Order by disorder in frustrated magnetic systems

Bachelor's thesis
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June 13, 2018

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Abstract

In this thesis the theory of ordering due to disorder will be investigated and reproduced as forumulated by C. L. Henley in Ref. [1]. The ground state of the two-dimensional square lattice with nearest (J_1) and next-nearest (J_2) neighbour exchange interactions will be determined. The special case of $\frac{J_2}{|J_1|} > \frac{1}{2}$ will be treated and it will be shown that this case leads to two antiferromagnetic sublattices, the alignment of which is seperated by an angle ϕ. However this ϕ will not be present in the ground state energy leading to a frustrated system degenerate in ϕ.

It will thereafter be shown that different effects will break this frustration under the expansion of random spin deviations. Thermal fluctuations will break this degeneracy at a finite temperature due to the entropy of the system. This will lead to the system being in collinear states. Dilution of the lattice will also break the degeneracy leading to the system being in anticollinear states. It will be shown that the spin deviations that minimize the energy of the diluted lattice are not random, but specific values. The diluted lattice will be investigated numerically and it will be reinforced that the energy of a lattice with random spin deviations is higher than that of a diluted lattice with the specific spin deviations.

Contents

1 Introduction

The symmetry, or lack thereof, of the particles in liquid and solid materials has always been an intriguing subject in the field of condensed matter physics. The concept of order is mostly associated with stable states or phase transitions to neatly organized systems (such as ferromagnetic or antiferromagnetic systems, henceforth abbreviated by FM and AFM respectively). Disorder is generally linked to the complete opposite, namely chaotic or cluttered states. The theory of order by disorder completely goes against this intuition for the terms.

The theory was first formulated by J. Villain, [2] and later explored by, among others, C. L. Henley. This thesis is based on the results of the latter. The theory shows how a system, which is originally frustrated, will have this frustration broken by disorder of the system. A frustrated system is characterized by not having one unique determinable ground state - several configurations give the same small energy for the system, so the system is degenerate in some parameter.

Ordering due to disorder, as devised by Henley in Ref. [1] has been used to examine a wide variety of subjects. For instance different kinds of transport of doped materials with frustrated ground states, such as $\mathrm{CuCr_{1\text{-}x}Mg_xO_2}$ [3], or the search for new types of non-Abelian topological superconductors [4]. Generally the theory has proved useful when dealing with systems with magnetically frustrated ground states.

The purpose of this thesis is to gain understanding of the theory in depth, which will be done by considering thermal fluctuations and dilution of the lattice characterizing a material. Dilution signifies the removal of atoms from some lattice sites, leaving them empty. One could think that these perturbations of the system would leave the system disordered and chaotic. In fact the exact opposite happens, as will be shown in this thesis. The disordering of the system will lead to energies characterized by an angle ϕ (a parameter depending on the structure of the spins of the lattice) and a consequence of this is that the energy of the system will be minimized at a certain angle ϕ. In fact, as we will see in section 5, thermal fluctuations will lead to the system being in some so-called collinear states while dilution of the lattice will lead to the system being in anticollinear states, which will be shown in section 6.

2 The two-dimensional square lattice

Crystalline materials are characterized by periodic arrays of atoms. In this thesis the two-dimensional square lattice with an effective spin at each lattice point will be considered, as depicted in Fig. 1. The lattice points are equally spaced in the x- and y-direction, resulting in lattice constants $a_x = a_y = a$. These lengths are illustrated in Fig. 3. For simplicity the considered lattice will be constructed to have $a = 1$.

2.1 Exchange constants

The exchange interaction between atoms located at different lattice points is characterized by the exchange constant J_{ij} between sites i and j [5]. This constant describes the strengths of the bonds between sites at differents distances from each other. The atoms of the lattice can interact with every other atom in the lattice, leading to many different exchange constants, but this interaction is symmetric so that $J_{ij} = J_{ji}$. In this thesis only nearest (J_1) and next-nearest (J_2) neighbour interactions will be considered, the bonds of which are illustrated in Fig. 1. The ground state of this system will be determined in section 3.

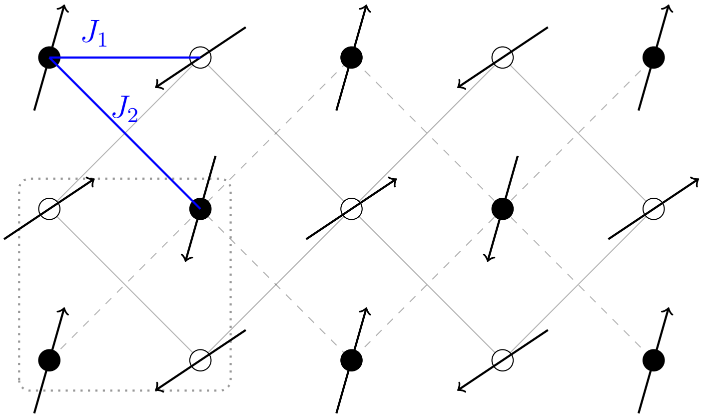


Fig. 1: A two-dimensional square lattice consisting of two AFM sublattices, the spins of one are connected by filled lines, while the spins of the other are connected by dashed lines. The exchange constants between nearest neighbouring sites (J_1) and next-nearest neighbouring sites (J_2) are illustrated in blue. The dotted square encloses the lattice points shown in Fig. 3.

2.2 Brillouin Zones

When examining lattices it is useful to be aware of the related reciprocal lattice. The Fourier transform of the lattice in real space yields the structure of the lattice in reciprocal space. The two-dimensional square lattice has the same structure in real space as in reciprocal space except that the spacing between lattice points in the reciprocal lattice is $\frac{2\pi}{a}$. The First Brillouin zone is the area in reciprocal space in which all physically distinct values for the wave vector $\mathbf{q}$ is contained [6]. It is made up of the Wigner-Seitz unit cell of the reciprocal lattice.

The reciprocal lattice is periodic in $\mathbf{q} \to \mathbf{q} + \frac{2\pi}{a}$ so that every $\mathbf{q}$ outside of the first Brillouin zone describes exactly the same wave as one of the $\mathbf{q}$'s in the first Brillouin zone. This means that when summing (or integrating) over $\mathbf{q}$ it is sufficient to sum over every $\mathbf{q}$ in the first Brillouin Zone. Therefore sums (or integrals) of this form in this thesis will be denoted by only $\mathbf{q}$ but it is implicit that this means $\mathbf{q} \in 1^{\text{st}}\text{BZ}$.

