Bachelor Thesis Project

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↑↓ Characterization of "J-Q" Classical Magnets ↓↑

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What one man calls God, another calls the laws of physics.

- *Nikola Tesla*

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1. INTRODUCTION

Magnetism in a matter is born out of quantum mechanics of atoms and molecules. Almost every system exhibits some kind of magnetism - weak or strong. Magnetic systems can sometimes be described by classical Heisenberg model ([1], [2]) in which the Hamiltonian (for a 0 external magnetic field) is given by the following equation:

$$\mathcal{H} = \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} J_{ij} \mathbf{S}_i . \mathbf{S}_j \tag{1.1}$$

In the above equation, J_{ij} is the coupling constant whereas $\mathbf{S}_i$ is the unit spin vectors at the lattice point i. The factor of $\frac{1}{2}$ is introduced to check the double counting. Based on the value of the coupling constant magnetism can be classified into two types: (i) Ferromagnetism ($J_{ij} < 0$) and (ii) Antiferromagnetism ($J_{ij} > 0$) (other types of magnetism also exists). In ferromagnets, due to negative value of J_{ij} all the spins align themselves in the same direction to minimise the energy of the system. The properties of ferromagnetic materials have been studied in the past and is very well understood.

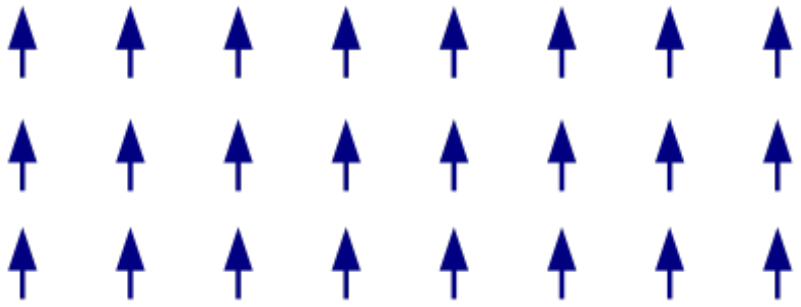


Fig. 1.1.: Ferromagnetism ($J_{ij} < 0$)

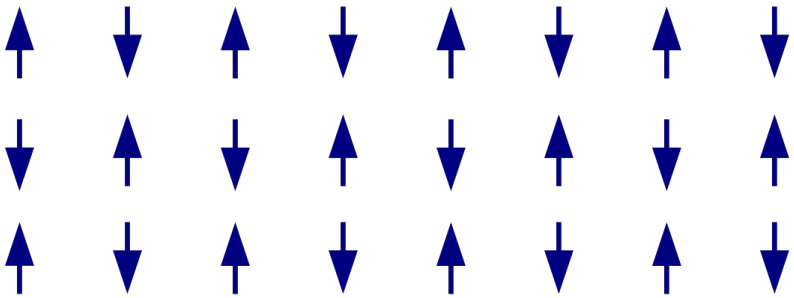
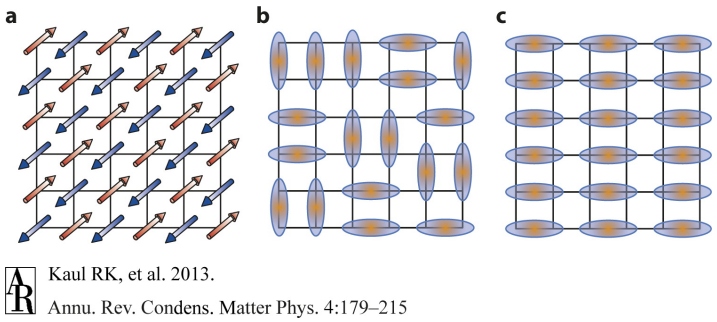
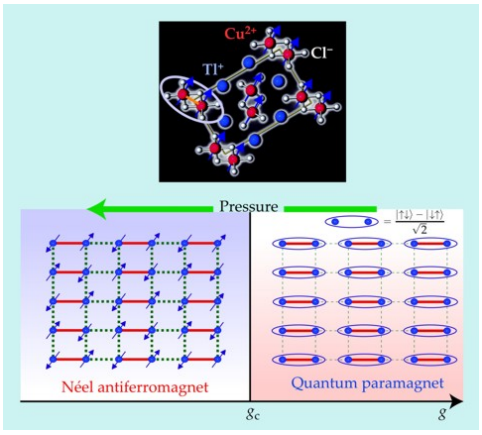


Fig. 1.2.: Anti-ferromagnetism ($J_{ij} > 0$)

Antiferromagnetism ($J_{ij} > 0$) is one of the kinds of magnetism that matter exhibits which was first discovered by M. Louis Néel [3]. When no external magnetic field is acting upon the crystal, the atomic spins get themselves aligned in the direction opposite to the direction of nearest neighbouring spins. This makes the net magnetic moment of the crystal equal to 0. However, in small crystals, due to defects, deviation from the configuration could take place giving birth to a small magnetic moment. Also, above Neel temperature (Curie temperature for anti-ferromagnetic materials), the antiferromagnetic substance loses its configuration as the heat energy disorders the atomic spins.



(a) *Source:* Fig 2, Kaul RK, 2013, *Ann. Rev. Cond. Matter Phys. 4:179-215*, [4]



(b) *Source:* Fig 2, Keimer, 2011, *Phys. Today*, [5]

Fig. 1.3.: Quantum Critically

$$H = \frac{1}{2} \sum_{\langle i,j,k,l \rangle} Q_{ijkl}(1 - \mathbf{S}_i.\mathbf{S}_j)(1 - \mathbf{S}_k.\mathbf{S}_l) \tag{1.2}$$

Quantum Criticality is defined as continuous phase transition at absolute 0 K. In this project, we study this criticality in classical regime (Eq. (1.2)) (Equation 17 & 19, [4]). We start with studying ferromagnetic and antiferromagnetic systems using classical Heisenberg Model. Then we try to understand the Luttinger-Tisza Method and obtain reciprocal lattice vector for various ground state configuration obtained at $T = 0K$. After verifying our results with previously formulated results we move forward to minimise the Hamiltonian obtained by including factors of quantum criticality (Eq. (1.2)).

All the simulations have been done on a two-dimensional crystal which has 4×4 lattice points with periodic boundary conditions to mimic the crystal up to infinity. The magnitude of $\mathbf{S}_i$ has been always taken unity to classically mimic the actual quantum system. The spins do have degree of freedom to rotate in all the 3-dimensions, but we have also included the case of 2-dimensional constrained spins.

Interactions only up to second nearest neighbouring atom have been considered for the sake of simplicity. We also assume that the coupling constant is same for the same kind of neighbours for all the spins, that is, for nearest neighbouring spins, value of J_{ij} is same for all the lattice points in the crystal and similarly, for next nearest neighbours, the coupling constant value is same for all.

2. ITERATIVE MINIMISATION

To find and understand the ground state spin configuration of a lattice we first follow the method of iterative minimization. This method, for a given state of the lattice, run for given number of iterations and relaxes the randomly chosen spin of the lattice to their ground state according to their local magnetic field. The procedure can be described by the following flowchart:

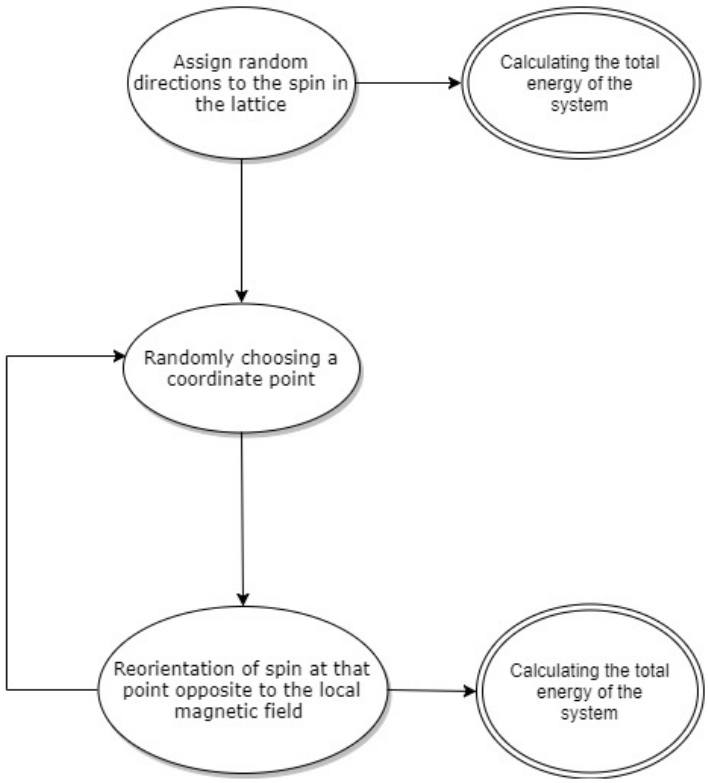


Fig. 2.1.: *Flowchart:* Method of Iterative Minimisation

The above flowchart is described as follows:

1. Firstly, we assign random directions to all the spin in the lattice. The magnitude of all the spins is always kept 1.

2. We then calculate the total energy of the system and after every iteration.

3. A lattice point is randomly chosen and for that point, the local magnetic field is calculated due to all the surrounding 8 spins.

4. The direction of randomly selected spin is reorientated in the direction opposite to the local magnetic field to minimize the energy.

5. The above process is repeated again from step 2 till the given number of iterations. The total number of iterations is kept between 300 - 1500, to ensure the minimization of the total energy of the system

We calculate the total energy of the system to ensure the convergence of the system to its ground state. The energy is calculated after each reorientation of the spins and plotted against the i^{th} iteration.

2.1 Local Magnetic Field & Spin Orientation

For our simulations, since we have taken spin-spin interactions only up to next nearest neighbors, local magnetic field at the location of randomly chosen spin is given as follows:

$$\mathbf{B} = J_1.\big(\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4\big) + J_2.\big(\mathbf{S}_5 + \mathbf{S}_6 + \mathbf{S}_7 + \mathbf{S}_8\big) \tag{2.1}$$

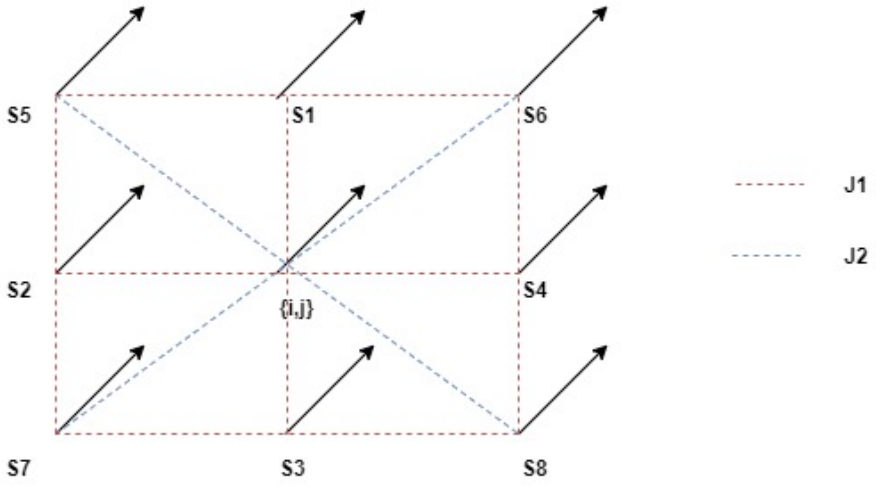


Fig. 2.2.: Local Magnetic Field at randomly chosen (i,j) due to interaction with its nearest 8-neighboring spins

