

## Chapter 5

# Thermal fluctuations of classical Heisenberg magnets

For Heisenberg models that possess long-range order at zero temperature, thermal fluctuations tend to reduce magnetic order. In three dimensions, long-range order is destroyed above a critical temperature  $T_c > 0$ , while in two dimensions the Mermin-Wagner theorem shows that there cannot be long-range order at any temperature  $T > 0$ . In these circumstances, one might be tempted to believe that, in frustrated models for which the classical ground is infinitely degenerate, hence disordered, thermal fluctuations can only make things worse, and that such systems will remain disordered at any temperature. This conclusion turns out to be *completely wrong*. Indeed, Heisenberg systems have low-energy configurations around any ground state, and thermal fluctuations induced by these low-energy configurations must be taken into account when minimizing the free energy. But different states that have the same energy can have very different low-energy configurations surrounding them. As we shall see, this implies that a selection mechanism can be induced by thermal fluctuations, potentially leading to some form of order, an effect known as "order by disorder". In 3D, this can be true long-range order persisting up to a critical temperature  $T_c > 0$ , as in non-frustrated models whereas, for the 2D models that we will consider in this chapter, long-range order will strictly speaking only emerge in the limit  $T \rightarrow 0^+$ . Still, if a selection mechanism operates, the low temperature properties are expected to be similar to those of a non-frustrated Heisenberg model, with a correlation that diverges exponentially with the inverse temperature.

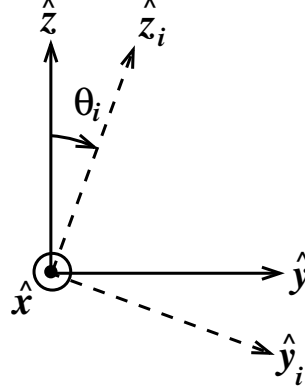


Figure 5.1: Definition of the local reference frame for a coplanar magnet.

## 5.1 Expansion around coplanar ground states

The basic idea to expand the energy around an ordered state where the spin is given by  $\vec{S}_i$  at site  $i$  is to express the scalar products that enter the energy in terms of spin components  $S_i^{x_i}, S_i^{y_i}, S_i^{z_i}$  in a local reference frame  $(\hat{x}_i, \hat{y}_i, \hat{z}_i)$  such that  $\vec{S}_i$  is parallel to  $\hat{z}_i$ , and to expand in the components perpendicular to  $\hat{z}_i$ . For simplicity, let's see how this works for coplanar states. One can choose a common axis, say  $\hat{x}_i = \hat{x}$ , and describe the ground state with local axes  $\hat{y}_i$  and  $\hat{z}_i$  rotated by  $\theta_i$  around  $\hat{x}$  (see Fig.5.1). Then, the spin at site  $i$  can be expressed as

$$\vec{S}_i = S_i^x \hat{x} + S_i^{y_i} \hat{y}_i + S_i^{z_i} \hat{z}_i$$

and the scalar product takes the form

$$\vec{S}_i \cdot \vec{S}_j = S_i^x S_j^x + S_i^{y_i} S_j^{y_j} \hat{y}_i \cdot \hat{y}_j + S_i^{z_i} S_j^{z_j} \hat{z}_i \cdot \hat{z}_j + S_i^{y_i} S_j^{z_j} \hat{y}_i \cdot \hat{z}_j + S_i^{z_i} S_j^{y_j} \hat{z}_i \cdot \hat{y}_j$$

or, since

$$\hat{z}_i = \hat{z} \cos \theta_i + \hat{y} \sin \theta_i, \quad \hat{y}_i = -\hat{z} \sin \theta_i + \hat{y} \cos \theta_i,$$

the following form in terms of the angles  $\theta_i$ ,

$$\vec{S}_i \cdot \vec{S}_j = S_i^x S_j^x + (S_i^{y_i} S_j^{y_j} + S_i^{z_i} S_j^{z_j}) \cos(\theta_i - \theta_j) + (S_i^{y_i} S_j^{z_j} - S_i^{z_i} S_j^{y_j}) \sin(\theta_i - \theta_j).$$

