Models and methods for classical spin systems

Submitted by

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Certificate

This is to certify that the dissertation titled "Models and methods for classical spin systems" submitted by Sameep Chandel (Reg. No. MS07021) for the partial fulfilment of BS-MS dual degree programme of the Institute, has been examined by the thesis committee duly appointed by the Institute. The committee finds the work done by the candidate satisfactory and recommends that the report be accepted.

Dr. Yogesh Singh **Dr. Ananth Venkatesan** **Dr. Sanjeev Kumar**

(Supervisor)

Dated: May 9, 2012

Declaration

The work presented in this dissertation has been carried out by me under the guidance of Dr. Sanjeev Kumar at the Indian Institute of Science Education and Research Mohali. This work has not been submitted in part or in full for a degree, a diploma, or a fellowship to any other university or institute. Whenever contributions of others are involved, every effort is made to indicate this clearly, with due acknowledgement of collaborative research and discussions. This thesis is a bonafide record of original work done by me and all sources listed within have been detailed in the bibliography.

Sameep Chandel

(Candidate)

Dated: May 9, 2012

In my capacity as the supervisor of the candidate's project work, I certify that the above statements by the candidate are true to the best of my knowledge.

Dr. Sanjeev Kumar

(Supervisor)

Acknowledgement

Apart from my efforts, the success of this project depends largely on the encouragement and guidelines of many others. I take this opportunity to express my gratitude to the people who have been instrumental in the successful completion of this project.

I would like to show my deepest appreciation to Dr. Sanjeev Kumar. I can't say thank-you enough for his tremendous support and guidance. I felt motivated and encouraged every time I met him.

I am also thankful to Dr. Rajeev Kapri for his help in installing some needed library packages.

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Abstract

We model certain real systems using classical spins with some suitable spin interaction Hamiltonian. In all the simulations, Classical Monte Carlo method is used to extract expectation value of observables like Energy, Magnetisation, Specific Heat and Susceptibility from a large periodic spin lattice at a particular temperature. The spins interact via a particular model as if they are mimicing a corresponding real system (some Magnetic material). In the initial chapters we discuss how the Classical Monte Carlo method is the preferable one. Then in the later chapters we mainly deal with two types of models on large periodic spin lattices:

1. Triangular lattice model with site distortions: Here, we apply the Heisenberg model on triangular lattice. This model also demonstrates geometrical frustration. We divide this discussion into two parts, one with lattice distortion and the other without lattice distortion.

2. Heisenberg Kitaev model (Honey Comb lattice): Here, we deal with spin interactions on Honeycomb lattice. We see variation in the magnetic order of the ground state spin configuration with the relative variation of the parameters values of the model.

Under a particular model of spin interations, we see how the magnetic phase of our lattice makes transitions with changes in temperature. The task is to find the values of the parameters of a given model and temperatures for which the system attains magnetic ordering i.e. it settles to a phase.

Chapter 1

Introduction

The diversity of systems and phenomena available for study makes Condensed Matter physics the most active field of contemporary physics[1][2]. We know that Condensed Matter Physics deals with the physical properties of condensed phases of matter[13]. The most familiar condensed phases are solids and liquids.

Of the various physical properties, magnetic properties of systems are of significant importance and have wide applications. Materials with magnetic properties are understood mostly through spin models.

We use suitable classical spin models to study such systems. Also, magnetic phase transition is a very common phenomena in such systems. We track the magnetic ordering of our system at various temperatures using structure factor calculations. This gives us idea about the manner in which phase change is happening with temperature. We also look at the ground state spin configurations of our system for different values of the model parameters to get further insight about the real systems. This enables us to make better predictions about the behaviour of real systems under different conditions.

In this chapter we understand what are models and how they are important in Condensed Matter Physics. We further discuss how computer simulations are of great help nowadays.

1.1 Models

As we know, the way science understands nature is by giving a theory in the form of some model and applying it to nature. We need to understand the functioning of the real systems involved to explain a physical phenomena. A good model can

represent the physical system to a great extent. A model consist of parts which interact in certain ways. For example, Ising model, which is a spin model, is used to study phase transition in Ferromagnets.

Models are often systems for which certain quantities can be computed exactly or atleast can be reduced to simpler forms. Such techniques are very specialized and only work in certain special cases[7].

We, in particular, deal with spin models. Many real systems can be modelled in terms of classical spins on different types of lattices. Examples,

- $AEMnO_3$: In such materials, Mn moments sits on Cubic lattice.
- $RE_2M_2O_7$: In such materials, magnetic moments sits on Pyrochlore lattice.

1.2 Computer Simulations

Physics was first known as 'natural philosophy' historically. Pure theoretical (or philosophical) investigation was the way of doing research. Whether a given theory really applies to nature or not was not known. This lack of real knowledge limited the true progress. Experimental investigation, eventually, became an accepted form of research. Although physicist's ability to prepare a sample for study or to devise techniques to probe for the desired properties always limited it.

Direct comparison between analytical theory and experiment is inconclusive in numerous situations. For example, the theory of phase transitions in condensed matter must begin with the choice of a Hamiltonian, and to what extent a particular model actually represents a real material on which experiments are done is seldom clear. Since mathematical approximations are also usually required in analytical treatments, whose accuracy is difficult to control or assess, one does not know whether discrepancies between theory and experiment should be attributed to the approximations, shortcomings of the model, or both.

With the advent of *computers* it became possible to carry out *simulations* of models which were intractable using 'classical' theoretical techniques. In many cases computers have enabled physicists to invent new models for various aspects of nature and to solve those same models without substantial simplification. Computer power has increased quite dramatically in recent years. Access to computers is becoming both easier and more common (e.g. with personal computers and workstations) and computer simulation methods have also been steadily refined.

As a result computer simulations have become another way of doing physics research. In some cases simulations provide a theoretical basis for understanding experimental results, and in other instances simulations provide 'experimental' data with which theory may be compared[8].

Chapter 2

Method and Simulation of the Spin System

In this chapter we introduce the main concept of Metropolis algorithm which involves Classical Monte Carlo method. We also discuss how the method and algorithm are implimented in our simulation programs.

2.1 Classical Monte Carlo Method

If we want to find the *expectation value* of an observable A for a system that has a discrete number of states, we could, using a computer, calculate A for each state and weight these values by their Boltzman factors.

$$\langle A \rangle = \frac{\sum_r A_r e^{-\beta E_r}}{\sum_r e^{-\beta E_r}}, \tag{2.1}$$

where A_r is the value of A for the state r.

This might be feasible for a system with a small number of states, but if we have a 20×20 spin lattice interacting via the Ising model, there are 2^{400} states, so we cannot possibly examine all of them. We can also approximate the calculation by sampling some of the states.

Here "Monte Carlo" part comes in. Named for the Mediterranean casino town, a *Monte Carlo method* is any algorithm that involves a pseudorandom number generator[9].

2.2 Metropolis Algorithm

One way of using random numbers would be to randomly pick a lot of states, measure A for each of them, and weight these values of A by their Boltzman factors. If we sample a lot of states we might get close to the right answer, but it would take a lot of time calculating A for states that contribute very little to the final result. It is because an Ising lattice at very high temperature is less likely to be in the state with all spins pointing in one direction.

Instead of sampling (measuring parameters like A for) a lot of states and then weighting them by their Boltzman factors, it is better to choose states based on their Boltzman factors and to then weight them equally. This is known as the *Metropolis algorithm* and it is an important sampling technique[9].

For our system lying in a particular spin configuration, as shown in figure 2.1, one pass through the algorithm is as follows:

1. A trial configuration is made by choosing one spin and randomly modifying it, i.e., assigning a new value.

2. The energy difference of this trial state (i.e., the new configuration with the modified spin) relative to the initial state, δE is calculated.

3. If $\delta E \leq 0$, the trial state is accepted as it is energetically favorable. Otherwise, a random number $0 \leq \eta \leq 1$ is generated, and the new state is only accepted if $e^{-\beta\delta E} > \eta$. This condition can be rewritten as $-\beta\delta E > \log\eta$, which is used in the code[9].

2.3 Program Outline

In the program we have a general $m \times n$ spin lattice. The spins at each lattice site can, in general, point in a direction, discretely, in 3-D space. We initialize our system with some spin configuration.

