



FRUSTRATION IN CLASSICAL SPIN SYSTEMS

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An abstract geometric diagram consisting of several overlapping circles and lines, rendered in a light gray color. The diagram is positioned on the right side of the page, partially overlapping the text 'UNIVERSITY OF COPENHAGEN'.



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Abstract

A model of classical spins on Bravais lattices with geometrical frustration is studied. A way of determining the ground state spin configurations as a helical order is argued along with a way of classifying these according to their ground state pitch vectors. Taking up to second nearest neighbouring spins into account parametrised continuous ground state degeneracies with certain values of the interaction constants are shown in the triangular and square lattices. It is shown that due to an *order by disorder* effect these degeneracies are lifted at finite temperature. A third nearest neighbour interaction is added in the square lattice and it is shown that with this being ferromagnetic an infinite degeneracy is reduced to a parametrised one in the case of an antiferromagnetic second nearest neighbour interaction being half of an antiferromagnetic nearest neighbour interaction.

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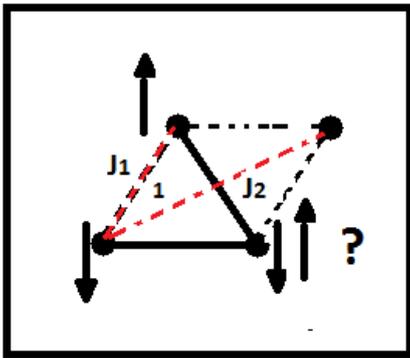
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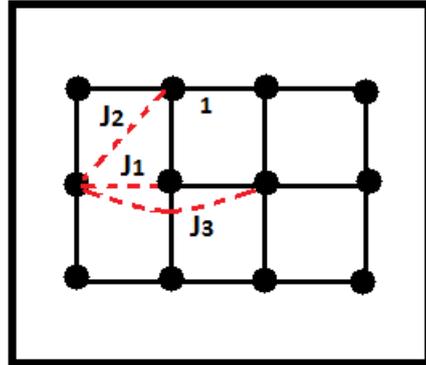
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1 Introduction

Frustration in exchange coupled spin systems oftentimes brings about interesting phenomena because it can lead to quite complex spin configurations and rich phase diagrams. The term "frustration" is introduced when it is impossible to simultaneously satisfy all the exchange processes in a system. In periodic lattices "geometrical frustration" would be more exact. It occurs when the geometry of the lattice makes it impossible locally to make a simple spin pattern that would minimise the energy. When introducing geometrical frustration it is quite common to use a triangular lattice with antiferromagnetic (henceforth AFM) nearest neighbor interactions as seen in figure 1. The triangle is such a geometrical shape that we only need the nearest neighbour AFM bond to easily realise that the energy contributions from all the spin interactions can not simultaneously be minimised. Through this example we can generalise and say that a necessary condition for frustration is that at least one interaction is AFM. It is illustrated in figure 1(a). So what will the ground state configuration in this case look like? this question and more will be studied in this thesis.



(a) Plaquettes of a triangular lattice



(b) Plaquettes of a square lattice

Figure 1: A small number of plaquettes in a triangular and square lattice to illustrate that every interaction process can not be satisfied simultaneously. We will take into account up to second nearest neighbour bond in the triangular lattice and set lattice constants to 1

Only classical spins on a square and a triangular lattice will be dealt with and a way of determining the ground state configurations of frustrated spin systems will be argued. This is done in chapter 3. A way of classifying these ground states is developed in chapter 4. This constitutes a theoretical background of performing calculations on concrete lattice structures with well defined interaction parameters that in general could be defined by a vector,

$$\mathbf{J} = (J_1, J_2, \dots, J_N), \quad (1.1)$$

with in this case N different interactions between the particles of the sites of the lattice.

Next we will use the triangular and square lattices with nearest and second nearest neighbour interactions as concrete examples. When dealing with frustrated systems one

can encounter a continuous manifold of degenerate ground states at zero temperature as we shall see examples of. These degeneracies can be lifted due to a mechanism called "order by disorder" which we will also see examples of. Next we take fluctuations into account and show how a spectrum of these can be found.

All figures in this thesis are self-made. Plots and numerical calculations have been made using MathematicaTM.

2 The Heisenberg model

The general model under consideration is the Heisenberg model given by the Hamiltonian

$$\mathcal{H} = \frac{1}{2} \sum_{ij} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j. \quad (2.1)$$

The prefactor of $\frac{1}{2}$ in 2.1 corrects for double counting, and the sum is to be taken over pairs of spins $\langle ij \rangle$. The symmetric exchange interaction integrals, $J_{ji} = J_{ij}$, we will take to be functions of real space positions only i.e. $J_{ij} = J_n(\mathbf{R}_i - \mathbf{R}_j)$, where the J_n is the n 'th interaction constant with the corresponding distance $(\mathbf{R}_i - \mathbf{R}_j)$. The sign of these determine whether the spins favour a parallel or antiparallel configuration. 2.1 will for example be minimized with an antiparallel configuration if the $J_{ij} > 0$. The spins, \mathbf{s}_i , are also functions of real space. We want to impose the local constraint that

$$\mathbf{s}_i \cdot \mathbf{s}_i = 1, \quad (2.2)$$

at each of the, \mathcal{N} , sites of the lattice. The spins under consideration in this thesis are situated on periodic triangular or square lattices where we through every calculation define the lattice constant to be 1. When doing thermodynamic calculations we have to assume that the systems are in the thermodynamic limit, hence $\mathcal{N} \rightarrow \infty$.

The translational invariance makes it convenient to introduce the Fourier transform of the spins,

$$\mathbf{s}_i = \frac{1}{\mathcal{N}} \sum_{\mathbf{q}} \mathbf{S}_{\mathbf{q}} e^{i\mathbf{R}_i \cdot \mathbf{q}}. \quad (2.3)$$

When 2.3 is used in 2.1 we obtain

$$\begin{aligned} \mathcal{H} &= \frac{1}{2} \sum_{\mathbf{q}\mathbf{q}'} \mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{\mathbf{q}'} \sum_{ij} J_{ij} e^{i(\mathbf{R}_i \cdot \mathbf{q} + \mathbf{R}_j \cdot \mathbf{q}')} \\ &= \frac{1}{2} \sum_{\mathbf{q}\mathbf{q}'} \mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{\mathbf{q}'} \sum_{ij} J_{ij} e^{i\mathbf{R}_i \cdot (\mathbf{q} + \mathbf{q}')} e^{-i(\mathbf{R}_i - \mathbf{R}_j) \cdot \mathbf{q}'} \\ &= \frac{1}{2} \sum_{\mathbf{q}\mathbf{q}'} \mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{\mathbf{q}'} \sum_{ij} J_{ij} e^{-i(\mathbf{R}_i - \mathbf{R}_j) \cdot \mathbf{q}'} \sum_i e^{i\mathbf{R}_i \cdot (\mathbf{q} + \mathbf{q}')} \end{aligned} \quad (2.4)$$

$$= \frac{1}{2} \sum_{\mathbf{q}} J(\mathbf{q}) \mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{-\mathbf{q}}, \quad (2.5)$$

where we have defined

$$J(\mathbf{q}) = \sum_{ij} J_{ij} e^{i(\mathbf{R}_i - \mathbf{R}_j) \cdot \mathbf{q}}, \quad (2.6)$$

which can be used to calculate the energy spectrum in momentum space. This will be used extensively through the thesis.

