Bachelor Thesis Project

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↑↑ Characterization of 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 minimize the energy of the system. The properties of ferromagnetic materials have been studied in the past and is very well understood.

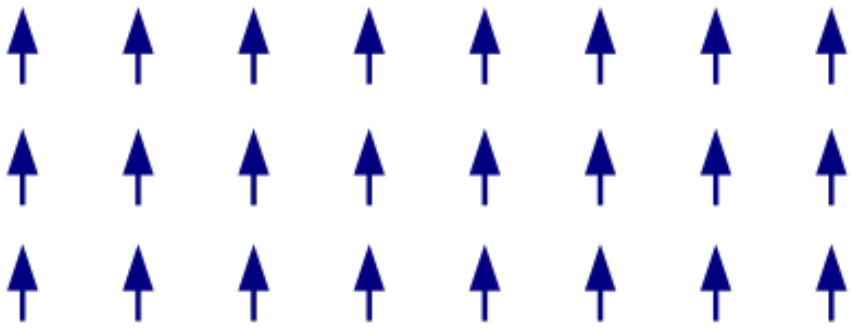


Fig. 1.1.: Ferromagnetism ($J_{ij} < 0$)

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.

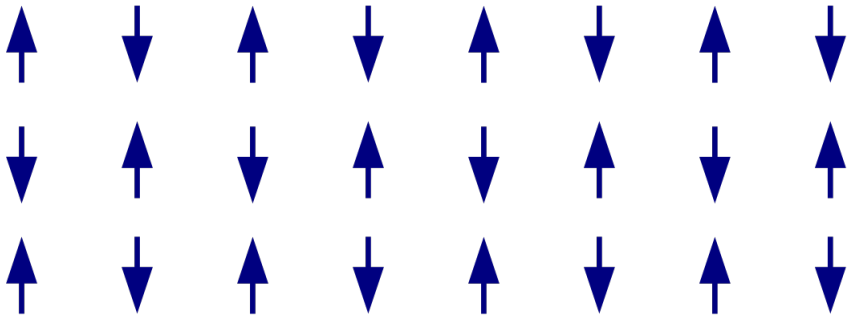


Fig. 1.2.: Anti-ferromagnetism ($J_{ij} > 0$)

In this project, we have done work on antiferromagnetic systems (though it has been done in a generalized way so that it could be applied to ferromagnetic systems also). 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-dimensionally 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 neighbors for all the spins, that is, for nearest neighboring spins, value of J_{ij} is same for all the lattice

points in the crystal and similarly, for next nearest neighbors, the coupling constant value is same for all.

To understand the spin-spin interaction in antiferromagnetic crystals, we first use method of Iterative Minimization and then later we use Luttinger-Tisza Method to verify our results obtained via iterative minimization (for various values of the coupling constant).

In Luttinger-Tisza Method, we also introduce spin structure factor $S(\mathbf{q})$ which is the Fourier transform of the actual spins. The spin structure factor eases our way in finding the values of $\mathbf{q}$ which gives us the ground state spin configuration of the lattice.

2. ITERATIVE MINIMIZATION

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:

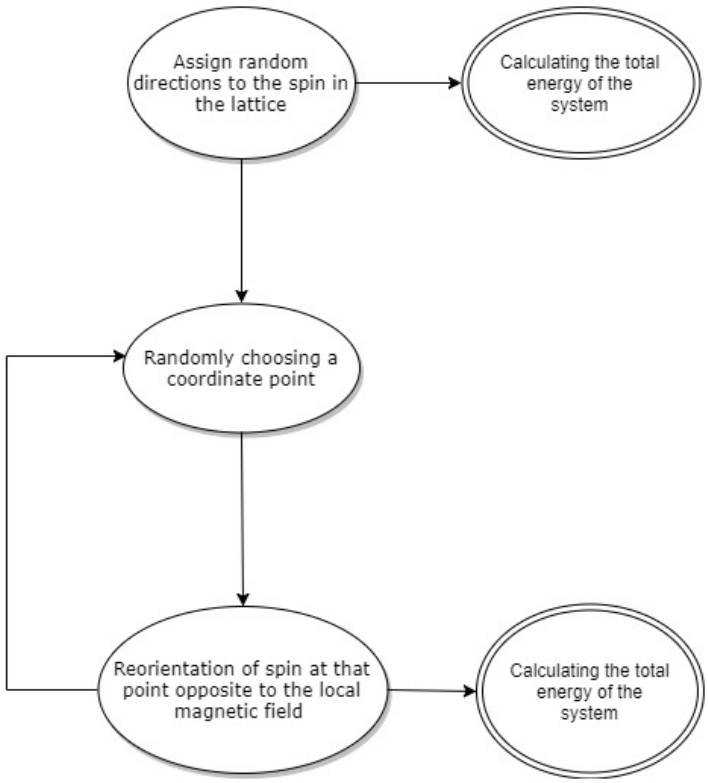


Fig. 2.1.: *Flowchart:* Method of Iterative Minimization

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:

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

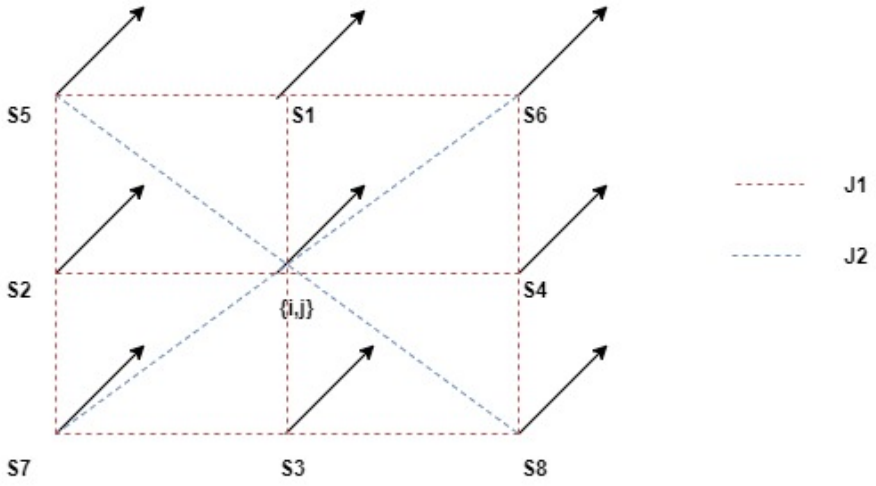


Fig. 2.2.: Local Magnetic Field at randomly chosen (i,j) due to interaction with its nearest 8-neighboring spins

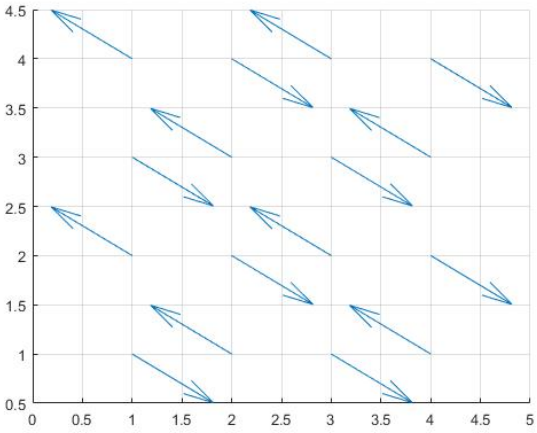
The randomly chosen spin $\left(\mathbf{S}_{ij}\right)$ is then orientated opposite to the direction of the magnetic field. Hence,