Starting at the given high temperature, our system is continuously modified by reassigning a new value to one spin at a time, i.e. one pass through the Metropolis algorithm as discribed in section 2.2. We move to next spin keeping all the previous changes whether accepted or rejected. Whenever we modify any spin, as needed by the Metropolis algorithm, we calculate and compare the energy of the whole system, i.e., of all spins in total, of the modified state with the previous state. When this spin-by-spin updation process, beginning from the first spin,

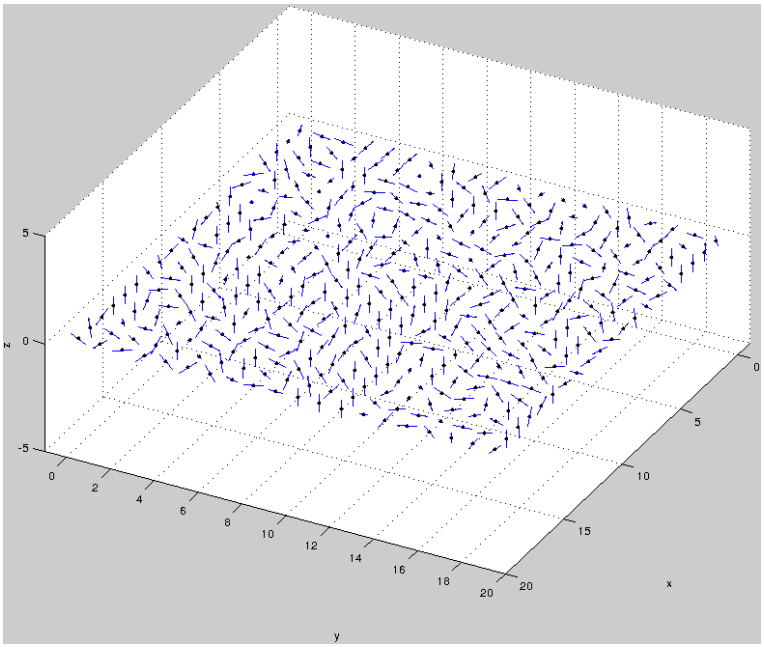

Figure 2.1: A random spin configuration on a 20×20 lattice

reaches the last spin of the configuration of $m \times n$ spin lattice, it is refered to as one *simulation step* in the program. In other words, updating the whole spin lattice one spin at a time is a single simulation step.

So, starting from the given high temperature, or at any temperature in general, the system goes through 1000 such steps of updation without other calculations besides energy which is a requirement of the algorithm. But these energies are not recorded. These simulation steps are refered to as *equilibration steps*.

After these 1000 equilibration steps it is expected that the spin configuration would be reflection the spin state of the real system we are modeling. So now, for the next 1000 steps, we calculate observables like Energy and Magnetisation. These simulation steps are refered to as *averaging steps* because at the end of these 1000 steps we take the averages of these observables to calculate the expectation values of Energy, Magnetisation, Specific heat and Susceptibility.

The calculation of the Energy depends on the type of model under consideration. A particular model has a specific hamiltonian which accounts for the interation of a spin with its neighbouring spins. The interactions can be either magnetic or due to their relative positions or both.

After these 1000 equilibration and 1000 averaging steps, the temperature parameter is reduced by a fixed amount and similar simulation process is repeated again at this temperature. This process continues till the system reaches the given low temperature. At the end of last 1000 + 1000 steps at the lowest temperature the state of the system is refered to as *ground state* and is ploted in the later chapters.

2.4 Key Observables

Mainly we are concerned with Energy, Magnetisation, Specific heat and Susceptibility of the system at some temperature. We can measure the magnetization by taking the sum of all the spins in the lattice, and we can calculate the energy by determining the energy for each spin and dividing by two for double counting. Other quantities can be calculated using the following formulae:

Specific Heat,

$$C_V = \frac{\beta}{T}[\langle E^2 \rangle - \langle E \rangle^2] \tag{2.2}$$

Susceptibility,

$$\chi = \beta[\langle M^2 \rangle - \langle M \rangle^2] \tag{2.3}$$

Chapter 3

Heisenberg Model on Square Lattice

Now lets work out a basic model, the Heisenberg model. In this model, spins can orient in 3D space and are fixed on their lattice sites. The Hamiltonian for the near neighbour spin interactions is given by,

$$H = J \sum_{\langle ij \rangle} \overrightarrow{S_i} \cdot \overrightarrow{S_j} \tag{3.1}$$

The program is run for the following parameters:

- $J = 1$ which is for a antiferromagnet.
- 10×10 spin lattice
- High temperature = $6J$, Low temperature = $0.25J$
- Temperature step size = $0.25J$
- Equilibration steps = 2500, Averaging steps = 2500

Following are the results and the plots of the key observables, as shown from table 3.1 to figure 3.4

THE MAIN PROPERTIES				
T	E_{avg}	M_{avg}	C_V	χ
6	-0.352593	0.120496	0.000619643	0.00135794
5.75	-0.370344	0.126728	0.000719426	0.00160135
5.5	-0.383642	0.126568	0.00077537	0.00155246
5.25	-0.399834	0.129408	0.000857852	0.00179112
5	-0.428004	0.135304	0.000980088	0.00206686
4.75	-0.451999	0.14052	0.00108136	0.00239695
4.5	-0.477965	0.149288	0.00131892	0.00277512
4.25	-0.511748	0.155288	0.00146137	0.00309777
4	-0.554348	0.171256	0.00178541	0.00413061
3.75	-0.59083	0.17688	0.00216569	0.00452776
3.5	-0.659974	0.196768	0.00229074	0.00602949
3.25	-0.723313	0.225672	0.0033828	0.00826355
3	-0.81461	0.263575	0.00395837	0.0110699
2.75	-0.949633	0.354264	0.00661012	0.0185852
2.5	-1.19539	0.546353	0.0108968	0.0255181
2.25	-1.48033	0.754822	0.0130588	0.0192151
2	-1.74234	0.910735	0.00742561	0.00347927
1.75	-1.86959	0.960717	0.00446141	0.00103082
1.5	-1.94924	0.985801	0.0020824	0.000314633
1.25	-1.98127	0.995109	0.00101227	9.88007e-05
1	-1.99133	0.99779	0.00071907	5.1558e-05
0.75	-1.99237	0.998079	0.00114441	5.82536e-05
0.5	-1.99307	0.998247	0.00246716	8.51154e-05
0.25	-1.99231	0.998071	0.0105515	0.000178099

Table 3.1: Observables–Energy, Magnetisation, Specific Heat and Susceptibility, for Heisenberg Model on a 10×10 lattice, for $J = 1$

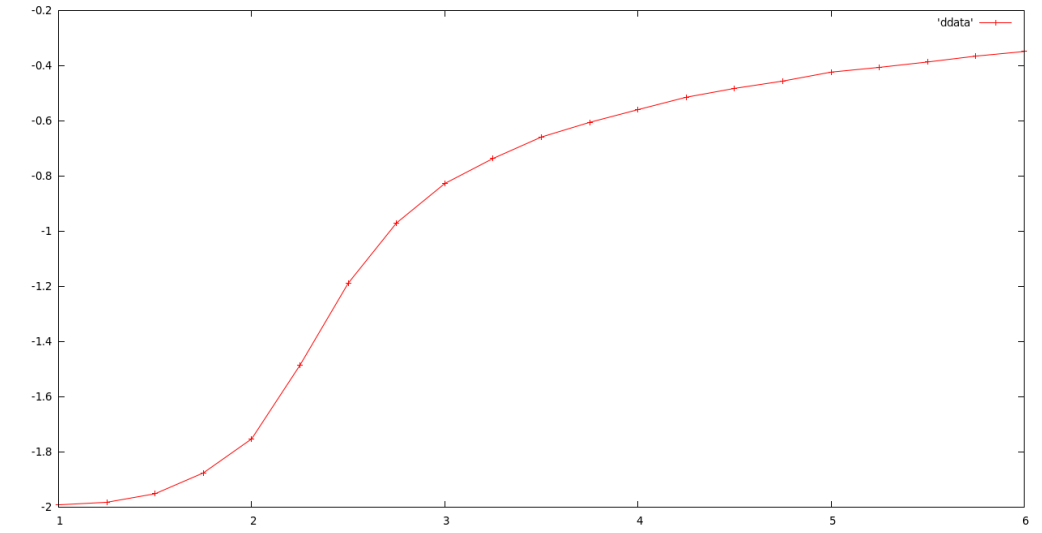

Figure 3.1: Energy as a function of Temperature, for Heisenberg Model on a 10×10 lattice, for $J = 1$

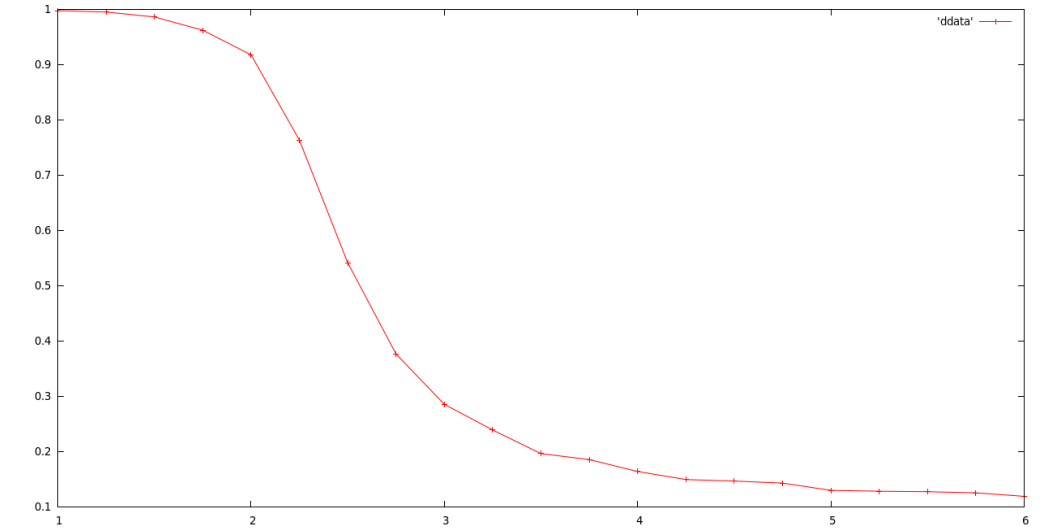

Figure 3.2: Magnetization as a function of Temperature, for Heisenberg Model on a 10×10 lattice, for $J = 1$