3 Spin configurations of ground states

In this thesis the two-dimensional square lattice, described by the Heisenberg Hamiltonian

$$\hat{\mathcal{H}} = \frac{1}{2}\sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j, \tag{3.1}$$

with nearest (J_1) and next-nearest (J_2) neighbour couplings will be considered as seen in Fig. 1. It is useful to determine the ground state of the given system. Both J_1 and J_2 can be FM ($J < 0$) or AFM ($J > 0$). Different combinations of J_1 and J_2 couplings give different ground states. To determine the ground state it is convenient to insert the Fourier transform of the spins $\mathbf{S}_i = \frac{1}{\sqrt{N}}\sum_{\mathbf{q}} \mathrm{e}^{i\mathbf{R}_i\cdot\mathbf{q}}\mathbf{S}_{\mathbf{q}}$ to obtain an expression for $\hat{\mathcal{H}}(\mathbf{q})$ while also exploiting the fact that this system only has exchange interactions between nearest neighbours and next-nearest neighbours, so that

$$\begin{aligned}
\hat{\mathcal{H}} &= \frac{1}{2}\sum_{ij}\sum_{\mathbf{q},\mathbf{q'}} J_{ij}\mathrm{e}^{i\mathbf{R}_i\cdot\mathbf{q}}\mathrm{e}^{i\mathbf{R}_j\cdot\mathbf{q'}}\mathbf{S}_{\mathbf{q}}\cdot\mathbf{S}_{\mathbf{q'}} \\
&= \frac{1}{2}\sum_{\mathbf{R}_i}\sum_{\mathbf{q},\mathbf{q'}} \mathbf{S}_{\mathbf{q}}\cdot\mathbf{S}_{\mathbf{q'}}\mathrm{e}^{i\mathbf{R}_i\cdot\mathbf{q}}\Big[J_1\left(\mathrm{e}^{i(\mathbf{R}_i+(0,a))\cdot\mathbf{q'}} + \mathrm{e}^{i(\mathbf{R}_i+(0,-a))\cdot\mathbf{q'}} + \mathrm{e}^{i(\mathbf{R}_i+(a,0))\cdot\mathbf{q'}} + \mathrm{e}^{i(\mathbf{R}_i+(-a,0))\cdot\mathbf{q'}}\right) \\
&+ J_2\left(\mathrm{e}^{i(\mathbf{R}_i+(a,a))\cdot\mathbf{q'}} + \mathrm{e}^{i(\mathbf{R}_i+(a,-a))\cdot\mathbf{q'}} + \mathrm{e}^{i(\mathbf{R}_i+(-a,a))\cdot\mathbf{q'}} + \mathrm{e}^{i(\mathbf{R}_i+(-a,-a))\cdot\mathbf{q'}}\right)\Big] \\
&= \sum_{\mathbf{R}_i}\sum_{\mathbf{q},\mathbf{q'}} \mathbf{S}_{\mathbf{q}}\cdot\mathbf{S}_{\mathbf{q'}}\mathrm{e}^{i\mathbf{R}_i\cdot(\mathbf{q}+\mathbf{q'})}\left[J_1\left(\cos(q'_x a) + \cos(q'_y a)\right) + 2J_2\cos(q'_x a)\cos(q'_y a)\right],
\end{aligned} \tag{3.2}$$

where the sum $\sum_{\mathbf{R}_i}\mathrm{e}^{i\mathbf{R}_i\cdot(\mathbf{q}+\mathbf{q'})}$ is only nonzero for $\mathbf{q} = -\mathbf{q'}$, so the Heisenberg Hamiltonian can be rewritten to

$$\hat{\mathcal{H}} = \sum_{\mathbf{q}} J_{\mathbf{q}}\mathbf{S}_{\mathbf{q}}\cdot\mathbf{S}_{-\mathbf{q}}, \tag{3.3}$$

where $J_{\mathbf{q}} = J_1\left[\cos(q_x a) + \cos(q_y a)\right] + 2J_2\cos(q_x a)\cos(q_y a)$. If the Hamiltonian is given by 3.3 under the restriction $\mathbf{S}_i^2 = 1$ the energy of the system can be described by [7]

$$E(\mathbf{q}) = J_{\mathbf{q}}N, \tag{3.4}$$

where N is the total number of lattice points. The spins are given by

$$\mathbf{S}_i = \hat{x}\sin(\mathbf{q}_0\cdot\mathbf{R}_i) + \hat{y}\cos(\mathbf{q}_0\cdot\mathbf{R}_i). \tag{3.5}$$

So the ground state energy is given by the set of $\mathbf{q}$-vectors that minimize Eq. 3.4, namely the pair $\pm\mathbf{q}_0$. In nature it is most common that only one $\mathbf{q}_0$-vector minimizes the energy [8], but as will be seen this is not always the case. For the different combinations of FM and AFM exchange couplings the ground state will now be determined.

3.1 FM J_1 and FM J_2 & AFM J_1 and FM J_2

These two cases are fairly simple and intuitively straightforward. To find the spin configuration of the ground state $J_{\mathbf{q}}$ is minimized with respect to $\mathbf{q}$. The energy of the ground state of the first case where both J_1 and J_2 are FM is unsurprisingly achieved when $\mathbf{q}_0 = (0, 0)$ resulting in a perfect ferromagnet since the spins will be

$$\mathbf{S}_i = \hat{y}, \tag{3.6}$$

that is completely unchanged over the entire lattice.

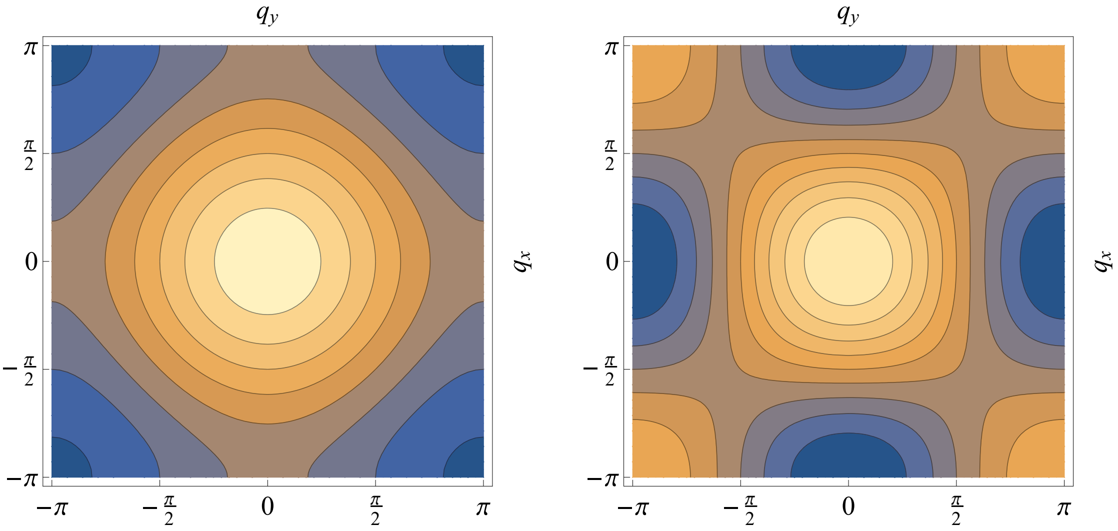
For the other case with AFM J_1 and FM J_2 the energy is minimized for $\mathbf{q}_0 = (\pi, \pi)$ and $\mathbf{q}_0 = (\pi, -\pi)$ resulting in the spins being

$$\mathbf{S}_i = \hat{y}\cos(\pi x_i \pm \pi y_i), \tag{3.7}$$

i.e. alternating in both the x- and y-direction, i.e. a perfect antiferromagnet for both plus and minus. Thus both signs describe the same configuration.

3.2 FM J_1 and AFM J_2 & AFM J_1 and AFM J_2

The two cases with AFM J_2 and corresponding J_1's have less self-evident results than the previously discussed cases. Here the exchange couplings are conflicting and cannot both be satisfied. By varying the exchange couplings it can be seen that a shift of the $J_\mathbf{q}$ function happens at a certain J_2. For small J_2 both cases are dominated by the J_1 exchange (completely FM or AFM). When $\frac{J_2}{|J_1|} > \frac{1}{2}$ the minimum of $J_\mathbf{q}$ shifts to $\mathbf{q}_0 = (\pi, 0)$ and $\mathbf{q}_0 = (0, \pi)$ for both cases. This is illustrated in Fig. 2.



