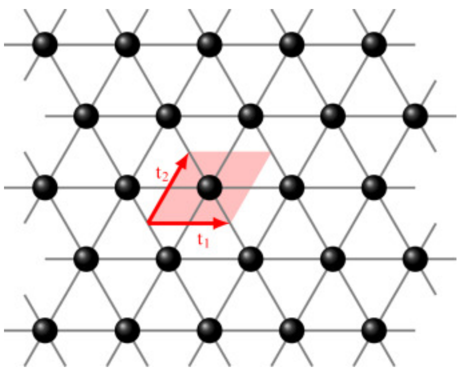
Triangular lattice summary

June 5, 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

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

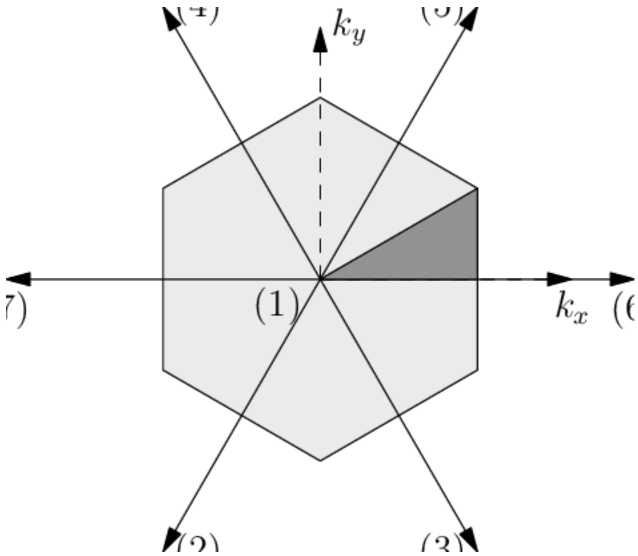


By definition one gets the reciprocal lattice with primitive vectors

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

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:

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

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

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

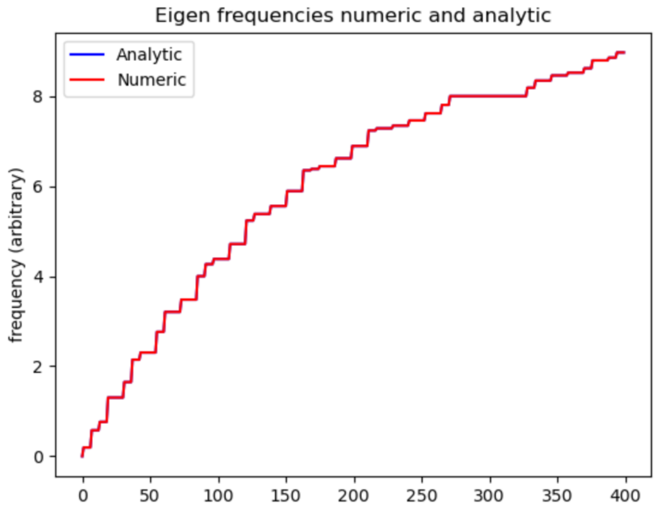
meaning in BZ1 of our lattice

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

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



Here we can see the eigen values are the same up to floating point error (order of 10^{-15}) and we consider this an exact match.
Recall that while calculating the analytical solution we assumed $u = Re(Ae^{i(\omega t - kr)})$ meaning solutions are linear combinations of:

$$cos(\omega t - kr), sin(\omega t - kr)$$

In order to varify that the numeric solutions are also of this form we recall a theorem from linear algebra.
1. (find exact theorem) Let A,B be two linearly independent sets with the same cardinality, if $B \subset SpanA$ then $A \subset SpanB$
2. Let $a_1, ..., a_n$ be an orthonormal basis and $b = \sum b_i a_i$ then $\langle b, a_i \rangle = b_i$ further $||b||^2 = \sum_{j=1}^{n} |\langle b, a_i \rangle|^2$
By using the orthonormal set of vectors supplied numerically we can show that the planar wave solutions are equivalent to the numeric one iff for a set $\{v_1, ...v_n\}$ eigenvectors with the same eigen values and the set $\{u_1, ...u_n\}$ of normalized planar waves with momentum k corresponding to the same eigen value the following equation holds for all $i \in [n]$:

$$\sum_{j=1}^{n} |\langle v_j, u_i \rangle|^2 = 1$$

Indeed checking each eigenvalue and all coresponding k values we conclude that the above equation hold for all k values.