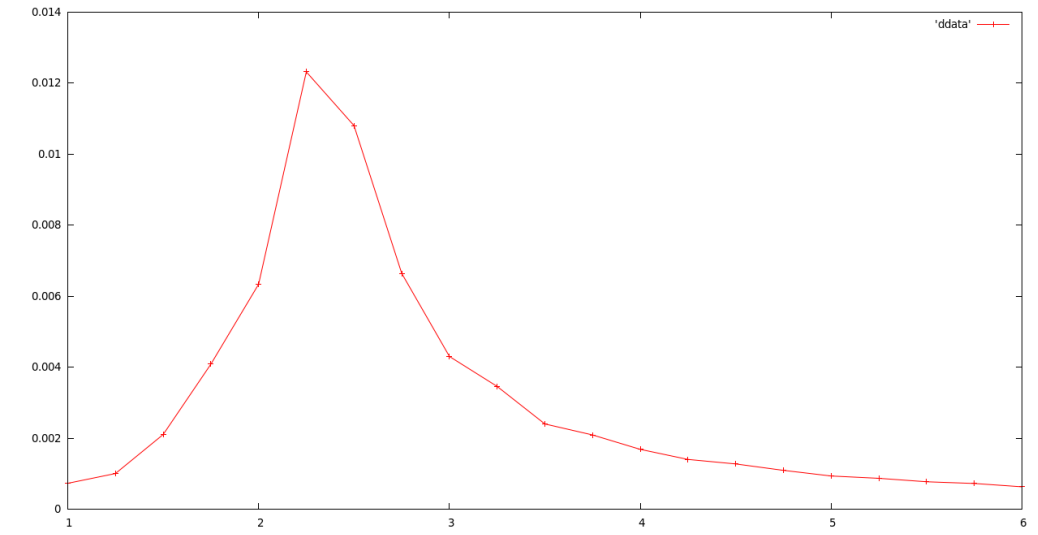

Figure 3.3: Specific Heat as a function of Temperature, for Heisenberg Model on a 10×10 lattice, for $J = 1$

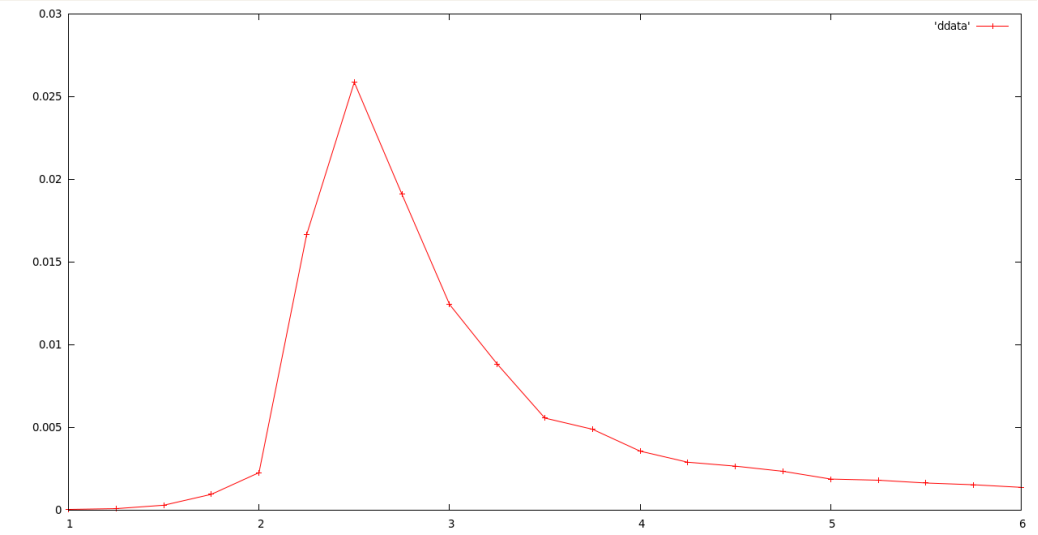

Figure 3.4: Susceptibility as a function of Temperature, for Heisenberg Model on a 10×10 lattice, for $J = 1$

The program is also run for 10×10, 40×40 and 80×80 spin lattices with the following parameters:

- $J = 1$ which is for a antiferromagnet.

- High temperature = 2, Low temperature = 0.05
- Temperature step size = 0.05
- Equilibration steps = 10000, Averaging steps = 10000

The following plot, figure 3.5, is the Magnetisation versus Temperature plot for different lattice sizes. It shows that phase transition is sharp for bigger lattice sizes.

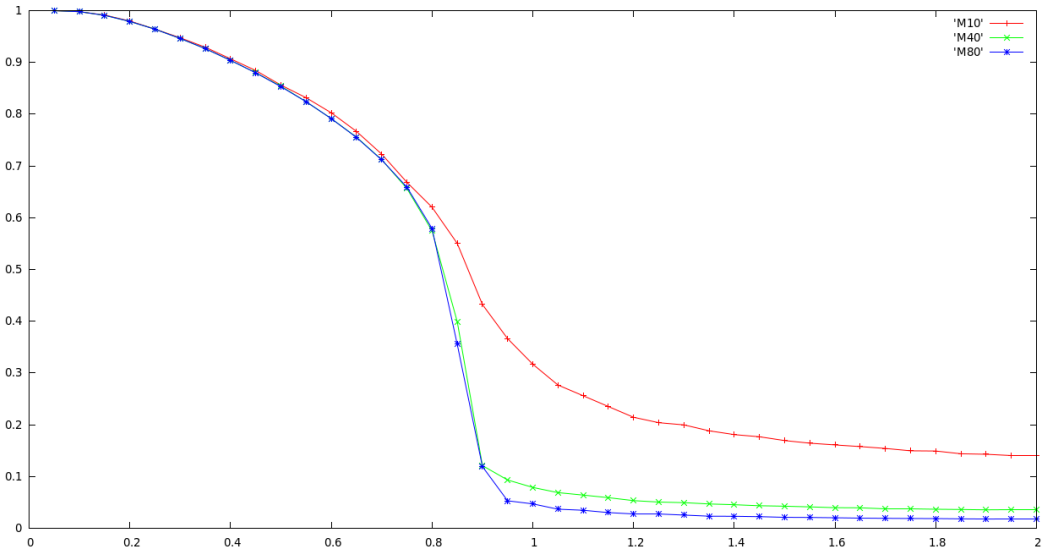

Figure 3.5: Magnetization as a function of Temperature, for Heisenberg Model on 10×10, 40×40 and 80×80 lattices, for $J = 1$

Chapter 4

Triangular lattice Model

In this chapter we deal with the triangular lattice model with and without lattice distortions. Examples of real systems where such models can be applied are $LiMnO_2$ and $NiGaS_4$.

Figure 4.1 shows the actual triangular lattices and figure 4.2 shows how it can be interpreted while making a program. In other words, a triangular lattice can be modeled as a square lattice with an extra diagonal interaction.

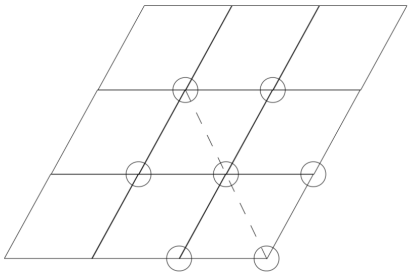

Figure 4.1: Triangular lattice

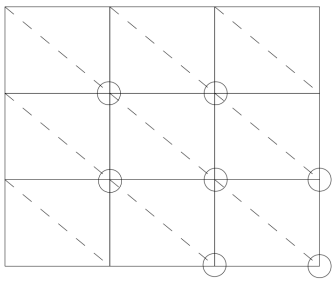

Figure 4.2: Equivalent square lattice

Thus, Hamiltonian for this model is similar to Heisenberg model but here i and j also goes over one of the diagonal neighbouring spins.

$$H = J \sum_{\langle ij \rangle} \vec{S_i} \cdot \vec{S_j} \tag{4.1}$$

Also we only deal with the case when spins can only be in a plane. So we are having an $X - Y$ model. An important point to notice for such model is that if we take J as -1, i.e., as in ferromagnetic case, then ground state is obviously a ferromagnet. Because in ferromagnetic configuration, all spins in one direction is

the favourable case with minimum energy.

But if we take J as +1, then ground state cannot be an antiferromagnet due to an apparent *strain* that any spin can feel because of the neighbouring spins at triangular position. Figure 4.3 shows how spin-a cannot anti-allign with either of spin-b and spin-c, as in one case it minimizes energy but in other case that orientation costs too much energy.

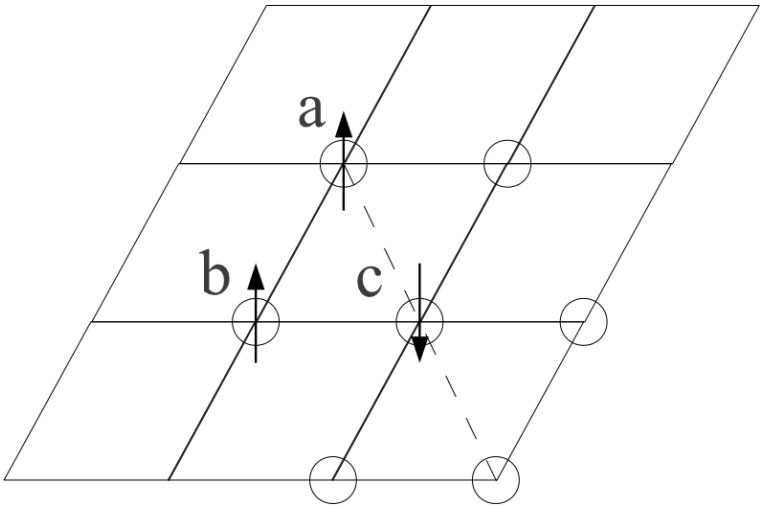

Figure 4.3: Demonstration of frustration on a triangle of spins

Hence $J = +1$ is an interesting case to see which is what we see in the following sections. This case serves to demonstrate *geometrical frustration*. Geometrical frustration is one of the key concepts in modern condensed matter theory. It is related to the impossibility of simultaneously minimizing the energy for all constituents of a system due to geometrical constraints[10].