3 Spin configuration in the classical Ground State at zero temperature

As stated earlier frustration is equivalent to saying that it is impossible for all the terms in 2.1 simultaneously to be minimized and it is hence not obvious what the ground state configuration looks like. In this section a method of rigorously determining the ground state spin configuration for some system is taken into account as it will be essential to the rest of the thesis. Ref. 5 is followed in the pursuit of finding a minimum of the energy.

We want to find the minimum of the energy and still have the the strong, local constraint given in 2.2 satisfied. When using the Lagrange multiplier method this gives rise to a condition for every site of the lattice, i.e. we would have \mathcal{N} Lagrange multipliers, which makes the task of hopeless. We take another approach and begin with merely satisfying the weaker constraint given by

$$\sum_i \mathbf{s}_i^2 = \mathcal{N}. \quad (3.1)$$

That a spin configuration satisfies this weak constraint is a necessary but not a sufficient condition for it to satisfy the strong condition. Replacing the strong condition by the weak condition is equivalent to the Lagrange multipliers being independent of the site at which it is supposed to ensure the size of its spin. This problem is a much simpler one and we start by solving that.

We can now write the stationarity condition with respect to the set of variables (\mathbf{s}_i, λ) for each component $\alpha = x, y, z$ as

$$0 = \frac{\partial}{\partial s_i^\alpha} \left[\sum_{ij} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j - \lambda \left(\sum_i \mathbf{s}_i^2 - \mathcal{N} \right) \right], \quad (3.2)$$

which implies

$$\sum_j J_{ij} s_j^\alpha = 2\lambda s_i^\alpha. \quad (3.3)$$

This is a set of three independent eigenvalue problems. The translational symmetry of J_{ij} makes,

$$s_j^\alpha = A_\alpha \cos [\mathbf{Q} \cdot \mathbf{R}_j + \phi_\alpha], \quad (3.4)$$

a good ansatz for a solution where \mathbf{Q} is some particular wave vector. We get

$$\sum_j J_{ij} s_j^\alpha = A_\alpha \sum_j J_{ij} \cos [\mathbf{Q} \cdot \mathbf{R}_j + \phi_\alpha], \quad (3.5)$$

which upon Fourier transformation of J_{ij} becomes

$$\begin{aligned} &= A_\alpha \sum_j \frac{1}{\mathcal{N}} \sum_{\mathbf{q}} J_{\mathbf{q}} e^{i\mathbf{q} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \left(e^{i(\mathbf{Q} \cdot \mathbf{R}_j + \phi_\alpha)} + e^{-i(\mathbf{Q} \cdot \mathbf{R}_j + \phi_\alpha)} \right) \\ &= A_\alpha \frac{1}{\mathcal{N}} \sum_{\mathbf{q}} J_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{R}_i} \sum_j \left[e^{i(\mathbf{Q} - \mathbf{q}) \cdot \mathbf{R}_j + \phi_\alpha} + e^{-i((\mathbf{Q} + \mathbf{q}) \cdot \mathbf{R}_j + \phi_\alpha)} \right] \\ &= A_\alpha \frac{1}{\mathcal{N}} \sum_{\mathbf{q}} J_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{R}_i} \left[\delta_{\mathbf{q}, \mathbf{Q}} e^{\phi_\alpha} + \delta_{\mathbf{q}, -\mathbf{Q}} e^{-\phi_\alpha} \right] \\ &= A_\alpha J_{\mathbf{Q}} 2 \cos [\mathbf{Q} \cdot \mathbf{R}_i + \phi_\alpha]. \end{aligned} \quad (3.6)$$

Using the fact that $J_{\mathbf{Q}} = J_{-\mathbf{Q}}$. This means that the eigenvalues were given by $\lambda = J_{\mathbf{Q}}$. The energy of a state satisfying the stationarity condition with the weak constraint can now be found by picking the \mathbf{Q} that minimizes

$$E = \sum_{\mathbf{q}} J_{\mathbf{q}} |\mathbf{s}_{\mathbf{q}}|^2, \quad (3.7)$$

which only comprises to a single wave vector pair $\pm \mathbf{Q}$ and can therefore be reduced to

$$E = \mathcal{N} J_{\mathbf{Q}} \quad (3.8)$$

Having established a solutions that satisfy the weak constraint we can now among these pick out those that also satisfy the full local constraint. This is done by adjusting the six parameters $\{A^{1,2,3}, \phi_{1,2,3}\}$. We choose one of the A^α 's to be zero, the other two to be equal and the phases to be $\phi_1 = \phi, \phi_2 = \phi + \frac{\pi}{2}$ and we end up with a planar spiral solution

$$\mathbf{s}_i = \mathbf{e}_1 \cos [\mathbf{Q} \cdot \mathbf{R}_i] + \mathbf{e}_2 \sin [\mathbf{Q} \cdot \mathbf{R}_i] \quad (3.9)$$

Where we without loss of generality have put $\phi = 0$. This comes with the requirements

$$\mathbf{e}_1 \cdot \mathbf{e}_1 = \mathbf{e}_2 \cdot \mathbf{e}_2 = 1, \quad \mathbf{e}_1 \cdot \mathbf{e}_2 = 0 \quad (3.10)$$

This analysis has made it clear that to continue the search for ground state spin configurations in frustrated systems we need to understand how 3.9 looks with different \mathbf{Q} , which we will henceforth call pitch vectors.

4 Classification of ground states due to pitch vectors

In the following a way of classifying ground state spin configurations in accordance with the given pitch vector is introduced. We follow mostly ref. 8 in this endeavour and define a commensurate spin phase as one that has a periodicity of the spins of finite size in its ground state. An incommensurate spin phase is thus one that cannot be divided into a finite number of sublattices.

4.1 The 'star' of \mathbf{Q}

As we will see concrete examples of later some systems have more than one \mathbf{Q} (or its negative) minimising the energy. Two such \mathbf{Q} 's are said to be equivalent if their difference is a reciprocal lattice vector. The set of non-equivalent \mathbf{Q} 's is called the 'star' of \mathbf{Q} . The star of \mathbf{Q} consisting of only one element is the most common in nature. If for example $\mathbf{Q} = 0$ we have a ferromagnet.

When the star of \mathbf{Q} consists of more than one element eq. 3.9 does not necessarily contain all lowest energy states. When 3.9 comprises all lowest energy states the ground-state degeneracy is discrete. In the next section we will see examples where \mathbf{Q} 's can be combined to give ground states which are not comprised in 3.9.

In general \mathbf{Q} brings about incommensurate spin configurations. Our ground state spins given in 3.9 are periodic with 2π which means that incommensurate phases correspond to $n\mathbf{Q}$ not being equal to a reciprocal lattice vector for any $n \neq 0$. The reason is that if $n\mathbf{Q} = \mathbf{G}$, we could write $n\mathbf{Q} \cdot \mathbf{R}_i = \mathbf{G} \cdot \mathbf{R}_i = 2\pi m$ with $m \in \mathbb{Z}$ which means that whenever $\frac{m}{n}$ is an integer a spin will be back pointing in its original direction. This means that for infinitely large systems if $n\mathbf{Q} = \mathbf{G}$ with n being rational the configuration can in principle be broken up into a number of sublattices.

4.2 Pitch vectors of special interest

Let us now turn to look at some special points in first Brillouin zone. At certain positions, see figure 2, the groundstate degeneracy may be continuous. We shall be contented with two examples.