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

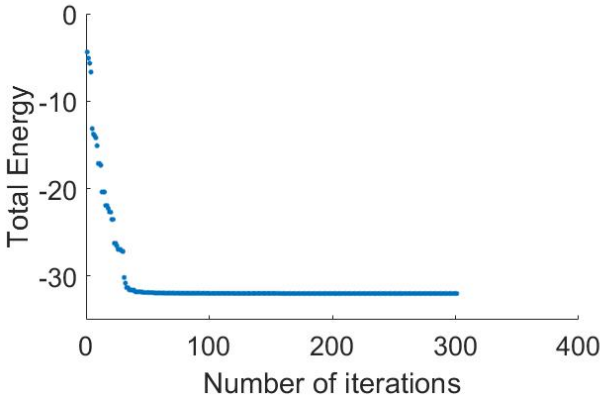
2.2 Simulations & Results

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



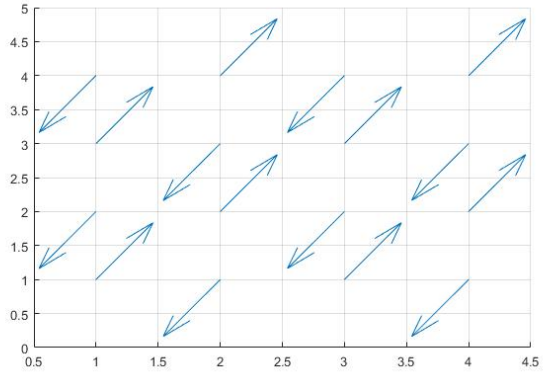
(b) Energy vs iterations

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

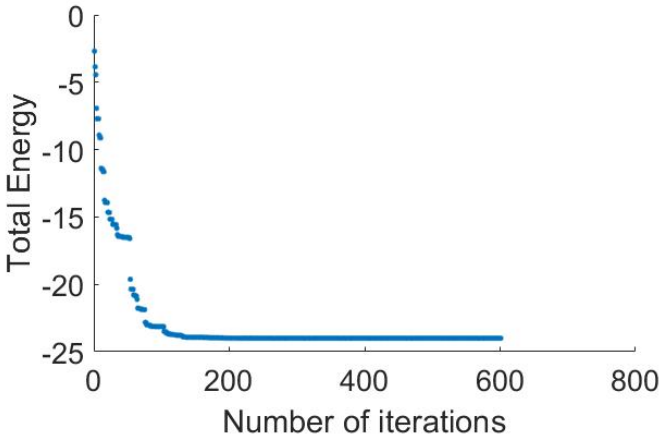
As the figure shows, when J_2 is equal to 0, all the spins align themselves opposite to the direction of neighboring spins. This is what we expect the orientation of spins for any anti-ferromagnetic crystal. As the energy vs number of iterations graph shows, our system have achieved is converging to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

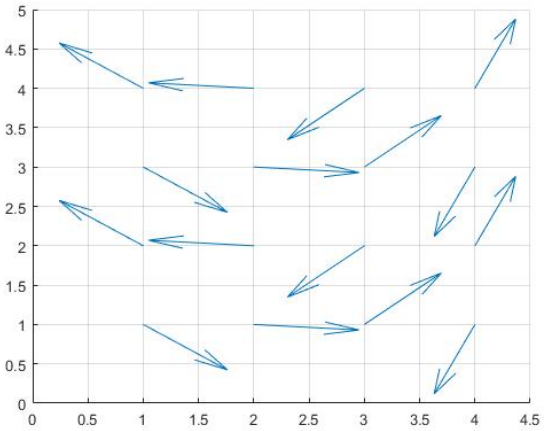


(b) Energy vs iterations

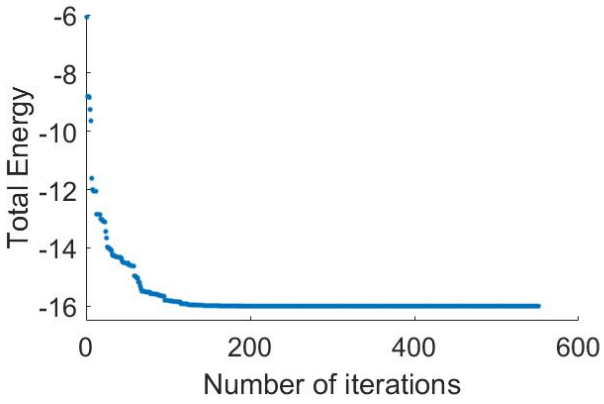
Fig. 2.4.: *Case 2.1:* Spins constrained in a plane, $J_2 = 0.25$ & $J_1 = 1$

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.