In one section spins in their ground state minimizes energy by orienting in a triangular fashion and in the next section we see that besides orienting this way, they also try to move to other locations to minimize energy.

We also calculate the Structure factor in the program. Lets first understand what it is. For a periodic lattice like ours, *structure factor* is simply the squared modulus of the *Fourier transform* of the lattice, and it is itself a periodic arrangement of points, known as the *reciprocal lattice*.

In single expression it can be written as,

$$S_{\vec{q}} = \sum_{\langle ij \rangle} (\vec{S}_i \cdot \vec{S}_j) e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)} \tag{4.2}$$

where $\vec{q}$ is the change in the wave vector or the scattering vector $\triangle\ k$ as in the context of X-ray diffraction by a crystal.

Structure factor can also be written as,

$$S_{\vec{q}} = f_x \cdot f_x^* + f_y \cdot f_y^* + f_z \cdot f_z^* \tag{4.3}$$

where $f's$ are given by,

$$f_x(q_x, q_y) = \sum_i S_i^x e^{i\vec{q}\cdot\vec{r}_i}, \tag{4.4}$$

$$f_y(q_x, q_y) = \sum_i S_i^y e^{i\vec{q}\cdot\vec{r}_i}, \tag{4.5}$$

$$f_x(q_x, q_y) = \sum_i S_i^z e^{i\vec{q}\cdot\vec{r}_i} \tag{4.6}$$

4.1 Triangular lattice without lattice distortion

If we are considering our lattice cannot distort, then the ground state results into spins aligned at 120° with the neighbouring spins as shown in figure 4.4. The program is run for the following parameters:

- $J = 1$
- 20×20 spin lattice
- High temperature = $5J$, Low temperature = $0.1J$
- Temperature step size = $0.1J$
- Equilibration steps = 1000, Averaging steps = 1000

From the data file generated, for $T = 0.2J$ (near ground state temperature), we get highest $S_{\vec{q}}$ value as 0.4287 for (q_x, q_y) = (2.19911, 2.19911) and (-2.19911, -2.19911). This corresponds to the $\frac{2\pi}{3}$ or 120° angle with which each spin is aligned to the neighbouring spin in the ground state.

Plots for C_V and $S_{\vec{q}}$ are also shown below.

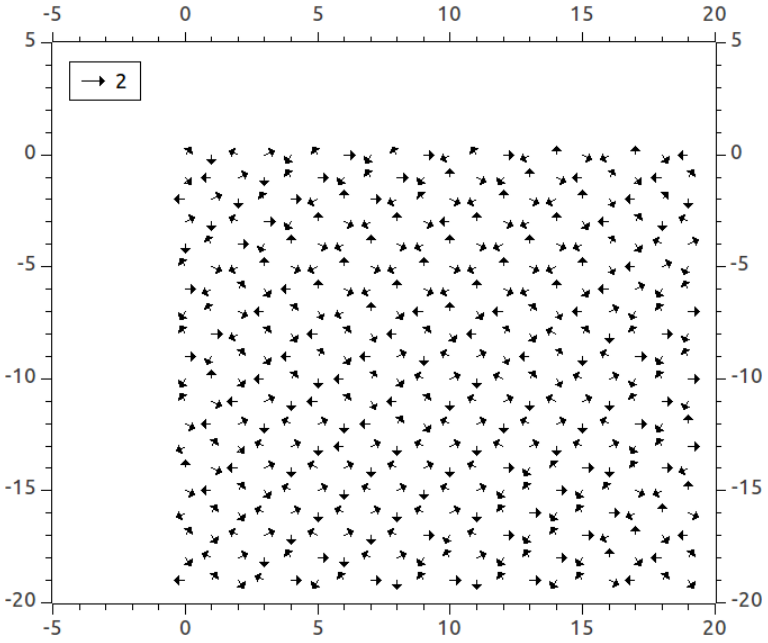

Figure 4.4: Ground state spin configuration, for Triangular lattice $X - Y$ model without distortion on a 20×20 lattice, for $J = 1$

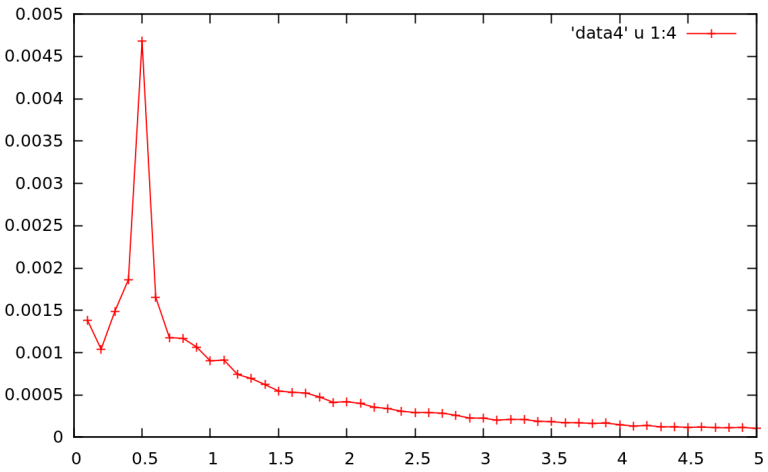

Figure 4.5: Specific Heat as a function of Temperature, for Triangular lattice $X-Y$ model without distortion on a 20×20 lattice, for $J = 1$

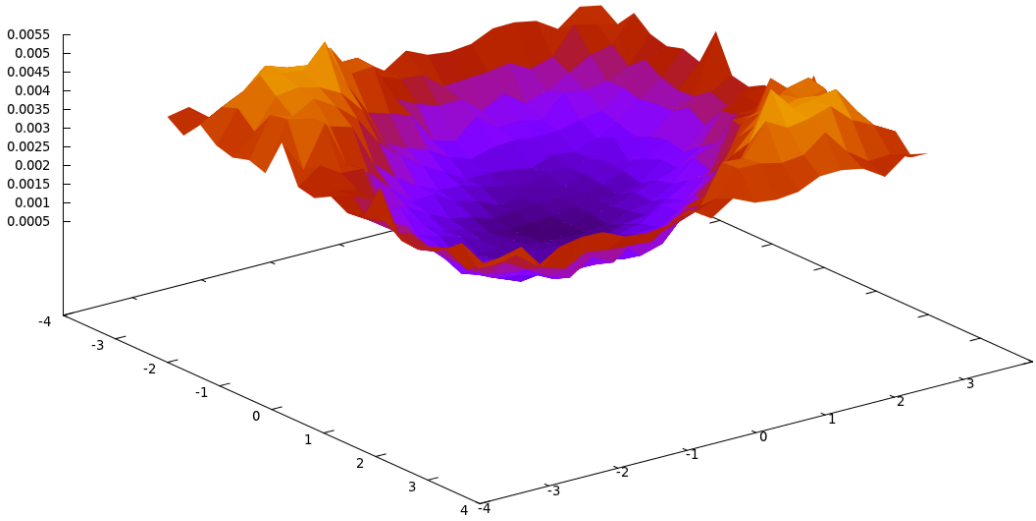

Figure 4.6: Structure factor at $T = 2$, plotted against the reciprocal lattice coordinates, for Triangular lattice $X - Y$ model without distortion on a 20×20 lattice, for $J = 1$

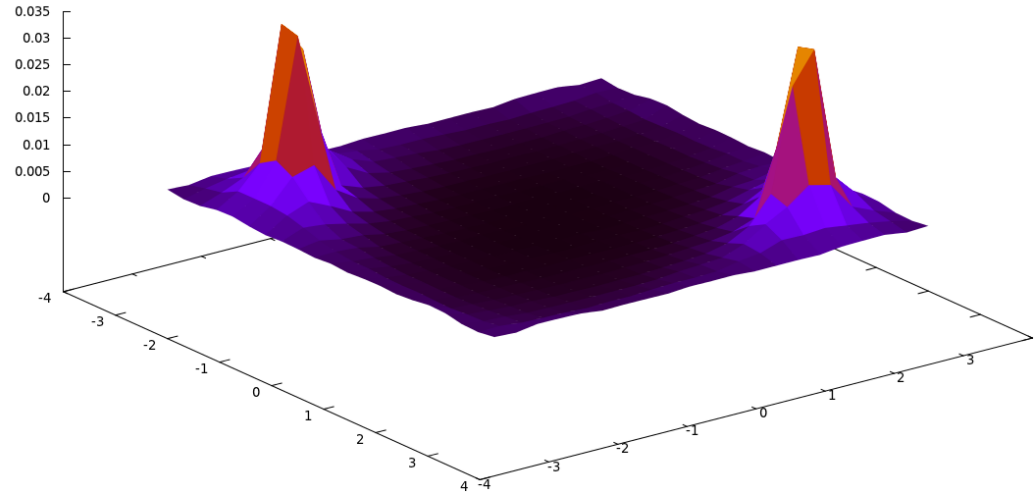

Figure 4.7: Structure factor at $T = 0.6$, plotted against the reciprocal lattice coordinates, for Triangular lattice $X - Y$ model without distortion on a 20×20 lattice, for $J = 1$