If we let the dimensionality of the spins be $n \geq 4$ one way of obtain a ground state which is not given by 3.9. The way in which this can be done is simply to add two configurations with \mathbf{Q}_1 and \mathbf{Q}_2 such that

$$\begin{aligned} \mathbf{s}_i = & [\mathbf{e}_1 \cos(\mathbf{Q}_1 \cdot \mathbf{R}_i) + \mathbf{e}_3 \sin(\mathbf{Q}_1 \cdot \mathbf{R}_i)] \cos \theta \\ & + [\mathbf{e}_2 \cos(\mathbf{Q}_2 \cdot \mathbf{R}_i) + \mathbf{e}_4 \sin(\mathbf{Q}_2 \cdot \mathbf{R}_i)] \sin \theta, \end{aligned} \tag{4.1}$$

where the \mathbf{e}_α 's are all orthogonal unit vectors in order to satisfy the local constraint. θ is an arbitrary phase which can be attached without violating any of constraints. A

special case is when $2\mathbf{Q} \equiv 0$. Or put in other words if $n = 2, m = 2$ and we hence have periodicity of 2 in the direction of \mathbf{Q} based on the argument above. The correspond in the square lattice to horizontal stripes, vertical stripes or the Néel state. Then 4.1 reduces to

$$\mathbf{s}_i = \mathbf{e}_1 \cos(\mathbf{Q}_1 \cdot \mathbf{R}_i) \cos \theta + \mathbf{e}_2 \cos(\mathbf{Q}_2 \cdot \mathbf{R}_i) \sin \theta, \quad (4.2)$$

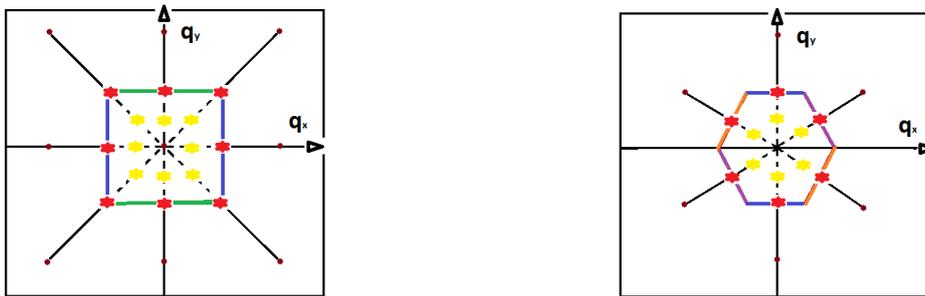
since the sine terms disappear and only two orthogonal unit vectors are needed. 4.2 thus gives us a groundstate that is not comprised in 3.9 for two dimensional spins. The θ could be any number we thereby have continuously degenerate ground state.

If $4\mathbf{Q} \equiv 0$ the ground state spins have periodicity 4 in the direction of \mathbf{Q} configuration consists of only vertical and horizontal spins. One can tilt globally the vertical or horizontal spins without energy costs which can be expressed as

$$\mathbf{s}_i = \mathbf{e}_1 [\cos(\mathbf{Q} \cdot \mathbf{R}_i) + \sin(\mathbf{Q} \cdot \mathbf{R}_i) \cos \theta] + \mathbf{e}_2 \sin(\mathbf{Q} \cdot \mathbf{R}_i) \sin \theta. \quad (4.3)$$

This is a legitimate ground state because the constraints 3.10 are still satisfied. We thus see that both 4.2 and 4.3 give continuous manifolds of ground states parametrised by the angle θ . We will later see examples of both in concrete examples of geometrical frustration.

Furthermore it is worth noticing that when the pitch vector, \mathbf{Q} , only has one nonzero component the spin configuration will be a one dimensional spiral in the case of a square lattice with ferromagnetic stripes on the axis corresponding to the zero component of \mathbf{Q} since the direction of the spins does not change along this direction. When \mathbf{Q} lies on the Brillouin zone edge boundary in the case of a triangular lattice this is configuration in which second nearest neighbouring spins would be either aligned or anti aligned. This is summed up in the figure below with special positions of the pitch vector



(a) First Brillouin zone of the square lattice with special \mathbf{Q} 's

(b) First Brillouin zone of the triangular lattices with special \mathbf{Q} 's

Figure 2: Brown dots are reciprocal lattice sites. Red spots: $\sim 0.5\mathbf{G}$ and coexisting spirals can occur. Yellow spots $\sim 0.25\mathbf{G}$ where every spin points vertically or horizontally. Dotted lines: $n\mathbf{Q} = \mathbf{G}$ corresponds possibly to commensurate states. The rest is incommensurate states

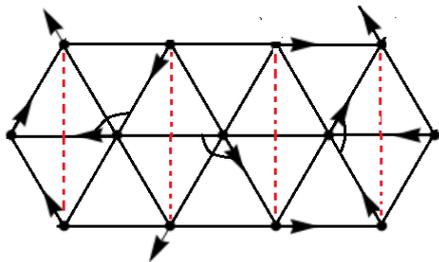
5 Frustration in the triangular lattice with J_1 and J_2 bonds

In this section geometrical frustration in a triangular lattice is considered. The geometry of the lattice gives frustration when only a nearest neighbour AFM coupling is taken into account. We will briefly show that the ground state configuration is the '120 deg.' three sublattice structure ordered ferromagnetically, thus answering the question posed in the introduction. Next we will introduce an AFM next nearest neighbour and look at cases of both a FM and AFM J_1 interaction. We will outline the phase diagram based on the first case and focus on some of the interesting values of J_2 . We will in the following define $\alpha \equiv \frac{J_2}{|J_1|}$ and use this as a tuning parameter.

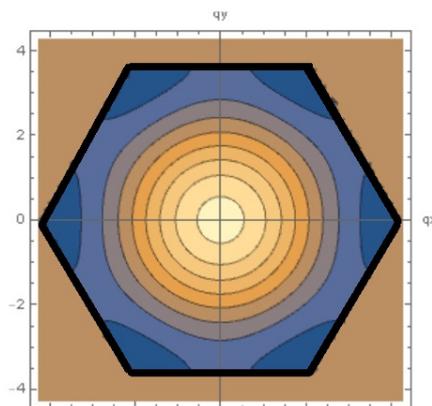
$$\frac{J_{\mathbf{q}}}{2J_1} = \cos [q_x] + 2 \cos \left[\frac{1}{2}q_x \right] \cos \left[\frac{\sqrt{3}}{2}q_y \right] + \alpha \left(\cos [\sqrt{3}q_y] + 2 \cos \left[\frac{3}{2}q_x \right] \cos \left[\frac{\sqrt{3}}{2}q_y \right] \right), \quad (5.1)$$

5.1 AFM nearest neighbour ($J_1 > 0$, $J_2 = 0$)

When $J_2 = 0$, 5.1 is minimised in the corners of the first Brillouin zone boundary which means that the 'star' of \mathbf{Q} is twofold. Figure 3 (b) shows a plot of the contours of the energy in momentum space. It also means that $3\mathbf{Q}$ is equivalent to a lattice site in reciprocal space and we should see a three sublattice structure. Using the pitch vectors in 3.9 gives a configuration seen in figure 3(a), where the alignment of the second nearest neighbour mentioned earlier is also marked by red dotted lines. It can be seen in the figure that this configuration corresponds to $\mathbf{Q} = (\frac{4\pi}{3}, 0)$ since we see the periodicity in the x direction. The energy of these ground states is $E_0 = -3J_1$.