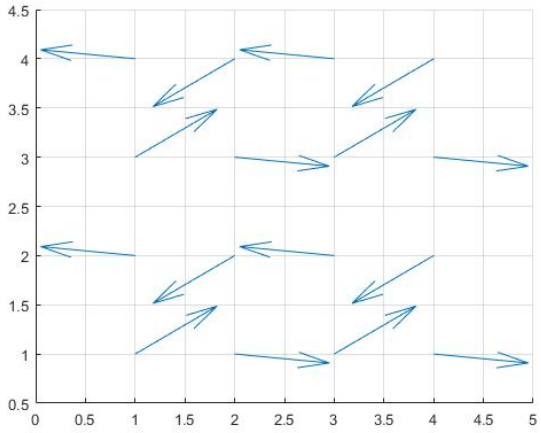


(a) Spin Orientations

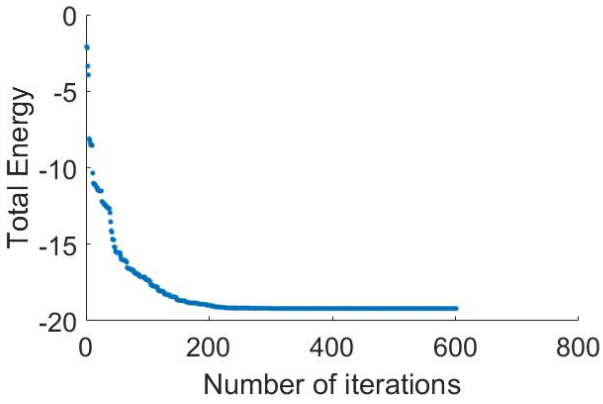


(b) Energy vs iterations

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



(a) Spin Orientations

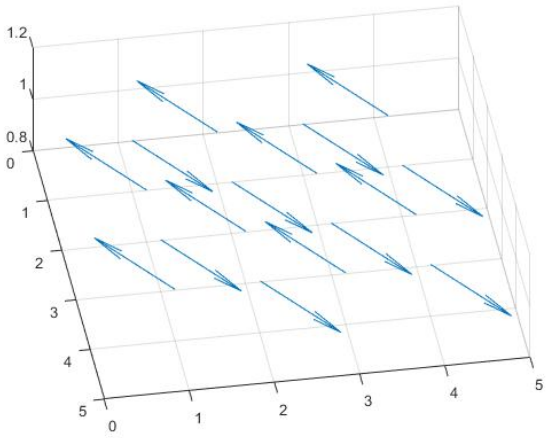


(b) Energy vs iterations

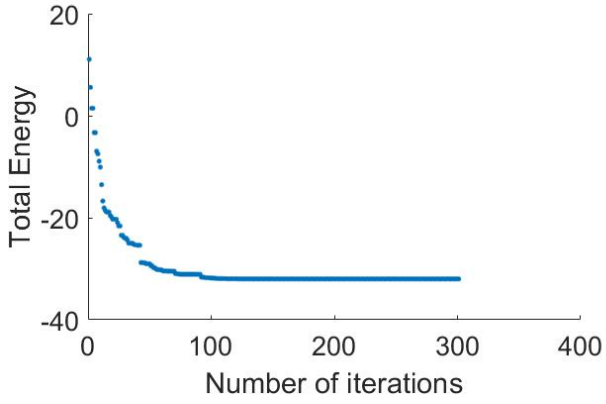
Fig. 2.6.: *Case 2.3:* Spins constrained in a plane, $J_2 = 0.6$ & $J_1 = 1$