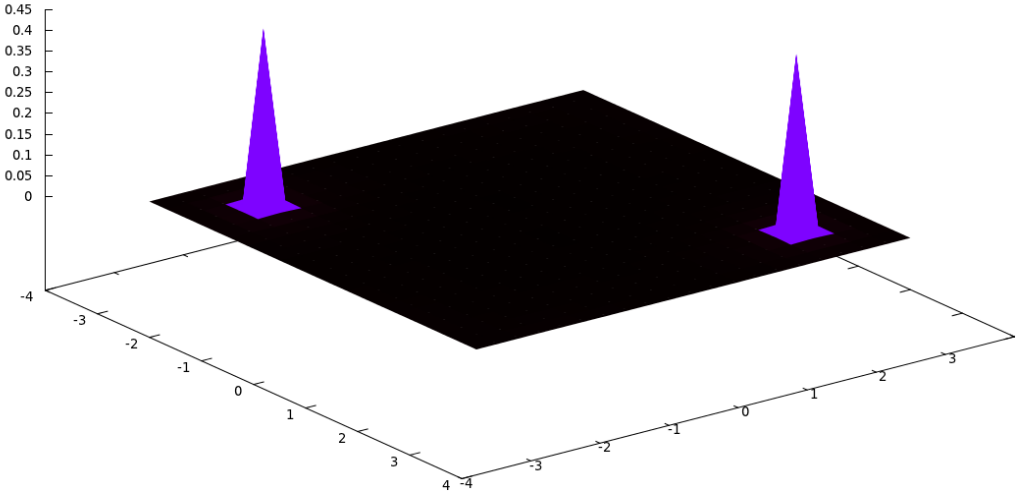

Figure 4.8: Structure factor at $T = 0.2$, plotted against the reciprocal lattice coordinates, for Triangular lattice $X - Y$ model without distortion on a 20×20 lattice, for $J = 1$

4.2 Triangular lattice with lattice distortion

If our lattice is allowed to distort, i.e., if spins can move by little amounts around their lattice sites, then we get our ground state which is a combination of both spin orientation in a nearly triangular fashion and spins shifted from their positions. We can also find the pattern of the spin shifts by finding the Structure factor for spin positions in the same way as it is calculated for spin directions. But this work is yet to be done and is in its partial stage.

The Hamiltonian in this case is given by,

$$H = \sum_{\langle ij \rangle} J_{ij} \, \vec{S_i} \cdot \vec{S_j} + \frac{1}{2} k \sum_i |u_i|^2, \tag{4.7}$$

where,

- $J_{ij} = J(1 - u_{ij})$
- u_{ij} is the increment in the distances between the two spins.
- u_i is the distance of the spin from its lattice site.

The program is run for the following parameters:

- $J = 1$
- 20×20 spin lattice
- High temperature = $5J$, Low temperature = $0.1J$
- Temperature step size = $0.1J$
- Equilibration steps = 1000, Averaging steps = 1000

Figure 4.9 and 4.10 shows the ground state after the simulations.

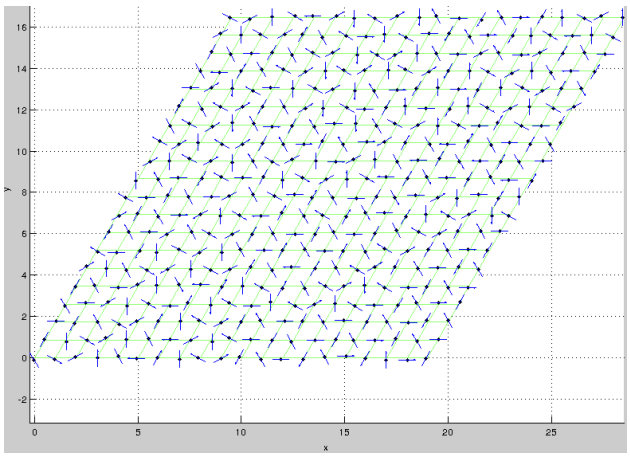

Figure 4.9: Ground state spin configuration, for Triangular lattice $X - Y$ model with distortion on a 20×20 lattice, for $J = 1$

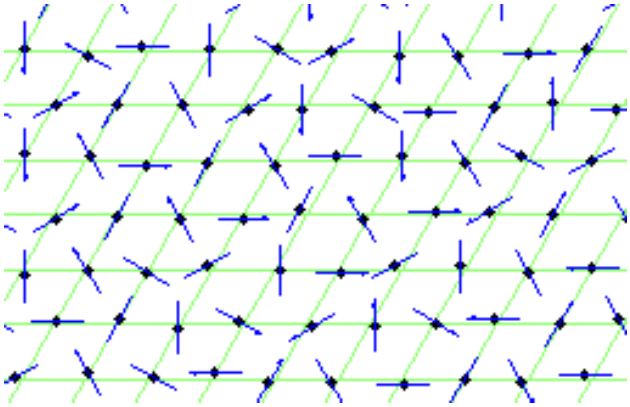

Figure 4.10: Close view of ground state spin configuration, for Triangular lattice $X - Y$ model with distortion on a 20×20 lattice, for $J = 1$

Chapter 5

Heisenberg Kitaev model

This chapter deals with *Heisenberg Kitaev model* in which our lattice is of the form of *honeycomb*, figure 5.1, but it can also be modeled in the form of a square lattice as in figure 5.2 for the simulation purpose. An example where this model is applicable is for Na_2IrO_3.

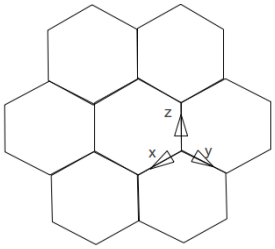

Figure 5.1: Honeycomb lattice

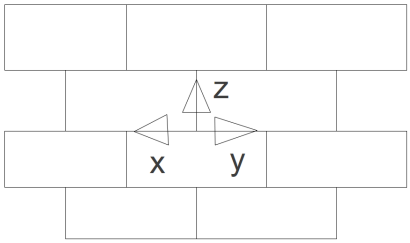

Figure 5.2: Equivalent square lattice

The interaction Hamiltonian has two kind of terms. One is the usual interation term with a coefficient α and other is the Kitaev term with coefficient β. The Hamiltonian is given as,

$$H = \alpha \sum_{\langle ij \rangle} \vec{S_i} \cdot \vec{S_j} - \beta \sum_{\langle ij \rangle} (S_i^x S_{i+x}^x + S_i^y S_{i+y}^y + S_i^z S_{i+z}^z) \tag{5.1}$$

In this model, as is shown in figure 5.1, there are three types of bonds– x, y and z and the pattern is repeated in a similar fashion. So if a bond is x-type, then, as in our Kitaev term, it interacts with the neighbouring spin via x component of spin. And similar are the interactions along y-type and z-type bonds. In this model, unlike triangular lattice model, spins are allowed to orient in 3-D space.

Figures from 5.3 to 5.11 are the Structure factor plots and the ground state spin

configurations for different values of α and β. The simulations were done for the following parameters:

- 20×20 spin lattice
- High temperature = $5J$, Low temperature = $0.1J$
- Temperature step size = $0.1J$
- Equilibration steps = 1000, Averaging steps = 1000

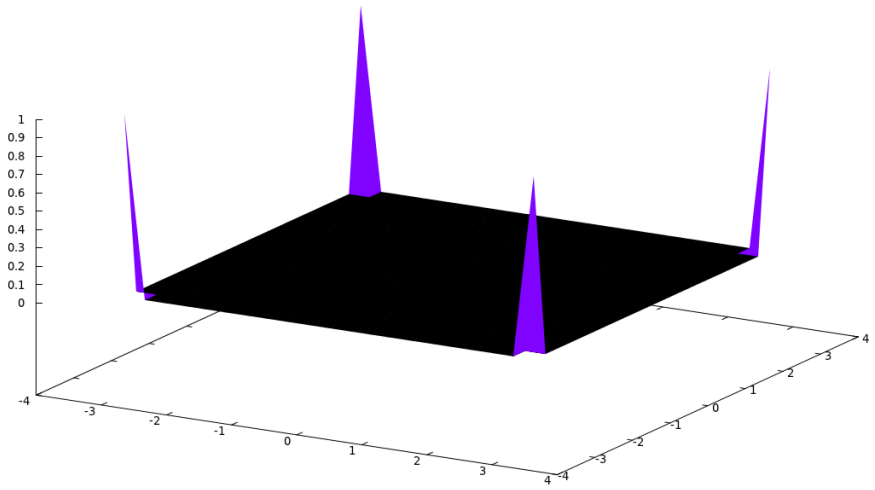

Figure 5.3: Structure factor for $\alpha = 1$, $\beta = 0$ and at $T = 0.1$, plotted against the reciprocal lattice coordinates, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