(a) A three sublattice structure with 120 deg. between them. The ground state with of the AFM nearest neighbour model on traingular lattice



(b) Plot of the contours in which it is seen that the corners of the first Brillouin zone define the pitch vectors.

Figure 3: Three sublattice structure in AFM nearest neighbour model on triangular lattice and contourplot of energy in first Brillouin zone

5.2 AFM J_1 and AFM J_2

An AFM next nearest neighbour bond is now added to the model. First we need to ask ourselves at what value of α the pitch vectors start change. Surely we expect 120 deg. state to be the ground state at small J_2 couplings. The energy at the corners of the Brillouin zone is $E(\alpha < \alpha_0) = -3 + 6\alpha$. It is easily checked by using contour plots such as the one in figure 3 (b) that the points at which 5.1 has its minimum changes for some value α_0 to become half reciprocal lattice vectors. The energy here is $E(\alpha > \alpha_0) = -2 - 2\alpha$ which means that $\alpha_0 = \frac{1}{8}$. When $\alpha > 1$ the pitch vectors begin moving along the reciprocal lattice vectors towards the origin corresponding possibly to commensurate spin configurations.

Looking for the minimum along the q_y -axis by setting the gradient of 5.1 to zero it is found that the distance d from the origin is $d(\alpha) = \frac{2}{\sqrt{3}} \arccos\left(-\frac{1+\alpha}{2\alpha}\right)$ with $\alpha \geq 1$. Notice now that $d(\infty) = \frac{1}{3} \frac{4\pi}{\sqrt{3}}$ is one third of the length a reciprocal lattice vector and we should expect a periodicity of 3 when $J_2 \gg J_1$. Indeed we see that in figure 5 (b) along the marked lines and in the horizontal direction. This analysis is summed up in figure 4.

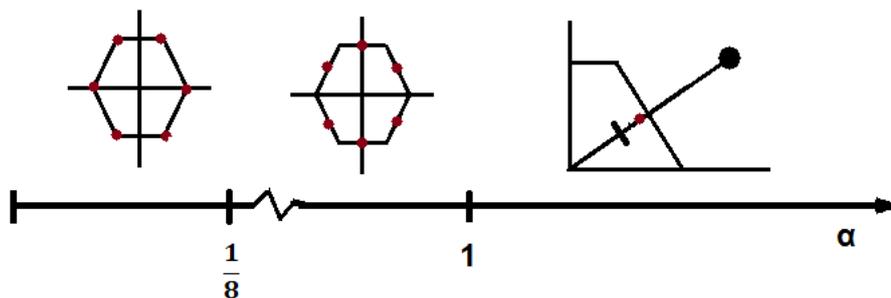


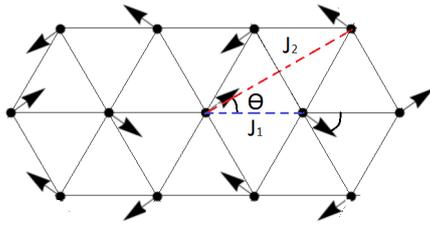
Figure 4: With $\alpha < \frac{1}{8}$ the pitch vectors (represented by brown dots) point to the corners of the first Brillouin zone and the ground state configuration is like that of the case of only nearest neighbour AFM bonds. With $\frac{1}{8} < \alpha < 1$, \mathbf{Q} 's are half reciprocal lattice vectors $\alpha > \frac{1}{8}$ the \mathbf{Q} 's move towards origin and saturates at $\frac{1}{3}\mathbf{G}$.

The fact that the pitch vectors are half reciprocal lattice vectors in the interval $\frac{1}{8} < \alpha < 1$ means according to the argument in section 4 that we find a continuous manifold of ground states on the form 4.2 parametrised by an angle θ as seen figure 5(a).

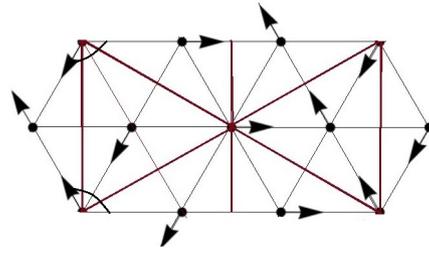
We will show later that when we add fluctuations and do thermodynamic calculations the entropy per site depends on θ and specific values are chosen thus lifting this ground state manifold due to an order by disorder mechanism.

5.3 FM J_1 and AFM J_2

In the case where we have a FM J_1 and an AFM J_2 we have one pitch vector, $\mathbf{Q} = (0, 0)$, at small values of $\alpha \equiv \frac{J_2}{|J_1|}$ which is not surprising since this corresponds to a ferromagnet. However, when α is increased the \mathbf{Q} 's begin moving away from the origin along the lines of $\mathbf{Q} = n\mathbf{G}$. The distance from the origin is this time given by

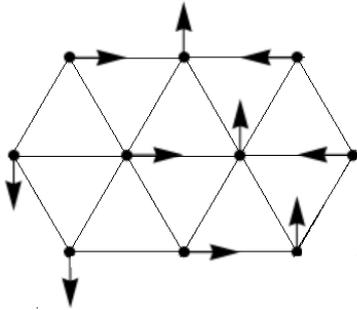


(a) Ground state on the form 4.2 with AFM J_2 and $\frac{1}{8} < \alpha < 1$ and an angle, θ , can be used as shown without energy cost

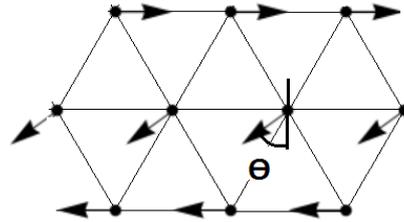


(b) $\alpha \rightarrow \infty$: $\mathbf{Q} = \frac{1}{3}\mathbf{G}$. The ground state again becomes a three sublattice 120 deg. structure between the next nearest neighbouring spins

Figure 5: Ground state spin configurations in the AFM J_1 - AFM J_2 model



(a) Ground state with $4\mathbf{Q} \equiv 0$ as is the case with FM J_1 and AFM J_2 when $\alpha = 1$ a periodicity of 4 is seen. The spins are pointing only along the horizontal axes, as depicted also



(b) Ground state configuration with $J_1 = -1$ $J_2 = 1$. The ground states can be parametrised by an angle θ

Figure 6: Ground state spin configurations with FM J_1 and AFM J_2 and $\alpha = 1$

$d(\alpha) = \frac{2}{\sqrt{3}} \arccos\left(\frac{1-\alpha}{2\alpha}\right)$ which gives real values when $\alpha \geq \frac{1}{3}$. So a smooth transition happens here according to our calculations. We notice now that $(0, 4d(1)) \equiv 0$ which is a point of interest. This is to say that when the couplings are equal in size but opposite we have six non-equivalent pitch vectors corresponding to states where the spins are only pointing along \mathbf{e}_1 or \mathbf{e}_2 and ground states are given by 4.3. We again have a continuous ground state manifold. This is shown in figure 6.

In the limit we of course still have $(0, 3d(\infty)) = \mathbf{G}$ just like we had in the case of AFM J_1 and AFM J_2 .