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

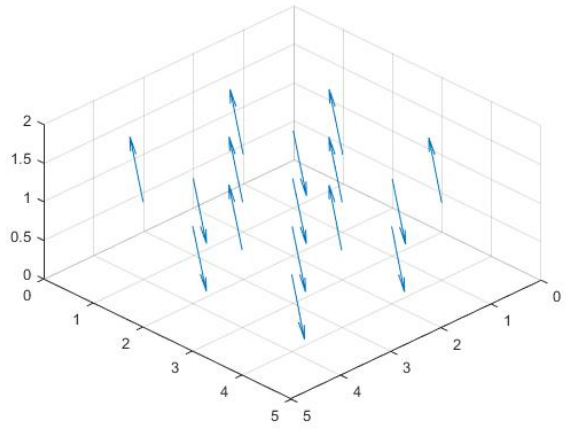


(b) Energy vs iterations

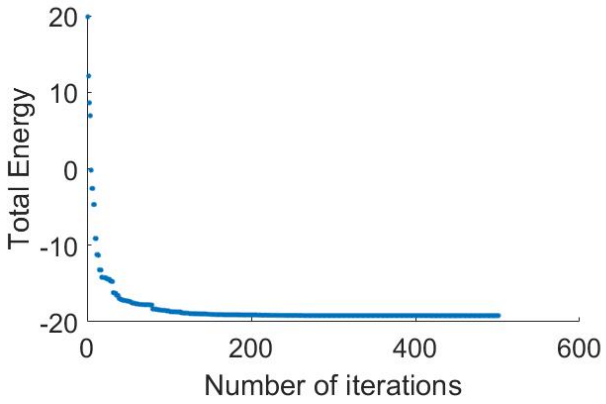
Fig. 2.7.: *Case 3:* Spins are free to rotate in 3-dimension, $J_2 = 0$ & $J_1 = 1$

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 $J_2 \neq 0$:

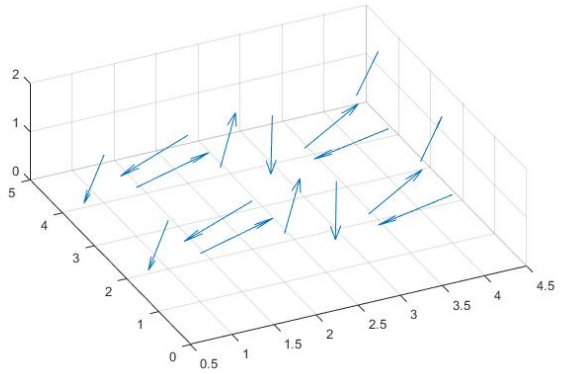


(a) Spin Orientations

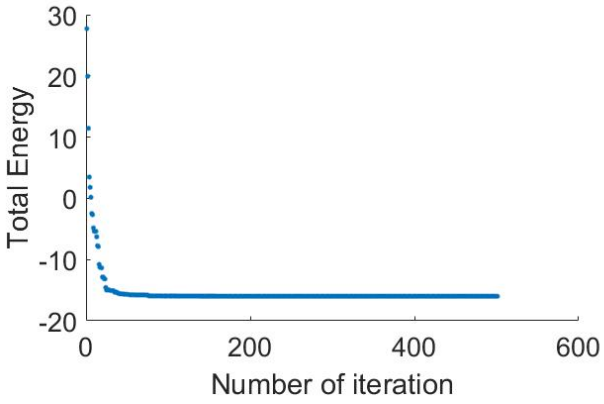


(b) Energy vs iterations

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



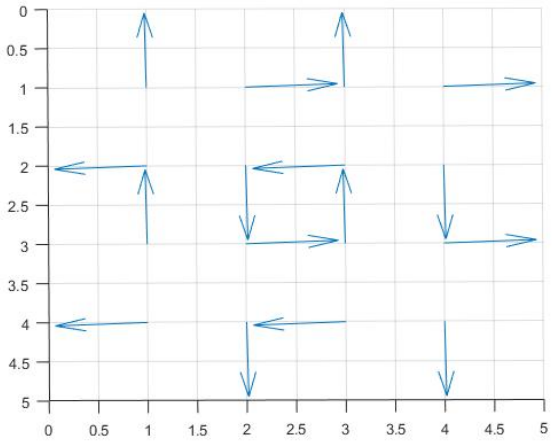
(a) Spin Orientations



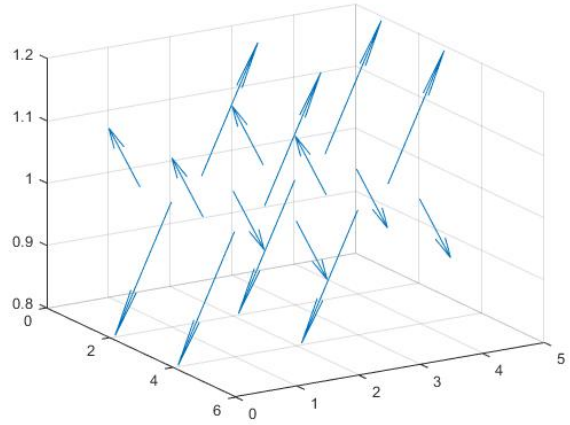
(b) Energy vs iterations

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

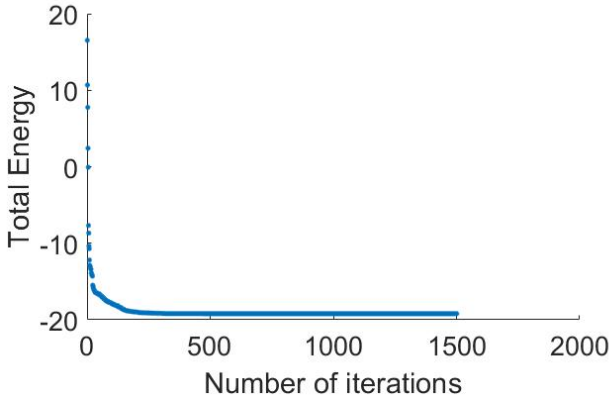
When spin rotors are free to rotate in space, then the simulation results shows similarity with case for two dimensionally constrained spins when $J_2 \neq 0$ in theri respective ground states.



(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 [4] 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 [5] to the following:

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

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

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

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)

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

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)	2J1
-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

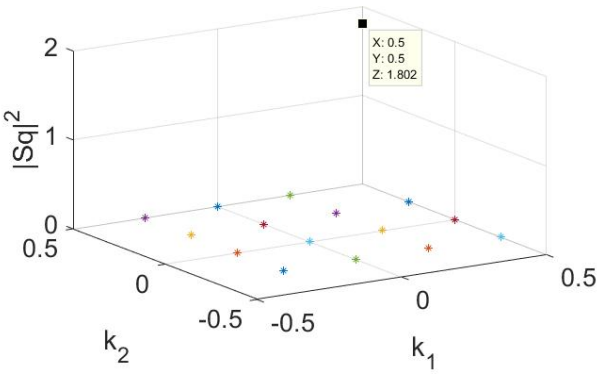
For all the values of k_1 & k_2, the value of the equation 3.12 has been tabulated in Table 3.1 Now for the different values of the ratio $\frac{J_2}{J_1}$, the value of k_1 and k_2 (thus corresponding q) for which $J_{\mathbf{q}}$ is minimum is tabulated in Table 3.2

$\frac{J_2}{J_1}$	(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	$(0, \frac{1}{2})$,$(\frac{1}{2}, 0)$

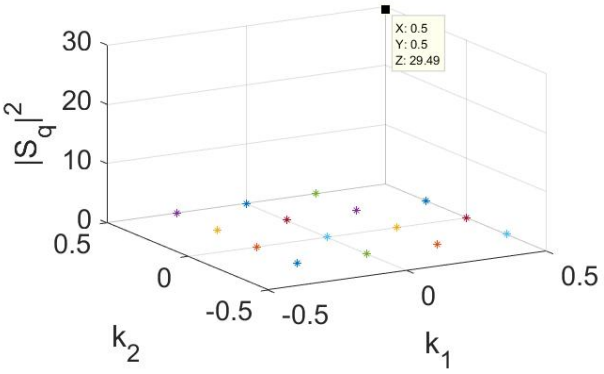
Table 3.2: k_1 and k_2 corresponding to minimum value of $J_{\mathbf{q}}$