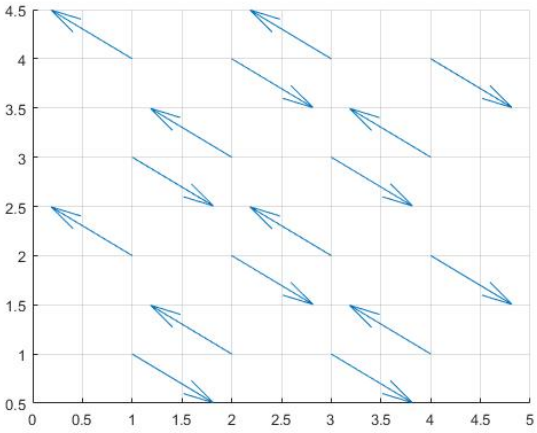
The randomly chosen spin $\left(\mathbf{S}_{ij}\right)$ is then orientated opposite to the direction of the magnetic field. Hence,

$$\widehat{\mathbf{S}}_{ij} = -\widehat{\mathbf{B}} \tag{2.2}$$

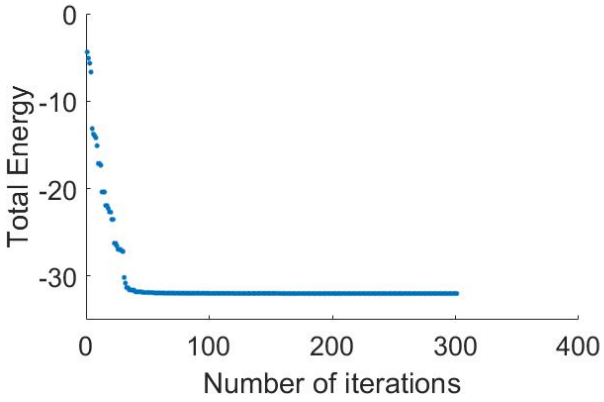
2.2 Simulations & Results

All the simulations were done for spin fixed in a 2-dimensional plane as well as for spins free to rotate in all the directions. The simulations were done for two cases in each of the above conditions- (i) $J_2 = 0$ and (ii) $J_2 \geq 0$, where J_1 was always kept greater than 0. The results of the simulations are as below.

Case 1: Spin constrained in a plane and $J_2 = 0$:



(a) Spin Orientations



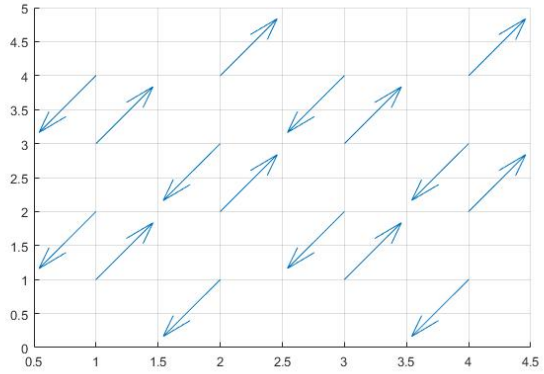
(b) Energy vs iterations

Fig. 2.3.: *Case 1:* Spins constrained in a plane, $J_2 = 0$ & $J_1 = 1$

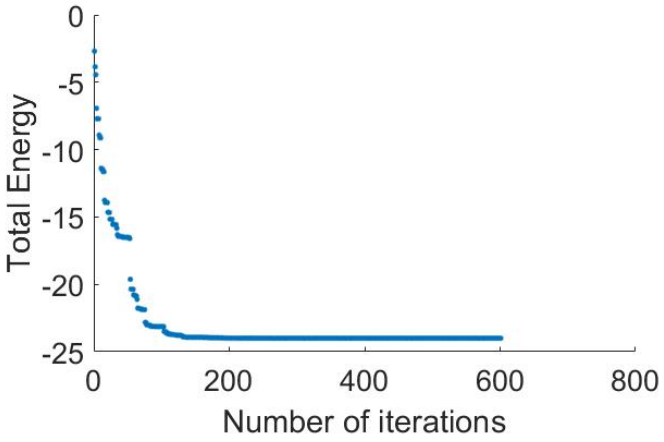
As the figure shows, when J_2 is equal to 0, all the spins align themselves opposite to the direction of neighboring spins. This is what we expect the orientation of spins for any anti-ferromagnetic crystal. As the energy vs number of iterations graph shows, our system have achieved is converging to ground state and has achieved it.

Case 2: Spin constrained in a plane and $J_2 \neq 0$:

Depending on the value J_2, the results of the simulation vary. If $J_2 < 0.4$ (approximately) then the ground state configuration of the spins remains almost same as the case when $J_2 = 0$.[1]



(a) Spin Orientations

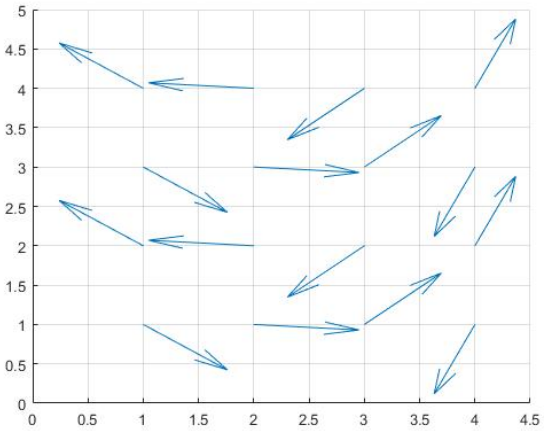


(b) Energy vs iterations

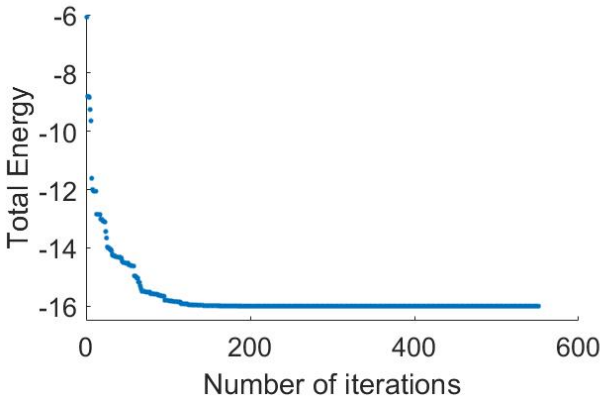
Fig. 2.4.: *Case 2.1:* Spins constrained in a plane, $J_2 = 0.25$ & $J_1 = 1$

For the case $J_2 > 0.4$, deviation from the ground state case of $J_1 = 0$ starts occurring, as shown below.

[1]In some of the cases, we have found that the total energy of the system increases with respect to the previous iteration for one to two points. This has been assumed to be a round-off error of MATLAB as the the increase in energy was of magnitude 0.01 units only.

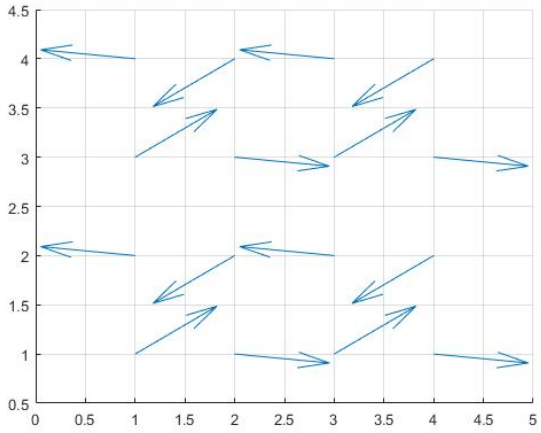


(a) Spin Orientations

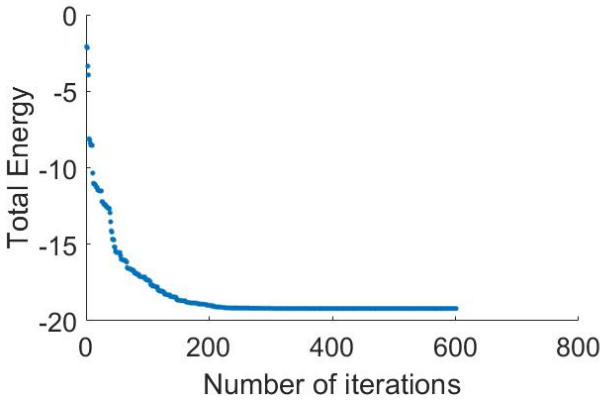


(b) Energy vs iterations

Fig. 2.5.: *Case 2.2:* Spins constrained in a plane, $J_2 = 0.5$ & $J_1 = 1$



(a) Spin Orientations

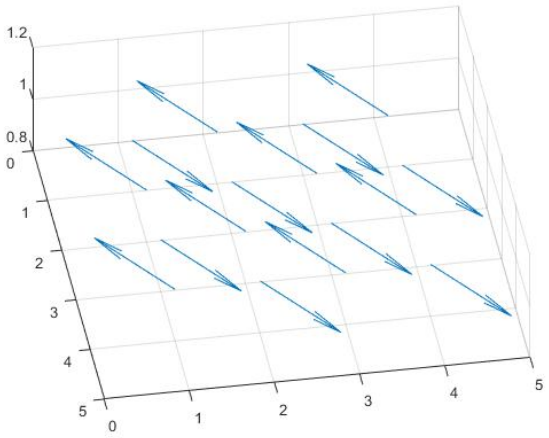


(b) Energy vs iterations

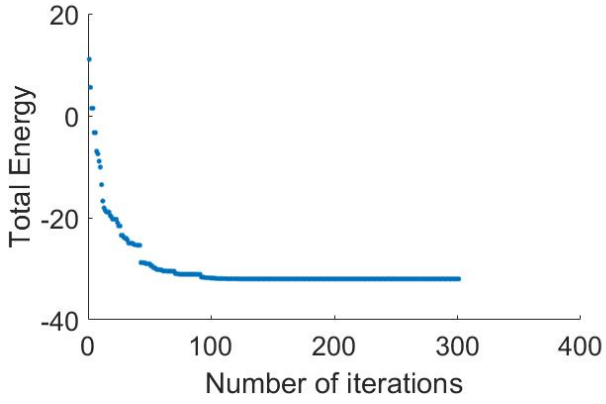
Fig. 2.6.: *Case 2.3:* Spins constrained in a plane, $J_2 = 0.6$ & $J_1 = 1$

In all the part(b) of the figures it has been shown that the system has achieved its ground state.

Case 3: Spin free in space and $J_2 = 0$:



(a) Spin Orientations

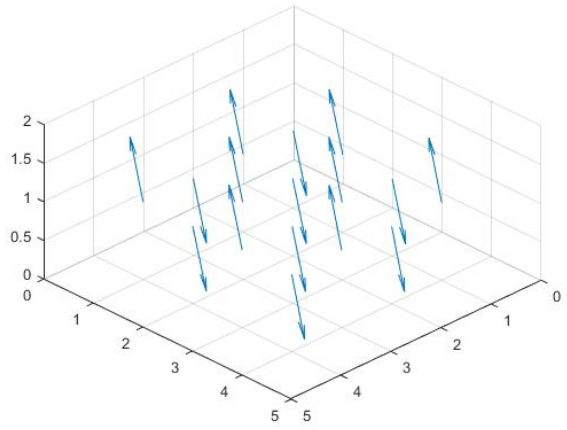


(b) Energy vs iterations

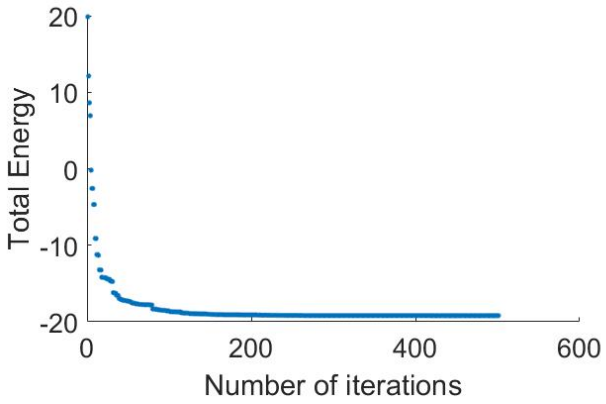
Fig. 2.7.: *Case 3:* Spins are free to rotate in 3-dimension, $J_2 = 0$ & $J_1 = 1$

Results here are similar to the case in 2-dimensionally constrained spins, that is, all are aligned opposite to their neighboring spins.