6 Frustration in a square lattice with AFM J_1 and AFM J_2 bonds

In this chapter we will discuss the square lattice with nearest and second nearest neighbour interaction. Although quite simple in appearance this model realizes some interesting phenomena of which the order from disorder mechanism is one. The energy spectrum in momentum space can be calculated using 2.6 and we get

$$\frac{J_{\mathbf{q}}}{2J_1} = \cos q_x + \cos q_y + 2\alpha \cos q_x \cos q_y, \quad (6.1)$$

Where $\alpha = \frac{J_2}{J_1}$. It is easily checked that for small values of α the pitch vectors are in the corners of the Brillouin zone i.e $\mathbf{Q} = (\pi, \pi)$ which this time itself is half a reciprocal lattice vector but has no non-equivalent \mathbf{Q} to coexist with. This corresponds to the Néel state. If we increase α , we get $\mathbf{Q}_1 = (\pi, 0)$ and $\mathbf{Q}_2 = (0, \pi)$. We have $J_{(\pi,\pi)} = -2 + 2\alpha$ and $J_{(\pi,0)} = -2\alpha$ which means that the transition happens at $\alpha = \frac{1}{2}$. But if we take some generic point on the Brillouin zone edge at $\alpha = \frac{1}{2}$, we get $J_{(a\pi,b\pi)} = -1$, where $-1 < b < 1$ if $a = 1$ and vice versa. We immediately see that $\alpha = \frac{1}{2}$ is a special value and we will deal with this later. In the following we briefly discuss the ground state degeneracy with $\alpha \geq \frac{1}{2}$

6.1 Degeneracy of the ground state configuration with $\alpha > \frac{1}{2}$

When $\alpha > \frac{1}{2}$ we have ordering vectors which are half a reciprocal lattice vector which means that states of lowest energy can be described by 4.2. The system thus breaks up in its ground state and becomes two sublattices each ordered antiferromagnetically as two interpenetrating decoupled Néel states as shown in figure 7.

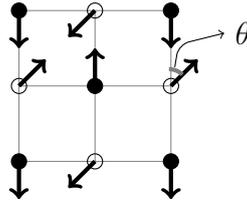


Figure 7: The spins in two interpenetrating sublattices each ordered antiferromagnetically with arbitrary angle θ

6.2 Degeneracy of the ground state configuration with $\alpha = \frac{1}{2}$

This is, as mentioned, a very special case since every point on the Brillouin zone boundary can be used as a pitch vector. The Hamiltonian can be rewritten in terms of a sum over square plaquettes of the lattice

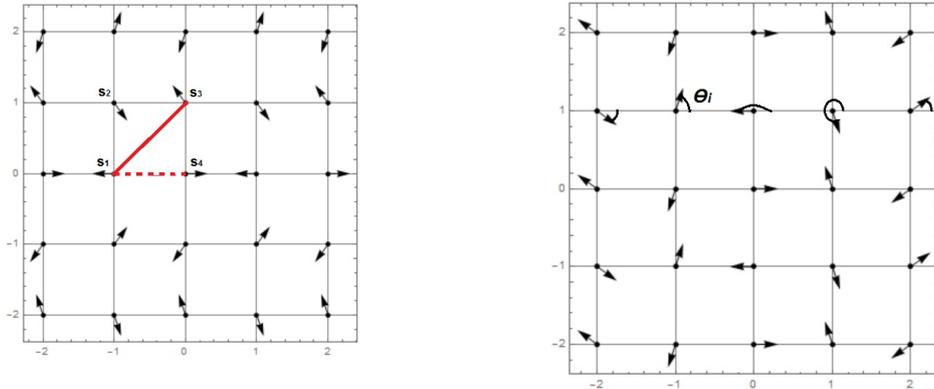
$$\begin{aligned} \mathcal{H} &= \sum_{\square} \mathcal{H}_{\square} \\ &= -4\alpha N_{\square} + \frac{1}{2}\alpha \sum_{\square} (\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4)^2, \end{aligned} \quad (6.2)$$

¹ keeping in mind that the J_1 bond is shared between two adjacent plaquettes and should only to be counted once, see figure 8 (a). N_{\square} is the number of square plaquettes in the system. We thus see that every state that satisfies the zero sum condition given by

¹Chandra et al. 1990

$$\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4 = 0, \quad (6.3)$$

on every square plaquette is a ground state of the system. With two dimensional spins this gives an infinite degeneracy of the ground states with AFM lines either vertically or horizontally as described in section 4. This is illustrated in figure 8 (b) where a ground state could be obtained by any set of $\{\theta_i\}$.



(a) The zero sum condition visualised with four spins on a plaquette summing to zero. The dotted red line is a J1 bond shared between two adjacent plaquettes and is only to be counted once

(b) The zero sum condition visualised with four spins on a plaquette summing to zero with AFM lines vertically. A ground state could be a set of θ_i 's.

Figure 8

In a later chapter we will see how adding a ferromagnetic third nearest neighbour coupling lifts this infinite degeneracy by fixing third nearest neighbour spins such that $\theta_{\mathbf{R}i} = \theta_{\mathbf{R}i+(2,0)} = \theta_{\mathbf{R}i+(0,2)}$ in the ground state.

7 Low temperature thermodynamics and Order by Disorder

Having established that a ground state at specific values of the coupling constants can have a continuous degeneracy let us now turn to look at the low temperature thermodynamics of such systems. Specifically we will calculate the spin wave spectra in the two cases considered above. We want to add small fluctuations from the ground state defined by the parameter θ to the Hamiltonian and expand around this configuration expressed by $\{\phi_i^0\}$ in terms of angles. We rewrite the ground state Hamiltonian 2.1 as,

$$\mathcal{H} = \frac{1}{2} \sum_{ij} J_{ij} \cos(\phi_i - \phi_j), \quad (7.1)$$

and introduce deviations by $\phi_i \rightarrow \phi_i^0 + \delta\phi_i$. Now we can expand to second order which gives

$$\begin{aligned}
\mathcal{H} &= \frac{1}{2} \sum_{ij} J_{ij} \cos(\phi_i^0 - \phi_j^0 + \delta\phi_i - \delta\phi_j) \\
&\approx \frac{1}{2} \sum_{ij} J_{ij} \left[\cos(\phi_i^0 - \phi_j^0) - \sin(\phi_i^0 - \phi_j^0) (\delta\phi_i - \delta\phi_j) - \frac{1}{2} \cos(\phi_i^0 - \phi_j^0) (\delta\phi_i - \delta\phi_j)^2 \right].
\end{aligned} \tag{7.2}$$

The first term inside the sum when summed over i and j is just the ground state energy. It follows from translational invariance that the second term vanishes because,

$$\begin{aligned}
\sum_{ij} J_{ij} \sin(\phi_i^0 - \phi_j^0) (\delta\phi_i - \delta\phi_j) &= \sum_i \sum_l J_l \sin(\Delta\phi_l) (\delta\phi_i - \delta\phi_{i+l}) \\
&= \sum_l J_l \sin(\Delta\phi_l) \left(\sum_i \delta\phi_i - \sum_i \delta\phi_{i+l} \right) \\
&= 0.
\end{aligned} \tag{7.3}$$

Because the last i sum may just be shifted by l . Had the linear term not been zero we could not be sure whether we were actually at a minimum. We have now that, $\mathcal{H} \approx \mathcal{H}^{(0)} + \delta\mathcal{H}_\theta$ where,

$$\delta\mathcal{H}_\theta = \frac{1}{4} \sum_{ij} J_{ij} \cos(\phi_i^0 - \phi_j^0) \left(2\delta\phi_i \delta\phi_j - \delta\phi_i^2 - \delta\phi_j^2 \right), \tag{7.4}$$

which upon Fourier transformation inside the sum, i.e., substituting in $\delta\phi_i = \frac{1}{N} \sum_{\mathbf{q}} \delta\theta_{\mathbf{q}} e^{i\mathbf{R}_i \cdot \mathbf{q}}$ into 7.4, can be linearised to give

$$\delta\mathcal{H}_\theta = \frac{1}{2} \sum_{\mathbf{q} \in BZ} A_{\mathbf{q}}(\theta) |\delta\phi_{\mathbf{q}}|^2. \tag{7.5}$$

The fluctuation spectrum $A_{\mathbf{q}}(\theta)$ can be obtained by inserting the J_{ij} which is a function of the geometry of the lattice. We also have to know what the ground state spin configuration looks like, which in our case, is the same as knowing the ground state parameter θ . Such a calculation is carried out in detail in 7.1.