(a) Plot of the contours of $J_\mathbf{q}$ with $J_1 = 1$ and $J_2 = 0.2$.

(b) Plot of the contours of $J_\mathbf{q}$ with $J_1 = 1$ and $J_2 = 2$.

Fig. 2: Plots of the contours of $J_\mathbf{q}$ showing the shift of $\mathbf{q}_0$ from (π, π) and $(\pi, -\pi)$ (Fig. (a)) to $(\pi, 0)$ and $(0, \pi)$ (Fig. (b)) as J_2 gets larger than $\frac{1}{2}J_1$.

Henceforth the case of $\frac{J_2}{|J_1|} > \frac{1}{2}$ will be considered and will be assumed to be the situation for the remainder of this thesis. In this case there is more than one vector $\pm\mathbf{q}_0$ that minimizes the energy, namely $\mathbf{q}_0^{(1)} = (\pi, 0)$ and $\mathbf{q}_0^{(2)} = (0, \pi)$. In fact this situation turns out to be a special case as described by [8]. Here $2\mathbf{q}_0 = (2\pi, 0)$ is a reciprocal lattice vector, as is $(0, 2\pi)$. Then, according to [8], the spins are given by

$$\mathbf{S}_i = \hat{x}\cos(\mathbf{q}_0^{(1)} \cdot \mathbf{R}_i)\sin(\theta) + \hat{y}\cos(\mathbf{q}_0^{(2)} \cdot \mathbf{R}_i)\cos(\theta). \tag{3.8}$$

By inserting the $\mathbf{q}_0$'s this becomes

$$\mathbf{S}_i = \hat{x}\cos(\pi x_i)\sin(\theta) + \hat{y}\cos(\pi y_i)\cos(\theta). \tag{3.9}$$

By varying θ it is clear that these spins lead to a split of the spins into two AFM sublattices with a free angle between them, as depicted in Fig. 1 with black dots making up one sublattice and white dots making up the other.

Different values for the angle between the sublattices is shown in Fig. 5 and Fig. 8. It is convenient to define a set of reference spins, for example at $[0,1]$ and $[0,0]$. Let the angle that these spins make with the y-axis be θ_a and θ_b respectively, as illustrated in Fig. 3. Now let $\theta_a - \theta_b = \phi$.

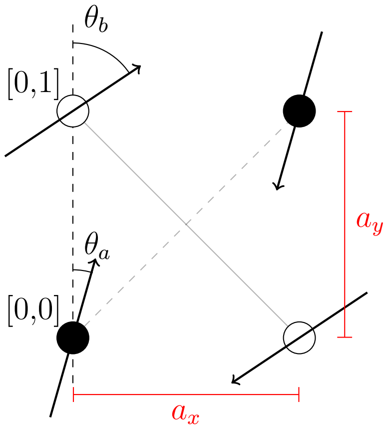


Fig. 3: A zoom in on four of the lattice points displayed in Fig. 1. The lenghts characterizing the two lattice constants a_x and a_y are shown as well as the angles between the two reference spins at [0,0] and [1,0] and the y-axis.

4 The Heisenberg model

The Heisenberg model can be used to describe the system introduced above. The general form of the classical Heisenberg model is given by Eq. 3.1. This model can be simplified by assuming that the spins $\mathbf{S}_i$ and $\mathbf{S}_j$ are effectively only in two dimensions, say x and y (and that their magnitude is equal for all i, j).The spins can then be treated as classical vectors $\mathbf{S}_i = S\,(\cos(\theta_i), \sin(\theta_i))$, where θ_i and θ_j are the angles between $\mathbf{S}_i$ and $\mathbf{S}_j$ and the y-axis, respectively. Then Eq. 3.1 can be reduced to the two-dimensional XY model, which is given by [9]

$$\hat{\mathcal{H}} = \frac{1}{2}S^2 \sum_{ij} J_{ij}\cos(\theta_i - \theta_j). \tag{4.1}$$

It is worth noting that, the two-dimensional XY model is oftentimes considered with regards to the Mermin-Wagner theorem and the Kosterlitz-Thouless transition (vortices and anti-vortices) [5] . In that case only nearest neighbour interactions are considered, so surely the circumstances of the instance with the addition of next-nearest neighbour interactions are different, and will not be considered in this thesis.

Since an atom in the lattice only couples to its nearest and next-nearest neighbours, $\theta_i - \theta_j$ can only take on three different values for each site. All next-nearest neighbours have $\theta_i - \theta_j = \pi$ since they form an AFM sublattice, as determined in section 3.2. The two nearest neighbours in the y-direction have $\theta_i - \theta_j = \theta_a - \theta_b = \phi$, while the two in the x-direction have $\theta_i - \theta_j = \theta_a - (\theta_b + \pi) = \phi - \pi$. Let $S^2 = 1$ for simplicity. The ground state energy of the system can now be determined to be

$$\begin{aligned}\hat{\mathcal{H}}^0 &= \frac{1}{2}\sum_i \left(2J_1\cos(\phi) + 2J_1\cos(\phi-\pi) + 4J_2\cos(\pi)\right)\\ &= -2NJ_2\\ &= E_0,\end{aligned} \tag{4.2}$$

where N is the number of atoms in the lattice. The ground state energy is independent of the orientation of the two sublattices, since there is no ϕ-dependency in Eq. 4.2. This leads to a degeneracy of the ground state energy in the angle ϕ and the ground state is therefore frustrated.

4.1 Spin deviations

A way to excite the system is to let the angles θ_i fluctuate, so the two sublattices no longer are perfectly AFM. The following derivations follow those of Ref. [1] in an attempt to do this. The excitation can be included by letting $\theta_i \to \theta_i^0 + \delta\theta_i$, so that

$$\begin{aligned}\hat{\mathcal{H}} &\to \frac{1}{2}\sum_{ij}\cos\left(\theta_i^0 + \delta\theta_i - \theta_j^0 - \delta\theta_j\right)\\ &\approx \frac{1}{2}\sum_{ij} J_{ij}\left[\cos\left(\theta_i^0-\theta_j^0\right) - (\delta\theta_i - \delta\theta_j)\sin\left(\theta_i^0-\theta_j^0\right) - \frac{1}{2}(\delta\theta_i-\delta\theta_j)^2\cos\left(\theta_i^0-\theta_j^0\right)\right].\end{aligned} \tag{4.3}$$

Here the cosine has been expanded to second order in $(\delta\theta_i - \delta\theta_j)$. So the addition to the Hamiltonian due to the deviations of the spins is

$$\begin{aligned}\delta\hat{\mathcal{H}} &\approx \hat{\mathcal{H}} - \hat{\mathcal{H}}^0\\ &= -\frac{1}{2}\sum_{ij} J_{ij}\left[(\delta\theta_i-\delta\theta_j)\sin\left(\theta_i^0-\theta_j^0\right) + \frac{1}{2}(\delta\theta_i-\delta\theta_j)^2\cos\left(\theta_i^0-\theta_j^0\right)\right],\end{aligned} \tag{4.4}$$

where $\hat{\mathcal{H}}^0$ is the Hamiltonian corresponding to the ground state energy from Eq. 4.2. As demonstrated in [10] the sine term vanishes due to translational invariance of the lattice, but it can also be seen that it disappears due to the possible values of $\theta_i - \theta_j$, the same way that the J_1 coupling terms cancels out in the ground state energy in Eq.