Case 4: Spin free in space and $J_2 \neq 0$:

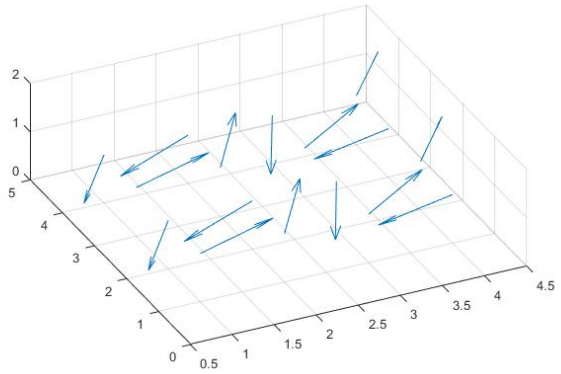


(a) Spin Orientations

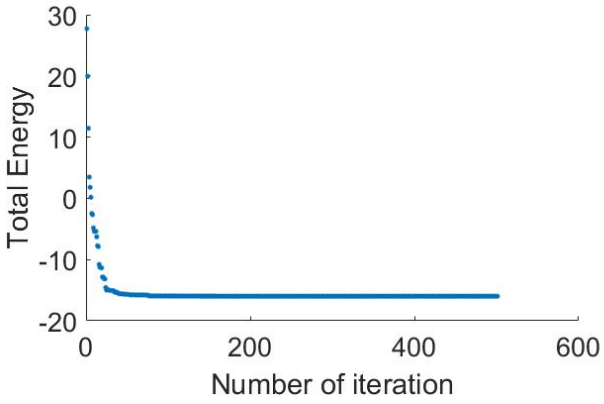


(b) Energy vs iterations

Fig. 2.8.: *Case 4.1:* Spins are free to rotate in 3-dimension $J_2 = 0.4$ & $J_1 = 1$



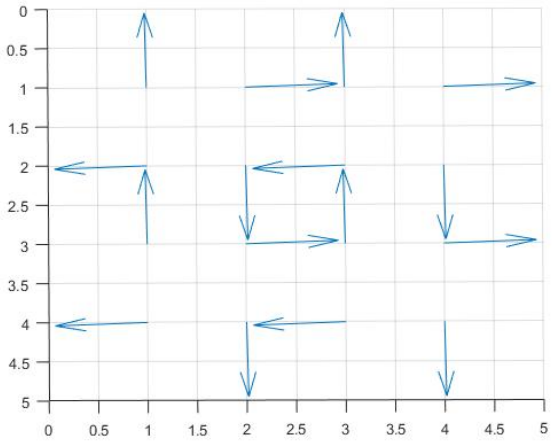
(a) Spin Orientations



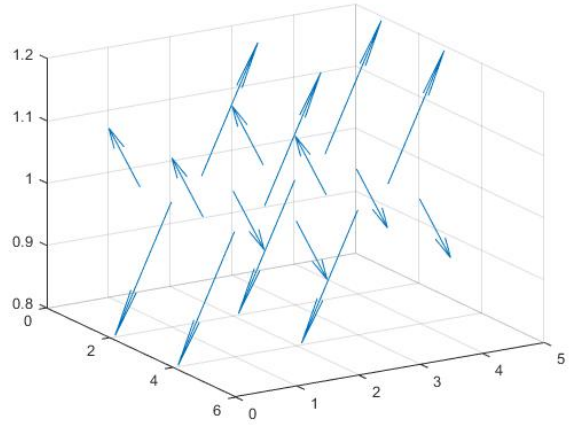
(b) Energy vs iterations

Fig. 2.9.: *Case 4.2:* Spins are free to rotate in 3-dimension, $J_2 = 0.5$ & $J_1 = 1$

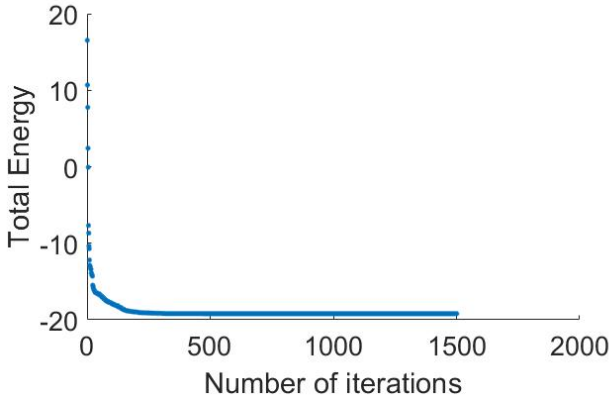
When spin rotors are free to rotate in space, then the simulation results shows similarity with case for two dimensionally constrained spins when $J_2 \neq 0$ in theri respective ground states.



(a) Spin Orientations



(b) Spin Orientations (another view)



(c) Energy vs iterations

Fig. 2.10.: *Case 4.3:*Spins are free to rotate in 3-dimension, $J_2 = 0.6$ & $J_1 = 1$

3. LUTTINGER-TISZA METHOD

3.1 Introduction

The Luttinger-Tisza (LT) method [6] was first proposed in 1946. The method is used for determining the minimum energy spin configuration in crystals for a given strong conditions. It can be used in any general lattice for a given spin arrangement interacting via a interaction.

In LT method, the Hamiltonian (1.1) is converted to its Fourier transform form. For this, the interaction coefficient and the spins - both are Fourier transformed [7] to the following:

$$J(\mathbf{q}) = \sum_{\substack{j \\ i \neq j}} J_{ij} \exp(-i\mathbf{q}.\mathbf{R}_{ij}) \tag{3.1}$$

The Fourier transform of the spins are also called as spin structure factor ($S(\mathbf{q})$) and is defined as:

$$\mathbf{S}_{\mathbf{q}} = N^{-1/2} \sum_{j} \mathbf{S}_j \exp(-i\mathbf{q}.\mathbf{R}_j) \tag{3.2}$$

Here N is the total number of atoms in the lattice and $\mathbf{q}$ is the crystal momentum. Also it is obvious that

$$\mathbf{S}_{-\mathbf{q}} = \mathbf{S}^*_{\mathbf{q}} \tag{3.3}$$

and

$$J(-\mathbf{q}) = J(\mathbf{q}) \tag{3.4}$$

Now the total Hamiltonian given by equation 1.1,

$$\mathcal{H} = \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} J_{ij} \mathbf{S}_i.\mathbf{S}_j \tag{3.5}$$

can be re-written as:

$$\mathcal{H} = \frac{1}{2} \sum_{\mathbf{q}} J(\mathbf{q}) \mathbf{S}_{\mathbf{q}}.\mathbf{S}_{\text{-}\mathbf{q}} \tag{3.6}$$

Now we need to minimize the equation (3.6) with respect to the condition $\mathbf{S}_j^2 = \text{constant}$ for all j (called stronger condition). But instead we impose the following milder condition for our problem:

$$\sum_j \mathbf{S}_j^2 = constant \tag{3.7}$$

which again can be written in its Fourier transformed as:

$$\sum_{\mathbf{q}} \mathbf{S_q}.\mathbf{S_{-q}} = \text{constant} \tag{3.8}$$

With this assumption, the minimum of the Hamiltonian (3.6) is achieved by taking that value of $\mathbf{q}$ for which $J(\mathbf{q})$ is minimum.

3.2 Applying the LT Method

In our simulations, we apply the Luttinger-Tisza Method to verify the results of our simulation. This is done by plotting the values of $|\mathbf{S_q}|^2$ against $\mathbf{q}$ and verifying if the value of $\mathbf{q}$ that light's up gives the minimum value of $J(\mathbf{q})$. The minimum value of $J(\mathbf{q})$ depends on the value of J_1 & J_2 and depending upon the ratio $\frac{J_2}{J_1}$ the corresponding value of $\mathbf{q}$ will vary.

So firstly, we would tabulate the values of $\mathbf{q}$ which would give the minimum value of $J(\mathbf{q})$ corresponding to a given $\frac{J_2}{J_1}$. Using the definition of $J(\mathbf{q})$ (3.1)

$$\begin{aligned} J(\mathbf{q}) &= \sum_{\substack{j \\ i \neq j}} J_{ij} \exp(-i\mathbf{q}.\mathbf{R}_{ij}) \\ &= J_1[\exp(-i\mathbf{q}.\mathbf{a}_1) + \exp(i\mathbf{q}.\mathbf{a}_1) + \exp(-i\mathbf{q}.\mathbf{a}_2) + \exp(i\mathbf{q}.\mathbf{a}_2)] \\ &\quad + J_2[\exp(-i\mathbf{q}.(\mathbf{a}_1 + \mathbf{a}_2)) + \exp(i\mathbf{q}.(\mathbf{a}_1 + \mathbf{a}_2)) + exp(-i\mathbf{q}.(\mathbf{a}_1 - \mathbf{a}_2)) \\ &\quad + exp(i\mathbf{q}.(\mathbf{a}_1 - \mathbf{a}_2))] \\ &= 2J_1[\cos(\mathbf{q}.\mathbf{a}_1) + \cos(\mathbf{q}.\mathbf{a}_2)] + 2J_2[\cos(\mathbf{q}.(\mathbf{a}_1 + \mathbf{a}_2)) + \cos(\mathbf{q}.(\mathbf{a}_1 - \mathbf{a}_2)] \end{aligned} \tag{3.9}$$

Here $\mathbf{a}_1$ & $\mathbf{a}_2$ are the lattice constants for our two-dimensional lattice. Also, $\mathbf{q}$ is the crystal momentum which can be written as:

$$\mathbf{q} = k_1\mathbf{b}_1 + k_2\mathbf{b}_2$$

Here k_1 and k_2 are the coefficients of the reciprocal lattice vectors . Their values varies as (for N_i = even case):

$$\begin{aligned} k_1 &= \frac{m_1}{N_1} \qquad \text{where} \quad m_1 = \frac{N_1}{2}, \frac{N_1}{2} - 1, ..., \frac{-N_1}{2} + 1 \\ k_2 &= \frac{m_2}{N_2} \qquad \text{where} \quad m_2 = \frac{N_2}{2}, \frac{N_2}{2} - 1, ..., \frac{-N_2}{2} + 1 \end{aligned} \tag{3.10}$$

Here, N_1 & N_2 are the total number of atoms in $\hat{\mathbf{a}}_1$ & $\hat{\mathbf{a}}_2$ directions respectively. The reciprocal lattice vectors ($\mathbf{b}_1$, $\mathbf{b}_2$) follows their rule of dot product with lattice constant, that is,

$$\mathbf{a}_i.\mathbf{b}_j = 2\pi\delta_{ij} \tag{3.11}$$

Now using equation 3.10 & 3.11 and substituting them in equation 3.9, we get:

$$J(\mathbf{q}) = 2\cos(2\pi k_1).(J_1 + J_2\cos(2\pi k_2)) + 2\cos(2\pi k_2).(J_1 + J_2\cos(2\pi k_1)) \tag{3.12}$$

Now for our case the value of k_1 and k_2 are:

$$\begin{aligned} k_1 &= \frac{1}{2}, \frac{1}{4}, 0, \frac{-1}{4} \\ k_2 &= \frac{1}{2}, \frac{1}{4}, 0, \frac{-1}{4} \end{aligned} \tag{3.13}$$

$\mathbf{k}_1 \backslash \mathbf{k}_2$	1/2	1/4	0	-1/4
1/2	-4($J_1 - J_2$)	-2J_1	-4J_2	-2J_1
1/4	-2J_1	0	2J_1	0
0	-4J_2	2J1	4(J_1+J_2)	2J_1
-1/4	-2J_1	0	2J_1	0

