectors in the disperssion relation we get all possible frequencies.

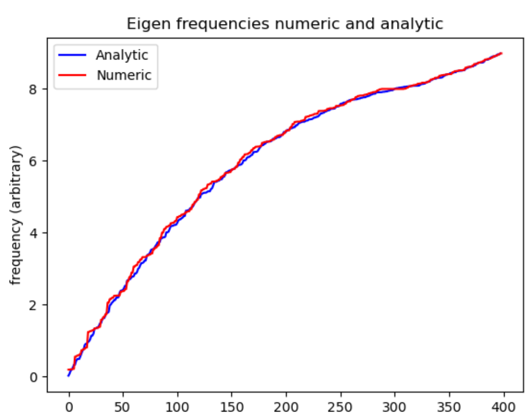
Results

Frequencies are sorted from smallest to largest as the numeric calculation does not use reciprocal lattice considerations



this is simillar but not great, using a uniform distribution around BZ1 yields the following results





this is better but the results are not exactly the same.
Next is a contour plot of the frequncies around BZ1