4.2. Also the next-nearest neighbour coupling term J_2 has $\sin(\theta_i - \theta_j) = \sin(\pi)$ and therefore the entire sine term vanishes. The remaining terms of $\delta\hat{\mathcal{H}}$ are then

$$\delta\hat{\mathcal{H}}_\phi = \frac{1}{4}\sum_{ij} J_{ij}\cos\left(\theta_i^0 - \theta_j^0\right)\left[-\delta\theta_i^2 - \delta\theta_j^2 + 2\delta\theta_i\delta\theta_j\right]. \tag{4.5}$$

One can now use the Fourier transform $\delta\theta_i = \frac{1}{\sqrt{N}}\sum_{\mathbf{q}} \mathrm{e}^{i\mathbf{R}_i\cdot\mathbf{q}}\delta\theta_{\mathbf{q}}$ to diagonalize this Hamiltonian. This yields

$$\begin{aligned}\delta\hat{\mathcal{H}}_\phi = -\sum_{\mathbf{R}_i}\sum_{\mathbf{q},\mathbf{q'}} \delta\theta_{\mathbf{q}}\delta\theta_{\mathbf{q'}}\mathrm{e}^{i\mathbf{R}_i\cdot(\mathbf{q}+\mathbf{q'})}\big[&J_1\cos(\phi)\left(\cos(aq'_x) - \cos(aq'_y)\right)\\ &+ J_2\left(-2 + 2\cos(aq'_x)\cos(aq'_y)\right)\big],\end{aligned} \tag{4.6}$$

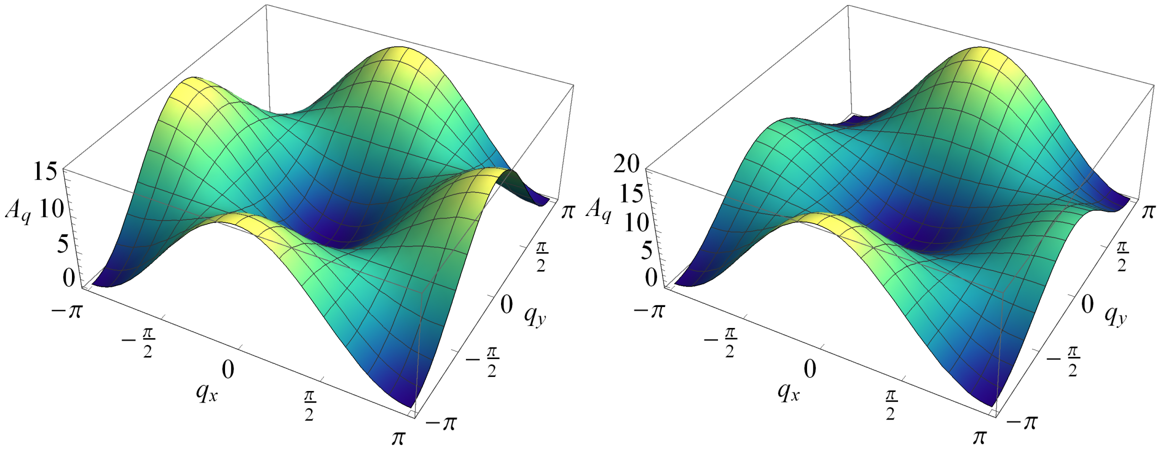
where the sum $\sum_{\mathbf{R}_i}\mathrm{e}^{i\mathbf{R}_i\cdot(\mathbf{q}+\mathbf{q'})}$ is only nonzero for $\mathbf{q} = -\mathbf{q'}$, so Eq. 4.6 can be simplified to

$$\delta\hat{\mathcal{H}}_\phi = \frac{1}{2}\sum_{\mathbf{q}} A_{\mathbf{q}}|\delta\theta_{\mathbf{q}}|^2, \tag{4.7}$$

where

$$A_{\mathbf{q}} = -\left[2J_1\cos(\phi)\left(\cos(aq_x) - \cos(aq_y)\right) + 4J_2\left(-1 + \cos(aq_x)\cos(aq_y)\right)\right]. \tag{4.8}$$

$A_{\mathbf{q}}$ is depicted for two different values of ϕ in Fig. 4. $A_{\mathbf{q}}$ is a measure of how costly the spin deviations are for the system for each $\mathbf{q}$.



(a) Plot of $A_{\mathbf{q}}$ with $J_1 = 1$ and $J_2 = 2$ for $\phi = \frac{\pi}{2}$. **(b)** Plot of $A_{\mathbf{q}}$ with $J_1 = 1$ and $J_2 = 2$ for $\phi = \pi$.

Fig. 4: Plots of $A_{\mathbf{q}}$ for different values of ϕ.

5 Thermal fluctuations

The system will now be considered at some finite temperature, leading to thermal fluctuations of the system to illustrate how this effect of disorder will lead to ordering of the frustrated system. In this case the partition function, determined by $Z = \mathrm{Tr}\left[\mathrm{e}^{-\beta\hat{\mathcal{H}}}\right]$, for the system is

$$\begin{aligned} Z &= \mathrm{e}^{-\beta E_0} \sum_{\delta\theta_{\mathbf{q}}} \mathrm{e}^{-\frac{\beta}{2}\sum_{\mathbf{q}} A_{\mathbf{q}}|\delta\theta_{\mathbf{q}}|^2} \\ &= \mathrm{e}^{-\beta E_0} \int \prod_{\mathbf{q}} (\mathrm{d}\delta\theta_{\mathbf{q}})\, \mathrm{e}^{-\frac{\beta}{2}\sum_{\mathbf{q}} A_{\mathbf{q}}|\delta\theta_{\mathbf{q}}|^2} \\ &= \mathrm{e}^{-\beta E_0} \prod_{\mathbf{q}} \left(\frac{2\pi}{\beta A_{\mathbf{q}}}\right)^{\frac{1}{2}}. \end{aligned} \tag{5.1}$$

Inserting this in $F = -\frac{1}{\beta}\ln(Z)$ to find the Helmholtz free energy, with $\beta = \frac{1}{Tk_b}$, k_b being Boltzmanns constant, which in the following will be neglected since it is of no conceptual importance to the result. Then one obtains

$$F = F_0 + \frac{1}{2\beta}\sum_{\mathbf{q}} \ln\left(\frac{\beta A_{\mathbf{q}}}{2\pi}\right), \tag{5.2}$$

where $F_0 = -\frac{1}{\beta}\ln\left(\mathrm{e}^{-\beta E_0}\right) = E_0$ is the ground state energy from Eq. 4.2. Subtracting this term yields

$$F - E_0 = -\frac{1}{2}T\ln(T)N + \frac{1}{2}T\sum_{\mathbf{q}} \ln\left(\frac{A_{\mathbf{q}}}{2\pi}\right). \tag{5.3}$$

If the lattice has periodic boundary conditions, so that site $(a + L_x, b + L_y)$, where L_x and L_y are the lengths of the lattice in the x- and y-direction, is exactly the same site as (a, b) then the sum over $\mathbf{q}$ can be approximated by an integral, so that $\sum_{\mathbf{q}} \to A\int(2\pi)^{-2}\mathrm{d}^2\mathbf{q}$, where A is the area of the lattice [6]. This integral can be evaluated numerically to

$$\begin{aligned} \frac{1}{2}T\sum_{\mathbf{q}} \ln(A_{\mathbf{q}}) &= \frac{TA}{8\pi^2}\int \ln(A_{\mathbf{q}})\,\mathrm{d}^2\mathbf{q} \\ &= \mathrm{const} - \frac{TN}{2} g_0\left(\frac{J_1\cos(\phi)}{2J_2}\right), \end{aligned} \tag{5.4}$$