Table 3.1: Value of $J(\mathbf{q})$ for all the values of k_1 and k_2

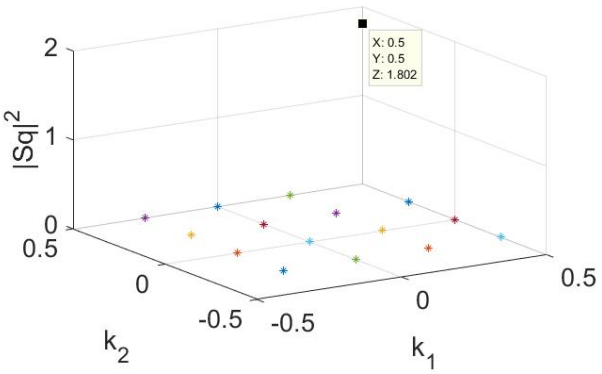
For all the values of k_1 & k_2, the value of the equation 3.12 has been tabulated in Table 3.1 Now for the different values of the ratio $\frac{J_2}{J_1}$, the value of k_1 and k_2 (thus corresponding q) for which $J_{\mathbf{q}}$ is minimum is tabulated in Table 3.2

$\frac{J_2}{J_1}$	(k_1,k_2)
< 0.5	$(\frac{1}{2}, \frac{1}{2})$
$= 0.5$	$(\frac{1}{2}, \frac{-1}{4})$,$(\frac{1}{2}, 0)$,$(\frac{1}{2}, \frac{1}{4})$,$(\frac{1}{2}, \frac{1}{2})$,$(\frac{1}{4}, \frac{1}{2})$,$(0, \frac{1}{2})$,$(\frac{-1}{4}, \frac{1}{2})$
> 0.5	$(0, \frac{1}{2})$,$(\frac{1}{2}, 0)$

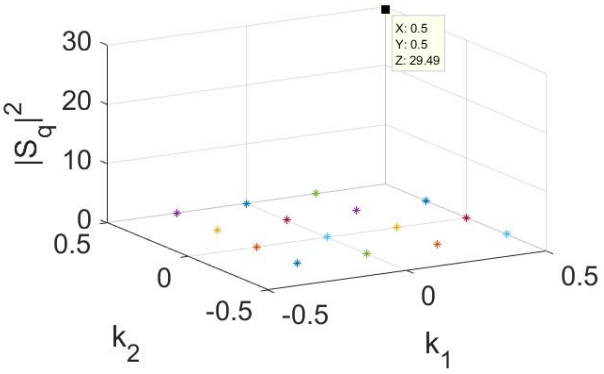
Table 3.2: k_1 and k_2 corresponding to minimum value of $J_{\mathbf{q}}$

3.3 Simulations for Luttinger-Tisza

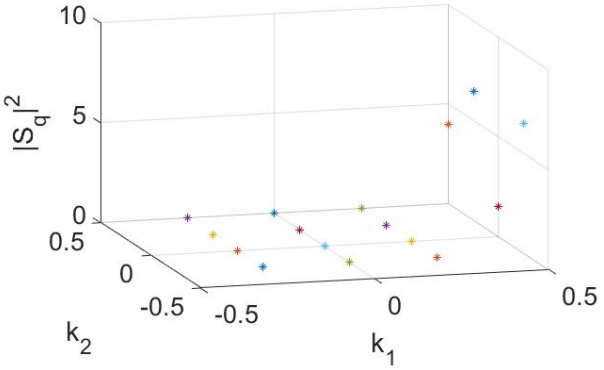
As said earlier, we use the LT method to verify the results of our simulations by plotting $|\mathbf{S_q}|^2$ against the different values $\mathbf{q}$. The following plots (figure 3.1 & 3.2) were obtained for all simulation results shown in the previous section.



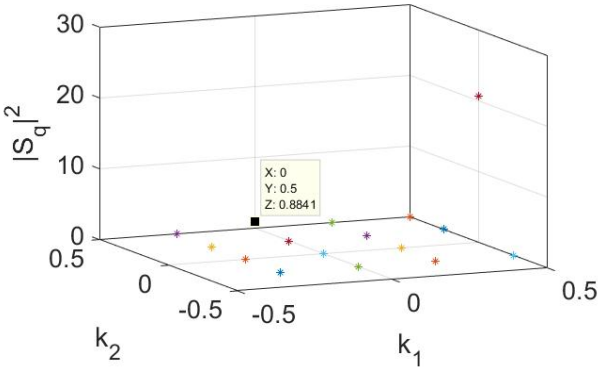
(a) 2D: $\frac{J_2}{J_1} = 0$



(b) 2D: $\frac{J_2}{J_1} = 0.25$

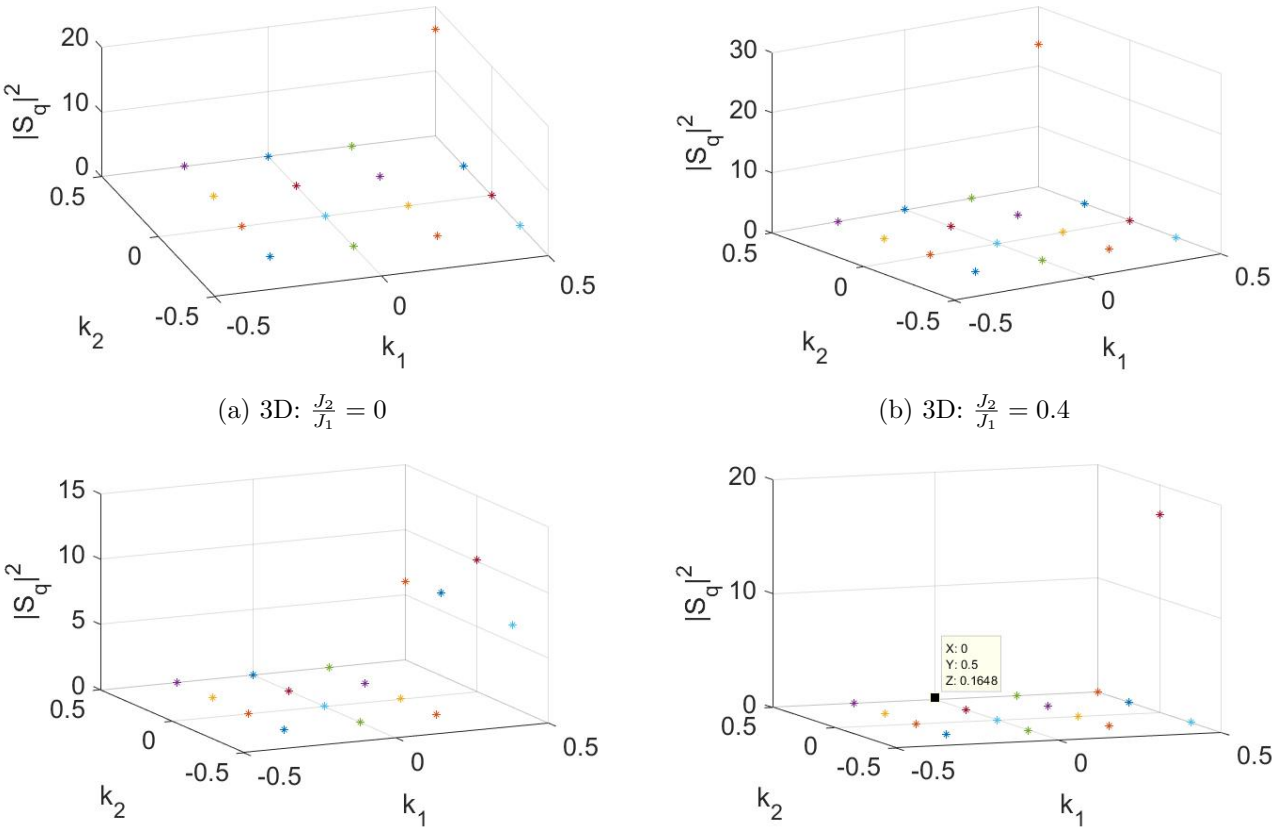


(c) 2D: $\frac{J_2}{J_1} = 0.5$



(d) 2D: $\frac{J_2}{J_1} = 0.6$

Fig. 3.1.: $|\mathbf{S}_q^2|$ vs k_1 and k_2 (thus $\mathbf{q}$) (Here, 2D means spins are constrained in 2-dimensional lattice plane)



(a) 3D: $\frac{J_2}{J_1} = 0$

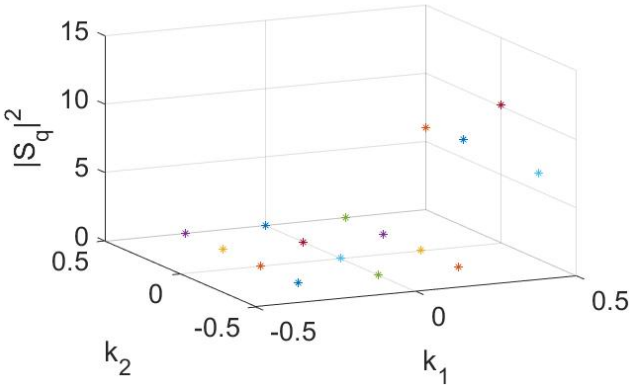
(b) 3D: $\frac{J_2}{J_1} = 0.4$

(c) 3D: $\frac{J_2}{J_1} = 0.5$

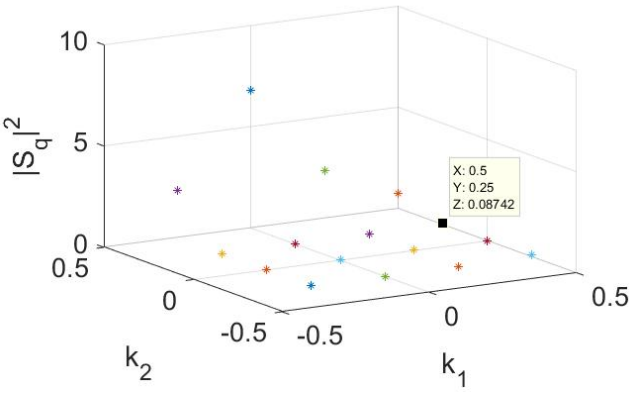
(d) 3D: $\frac{J_2}{J_1} = 0.6$

Fig. 3.2.: $|\mathbf{S}_q^2|$ vs k_1 and k_2 (Here, 3D means spins are free to rotate in 3-dimension)

The plots in figure 3.1 does gives us the expected result when compared with table 3.2 Some of the values of k_1 and k_2 are missing from plots (specially for $\frac{J_2}{J_1} = 0.5$). But statistically all the other values of k_1 and k_2 gets lighted up as it was found when the another simulation was run for the same value of $\frac{J_2}{J_1}$. This is shown in the figure 3.3



(a) 3D: $\frac{J_2}{J_1} = 0.5$ (same as fig. 3.1 (g))



(b) 3D: $\frac{J_2}{J_1} = 0.5$

Fig. 3.3.: Different value of k_1 and k_2 lights up in case of another simulation for the same value of$\frac{J_2}{J_1}$ ($= 0.5$ in this case)

In all the above figures, the plots are not to scale, i.e., magnitude of $|\mathbf{S}_q|^2$ does not bother us here as we are only looking for that values of k_1 and k_2 which are non-zero.

4. THE NEW HAMILTONIAN

We now investigate quantum criticality [4], [5] in the classical regime by an additional term in the Hamiltonian given by

$$H = \frac{1}{2} \sum_{\langle i,j,k,l \rangle} Q_{ijkl}(1 - \mathbf{S}_i.\mathbf{S}_j)(1 - \mathbf{S}_k.\mathbf{S}_l) \tag{4.1}$$

This makes our new Hamiltonian to be:

$$\mathcal{H} = \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} J_{ij}\mathbf{S}_i.\mathbf{S}_j + \frac{1}{2} \sum_{\langle i,j,k,l \rangle} Q_{ijkl}(1 - \mathbf{S}_i.\mathbf{S}_j)(1 - \mathbf{S}_k.\mathbf{S}_l) \tag{4.2}$$

We try to find the ground state of the lattice system at $T = 0K$ by same procedure as stated above - iterative minimisation and then study the corresponding reciprocal lattice vectors. These vectors are calculated by direct evaluation from the final obtained ground state configuration.