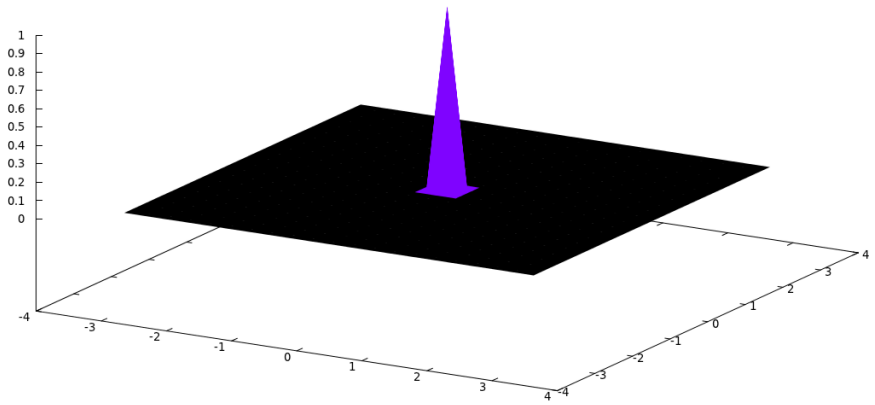

Figure 5.4: Structure factor for α = -1, $\beta = 0$ and at $T = 0.1$, plotted against the reciprocal lattice coordinates, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

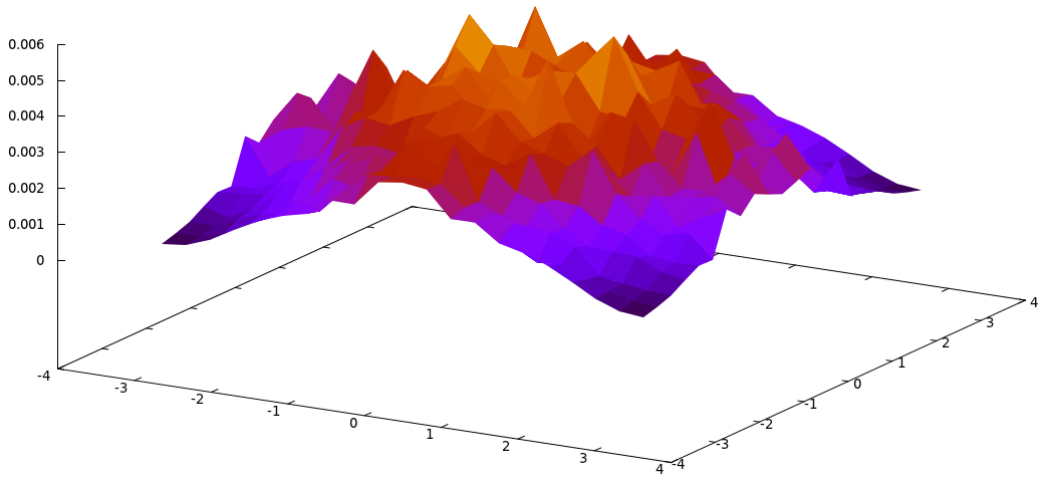

Figure 5.5: Structure factor for $\alpha = 0,\ \beta = 1$ and at $T = 0.1$, plotted against the reciprocal lattice coordinates, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

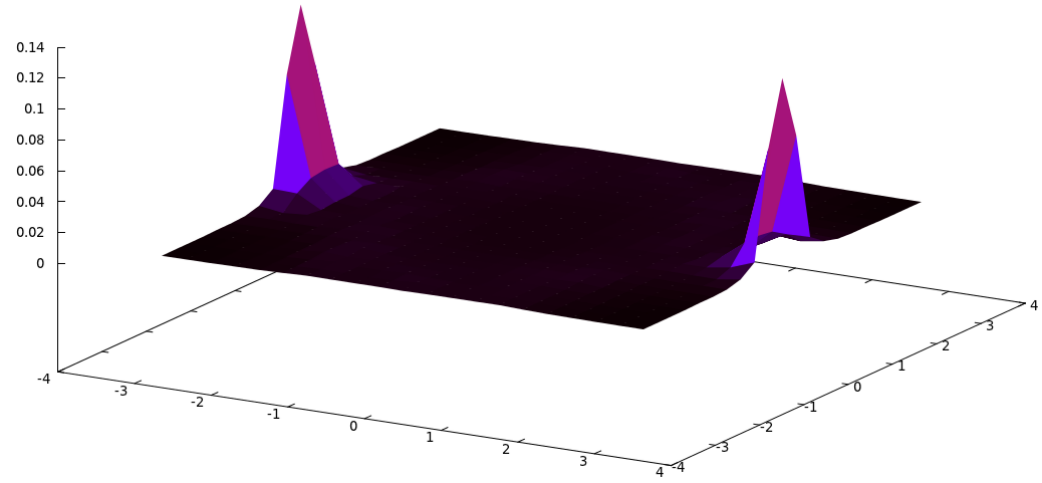

Figure 5.6: Structure factor for $\alpha = 0.1,\ \beta = 1$ and at $T = 0.1$, plotted against the reciprocal lattice coordinates, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

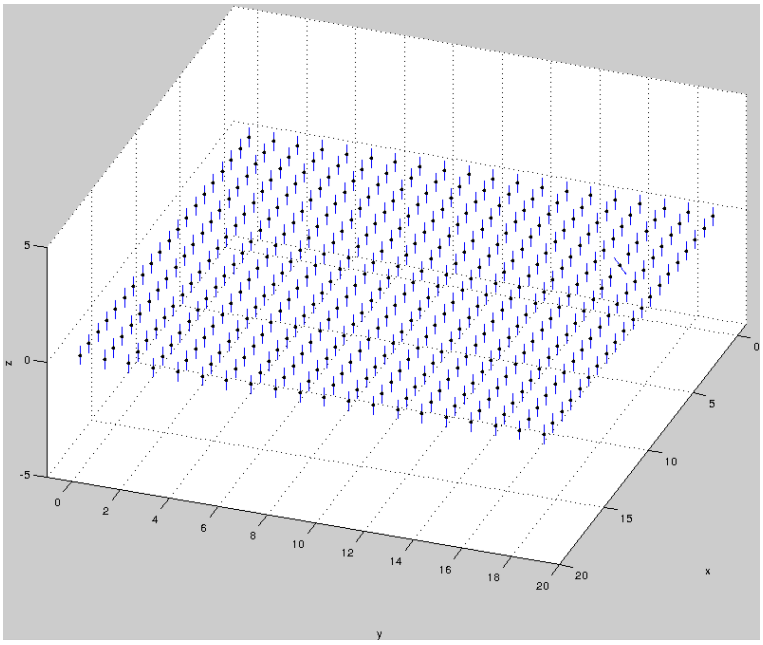

Figure 5.7: Ground state spin configuration for $\alpha = 1$ and $\beta = 0$, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

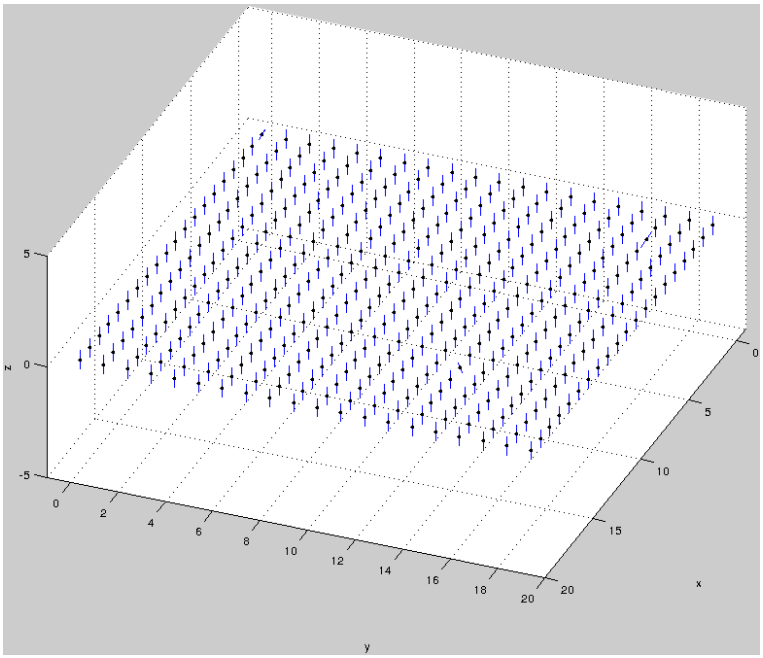

Figure 5.8: Ground state spin configuration for α = -1 and $\beta = 0$, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

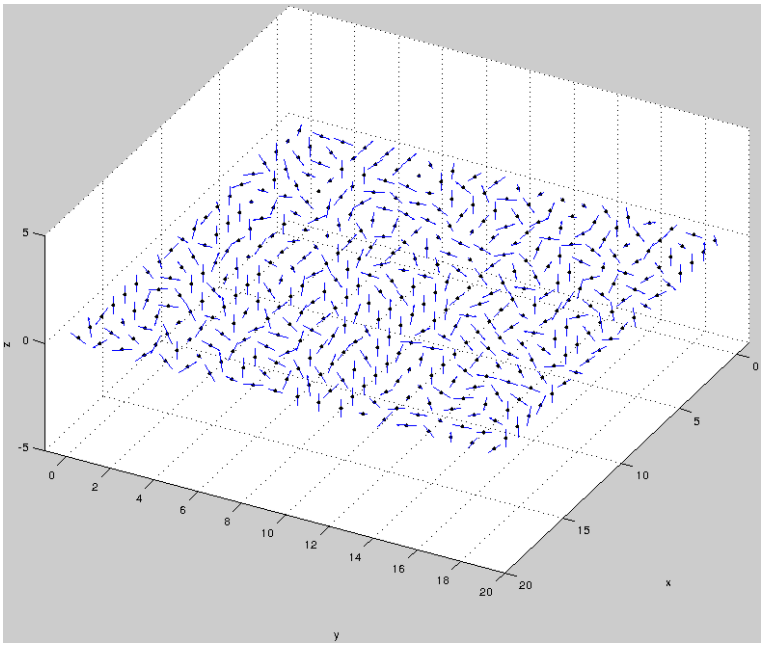

Figure 5.9: Ground state spin configuration for $\alpha = 0$ and $\beta = 1$, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