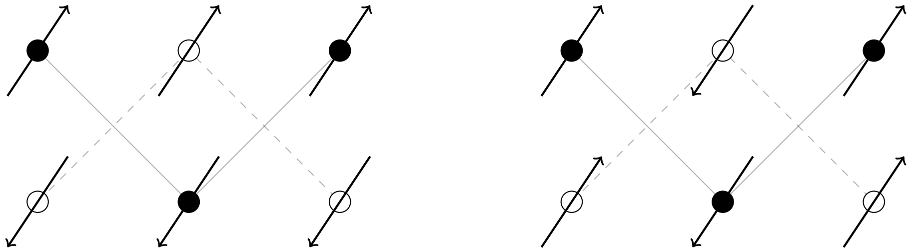
where $g_0(x) = 0.220 + 0.318x^2$. So the free energy is then

$$F - E_0 = -\frac{1}{2}TN\ln(T) - \frac{1}{2}TN\ln(2\pi) + \mathrm{const} - \frac{TN}{2}g_0\left(\frac{J_1\cos(\phi)}{2J_2}\right). \tag{5.5}$$

The only variable in Eq. 5.5 is the angle between the two AFM sublattices ϕ. The energy of the system in the presence of thermal fluctuations is minimized when $\phi = n\pi$, $n \in \mathbb{Z}$. The two sublattices will therefore select a collinear state, where the axis of the spins is the same for all lattice sites, as illustrated in Fig. 5.

Eq. 5.5 can be rewritten in terms of the entropy as

$$F - E_0 = -\frac{1}{2}N - TS(\phi), \tag{5.6}$$



(a) A collinear state with $\phi = 0$. **(b)** A collinear state with $\phi = \pi$.

Fig. 5: Collinear states for the two-dimensional square lattice with two AFM sublattices, characterized by the angle between the alignment of the two sublattices $\phi = n\pi$, $n \in \mathbb{Z}$.

since the entropy is given by

$$\begin{aligned} S &= \ln(Z) - \beta \frac{\partial \ln(Z)}{\partial \beta} \\ &= -\frac{1}{2} \sum_{\mathbf{q}} \ln\left(\frac{\beta A_{\mathbf{q}}}{2\pi}\right) + \frac{1}{2} N. \end{aligned} \tag{5.7}$$

When the system is subject to thermal fluctuations, an effect that leads to disordering of the lattice, the spins of the lattice will thus align themselves by these collinear states to minimize the free energy of the system. Hence a kind of ordering by disorder arises, leading to the name of this mechanism. The fact that the angle between the alignment of the sublattices minimizes the energy means that this type of fluctuation breaks the original frustration of the ground state because of the contribution of the entropy. The energy of the system is no longer degenerate in ϕ, since there clearly is a ϕ-dependency now, and a set of angles that minimize the energy of the system.

6 Dilution

Another type of disordering of the system is the effect of dilution. Diluting a lattice signifies the complete removal of spins from a number of lattice sites, so that they are empty. A diluted lattice therefore has unoccupied sites. By following Ref. [1] and Ref. [11] it will now be shown that this effect leads to a different type of ordering, namely the anticollinear state with $\phi = \frac{n\pi}{2}$, $n \in \mathbb{Z}$.

6.1 Site occupancy

Since not all sites are occupied the occupation parameter ϵ_i is introduced to account for this. If site i is occupied $\epsilon_i = 1$ and if it is empty then $\epsilon_i = 0$. The dilution of the lattice happens at random, so that the occupation parameters of different sites are random and independent of each other for each configuration. This implies that $\langle \epsilon_i \epsilon_j \rangle_\epsilon = \langle \epsilon_i \rangle \langle \epsilon_j \rangle_\epsilon$ for $i \neq j$, where $\langle \rangle_\epsilon$ signifies the action of averaging over configurations. For a known occupied fraction p of the lattice $\langle \rangle_\epsilon$ signifies averaging over every configuration with same p. If the lattice is diluted so that it has n unoccupied sites clearly $p = \frac{N-n}{N}$ with N being the total number of sites in the lattice.

The amount of ways n unoccupied sites can be arranged in a lattice of N points is given by the binomial coefficient $\binom{N}{n}$. For every configuration with site i occupied $\epsilon_i = 1$, and $\epsilon_i = 0$ otherwise, which means that averaging ϵ_i over configurations corresponds to the amount of configurations with site i occupied (since these are the only configurations that contribute with a nonzero value of ϵ_i) divided by the total number of configurations with n sites of the lattice empty. The amount of configurations with site i occupied must correspond to the total amount of configurations minus the amount of configurations with site i unoccupied. This is equivalent to placing the first empty site out of n at site i and then calculating how many ways the other $n-1$ empty sites can be placed at the remaining $N-1$ sites. This leads to the equation

$$\langle \epsilon_i \rangle = \frac{\binom{N}{n} - \binom{N-1}{n-1}}{\binom{N}{n}} = \frac{N-n}{N} = p. \tag{6.1}$$

Also $\langle \epsilon_i \epsilon_j \rangle_\epsilon = p^2$. Since $\epsilon_i = 1 \vee \epsilon_i = 0$ then $\epsilon_i^2 = 1 \vee \epsilon_i^2 = 0$, so $\langle \epsilon_i \epsilon_i \rangle_\epsilon = \langle \epsilon_i \rangle_\epsilon = p$.

It is convenient to define

$$\eta_{ij} = \epsilon_i \epsilon_j - p^2, \tag{6.2}$$

so that averaging η_{ij} over configurations yields $\langle \eta_{ij} \rangle_\epsilon = 0$. Because of the abovementioned results it follows that

$$\langle \eta_{ij} \eta_{kl} \rangle = \begin{cases} p^2(1-p^2) & \text{if the } i-j \text{ and } k-l \text{ bonds are the same bond} \\ p^3(1-p) & \text{if the } i-j \text{ and } k-l \text{ bonds share one site} \\ 0 & \text{if the } i-j \text{ and } k-l \text{ bonds share no sites} \end{cases}. \tag{6.3}$$

6.2 Spin deviations

The introduction of ϵ_i leads to the substitution

$$J_{ij} \to \epsilon_i \epsilon_j J_{ij}, \tag{6.4}$$

which can be rewritten to

$$J_{ij} \to p^2 J_{ij} + \eta_{ij} J_{ij}, \tag{6.5}$$

so that the Hamiltonian from Eq. 4.1 becomes

$$\hat{\mathcal{H}} = \frac{1}{2} \sum_{ij} \left(p^2 + \eta_{ij} \right) J_{ij} \cos\left(\theta_i - \theta_j \right). \tag{6.6}$$