4.1 Simulation Results

We study the Hamiltonian in primarily three different cases ($J_2 = 0$ in every case):

(i) $J_1 >> 0$ and $Q > 0$ such that $|J_1| >> Q$

(ii) $J_1 << 0$ and $Q > 0$ such that $|J_1| >> Q$

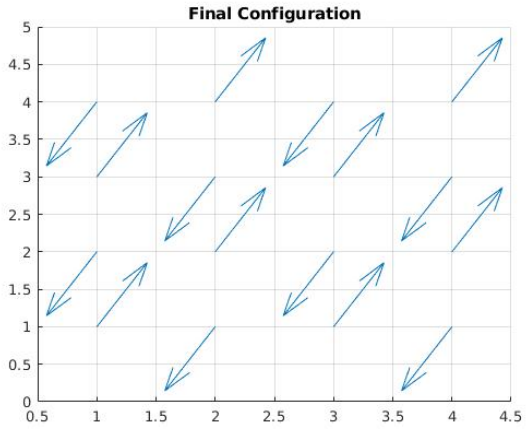
(iii) $J_1 > 0$ and $J_1 \sim Q > 0$

(iv) $J_1 \geq 0$ and $Q < 0$

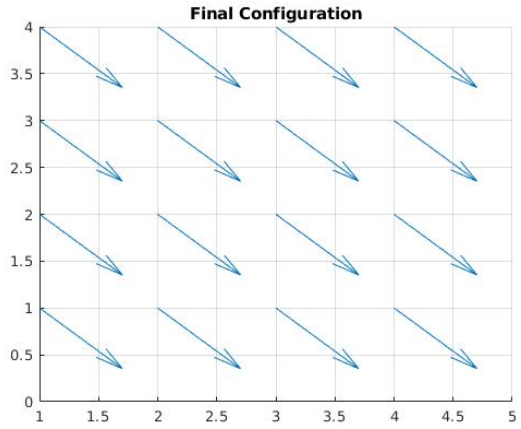
(v) $J_1 << 0$ and $Q < 0$ such that $|J_1| >> Q$

(vi) $J_1 < 0$ and $Q < 0$ such that $|J_1| \sim Q$

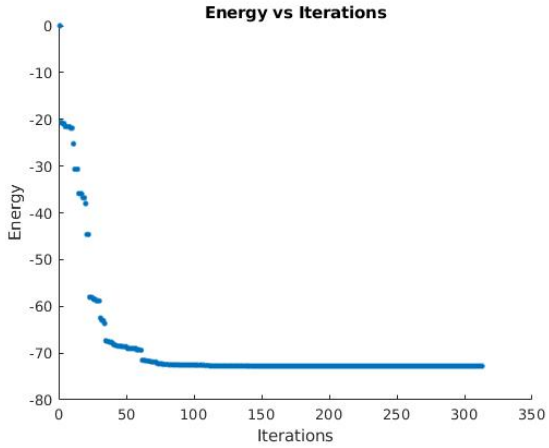
In the first two limiting cases, the results are as expected. The J term dominates over Q and the system reaches a anti-ferromagnetic (and ferromagnetic) ground state, respectively. This is shown in figure below (Fig.4.1).



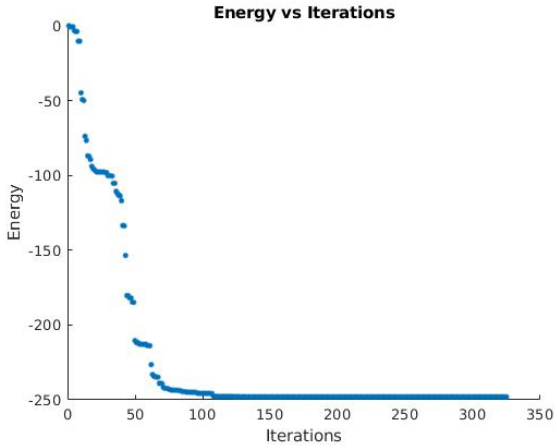
(a) Ground state configuration at T = 0K for $J_1 = 3$, $J_2 = 0$ and $Q = 0.1$



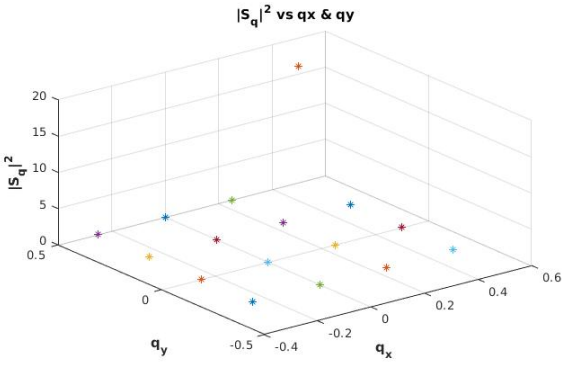
(b) Ground state configuration at T = 0K for $J_1 = -5$, $J_2 = 0$ and $Q = 1$



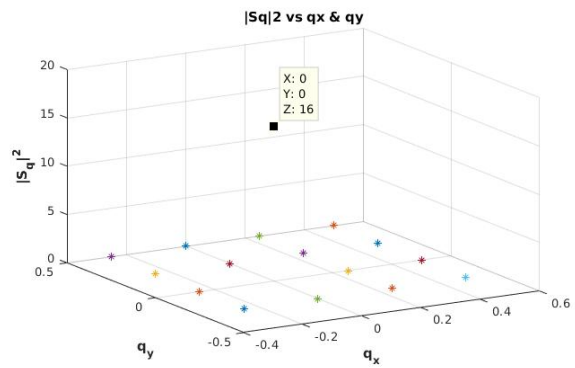
(c) Energy vs iteration number curve showing the stability of the system, $J_1 = 3$, $J_2 = 0$ and $Q = 0.1$



(d) Energy vs iteration number curve showing the stability of the system, $J_1 = -5$, $J_2 = 0$ and $Q = 1$



(e) Corresponding non-zero reciprocal lattice vector, Energy vs iteration number curve showing the stability of the system, $J_1 = 3$, $J_2 = 0$ and $Q = 0.1$



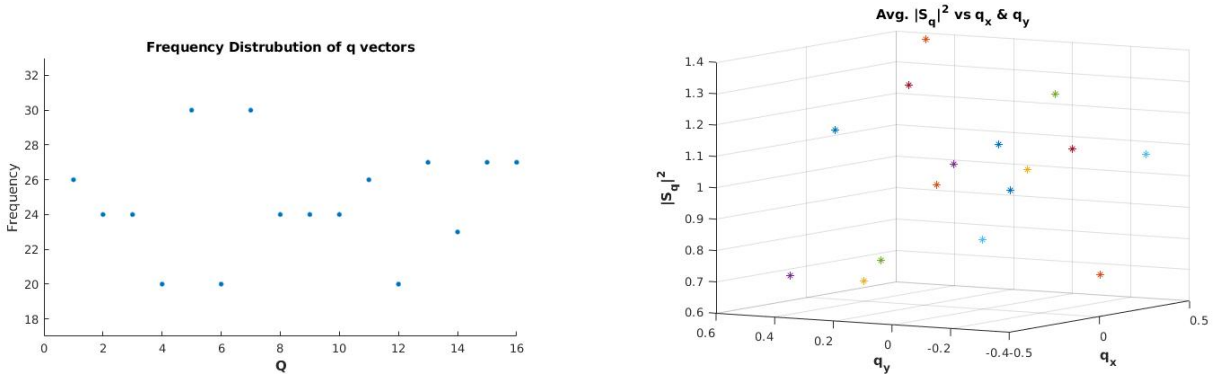
(f) Corresponding on-zero reciprocal lattice vector, Energy vs iteration number curve showing the stability of the system, $J_1 = -5$, $J_2 = 0$ and $Q = 1$

Fig. 4.1.: GS configuration, energy and reciprocal lattice vector for case (i) and (ii)

In case (iv), from intuition we expected the ground state configuration to be anti-ferromagnetic which it was indeed. In case (v), the result was expected to be a ferromagnetic systems. These are two cases are shown in the Fig. 4.2.

The most interesting case is (iii) and (iv) where $|J_1|$) is comparable to $|Q|$. The system exhibits different ground state configuration in different runs of the simulations giving rise to degeneracy in the system.

In the figure below (Fig: 4.3), for $J_1 = 0.5, J_2 = 0$ and $Q = 1$, we run the simulation for 50 iterations and present the statistics of it in the frequency distribution and average value of $|\mathbf{S}_q|^2$. One of the configuration and its corresponding parameters are shown in the figure.



(a) Frequency distribution of $\mathbf{q}$ for n = 50 runs

(b) Average value of $|\mathbf{S}_q|^2$ for the obtained frequency distribution

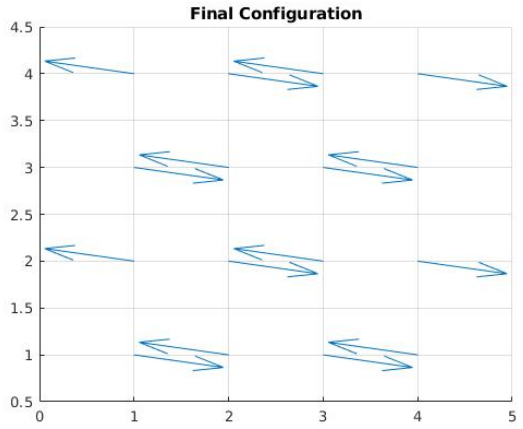
Fig. 4.3.: For $J_1 = 0.5$, $J_2 = 0$ and $Q = 1$, 50 iteration were run to obtain the frequency distribution of $\mathbf{q}$ (figure (a)) and corresponding average value of $|\mathbf{S}_q|^2$ (figure (b)).

In the figure (Fig. 4.4) below we show one of the 50 outcomes of the iteration. From the $|\mathbf{S}_q|^2 vs \mathbf{q}_x and \mathbf{q}_y$ plot, it is clear that in this outcome many possible values of q is 0 which was not necessarily the case in other 49 outcomes which is also seen in the figure 4.2, where all the reciprocal lattice vectors, $\mathbf{q}$, did have non-zero frequency.

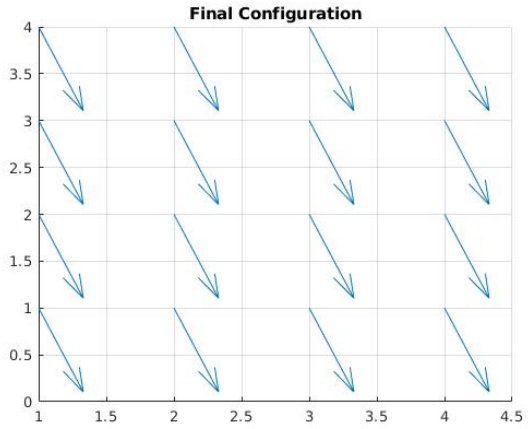
Now in a very special case, when $Q = J_1$, ($J_2 = 0$), expanding the Hamiltonian (Eq.(4.2)), we get:

$$\mathcal{H} = \sum_{\langle i,j,k,l \rangle} Q(\mathbf{S}_i.\mathbf{S}_j)(\mathbf{S}_k.\mathbf{S}_l) + \sum_{\langle k,l \rangle} Q(\mathbf{S}_k.\mathbf{S}_l) + \sum_i Q$$

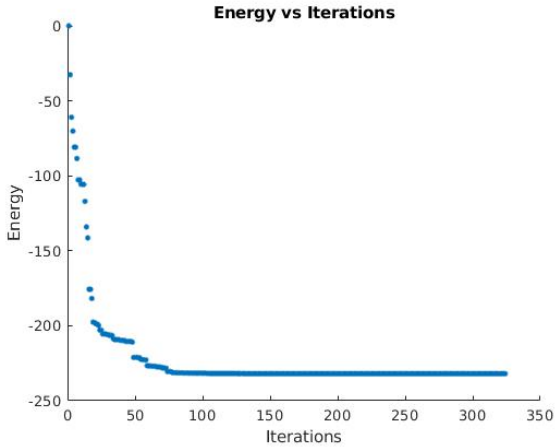
Ignoring the last two terms in the above Hamiltonian leads to a very interesting phenomena which is discussed in the next section. It is this factor which gives extensive degeneracy to the system in it's ground state at $T = 0K$.