We can now calculate the partition function by evaluating the integral

$$Z = e^{-\beta E_0} \int \prod_{\mathbf{q}} (d\delta\theta_{\mathbf{q}}) e^{-\frac{1}{2}\beta \sum_{\mathbf{q}} A_{\mathbf{q}} |\delta\theta_{\mathbf{q}}|^2}, \tag{7.6}$$

which is a product of Gaussian integrals and can readily be carried out

$$Z = e^{-\beta E_0} \prod_{\mathbf{q}} \left(\frac{\beta A_{\mathbf{q}}}{2\pi} \right)^{-\frac{1}{2}}. \tag{7.7}$$

The Helmholtz free energy can be found by calculating $F = -\frac{1}{\beta} \ln(Z)$ which yields

$$F(\theta, T) = E_0 + \frac{1}{2}T \sum_{\mathbf{q} \in BZ} \ln \frac{A_{\mathbf{q}}}{2\pi T}. \quad (7.8)$$

The entropy can now be calculated as $S = \ln(Z) - \frac{\beta}{Z} \frac{\partial Z}{\partial \beta}$, which gives

$$S(\theta, T) = \frac{N}{2} - \frac{1}{2} \sum_{\mathbf{q} \in BZ} \ln \left(\frac{A_{\mathbf{q}}}{2\pi T} \right), \quad (7.9)$$

where the constant depends on the system size. We can thus write the free energy per site as

$$f(\theta, T) = \frac{E_0}{N} + \frac{1}{2}T - T \frac{S(\theta)}{N}. \quad (7.10)$$

7.1 Order by disorder with $\alpha > \frac{1}{2}$ in the J1-J2 square lattice model

Based on the above it is clear that if we want to say something about the behaviour of the ground state configuration when fluctuations are added to the system it is necessary to calculate 7.11 for a particular system. We Fourier transform inside the sum 7.4 to get

$$A_{\mathbf{q}}(\theta) = \frac{1}{2} \frac{1}{\mathcal{N}^2} \sum_{ij} J_{ij} \cos(\phi_i^0 - \phi_j^0) \left(2e^{i(\mathbf{R}_i \cdot \mathbf{q} + \mathbf{R}_j \cdot \mathbf{q}')} - e^{i\mathbf{R}_i \cdot (\mathbf{q} + \mathbf{q}')} - e^{i\mathbf{R}_j \cdot (\mathbf{q} + \mathbf{q}')} \right). \quad (7.11)$$

We can now insert

$$J_{ij} = J_1 \left(\delta_{\mathbf{R}_j, \mathbf{R}_i \pm (1,0)} + \delta_{\mathbf{R}_j, \mathbf{R}_i \pm (0,1)} \right) + J_2 \left(\delta_{\mathbf{R}_j, \mathbf{R}_i \pm (1,1)} + \delta_{\mathbf{R}_j, \mathbf{R}_i \pm (1,-1)} \right), \quad (7.12)$$

when doing the sums. In figure 7 we see that the angles between the i 'th spin and its neighbours in the ground state are ϕ , π and $\pi - \phi$. We thus get

$$\begin{aligned} A_{\mathbf{q}}(\theta) = & \frac{1}{2} \frac{1}{\mathcal{N}^2} \sum_{ij} J_1 \left[2 \cos(\theta) e^{i\mathbf{R}_i \cdot (\mathbf{q} + \mathbf{q}') + \mathbf{q}' \cdot (1,0)} - e^{i\mathbf{R}_i \cdot (\mathbf{q} + \mathbf{q}')} - e^{i\mathbf{R}_i \cdot (\mathbf{q} + \mathbf{q}') + (\mathbf{q} + \mathbf{q}') \cdot (1,0)} \right] \\ & + J_1 \left[2 \cos(\pi - \theta) e^{i\mathbf{R}_i \cdot (\mathbf{q} + \mathbf{q}') + \mathbf{q}' \cdot (0,1)} - e^{i\mathbf{R}_i \cdot (\mathbf{q} + \mathbf{q}')} - e^{i\mathbf{R}_i \cdot (\mathbf{q} + \mathbf{q}') + (\mathbf{q} + \mathbf{q}') \cdot (0,1)} \right] + \dots \end{aligned} \quad (7.13)$$

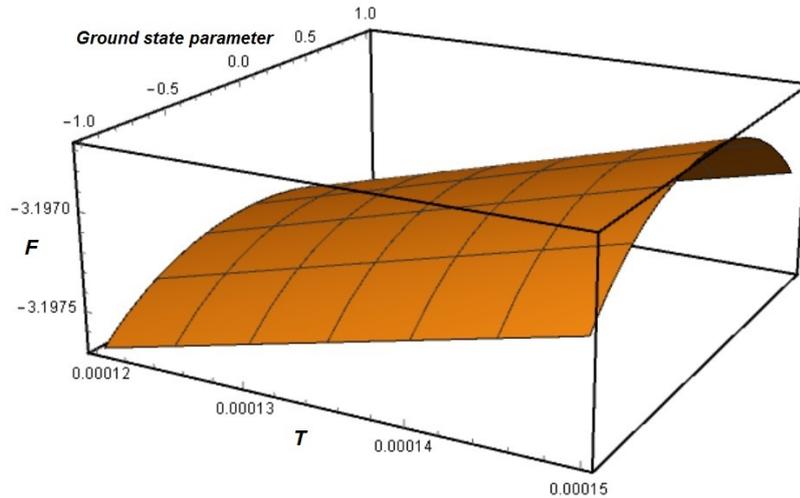


Figure 9: Plot of the free energy obtained by eq. 7.8 in a small temperature interval for the $\alpha > \frac{1}{2}$ square lattice. It is seen that minimisation of the free energy picks out -1 and +1 for the ground state parameter. $J_1 = 1$ and $J_2 = 0.8$.

We leave the full calculation undone because the expressions become very lengthy. After summing over i which gives delta functions $\delta_{\mathbf{q},-\mathbf{q}'}$ in every term we end up getting

$$A_{\mathbf{q}}(\xi) = 4J_2(1 - \cos q_x \cos q_y) + 2J_1(\cos q_x - \cos q_y)\xi, \quad (7.14)$$

because $\delta\theta_{\mathbf{q}}\delta\theta_{-\mathbf{q}} = |\delta\theta_{\mathbf{q}}|^2$ where we have set $\xi = \cos\theta$. We can now calculate how large scale thermodynamic properties behave under small fluctuations from the ground state as a function of the ground state parameter.