Now, we want to describe fluctuations around a state where  $S_i^{z_i} \simeq 1$ . So we write

$$\vec{S}_i = \begin{pmatrix} x_i \\ y_i \\ \sqrt{1 - x_i^2 - y_i^2} \end{pmatrix} \quad (5.1)$$

in the local basis, and we expand the square root in  $x_i$  and  $y_i$ :

$$\sqrt{1 - x_i^2 - y_i^2} \simeq 1 - \frac{x_i^2}{2} - \frac{y_i^2}{2}$$

to get

$$\begin{aligned} \vec{S}_i \cdot \vec{S}_j &= x_i x_j + y_i y_j \cos(\theta_i - \theta_j) \\ &+ \left(1 - \frac{x_i^2}{2} - \frac{y_i^2}{2}\right) \left(1 - \frac{x_j^2}{2} - \frac{y_j^2}{2}\right) \cos(\theta_i - \theta_j) \\ &+ \left[ y_i \left(1 - \frac{x_j^2}{2} - \frac{y_j^2}{2}\right) - y_j \left(1 - \frac{x_i^2}{2} - \frac{y_i^2}{2}\right) \right] \sin(\theta_i - \theta_j). \end{aligned}$$

This expression contains a term linear in  $y_i$  of the form  $y_i \sin(\theta_i - \theta_j)$ , leading to linear terms in the energy of the form

$$y_i \sum_j J_{ij} \sin(\theta_i - \theta_j).$$

Now, if we expand around a classical ground state, the energy has to be minimal. But the energy is given by

$$E = \frac{1}{2} \sum_{i,j} J_{ij} \vec{S}_i \cdot \vec{S}_j = \frac{1}{2} \sum_{i,j} J_{ij} \cos(\theta_i - \theta_j).$$

The minimisation of this energy with respect to the angles  $\theta_j$  leads to

$$\frac{\partial E}{\partial \theta_i} = -\frac{1}{2} \sum_{i,j} J_{ij} \sin(\theta_i - \theta_j) = 0.$$

So the coefficients of the linear terms vanishes, and up to order 2 we are left, up to a constant, with a quadratic expression in  $x_i$  and  $y_i$ :

$$\begin{aligned} \vec{S}_i \cdot \vec{S}_j &\simeq S_i^x S_j^x + (S_i^{y_i} S_j^{y_j} + S_i^{z_i} S_j^{z_j}) \cos(\theta_i - \theta_j) \\ &= \cos(\theta_i - \theta_j) + x_i x_j + \cos(\theta_i - \theta_j) \left( y_i y_j - \frac{x_i^2}{2} - \frac{y_i^2}{2} - \frac{x_j^2}{2} - \frac{y_j^2}{2} \right). \end{aligned}$$

Let us look at two specific examples.

### 5.1.1 Helical states

For a helical state of vector  $\vec{Q}$ , the energy can be written

$$E = \frac{1}{2} \sum_i \sum_{\vec{R}_n} J_{\vec{R}_n} [S_i^x S_{i+\vec{R}_n}^x + (S_i^y S_{i+\vec{R}_n}^y + S_i^z S_{i+\vec{R}_n}^z) \cos \vec{Q} \cdot \vec{R}_n]$$

or, after expanding it to second order in the transverse components of the spins,

$$\begin{aligned} E = & \frac{1}{2} \sum_i \sum_{\vec{R}_n} J_{\vec{R}_n} [y_i y_{i+\vec{R}_n} \cos \vec{Q} \cdot \vec{R}_n + x_i x_{i+\vec{R}_n} \\ & + \cos \vec{Q} \cdot \vec{R}_n - \frac{1}{2} \cos \vec{Q} \cdot \vec{R}_n (x_i^2 + y_i^2 + x_{i+\vec{R}_n}^2 + y_{i+\vec{R}_n}^2)] \end{aligned}$$

Let's introduce Fourier transforms:

$$\begin{aligned} x_{\vec{q}} &= \frac{1}{\sqrt{N}} \sum_i x_{\vec{r}_i} e^{i\vec{q}\vec{r}_i}, & x_i &= \frac{1}{\sqrt{N}} \sum_{\vec{q}} e^{-i\vec{q}\vec{r}_i} x_{\vec{q}} \\ y_{\vec{q}} &= \frac{1}{\sqrt{N}} \sum_i y_{\vec{r}_i} e^{i\vec{q}\vec{r}_i}, & y_i &= \frac{1}{\sqrt{N}} \sum_{\vec{q}} e^{-i\vec{q}\vec{r}_i} y_{\vec{q}} \\ J_{\vec{k}} &= \sum_{\vec{R}_n} J_{\vec{R}_n} e^{-i\vec{k}\vec{R}_n}, & J_{\vec{R}_n} &= \frac{1}{N} \sum_{\vec{k}} J_{\vec{k}} e^{i\vec{k}\vec{R}_n} \end{aligned}$$