Once again allowing spin deviations of the form $\theta_i \to \theta_i^0 + \delta\theta_i$ and expanding the cosine function to second order in $(\delta\theta_i - \delta\theta_j)$ gives

$$\begin{aligned}\hat{\mathcal{H}} &= \frac{1}{2}\sum_{ij}\left(p^2+\eta_{ij}\right)J_{ij}\cos\left(\theta_i^0+\delta\theta_i-\theta_j^0-\delta\theta_j\right)\\ &\approx \frac{1}{2}\sum_{ij}(p^2+\eta_{ij})J_{ij}\Bigg[\cos(\theta_i^0-\theta_j^0)-(\delta\theta_i-\delta\theta_j)\sin(\theta_i^0-\theta_j^0)\\ &\underbrace{-\frac{1}{2}(\delta\theta_i-\delta\theta_j)^2\cos(\theta_i^0-\theta_j^0)}_{(*)}\Bigg].\end{aligned} \tag{6.7}$$

p^2 is simply a number independent of the spin configuration. Hence if Eq. 6.7 is split into terms multiplied by p^2 and terms multiplied with η_{ij}, the p^2-terms will just simplify as in section 4 to $p^2\hat{\mathcal{H}} = p^2\left(\delta\hat{\mathcal{H}}_\phi+\hat{\mathcal{H}}^0\right)$. When examining the terms multiplied with η_{ij} one can choose to disregard the last cosine term (the term in $(*)$) since this term is proportional to $p^2\delta\theta_i^2$ both of which are small numbers, so this term is vanishingly small. The remaining terms can then be expressed as

$$\hat{\mathcal{H}} = p^2\left(\hat{\mathcal{H}}^0+\delta\hat{\mathcal{H}}_\phi\right)+\delta\hat{\mathcal{H}}', \tag{6.8}$$

where $\delta\hat{\mathcal{H}}' = \frac{1}{2}\sum_{ij}\eta_{ij}J_{ij}\left[\cos(\theta_i^0-\theta_j^0)-(\delta\theta_i-\delta\theta_j)\sin(\theta_i^0-\theta_j^0)\right]$. Since the lattice contains empty sites there is no longer translational invariance, so the sine term obviously does not vanish as it did in the case of thermal fluctuations. As a result of the structure of the lattice and the arrangement of angles θ_i^0 when a site has a next-nearest neighbour at an empty site this will yield one less factor of $-J_2$ than if all next-nearest neighbours had been present. If a site has a nearest neighbour at an empty site it will give an excess of $\pm\cos(\phi)$ and $\pm\sin(\phi)$, the sign depending on whether the empty neighbouring site is in the x- or the y-direction. So these terms that cancelled out before due to the structure of the sublattices no longer vanish. Because of this $\delta\hat{\mathcal{H}}'$ can be written as

$$\delta\hat{\mathcal{H}}' = -\frac{1}{2}\cos(\phi)\tilde{H} - J_1\sin(\phi)\sum_i\delta\theta_i\gamma_i - \frac{1}{2}\sum_{ij}\eta_{ij}J_2, \tag{6.9}$$

where the J_2-term is simply a constant, which in the following will be disregarded. Here

$$\tilde{H} = J_1\sum_{ij}\eta_{ij}(-1)^{y_i-y_j}, \tag{6.10}$$

$$\gamma_i = \sum_j\eta_{ij}(-1)^{x_i+y_j}. \tag{6.11}$$

Both are factors accounting for the sign of the extra sine/cosine terms due to empty neighbouring sites.

Fourier transforming the sine term of Eq. 6.9 gives

$$J_1\sin(\phi)\sum_i\delta\theta_i\gamma_i = J_1\sin(\phi)\sum_{\mathbf{q}}\delta\theta_{\mathbf{q}}\gamma_{-\mathbf{q}}. \tag{6.12}$$

Using this and inserting $\delta\hat{\mathcal{H}}'$ in $\delta\hat{\mathcal{H}} = \hat{\mathcal{H}} - p^2\delta\hat{\mathcal{H}}^0$ gives

$$\delta\hat{\mathcal{H}} = p^2\delta\hat{\mathcal{H}}_\phi - \frac{1}{2}\cos(\phi)\tilde{H} - J_1\sin(\phi)\sum_{\mathbf{q}}\delta\theta_{-\mathbf{q}}\gamma_{\mathbf{q}}. \tag{6.13}$$

6.2.1 Averaging over configurations

Both factors from Eq. 6.10 and Eq. 6.11 average to zero over configurations since they contain η_{ij}. But $\langle\tilde{H}^2\rangle_\epsilon$ and $\langle|\gamma_{\mathbf{q}}^2|\rangle_\epsilon$ both contain $\sum_{ij}\sum_{kl}\langle\eta_{ij}\eta_{kl}\rangle_\epsilon$, so it follows from Eq. 6.3 that these quantities contain terms that are not zero. They are

$$\langle\tilde{\mathcal{H}}^2\rangle_\epsilon = J_1^2\sum_{ij}\sum_{kl}(-1)^{y_i-y_j+y_k-y_l}\langle\eta_{ij}\eta_{kl}\rangle, \tag{6.14}$$

$$\langle|\gamma_{\mathbf{q}}^2|\rangle_\epsilon = \sum_i\sum_k \mathrm{e}^{-i\mathbf{q}\cdot(\mathbf{r}_k-\mathbf{r}_i)}\sum_j\sum_l\langle\eta_{ij}\eta_{kl}\rangle(-1)^{x_i+y_j+x_k+y_l}. \tag{6.15}$$

To carry out the calculations of these sums it is important to note the many different ways to satisfy the conditions for the nonzero results in Eq. 6.3. Since both $\tilde{\mathcal{H}}$ and $\gamma_{\mathbf{q}}$ only contain J_1-couplings it is only necessary to consider nearest neighbour couplings.

For the $i-j$ and $k-l$ bond to be exactly the same bond there are two options: $i=k\wedge j=l$ or $i=l\wedge j=k$ (four of each for each occupied site i with all nearest neighbouring sites occupied), see Fig. 6.

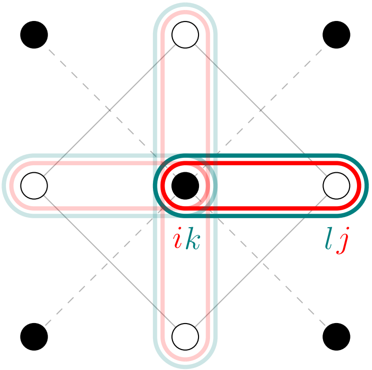


Fig. 6: $i-j$ (red) and $k-l$ (dark green) bonds are the same bond, with $i=k\wedge j=l$. This is also possible for $i=l\wedge j=k$. For each site i there are four possible configurations of the two bonds that satisfy either of the cases, all of which are illustrated by the opaque red and dark green lines encircling these.

There are four ways for them to have just one site in common; (1) $i=k\wedge j\neq l$, (2) $i=l\wedge j\neq k$, (3) $i\neq k\wedge j=l$ and (4) $i\neq l\wedge j=k$ (twelve of each for each occupied site i with all nearest neighbouring sites occupied), see Fig. 7.

In total there are 56 nonzero terms of $\sum_{ij}\sum_{kl}\langle\eta_{ij}\eta_{kl}\rangle_\epsilon$ which can be executed to give

$$\begin{aligned}\langle\tilde{\mathcal{H}}^2\rangle &= 8NJ_1^2p^3\left[1-2p+p^2\right]\\ &= 8NJ_1^2p^3(\delta p)^2\\ &\approx 8NJ_1^2(\delta p)^2.\end{aligned} \tag{6.16}$$

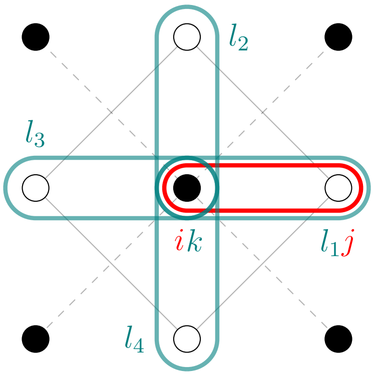


Fig. 7: $i-j$ (red) and $k-l$ (dark green) bonds share one site, here $i=k \wedge j \neq l$, but this is also possible for three other combinations of i, j, k and l. For each $i-j$ bond the $k-l$ bond have three possible configurations that satisfies the condition, as illustrated by the dark green lines encircling the possible bonds. This leads to a total of 12 combinations of j, k and l per i per satisfactory combination of these.