The selecting free energy and entropy can be calculated by using eq. 7.8 as a numerical integral over the first Brillouin zone. In figure 9 we show a plot of the free energy as a function of temperature and ground state parameter. It shows that at finite temperature the free energy is minimised at $\xi = \pm 1$ which corresponds to collinear states (see figure 7)

This shows that a collinear state in which the two sublattices line up is preferred at finite temperature. This is thus an archetypal example of the order by disorder mechanism and confirms results obtained by Henley 1989 [3].

7.2 Order by disorder in the case of AFM J_1 and AFM J_2 with $\frac{1}{8} < \alpha < 1$

By the same means as above we calculate the fluctuation spectrum. In the case of a triangular lattice with nearest and second nearest neighbour bonds we can, when summing over j insert,

$$J_{ij} = J_1 \left(\delta_{\mathbf{R}_j, \mathbf{R}_i \pm (1,0)} + \delta_{\mathbf{R}_j, \mathbf{R}_i \pm (\frac{1}{2}, \frac{\sqrt{3}}{2})} + \delta_{\mathbf{R}_j, \mathbf{R}_i \pm (-\frac{1}{2}, \frac{\sqrt{3}}{2})} \right) + J_2 \left(\delta_{\mathbf{R}_j, \mathbf{R}_i \pm (\frac{3}{2}, \frac{\sqrt{3}}{2})} + \delta_{\mathbf{R}_j, \mathbf{R}_i \pm (0, \sqrt{3})} + \delta_{\mathbf{R}_j, \mathbf{R}_i \pm (-\frac{3}{2}, \frac{\sqrt{3}}{2})} \right), \quad (7.15)$$

into 7.11. And with a configuration that looks like the one in figure 5 (a) with the ground state parameter denoted as $\xi = \cos(2\theta)$ we get

$$\frac{1}{2}A_{\mathbf{q}}(\xi) = J_1 \left[\xi a_{1,0} - \xi a_{\frac{1}{2}, -\frac{\sqrt{3}}{2}} - a_{\frac{1}{2}, \frac{\sqrt{3}}{2}} + 1 \right] - J_2 \left[a_{\frac{3}{2}, \frac{\sqrt{3}}{2}} + \xi a_{\frac{3}{2}, -\frac{\sqrt{3}}{2}} - \xi a_{0, \sqrt{3}} - 1 \right], \quad (7.16)$$

where we have invoked the notation $a_{\gamma_1, \gamma_2} = \cos(\gamma_1 q_x + \gamma_2 q_y)$. Again by using eq. 7.8 and numerical integration we get a free energy behaviour that is shown in figure 10

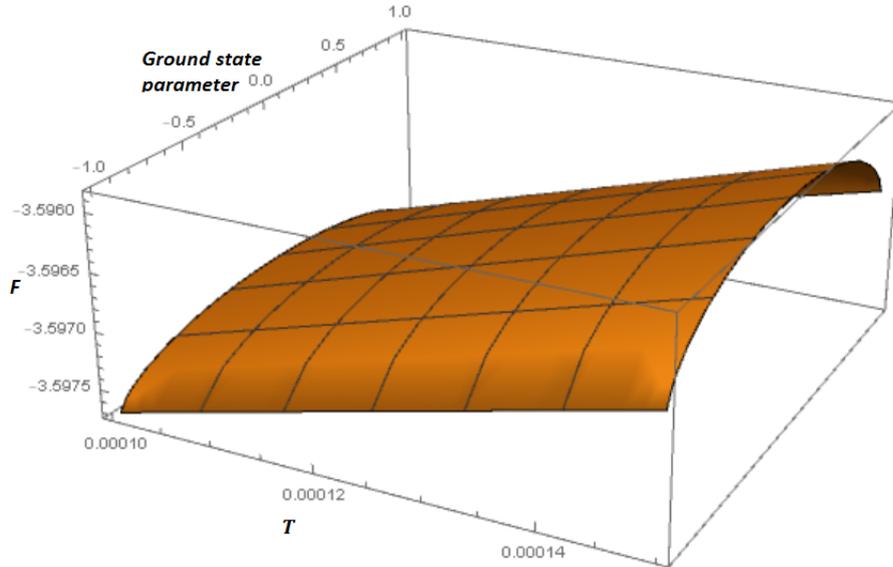


Figure 10: Plot of the free energy obtained by eq. 7.8 in a small temperature interval for the $\frac{1}{8} < \alpha < 1$ triangular lattice. It is seen that minimisation of the free energy picks out -1 and +1 for the ground state parameter. $J_1 = 1$ and $J_2 = 0.8$.

Again we see that at finite temperature it is minimised with $\xi = \pm 1$ which means that $\theta = \{0, \frac{\pi}{2}\}$. These values correspond again to stripes either horizontally or vertically. This confirms a result achieved by Joliceour et al..

8 Adding an AFM or FM third nearest neighbour in the square lattice.

In this section we will introduce a third nearest neighbour coupling and let this be both FM and AFM. We still define $\alpha = \frac{J_2}{J_1}$. We also introduce another tuning parameter given by $\beta = \frac{J_3}{J_1}$, which means that when we use the spiral method to draw a phase diagram this would now be two dimensional. The energy in momentum space is found by 2.6 and we get

$$\frac{J_{\mathbf{q}}}{2J_1} = \cos q_x + \cos q_y + 2\alpha \cos q_x \cos q_y + \beta (\cos 2q_x + \cos 2q_y). \quad (8.1)$$

8.1 The phase diagram with AFM $J_1 \equiv 1$ and J_2 and $J_3 \neq 0$.

Let us now obtain the phase diagram using the spiral method. We already know the phase diagram for the AFM J_1 - AFM J_2 model. What happens if we turn on an AFM J_3 ? Above a certain value of β in the two regions $\alpha < \frac{1}{2}$ and $\alpha > \frac{1}{2}$ the pitch vectors start to change positions and move towards the origin along the (π, π) direction. Searching for a minimum along this line by setting the gradient to zero it can be found that

$$\left(\cos(Q_x), \cos(Q_y) \right) = \left(-\frac{1}{2\alpha + 4\beta}, -\frac{1}{2\alpha + 4\beta} \right) \quad (8.2)$$

Which means that the two dimensional spiral states are bounded by the lines

$$\beta = \pm \left(\frac{1}{4} - \frac{\alpha}{2} \right) \quad (8.3)$$

According to arguments given in section 4 configurations corresponding to these \mathbf{Q}' s could be interpreted as two dimensional spiral states because moving a lattice site horizontally or vertically amounts to the same "twisting" of the spin direction. (see figure 11). In much literature this is called incommensurate spin states but in principle one might be able to see some periodicity if the amount with which the spin direction is "twisted" is a fraction of 2π .

When we turn on a FM J_3 it physically makes sense that we have no phase transition in the two regions $\alpha < \frac{1}{2}$ and $\alpha > \frac{1}{2}$ however large the FM J_3 may be. This means that we have three lines in parameter space separating the Néel phase, the stripe phases and the incommensurate phases. These are drawn in the phase diagram below

We thus have three lines the phase diagram that separate these three different phases. The red line in figure 11 corresponding to $J_2 = \frac{J_1}{2}$ and $J_3 < 0$ is of special interest. Here the infinite degeneracy of the ground states is lifted and we have three possible pitch vectors that can all coexist. This will be dealt with in the next section.