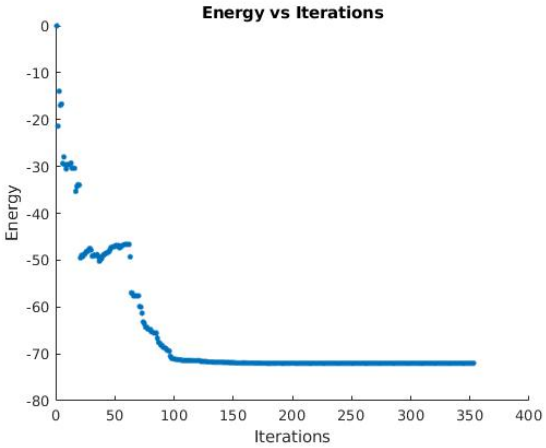
(a) Ground state configuration at T = 0K for $J_1 = 0$, $J_2 = 0$ and $Q = -1$. This will also be the case when $J_1 > 0$ as it will encourage anti-ferromagnetism in the system which is already there when $J_1 = 0$



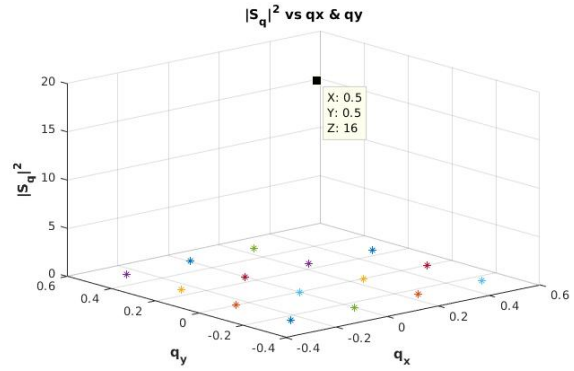
(b) Ground state configuration at T = 0K for $J_1 = -5$, $J_2 = 0$ and $Q = -1$



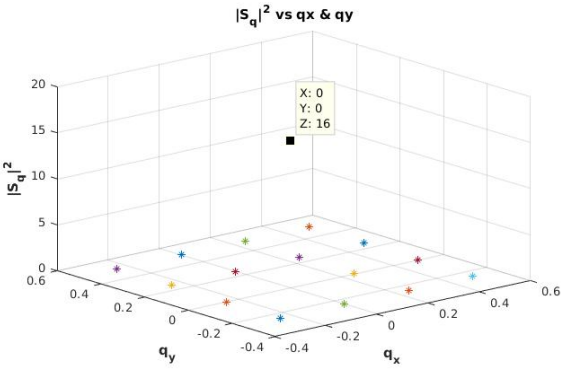
(c) Energy vs iteration number curve showing the stability of the system, $J_1 = 0$, $J_2 = 0$ and $Q = -1$



(d) Energy vs iteration number curve showing the stability of the system, $J_1 = -5$, $J_2 = 0$ and $Q = -1$

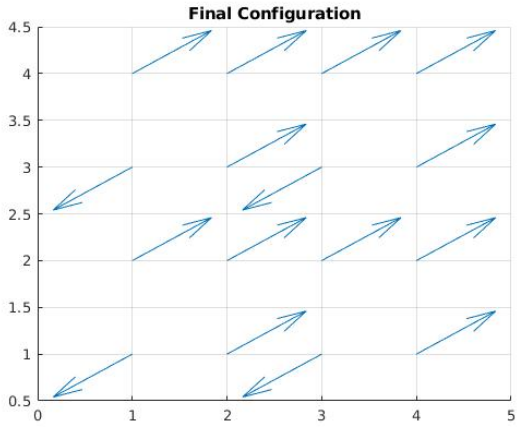


(e) Corresponding non-zero reciprocal lattice vector, $J_1 = 0$, $J_2 = 0$ and $Q = -1$

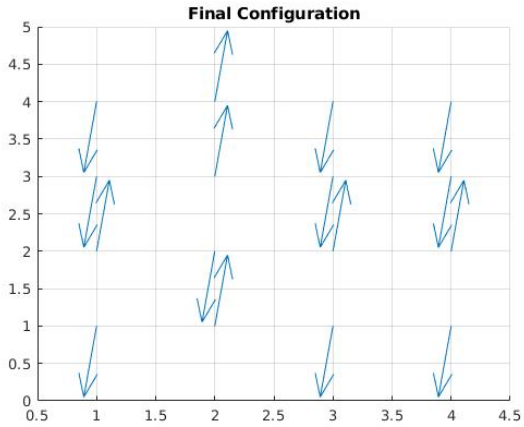


(f) Corresponding on-zero reciprocal lattice vector, $J_1 = -5$, $J_2 = 0$ and $Q = -1$

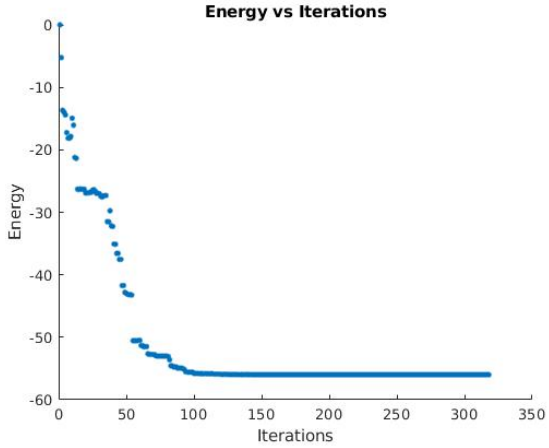
Fig. 4.2.: GS configuration, energy and reciprocal lattice vector for case (iv) and (v)



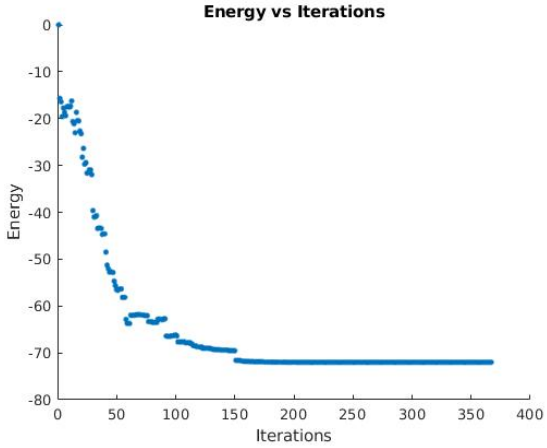
(a) Ground state configuration $J_1 = 0.5$ and $Q = 1$



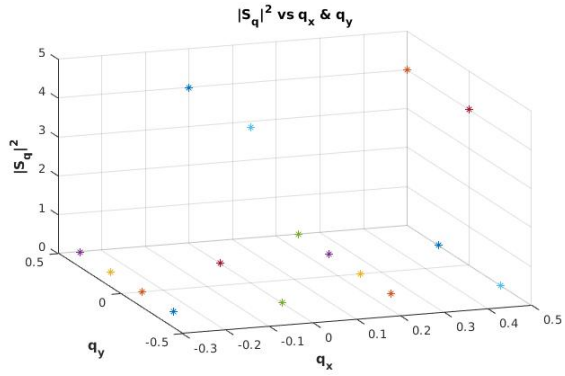
(b) Ground state configuration $J_1 = -1$ and $Q = -1$



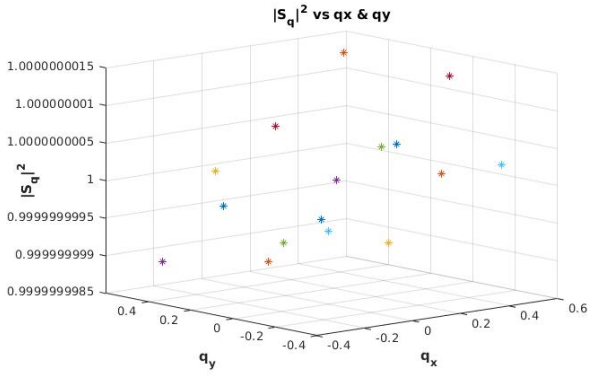
(c) Energy vs iteration number curve showing the stability of the system, $J_1 = 0.5$ and $Q = 1$



(d) Energy vs iteration number curve showing the stability of the system, $J_1 = -1$ and $Q = -1$



(e) Reciprocal lattice vector that are non zero for the obtained ground state $J_1 = 0.5$ and $Q = 1$



(f) Reciprocal lattice vector that are non zero for the obtained ground state $J_1 = -1$ and $Q = -1$

Fig. 4.4.: GS configuration, energy and reciprocal lattice vector for case (iii) (one of the 50 results) and (vi)

5. AN INTERESTING MAGNET!

Now we study and investigate the following Hamiltonian and understand from where extensive degeneracy comes from.

$$\mathcal{H} = \frac{1}{2}\sum_{\substack{i,j \\ i\neq j}} J_{ij}\mathbf{S}_i.\mathbf{S}_j + \frac{1}{2}\sum_{\langle i,j,k,l\rangle} Q(\mathbf{S}_i.\mathbf{S}_j)(\mathbf{S}_k.\mathbf{S}_l) \tag{5.1}$$

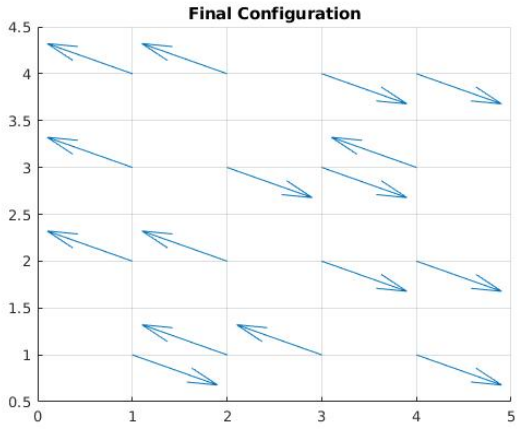
In it's extreme case where $|J_1| >> Q > 0$, the domination of the J term leads the magnet to be a anti-ferromagnetic and ferromagnetic in the ground state depending upon the sign of$J$. But as the J becomes comparable to Q, Q dominates the system as it is quadratic in $\mathbf{S}_i.\mathbf{S}_j$ whereas J is linear in the same.