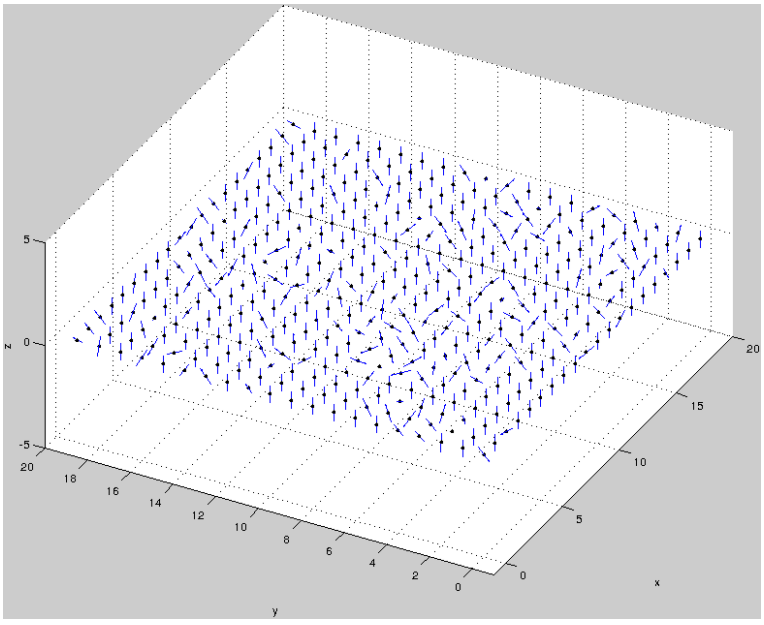

Figure 5.10: Ground state spin configuration for $\alpha = 0.1$ and $\beta = 1$, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

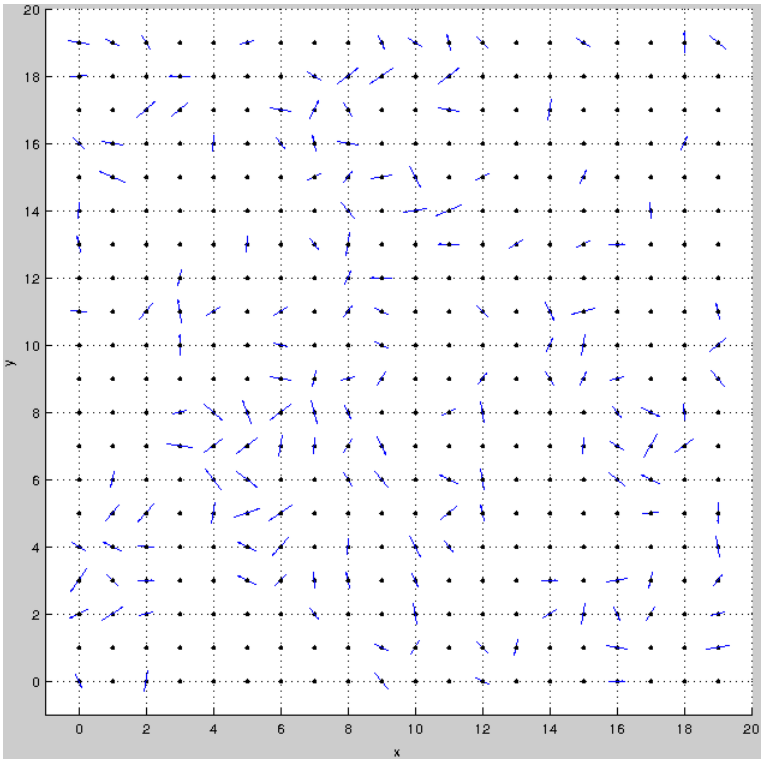

Figure 5.11: Top view of ground state spin configuration for $\alpha = 0.1$ and $\beta = 1$, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

Figures from 5.12 to 5.18 are the Structure factor plot and the ground state spin configurations for other different values of α and β. The simulations were done for the following parameters:

- 20×20 spin lattice
- High temperature = $3J$, Low temperature = $0.05J$
- Temperature step size = $0.05J$
- Equilibration steps = 5000, Averaging steps = 5000

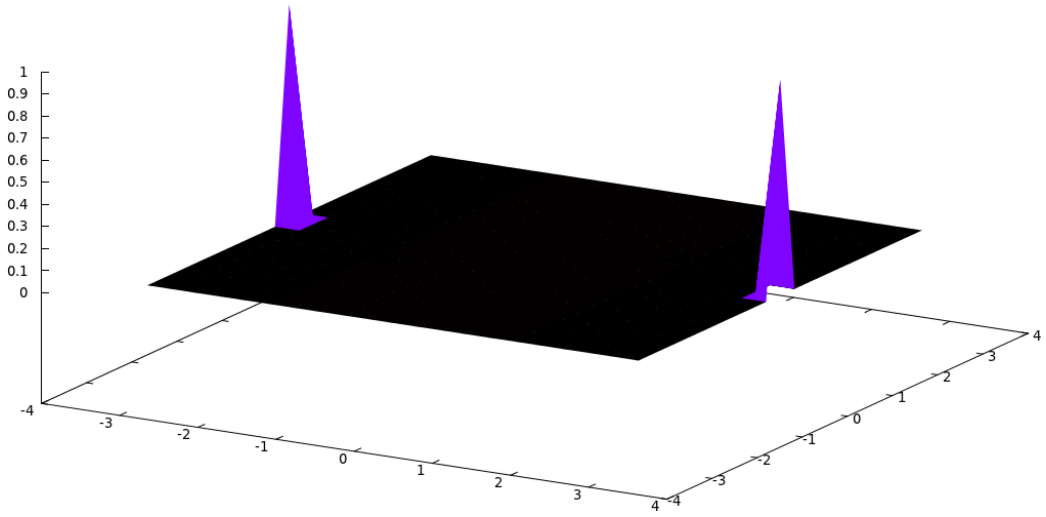

Figure 5.12: Structure factor for $\alpha = 0.1$, $\beta = 1$, and at $T = 0.05$, plotted against the reciprocal lattice coordinates, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice. Identical plots were obtained for $\alpha = 0.2, 0.3, 0.4, 0.5, 0.6$ and rest being the same.

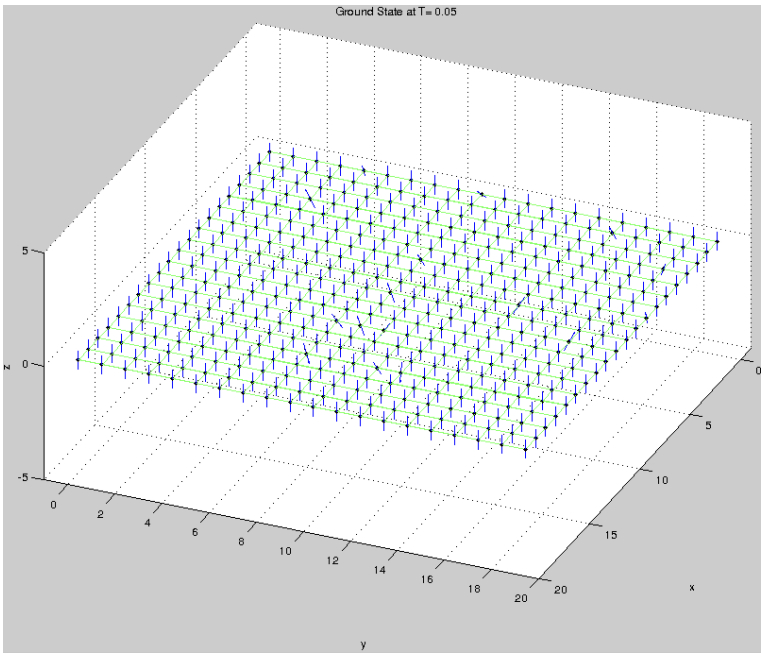

Figure 5.13: Ground state spin configuration for $\alpha = 0.1$ and $\beta = 1$, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