This result was obtained under the assumptions that the lattice can still be considered a two-dimensional square lattice, i.e. that the dilution of the lattice is small so that $p \approx 1$, while δp is the unoccupied fraction of the lattice, $\delta p = 1-p$. Eq. 6.15 yields

$$\begin{aligned}\langle|\gamma_{\mathbf{q}}^2|\rangle &= Np^3(1-p^2)2(2-\cos(q_x a)-\cos(q_y a)) + 2Np^4(1-p)\big[-2+2\cos(q_x a)\\ &\quad +2\cos(q_y a) - 4\cos(q_x a)\cos(q_y a) + \cos(2q_x a) + \cos(2q_y a)\big]\\ &\approx 2N\delta p\left[2+\cos(2q_x a)+\cos(2q_y a) - 4\cos(q_x a)\cos(q_y a)\right]\\ &= 4N\delta p\left(\cos(q_x a)-\cos(q_y a)\right)^2 .\end{aligned} \tag{6.17}$$

Exploiting the fact that $(1-p^2) = (1-p)(1+p) \approx 2\delta p$.

6.2.2 Minimizing the energy

The results from section 6.2.1 will now be used to minimize the energy of the system to determine the spin arrangement corresponding to the minimal energy state. Eq. 6.13 corresponds to an equation of the form $\delta\hat{\mathcal{H}}(x) = c - bx + ax^2$ where $x = \delta\theta_{\mathbf{q}}$. Minimizing this with respect to x trivially gives $x = \frac{b}{2a}$, that is

$$\delta\theta_{\mathbf{q}} = \frac{J_1 \sin(\phi)\gamma_{-\mathbf{q}}}{p^2 A_{\mathbf{q}}}, \tag{6.18}$$

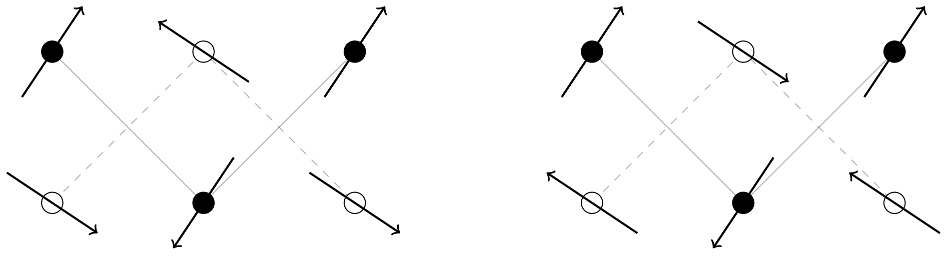
which is inconsistent with the result in [1]. Nonetheless the following results are consistent with the article, which could indicate that the dissimilarity is merely due to an erratum in the article. Inserting this value for $\delta\theta_{\mathbf{q}}$ in Eq. 6.13 and averaging over configurations, all the while ignoring the $\tilde{H}$-term (since $\tilde{H} \propto (\delta p)^2$, so this term vanishes for small δp, which is what is considered here), yields

$$\begin{aligned}\langle\delta\hat{\mathcal{H}}\rangle_\epsilon &= -\sum_{\mathbf{q}} \frac{\left(J_1\sin(\phi)\right)^2 \langle|\gamma_{\mathbf{q}}|^2\rangle_\epsilon}{2p^2 A_{\mathbf{q}}} \\ &= -\sum_{\mathbf{q}} \frac{(J_1\sin(\phi))^2 4N\delta p\left(\cos(aq_x)-\cos(aq_y)\right)^2}{2p^2 4J_2\left[\frac{2J_1}{4J_2}\cos(\phi)\left(\cos(aq_y)-\cos(aq_x)\right)+\left(1-\cos(aq_x)\cos(aq_y)\right)\right]},\end{aligned} \tag{6.19}$$

using $p \approx 1$. Here the limit $\frac{J_1}{J_2} \to 0$ is being considered which is merely a bit stricter than the original constraint $\frac{J_2}{|J_1|} > \frac{1}{2}$.

$$\begin{aligned}\langle\delta\hat{\mathcal{H}}(\phi)\rangle_\epsilon &\approx -\frac{J_1^2 N}{2J_2}\delta p\sin(\phi)^2\sum_{\mathbf{q}}\frac{(\cos(aq_x)-\cos(aq_y))^2}{1-\cos(aq_x)\cos(aq_y)} \\ &= -\frac{J_1^2 N}{2J_2}\delta p\sin(\phi)^2\int(2\pi)^{-2}\frac{(\cos(aq_x)-\cos(aq_y))^2}{1-\cos(aq_x)\cos(aq_y)}\,\mathrm{d}^2\mathbf{q} \\ &= -\frac{J_1^2 N}{2J_2}\delta p\sin(\phi)^2\cdot 0.7268.\end{aligned} \tag{6.20}$$

Eq. 6.20 is minimized when $\phi = \left(n+\frac{1}{2}\right)\pi, n \in \mathbb{Z}$, and therefore when the system is exposed to dilution of the lattice the two AFM sublattices will select an anticollinear state as illustrated in Fig. 8 for two different values of ϕ, and therefore the frustration of the ground state will be broken.



(a) An anticollinear state with $\phi = \frac{\pi}{2}$. **(b)** An anticollinear state with $\phi = \frac{3\pi}{2}$.

Fig. 8: Anticollinear states for the two-dimensional square lattice with two AFM sublattices, characterized by the angle between the alignment of the two sublattices $\phi = \left(n+\frac{1}{2}\right)\pi, n \in \mathbb{Z}$.

7 Numerical dilution

In section 6 the theoretical results for the orientation of the two AFM sublattices were found. This was the outcome of extensive calculations with a number of simplifications and approximations. It would be interesting to see these results, i.e. the selection of the anticollinear states for a diluted lattice, numerically. The purpose of this section is to compare the results of section 6 to those of a numerically diluted lattice.

A script in Mathematica$^{\mathrm{TM}}$ is set up to do this (the full script can be seen in appendix A). The script constructs a lattice with specified angles corresponding to all possible θ_i^0 but takes fluctuations at each site into account. These fluctuations consist of a random angle $\delta\theta_i \in \{-\frac{\pi}{8}, \frac{\pi}{8}\}$ at each lattice site, with the fluctuation being different from site to site.