5.1 Simulations for $Q \neq 0$ and $J = 0$

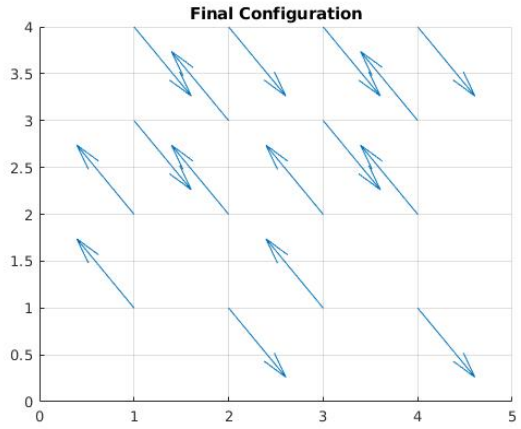
To understand the above Hamiltonian we first investigate the Q term only ($J = 0$). Then the Hamiltonian becomes:

$$\mathcal{H} = \frac{1}{2}\sum_{\langle i,j,k,l\rangle} Q_{ijkl}(\mathbf{S}_i.\mathbf{S}_j)(\mathbf{S}_k.\mathbf{S}_l) \tag{5.2}$$

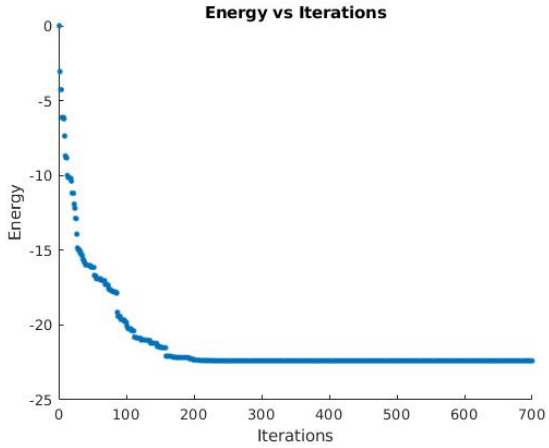
From simulation results, we find many possible configuration in GS at $T = 0K$. Few of the results are shown in the figure below (Fig. 5.1):



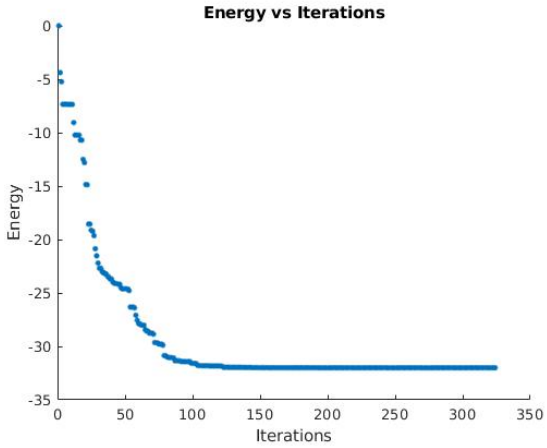
(a) $J_1 = 0$ and $Q = 0.35$



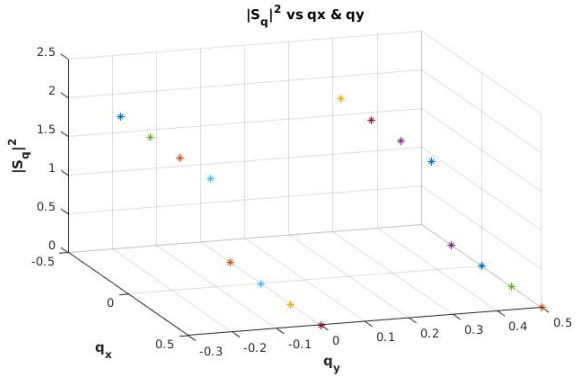
(b) $J_1 = 0$ and $Q = 0.5$



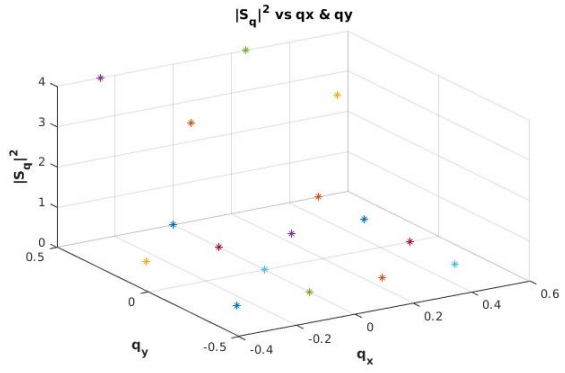
(c) Energy vs iteration number for $J_1 = 0$ and $Q = 0.35$



(d) Energy vs iteration number for $J_1 = 0$ and $Q = 0.5$

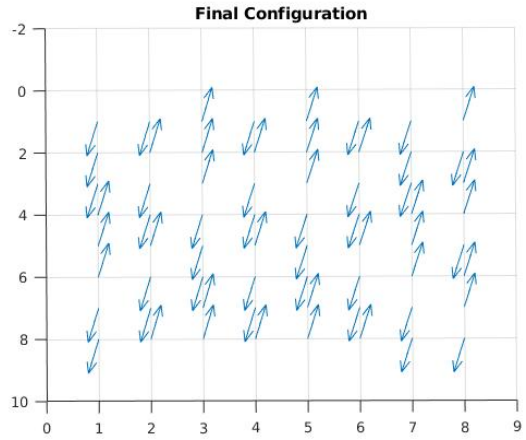


(e) Non zero reciprocal lattice vector ($\mathbf{q}$) for $J_1 = 0$ and $Q = 0.35$

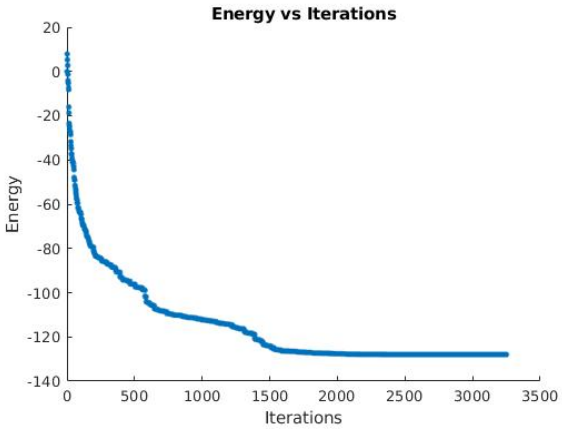


(f) Non zero reciprocal lattice vector ($\mathbf{q}$)for $J_1 = 0$ and $Q = 0.5$

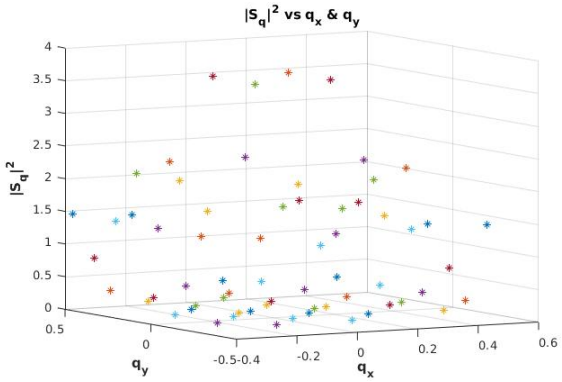
Fig. 5.1.: For $J_1 = 0$, $J_2 = 0$ and $Q = 0.35$ (a,c,e) & 0.5 (b,c,d), GS configuration, stability of system and non-zero $\mathbf{q}$ values. Note that if the ground state configuration would only depend on sign of Q not on its magnitude which will only scale the energy of the system.



(a) Ground state configuration for 8x8 lattice



(b) Energy vs iteration number



(c) Non zero reciprocal lattice vector

Fig. 5.2.: Simulation results for a 8x8 lattice for $J_1 = 0$, $J_2 = 0$ and $Q = 1$

5.2 Physical Interpretation of the Hamiltonian

For the equation 5.2 with $Q > 0$, if we chose a block of four neighbouring spins, then configuration that will generate minimum energy of the block must have 3 spins aligned in same direction and one in anti-parallel to the other three spins. This is because if we have alignment such that $\mathbf{S}_i$ and $\mathbf{S}_j$ which will make $\mathbf{S}_i.\mathbf{S}_j > 0$ and hence we must have $\mathbf{S}_k.\mathbf{S}_l < 0$, that is they must be anti-aligned to give a negative value. $\mathbf{S}_j$ and $\mathbf{S}_l$ also must be parallel because the block can also interact within itself in other way around: $(\mathbf{S}_i.\mathbf{S}_k)(\mathbf{S}_j.\mathbf{S}_l)$.

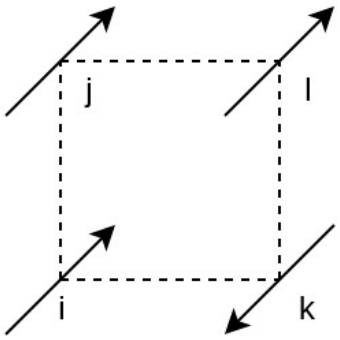


Fig. 5.3.: Ground state configuration for a block of four nearest neighbouring spins for Hamiltonian given by Eq. 5.2 for $Q \neq 0$ and $J = 0$

Now for a lattice, this minimisation needs to be extended to all the lattice points. The procedure to guess one of the many possible ground states is shown and described below.

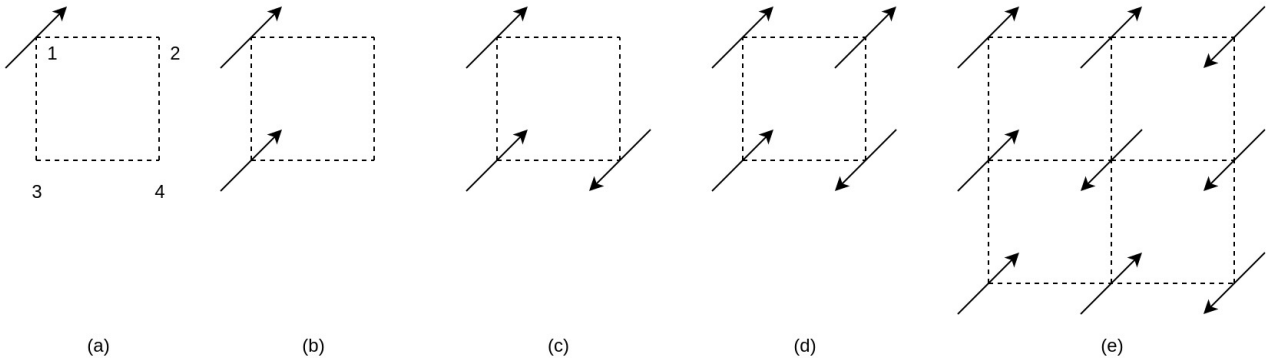


Fig. 5.4.: Step by step process to guess one of the possible ground state for $Q \neq 0$ and $J = 0$

(a) First, let's assume that spin at the position 1 in fig (a) is given in the shown direction.

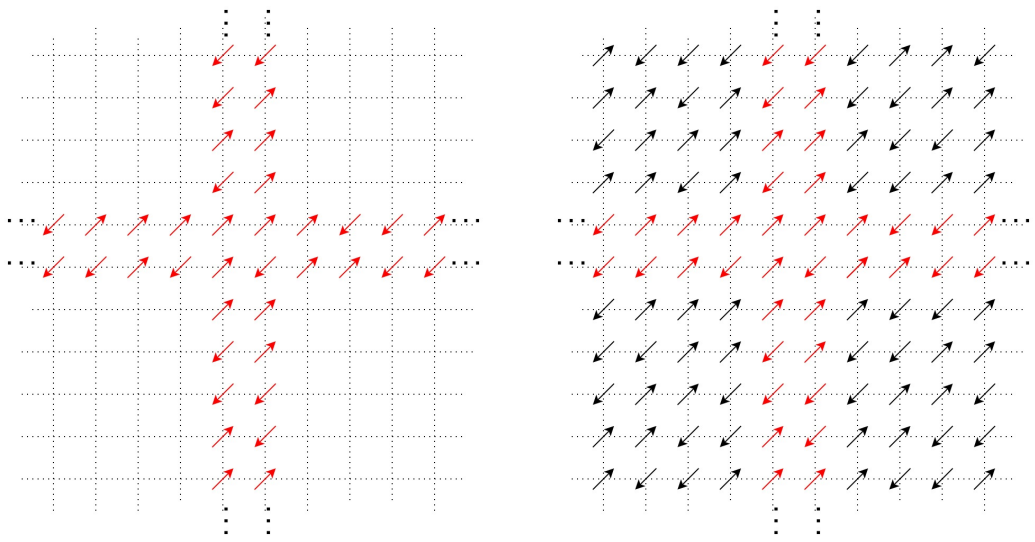
(b) Then let's decide the direction of spin at position 2. It doesn't matter which next position we chose to guess as the lattice is symmetric. At position 2, we can either have spin parallel to the spin at position 1 or anti-parallel to it.(Here we have 2 degree of freedom that can be present in the ground state) Let's chose it to be parallel to it. This is depicted in (b).

(c) Now at position 3, we again have the (2 degree) freedom to decide which way spin should be aligned with respect to the spin at position 2. This time we'll choose it to be anti-parallel as shown in (c)

(d) Since three of the four nearest spins have been constrained, the last spin, at position 4 must be in a such way that it minimises the Hamiltonian. This fixes the alignment at position 4 to be in parallel to spin at 1 and anti-parallel to 3(shown in (d))

(e) We can extend this analogy to map the spins of the whole lattice. But what we find that as we move along the any axis from the first block of four nearest spins, at each of the lattice points, we will have either freedom of spin to be parallel or anti-parallel with respect to surroundings or it is constrained to be in a specific direction again due to it's neighbours, in order to minimise the Hamiltonian, which gives rise to extensive degeneracy.