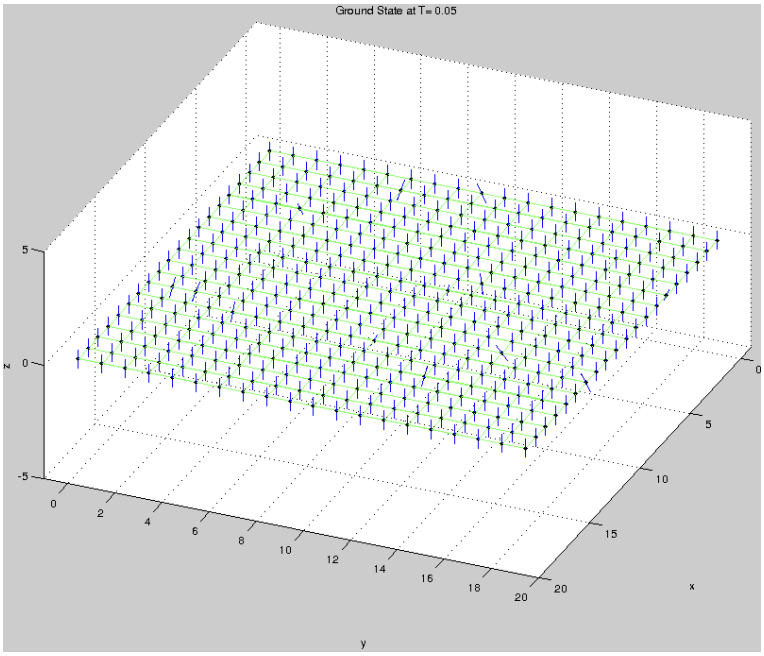

Figure 5.14: Ground state spin configuration for $\alpha = 0.2$ and $\beta = 1$, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

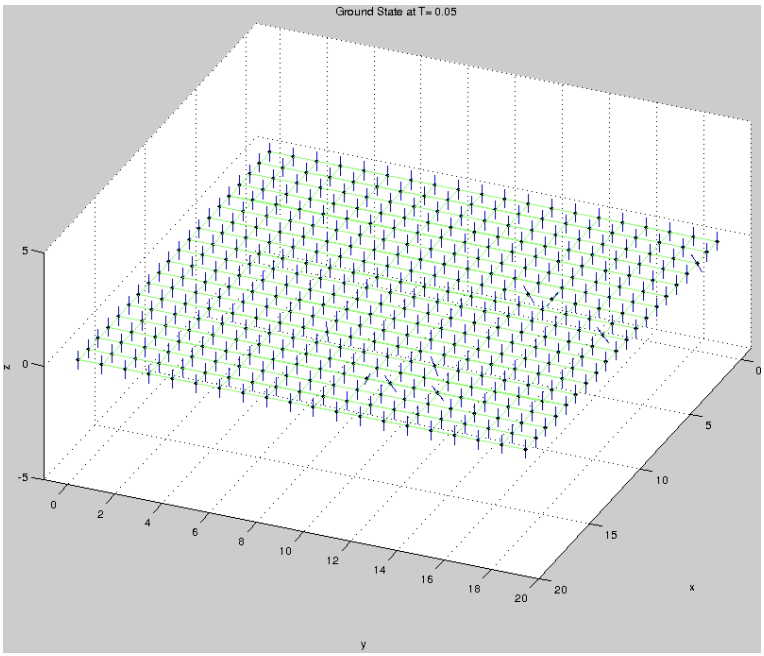

Figure 5.15: Ground state spin configuration for $\alpha = 0.3$ and $\beta = 1$, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

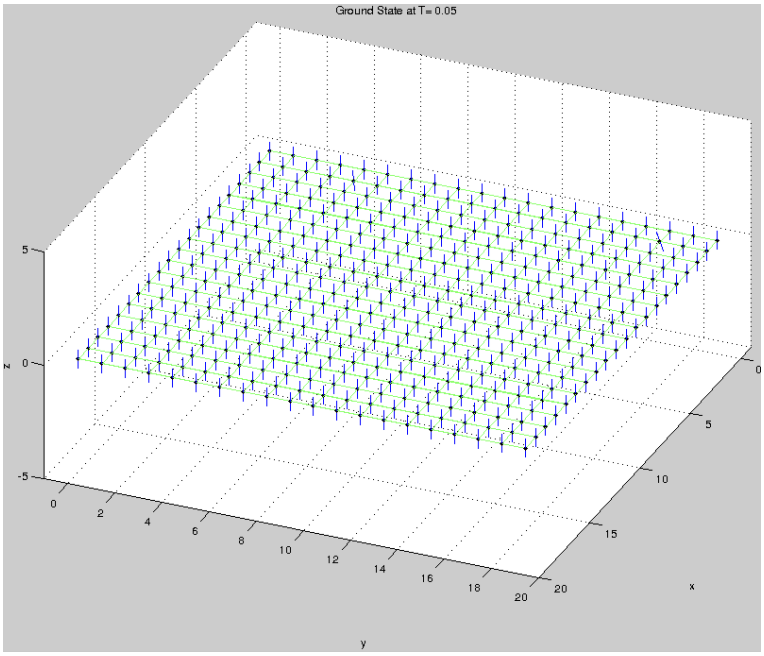

Figure 5.16: Ground state spin configuration for $\alpha = 0.4$ and $\beta = 1$, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

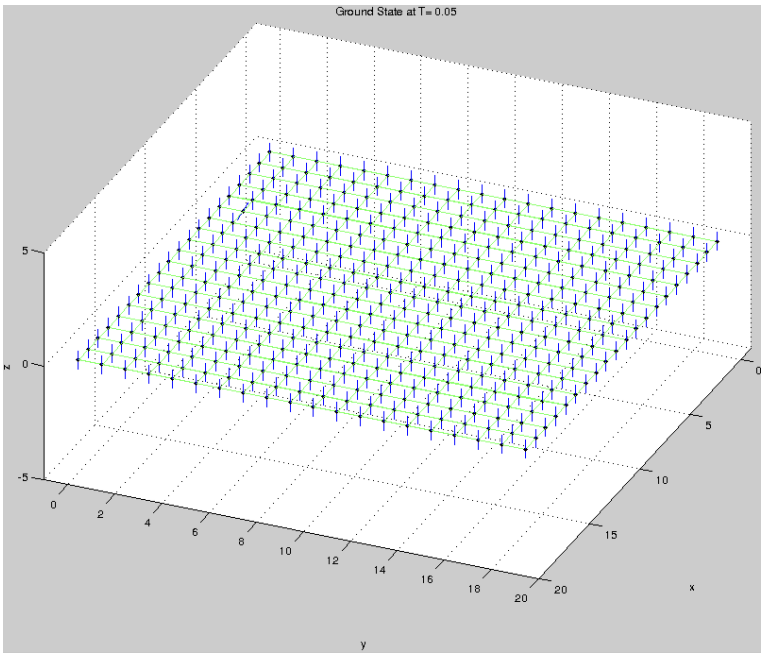

Figure 5.17: Ground state spin configuration for $\alpha = 0.5$ and $\beta = 1$, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

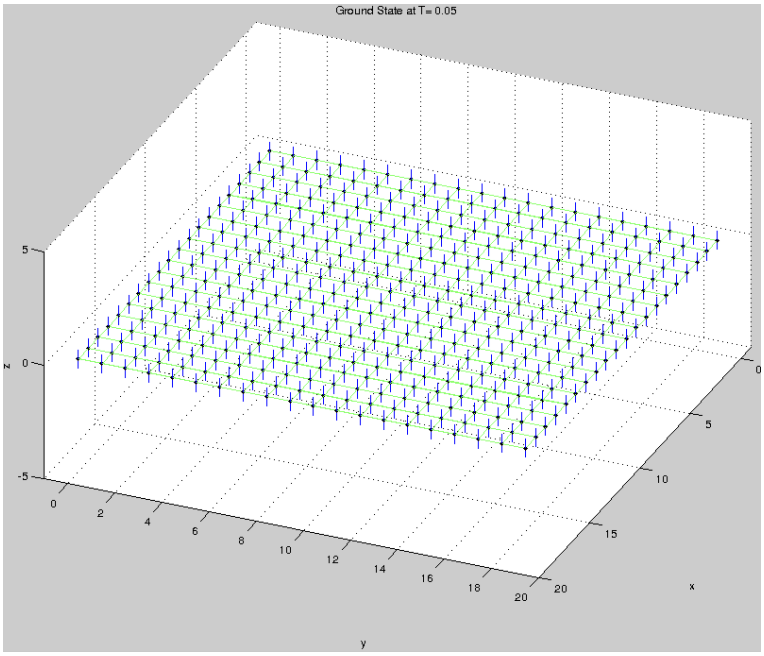

Figure 5.18: Ground state spin configuration for $\alpha = 0.6$ and $\beta = 1$, for Heisenberg-Kitaev model on a 20×20 honeycomb lattice

Chapter 6

Summary

From the models we have discussed so far it is clear that using Monte Carlo method with Metropolis algorithm is a very effective sampling technique.

In chapter 3, Heisenberg model on square lattice, we learn how the various observables can be calculated for a spin system at some temperature. We also see how the magnetic phase transition occurs as our system size grows.

In chapter 4, Triangular lattice model, we apply the Heisenberg model on triangular lattice. We construct an equivalent spin interaction structure of triangular lattice on square lattice for simulation purpose. Triangular lattice model also serves as a good example to demonstrate the possibility of geometrical frustration in spin systems. In the first part we do not allow lattice distortion. The structure factor calculations reveals that the ground state has a magnetic order in which adjacent spins align at 120 degree angle. In the second part, where we allow the lattice to distort, we observe that to minimize energy the spins also move from their locations, within the allowed limits.

In chapter 5, Heisenberg Kitaev model, we have different interaction between different neighbouring spins located on Honeycomb lattice. Again we construct an equivalent structure for square lattice and do the simulations for various parameter values of the model. We observe from the ground state spin configurations how the relative variation in the parameter values of the model affects the magnetic order of the system in the ground state.

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