Then it is easy to show that

$$\begin{aligned} \frac{1}{2} \sum_i \sum_{\vec{R}_n} J_{\vec{R}_n} x_i x_{i+\vec{R}_n} &= \frac{1}{2} \sum_{\vec{q}} J_{\vec{q}} x_{\vec{q}} x_{-\vec{q}} \\ \frac{1}{2} \sum_i \sum_{\vec{R}_n} J_{\vec{R}_n} y_i y_{i+\vec{R}_n} \cos \vec{Q} \cdot \vec{R}_n &= \frac{1}{2} \sum_{\vec{q}} \frac{J_{\vec{q}+\vec{Q}} + J_{\vec{q}-\vec{Q}}}{2} y_{\vec{q}} y_{-\vec{q}} \\ \frac{1}{2} \sum_i \sum_{\vec{R}_n} J_{\vec{R}_n} \cos \vec{Q} \cdot \vec{R}_n &= \frac{1}{2} N \frac{J_{\vec{Q}} + J_{-\vec{Q}}}{2} \\ -\frac{1}{4} \sum_i \sum_{\vec{R}_n} J_{\vec{R}_n} \cos \vec{Q} \cdot \vec{R}_n x_i^2 &= -\frac{1}{4} \frac{J_{\vec{Q}} + J_{-\vec{Q}}}{2} \sum_{\vec{q}} x_{\vec{q}} x_{-\vec{q}} \end{aligned}$$

where we have used  $\cos \vec{Q} \cdot \vec{R}_n = (e^{i\vec{Q}\vec{R}_n} + e^{-i\vec{Q}\vec{R}_n})/2$ .

Finally, the energy can be written

$$E = \frac{N}{2} J_{\vec{Q}} + \frac{1}{2} \sum_{\vec{q}} (\alpha_{\vec{q}} x_{\vec{q}} x_{-\vec{q}} + \beta_{\vec{q}} y_{\vec{q}} y_{-\vec{q}})$$

with

$$\alpha_{\vec{q}} = J_{\vec{q}} - J_{\vec{Q}}, \quad \beta_{\vec{q}} = \frac{J_{\vec{q}+\vec{Q}} + J_{\vec{q}-\vec{Q}}}{2} - J_{\vec{Q}}$$

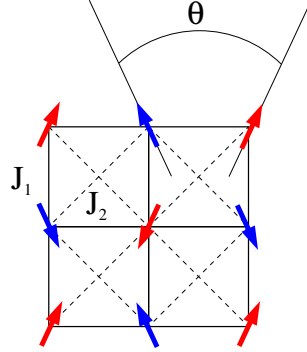


Figure 5.2: One of the ground states of the  $J_1 - J_2$  model on the square lattice when  $J_2 > J_1/2$ .

### 5.1.2 $J_1 - J_2$ model on the square lattice

In this section, we consider the  $J_1 - J_2$  model on the square lattice for  $J_2 > J_1/2$ . In this parameter range, two helical states with wave-vectors  $(\pi, 0)$  and  $(0, \pi)$  minimize the classical energy, but one can combine them because the pitch vectors differ by half a vector of the reciprocal lattice, leading to a continuous degeneracy defined by the angle  $\theta$  between the two  $J_2$  sublattices so that  $\cos(\theta_i - \theta_j)$  is equal to  $\cos \theta$  on horizontal  $J_1$  bonds,  $-\cos \theta$  on vertical  $J_1$  bonds, and  $-1$  on  $J_2$  bonds (see Fig. 5.2). The resulting energy in terms to  $x_i$  and  $y_i$  is periodic with one site per unit cell so that a simple Fourier transform can be performed, leading after some algebra to a similar expression

$$E = -2J_2N + \frac{1}{2} \sum_{\vec{q}} (\alpha_{\vec{q}} x_{\vec{q}} x_{-\vec{q}} + \beta_{\vec{q}} y_{\vec{q}} y_{-\vec{q}})$$

with

$$\begin{cases} \alpha_{\vec{q}} = 2J_1(\cos q_x + \cos q_y) + 4J_2 \cos q_x \cos q_y + 4J_2 \\ \beta_{\vec{q}} = 2J_1 \cos q_x \cos \theta - 2J_1 \cos q_y \cos \theta - 4J_2 \cos q_x \cos q_y + 4J_2 \end{cases}$$