We now claim that if we predefined two consecutive columns and rows of spins then the rest of the lattice points acquires constraints which fixes their orientation in the ground state (see Fig. 5.5). Thus the degeneracy of the whole lattice directly exists in two consecutive columns and rows while rest of the spin orientations is determined these four lines of spins.



(a) Predefining two consecutive columns and rows of spins

(b) Rest of the lattice gets fixed.

Fig. 5.5.: Analysing the spin configuration of full lattice

5.3 In the Fourier Space

To investigate the possible values of reciprocal lattice vector $\mathbf{q}$, we transform the Hamiltonian in the Fourier space and expanding it. The equation can be lengthen by writing spin interactions per block formed by four nearest spins(Fig. 5.6).

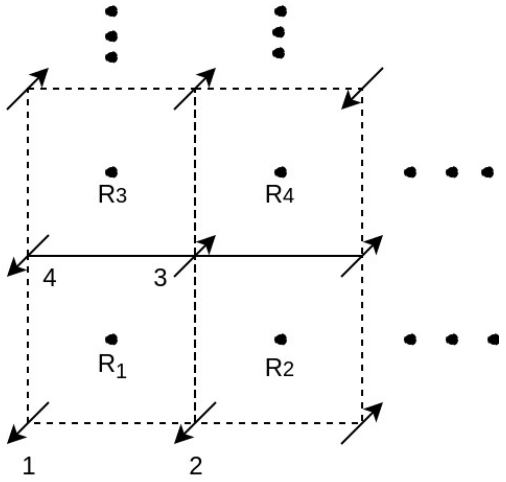


Fig. 5.6.: Blocks formed by four nearest spins and expanding the H per block

$$
\begin{aligned}
H &= \frac{1}{2}\sum_{\langle i,j,k,l\rangle} Q_{ijkl}(\mathbf{S}_i.\mathbf{S}_j)(\mathbf{S}_k.\mathbf{S}_l) \\
&= \frac{1}{2n^2}\sum_{\langle i,j,k,l\rangle} Q_{ijkl}\Bigg[\sum_{\mathbf{q}_1}\mathbf{S}_{\mathbf{q}_1}\exp^{i\mathbf{q}_1.(\mathbf{R}+\mathbf{d1})}.\sum_{\mathbf{q}_2}\mathbf{S}_{\mathbf{q}_2}\exp^{i\mathbf{q}_2.(\mathbf{R}+\mathbf{d2})}\Bigg]. \\
&\qquad\qquad \Bigg[\sum_{\mathbf{q}_3}\mathbf{S}_{\mathbf{q}_3}\exp^{i\mathbf{q}_3.(\mathbf{R}+\mathbf{d3})}.\sum_{\mathbf{q}_4}\mathbf{S}_{\mathbf{q}_4}\exp^{i\mathbf{q}_4.(\mathbf{R}+\mathbf{d4})}\Bigg]
\end{aligned}
\tag{5.3}
$$

$$
\begin{aligned}
H = \frac{1}{2n^2}\sum_{i}\sum_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3\mathbf{q}_4}\Big[&Q(\mathbf{a}_2)(\mathbf{S}_{\mathbf{q}_1}.\mathbf{S}_{\mathbf{q}_2})(\mathbf{S}_{\mathbf{q}_3}.\mathbf{S}_{\mathbf{q}_4})\exp^{i(\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3+\mathbf{q}_4).\mathbf{R}}\exp^{i(\mathbf{q}_1-\mathbf{q}_3).\mathbf{d}_1}\exp^{i(\mathbf{q}_2-\mathbf{q}_4).\mathbf{d}_2} \\
&+ Q(\mathbf{a}_1)(\mathbf{S}_{\mathbf{q}_1}.\mathbf{S}_{\mathbf{q}_4})(\mathbf{S}_{\mathbf{q}_2}.\mathbf{S}_{\mathbf{q}_3})\exp^{i(\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3+\mathbf{q}_4).\mathbf{R}}\exp^{i(\mathbf{q}_1-\mathbf{q}_3).\mathbf{d}_1}\exp^{i(\mathbf{q}_2-\mathbf{q}_4).\mathbf{d}_2}\Big]
\end{aligned}
\tag{5.4}
$$

Now, $\exp^{i(\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3+\mathbf{q}_4).\mathbf{R}} = \delta(\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3+\mathbf{q}_4)$, and swapping q_2 and q_4 in the second term:

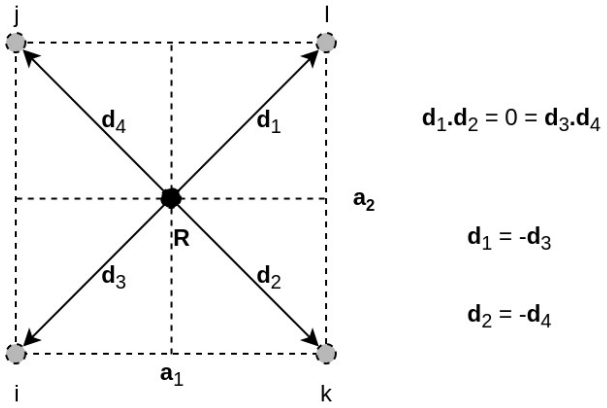


Fig. 5.7.: Calculation of Hamiltonian in Fourier space

$$H = \frac{1}{n}\sum_{i}\sum_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3\mathbf{q}_4} Q(\mathbf{S}_{\mathbf{q}_1}.\mathbf{S}_{\mathbf{q}_2})(\mathbf{S}_{\mathbf{q}_3}.\mathbf{S}_{\mathbf{q}_4})\Big(\exp^{i(\mathbf{q}_1-\mathbf{q}_3).\mathbf{d}_1}\exp^{i(\mathbf{q}_2-\mathbf{q}_4).\mathbf{d}_2} + \exp^{i(\mathbf{q}_1-\mathbf{q}_3).\mathbf{d}_1}\exp^{-i(\mathbf{q}_2-\mathbf{q}_4).\mathbf{d}_2}\Big)$$
$$= \frac{2}{n}\sum_{i}\sum_{\mathbf{q}_1\mathbf{q}_2\mathbf{q}_3\mathbf{q}_4} Q(\mathbf{a}_2)(\mathbf{S}_{\mathbf{q}_1}.\mathbf{S}_{\mathbf{q}_2})(\mathbf{S}_{\mathbf{q}_3}.\mathbf{S}_{\mathbf{q}_4})\Big(\exp^{i(\mathbf{q}_1-\mathbf{q}_3).\mathbf{d}_1}\cos\left((\mathbf{q}_2-\mathbf{q}_4).\mathbf{d}_2\right)\Big) \tag{5.5}$$

Now $\mathbf{q}_i = \alpha_i\mathbf{b}_1 + \beta_i\mathbf{b}_2$ where α_i and β_i can have values $\frac{2\pi}{a}$(-0.25,0.0,0.25,0.5), where $\mathbf{a}_i.\mathbf{b}_j = 2\pi\delta_{ij}$

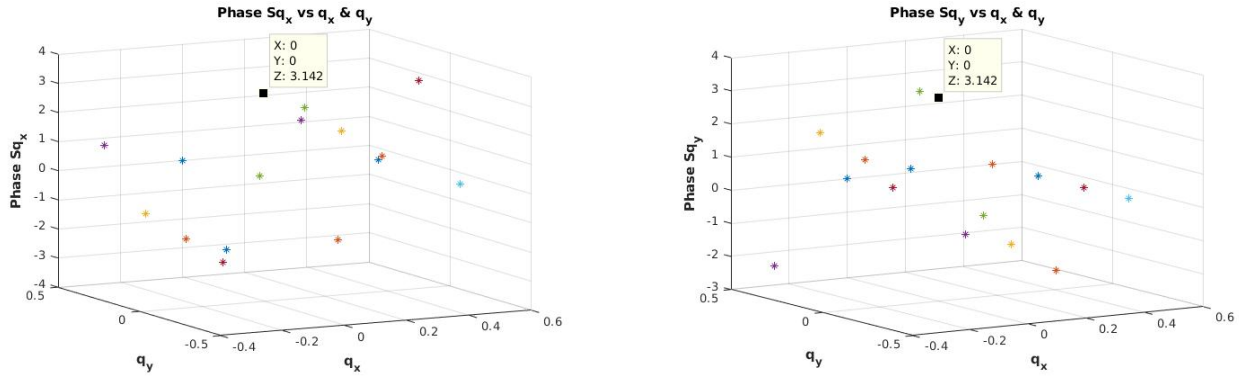
Also, $\mathbf{d}_1$ and $\mathbf{d}_2$ can be describe as:

$$\mathbf{d}_1 = \frac{\mathbf{a}_1 + \mathbf{a}_2}{2}$$

$$\mathbf{d}_2 = \frac{\mathbf{a}_1 - \mathbf{a}_2}{2}$$

Equation 5.5 tells us that Fourier transform of spin $\mathbf{S}_i$ can have complex value depending upon the phase value of the exponential term. This condition is applied for Hamiltonian to be remain real.

Since, $\mathbf{S}_q$ is complex too, it becomes computationally very complex to analyse equation 5.5 and find the possible values of $\mathbf{q}$.



(a) Phase of x-component of $\mathbf{S}_q$

(b) Phase of y-component of $\mathbf{S}_q$

Fig. 5.8.: $J_1 = 0$, $J_2 = 0$ and $Q = 1$: Components of $\mathbf{S}_q$ can have phases giving them complex values.

6. SUMMARY

The project was started with the aim of studying quantum criticality in the classical regime. We started with simulating and understanding the already formulated the Luttinger-Tisza analysis of Heisenberg model of ferromagnetic and anti-ferromagnetic systems via iterative minimisation. We then added another term to the Hamiltonian to simulate quantum criticality. It turns out the mathematics of it in Fourier space becomes computationally complex and there are extensive many possible ground state configurations possible giving rise all sorts of possible reciprocal lattice vectors at $T = 0K$.

We propose that one needs to study the Hamiltonian at $T \neq 0K$ using Monte-Carlo Simulations which is in itself can be treated as separate project. Meanwhile, studying this Hamiltonian at $T = 0K$ lead us to discover a very interesting and bizarre kind of magnet which shows extensive degeneracy and many possible ground state layout of the system with a very complex equation in Fourier space. One would also find the study of this Humiliation in quantum regime to be very interesting as it is itself in classical regime!

LIST OF REFERENCES

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[1] G. S. Joyce, "Classical heisenberg model," *Phys. Rev.*, vol. 155, pp. 478–491, Mar 1967.

[2] E. Ising, "Beitrag zur theorie des ferromagnetismus," *Zeitschrift für Physik*, vol. 31, pp. 253–258, Feb 1925.

[3] Nel, M. Louis, "Proprits magntiques des ferrites ; ferrimagntisme et antiferromagntisme," *Ann. Phys.*, vol. 12, no. 3, pp. 137–198, 1948.

[4] R. K. Kaul, R. G. Melko, and A. W. Sandvik, "Bridging lattice-scale physics and continuum field theory with quantum monte carlo simulations," *Annual Review of Condensed Matter Physics*, vol. 4, no. 1, pp. 179–215, 2013.

[5] S. Keimer, Bernhard; Sachdev, "Quantum criticality," *Physics Today*, vol. 64, p. 29, 2011.

[6] J. M. Luttinger and L. Tisza, "Theory of dipole interaction in crystals," *Phys. Rev.*, vol. 70, pp. 954–964, Dec 1946.

[7] T. Nagamiya, "Helical spin ordering1 theory of helical spin configurations," vol. 20 of *Solid State Physics*, pp. 305 – 411, Academic Press, 1968.