3.3 Simulations for Luttinger-Tisza

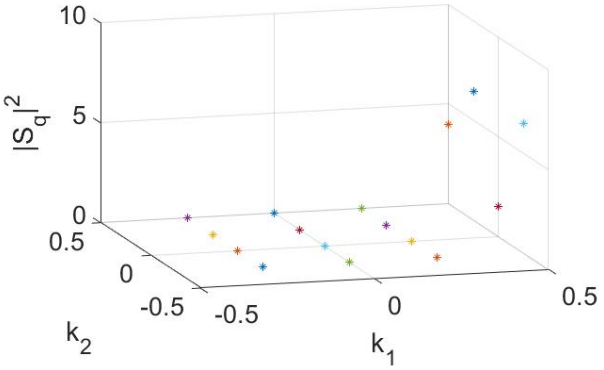
As said earlier, we use the LT method to verify the results of our simulations by plotting $|\mathbf{S_q}|^2$ against the different values $\mathbf{q}$. The following plots (figure 3.1 & 3.2) were obtained for all simulation results shown in the previous section.



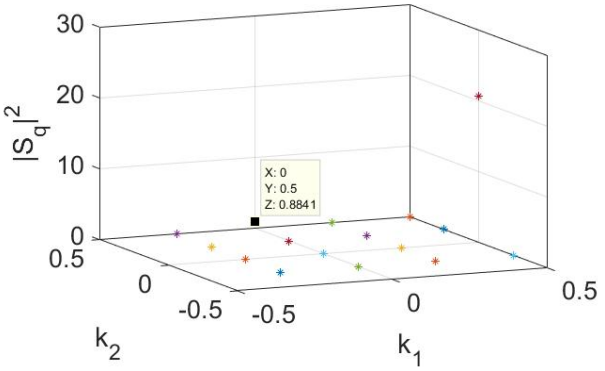
(a) 2D: $\frac{J_2}{J_1} = 0$



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

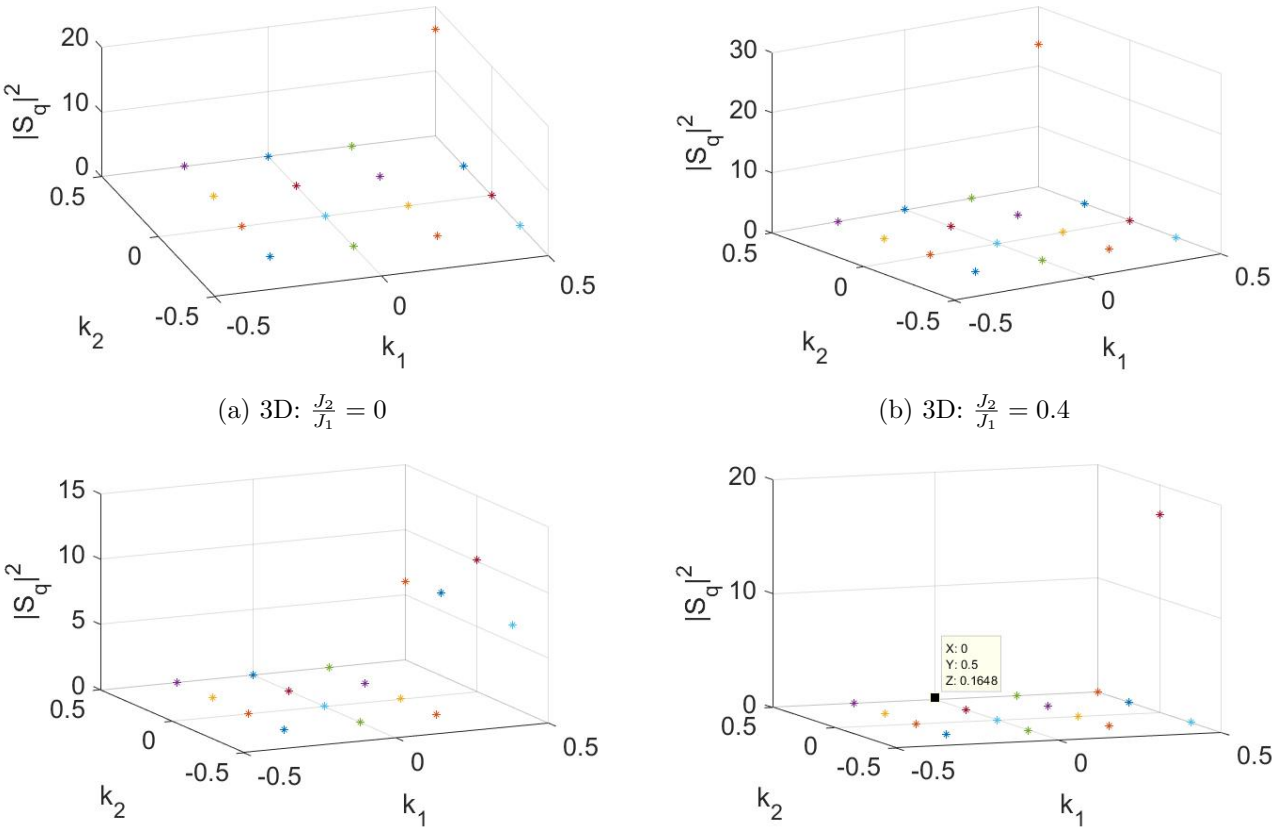


(c) 2D: $\frac{J_2}{J_1} = 0.5$



(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: $\frac{J_2}{J_1} = 0$

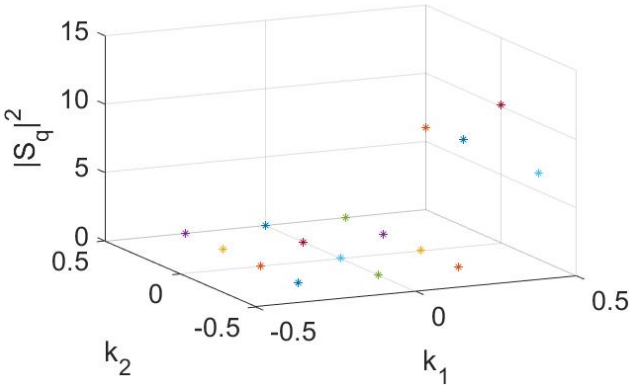
(b) 3D: $\frac{J_2}{J_1} = 0.4$

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

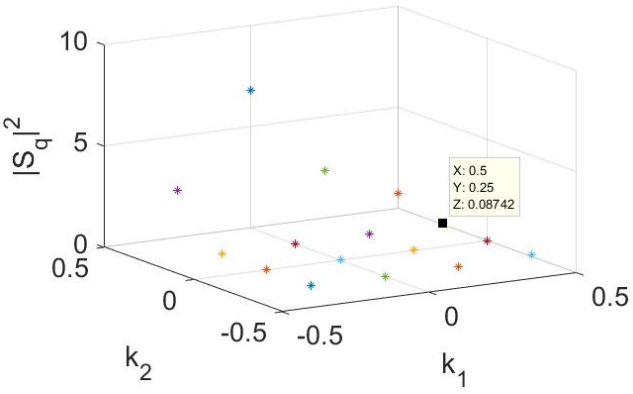
(d) 3D: $\frac{J_2}{J_1} = 0.6$

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. SUMMARY

The aim of our project for this semester was to simulate and understand the already formulated the methods of finding the ground state spin configurations in a given lattice. The iterative minimization always converges to the ground state configuration which is shown by the converging graph of the total energy of the system. For the cases where J_2 is small compared to J_1, the system configuration remain close to arrangement when J_2 is absent. However as J_2 increases its effect also increases which is shown in the results. The Luttinger-Tisza Method (and hence spin structure factor) is a very effective way to determine the ground state spin configurations although, here, we have used it only for verification of our results of our simulations via iterative minimizations.

In future we are planning to work on Hamiltonian which will also include a factor of two pair of coupled spins $[Q_{ijkl}(\mathbf{S}_i.\mathbf{S}_j)(\mathbf{S}_k.\mathbf{S}_l)]$. This is a new thing which we will try to do based on our current simulation and results.

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