When the lattice with spin deviations is fixed, the dilution takes place. A random selection of 99% of the lattice sites are kept in the lattice, while the rest are removed. When the lattice is diluted the energy of the system is calculated. Then a new random selection of lattice sites ensues, and the energy is determined again. This is done 1000 times. These energies are then averaged for some choice of exchange constants J_1 and J_2, and subsequently minimized with respect to ϕ. For a 40 × 40 lattice with $p = 0.99$ and exchange constants $J_1 = -1$ and $J_2 = 10$ the energy for the system is minimized at seemingly random ϕ. For even larger systems there is no systematical choice for ϕ. This shows that the choice of random spin deviations is not a good choice at all in terms of finding the minimal energy as predicted in 6. For the same choice of parameters this yields the theoretical and numerical energies respectively:

$$\langle \delta\hat{\mathcal{H}}(\phi)\rangle_\epsilon + E_0 = -32\,000.00036, \tag{7.1}$$

$$E_{min} = -28\,538.67272. \tag{7.2}$$

It can be seen that the energy from the script (Eq. 7.2) is considerably larger than the theoretical value for the anticollinear state (Eq. 7.1). Several factors can be the cause of this. Firstly, in section 6 it was seen that the spin deviations $\delta\theta_i$ are in fact not random at all; the minimal energy of the system occurs when the spin deviations take on some specific values given by Eq. 6.18. To determine the absolute minimum for the energy, as in section 6 this needs to be taken into account. Therefore the random spin deviations chosen here affect the system to a degree where a recurrent value of ϕ to minimize the energy is not determinable.

Secondly the averaging over configurations does not contain all configurations. As was shown, the amount of realizations for a given removal of a number of sites n is given by the binomial coefficient $\binom{N}{n}$. N need not be very large before this number gets enormous. For example; a 30 × 30 lattice with 1% of the sites removed yields

$$\binom{900}{891} = 1\,025\,634\,981\,654\,748\,129\,600 \tag{7.3}$$

different configurations, which is immensely challenging to generate and average over. To truly average over configurations the empty sites should not be selected at random, but instead systematically so that every configuration is represented once and only once.

Therefore this method does not find the minimum for the energy of the system as given in section 6 but it does show that completely random spin deviations yields a larger energy than the energy corresponding to the special $\delta\theta_{\mathbf{q}}$'s, which is in accordance with the theory and the results from section 6.

8 Conclusion

In an attempt to understand the results of Henley [1] the derivations were reproduced in this thesis. The two-dimensional square lattice with nearest (J_1) and next-nearest

(J_2) neigbour exchange interactions was considered. For different combinations of FM and AFM J_1 and J_2 the ground state spin configurations were determined by minimizing the exchange constant $J_{\mathbf{q}}$. It turned out that the special case of $\frac{J_2}{|J_1|} > \frac{1}{2}$ lead to a frustrated ground state. These exchange constants led to a split of the lattice into two AFM sublattices, the alignment of these seperated by an angle ϕ. Since the ground state energy had no ϕ-dependency the ground state of the system was frustrated. It could then be shown that different kinds of disorderings of the system would break this frustration.

The system was expanded to contain spin deviations, and the Hamiltonian was then diagonalized by Fourier transform of the spin fluctuations $\delta\theta_i$. Then the system was considered under thermal fluctuations. These fluctuations led to a contribution from the entropy to the free energy of the system. This energy could then be minimzed to reveal that the frustration of the ground state would be broken under the influence of thermal fluctuations. The free energy of the system was minimized by $\phi = n\pi$, $n \in \mathbb{Z}$, the system therefore selecting collinear states. Thus the entropy of the system broke the frustration of the ground state.

Subsequently the effect of dilution of the lattice was considered. The complete removal of spins from a fraction of the lattice sites lead to the translational invariance of the system being broken. Therefore the Hamiltonian had to be determined anew. To do this it was necessary to discover how the occupation parameter ϵ_i behaved under the act of averaging over spin configurations. This helped to arrive at a result for the Hamiltonian which could be minimized with respect to ϕ. In the proces of arriving at this result it could be seen that the energy was minimized for some specific values of the Fourier transform of the spin deviations $\delta\theta_{\mathbf{q}}$. These deviations, which had earlier been assumed to be random were in fact not random at all in the states with minimal energy. Thus the dilution of the lattice led to the frustration of the ground state being broken by a specific ϕ characterizing the minimal energy of the system. In this case ϕ turned out to be $\phi = \left(n + \frac{1}{2}\right)\pi, n \in \mathbb{Z}$ leading to a selection of anticollinear states.

In an attempt to support the results of dilution of the lattice a Mathematica$^{\text{TM}}$ script was created. The purpose of the script was to numerically dilute the lattice. However a few problems were encountered. Firstly, the spin deviations were assumed to be random, despite the fact that it was shown earlier not to be the case in the ground state of the diluted lattice. This meant that the resulting energy would not be the minimal energy. This was apparent in the results since the theoretically calculated energy was $\langle \delta\hat{\mathcal{H}}(\phi)\rangle_\epsilon + E_0 = -32\,000.00036$ and the numerically calculated energy was $E_{min} = -28\,538.67272$. Another obstacle was averaging over spin configurations. Since the amount of spin configurations was given by the binomial coefficient $\binom{N}{n}$, which quickly blows up, it was not possible to include all configurations.

As further work with the contents of this thesis it would be obvious to continue working with the numerical calculations. It is of great interest to see whether or not the effects of dilution can be shown numerically when the inadequacies of the results of this thesis are accounted for.

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Appendices

A Mathematica$^{\mathrm{TM}}$ script to numerically dilute a lattice

```
ClearAll["Global`*"]

Mx = 40;
My = Mx;(*The size of the lattice*)
p = 0.99; (*Occupied fraction of the lattice*)

Jfct[d_] := J1 * KroneckerDelta[d, 1] + J2 * KroneckerDelta[d, √2];
(*Exchange interaction function*)
θ[x_, y_] := If[OddQ[x] && OddQ[y], ϕ, 0] + If[EvenQ[x] && EvenQ[y], ϕ + π, 0] +
    If[OddQ[x] && EvenQ[y], π, 0] // N;(*Angle θ as a function of the coordinates of the site*)
δθ = Table[RandomReal[{-π/8, π/8}], {x, Mx}, {y, My}] // N;
(*Random spin deviations*)

Ham[J1_, J2_, ϕ_] =
  Flatten[
   Table[1/2 Jfct[√((i - k)^2 + (j - l)^2)] *
     (Cos[θ[i, j] - θ[k, l]] - (Part[δθ, i, j] - Part[δθ, k, l]) * Sin[θ[i, j] - θ[k, l]] -
       1/2 (Part[δθ, i, j] - Part[δθ, k, l])^2 * Cos[θ[i, j] - θ[k, l]]), {i, Mx}, {j, My},
    {k, Mx}, {l, My}]];
 (*The Hamiltonian*)

Etot[J1_, J2_, ϕ_] = Table[Total[RandomSample[Ham[J1, J2, ϕ], Round[p * (Mx * My)^2]]], 1000];
(*The total energy of 1000 spin configurations*)

J1 = -1;
J2 = 10;(*Exchange constants*)

Avg[ϕ_] = Mean[Etot[J1, J2, ϕ]];(*Averaging the energy*)

Minimum = Minimize[Avg[ϕ], ϕ] (*Minimizing the averaged energy. This yields the numerical energy*)

Int = 1/(2 π)^2 * NIntegrate[(Cos[qx] - Cos[qy])^2/(1 - Cos[qx] * Cos[qy]), {qx, -π, π}, {qy, -π, π}];
(*Integral used in the theoretical energy*)

dH[J1_, J2_, ϕ_, dp_, N_] := -2 * N * J2 - J1^2/(2 * J2) * dp * Int * Sin[ϕ]^2;
(*Theoretical energy plus E0*)

NumberForm[dH[J1, J2, π/2, (1 - p), Mx * My], 20]
(*The theoretical energy for the same parameters as the numerical energy*)
```