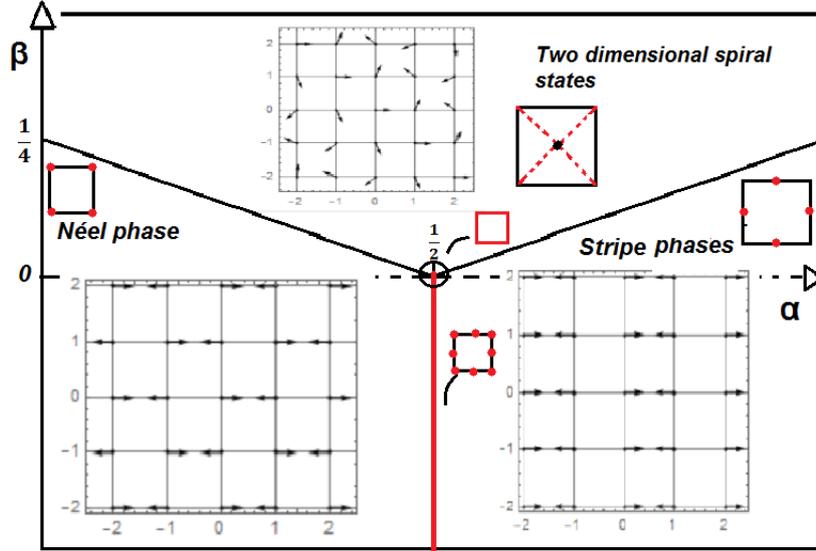


Figure 11: Phase diagram with AFM J_1 , AFM J_2 and AFM/FM J_3 obtained using the spiral method. Small squares with red dots or lines show where the pitch vectors lie.

8.2 The special case of $J_2 = \frac{J_1}{2}$ and $J_3 < 0$.

Our motivation for looking at this line in parameter space is, as touched up earlier the fact that we can use this as a tuning knob to lift the infinite degeneracy at $\alpha = \frac{1}{2}$.

Adding a ferromagnetic J_3 has a remarkable effect. The 'star' of \mathbf{Q} consists of $\mathbf{Q}_1 = (0, \pi)$, $\mathbf{Q}_2 = (\pi, 0)$ and $\mathbf{Q}_3 = (\pi, \pi)$. These all satisfy $2\mathbf{Q} \equiv 0$ and can thus all coexist if the spin dimensionality is $n \geq 3$.

$$\mathbf{s}_i = \mathbf{e}_1 \cos[\mathbf{Q}_1 \cdot \mathbf{R}_i] + \mathbf{e}_2 \cos[\mathbf{Q}_2 \cdot \mathbf{R}_i] + \mathbf{e}_3 \cos[\mathbf{Q}_3 \cdot \mathbf{R}_i] \quad (8.4)$$

The constraints given in 3.10 along with the zero sum condition still have to be satisfied for a ground state configuration. When $J_3 = 0$ a ground state can be denoted by $\{\theta_i, \phi_i\}$ in spherical coordinates where the i 's run over every square plaquette. This is illustrated in figure 8(b) where the spins are two dimensional i.e. we could think of it as the $\{\theta_i, 0\}$ groundstate.

The FM J_3 coupling fixes the third nearest neighbour spins in a ground state. When the third nearest neighbour is fixed so that it points in the same direction the energy contribution from the J_1 and J_2 bonds is minimized while maximally lowering the energy from the J_3 coupling.[2]. The sum of the spins on every square plaquette is vanishing in a ground state which means that a generic configuration for one plaquette could be

$$\mathbf{s}_1 = \{1, \theta, 0\}, \mathbf{s}_2 = \{1, \theta, \pi\}, \mathbf{s}_3 = \{1, \pi - \theta, \phi\}, \mathbf{s}_4 = \{1, \pi - \theta, \pi + \phi\} \quad (8.5)$$

If every alternating spin is fixed then every alternating plaquette is fixed. This is illustrated in figure 12 where the spins are symbolised at the sites by different shapes and alternating plaquettes are shaded. If the shaded plaquettes sum to zero the unshaded

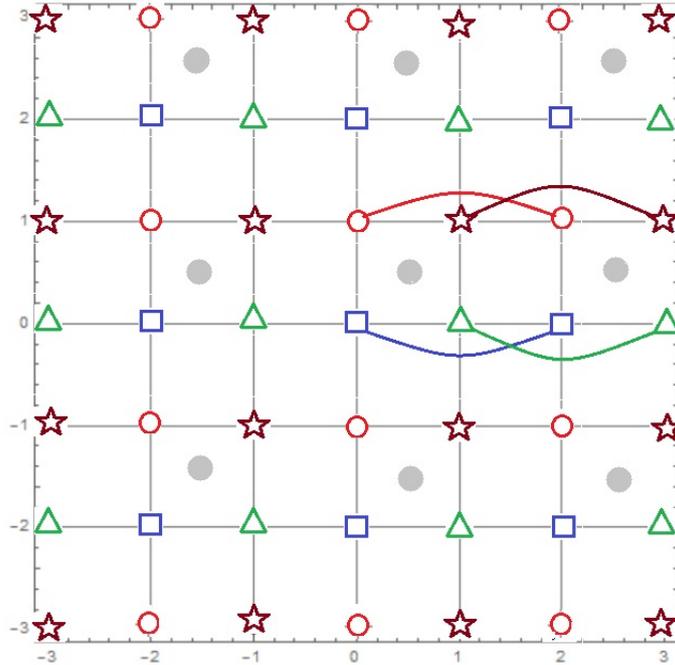


Figure 12: Visualisation of how adding a FM J3 fixes the spins on every alternating plaquette with the zero sum condition still satisfied

squares do to because they contain the same shapes in the corners. We then have a fixed ground state for the full lattice parametrised by this time two numbers $\{\theta, \phi\}$. Results regarding a free energy selection of specific values of θ and ϕ have been studied by Danu et al. 2016 [2]. They show that states with $\{\theta, \phi\} = \{0, 0\}$, $\{\theta, \phi\} = \{\frac{\pi}{2}, \pi\}$ and $\{\theta, \phi\} = \{\frac{\pi}{2}, 0\}$ are selected corresponding to horizontal stripes, vertical stripes and the Néel state respectively.

9 Conclusion

By realising that it is not easy to see what the ground state spin configurations in systems with geometrical frustration are we began our search for a way to do just that. The local constraint 2.2 forced the ground state spin configurations to be planar spiral pitched after a single vector \mathbf{Q} that minimises the energy. More than one of these can exist and if they are situated at special points in reciprocal space they can coexist. Coexistence of spirals lead to a continuous parametrised manifold of degenerate ground states. By calculating a spin wave spectrum after adding small fluctuations it was possible through thermodynamic calculations to show that the free energy and entropy depends on this parameter. It has been shown that at finite temperature free energy minimisation picks out specific values of the ground state parameter and the continuous ground state manifold is reduced to a discrete one. This is the order by disorder mechanism of which we have seen two examples in the square lattice and in the triangular lattice respectively. In the square lattice when only including the second nearest neighbour in the model we took a special point into consideration. When the interaction between the second nearest neighbour is half of what it is between the nearest neighbour the ground state had to satisfy a zero sum condition for every plaquette. This lead to

an infinitely degenerate ground state manifold. In an elegant way this could be lifted by introducing a ferromagnetic third nearest neighbour bond fixing every alternating plaquette and the ground state could again have a parametrisation as those looked at earlier this time with two parameters.

10 Acknowledgement

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