### 5.1.3 Free energy

In the case where there are several helical states, or a continuous family of states as for the  $J_1 - J_2$  model with  $J_2 > J_1/2$ , that minimize the ground state energy, one needs to compare the free energies calculated from fluctuations

around these states to find out which one is minimal. The free energy is defined by  $F = -k_B T \ln Z$ , with

$$\begin{aligned} Z &= \int e^{-\beta E(\{x_i, y_i\})} \prod_i dx_i dy_i \\ &= e^{-\beta E_0} \int \prod_i dx_i e^{-\frac{\beta}{2} \sum_{\vec{q}} \alpha_{\vec{q}} |x_{\vec{q}}|^2} \int \prod_i dy_i e^{-\frac{\beta}{2} \sum_{\vec{q}} \beta_{\vec{q}} |y_{\vec{q}}|^2} \end{aligned}$$

where  $E_0$  is the ground-state energy given by  $E_0 = \frac{N}{2} J_{\vec{Q}}$  for helical states and  $E_0 = -2J_2 N$  for the  $J_1 - J_2$  model.

To calculate these integrals, we need to change the variables of integration. Let's concentrate on the integral over the  $x_i$  variables for a moment.

### Proposition

$$\begin{aligned} &\int \prod_i dx_i e^{-\frac{\beta}{2} \sum_{\vec{q}} \alpha_{\vec{q}} |x_{\vec{q}}|^2} \\ &= 2^{N/2} \int \prod'_{\vec{q}} d\text{Re}(x_{\vec{q}}) e^{-\beta \sum'_{\vec{q}} \alpha_{\vec{q}} \text{Re}(x_{\vec{q}})^2} \int \prod'_{\vec{q}} d\text{Im}(y_{\vec{q}}) e^{-\beta \sum'_{\vec{q}} \alpha_{\vec{q}} \text{Im}(x_{\vec{q}})^2} \end{aligned}$$

where  $\prod'_{\vec{q}}$  and  $\sum'_{\vec{q}}$  correspond to products and sums over half the wave-vectors so that, for two vectors  $\vec{q}_1$  and  $\vec{q}_2$  entering the product or the sum,  $\vec{q}_1 \neq -\vec{q}_2$ .

### Proof

Since  $x_i$  is real,  $x_{-\vec{q}} = x_{\vec{q}}^*$ . So  $x_{\vec{q}} x_{-\vec{q}} = |x_{\vec{q}}|^2 = \text{Re}(x_{\vec{q}})^2 + \text{Im}(x_{\vec{q}})^2$ ,  $x_i$  can be expanded as

$$x_i = \frac{1}{\sqrt{N}} \sum'_{\vec{q}} (x_{\vec{q}} e^{-i\vec{q} \cdot \vec{r}_i} + \text{c.c.}) = \frac{2}{\sqrt{N}} \sum'_{\vec{q}} [\text{Re}(x_{\vec{q}}) \cos \vec{q} \cdot \vec{r}_i + \text{Im}(x_{\vec{q}}) \sin \vec{q} \cdot \vec{r}_i]$$

and

$$\text{Re}(x_q) = \frac{1}{\sqrt{N}} \sum_i x_i \cos \vec{q} \cdot \vec{r}_i, \quad \text{Im}(x_q) = \frac{1}{\sqrt{N}} \sum_i x_i \sin \vec{q} \cdot \vec{r}_i.$$

which implies

$$\frac{\partial \text{Re}(x_q)}{\partial x_i} = \frac{1}{\sqrt{N}} \cos \vec{q} \cdot \vec{r}_i, \quad \frac{\partial \text{Im}(x_q)}{\partial x_i} = \frac{1}{\sqrt{N}} \sin \vec{q} \cdot \vec{r}_i.$$

Now, if we have  $N$  sites, the sum  $\sum_q'$  will contain  $N/2$  terms. Let's denote by  $\vec{q}_j$ ,  $j = 1, \dots, N/2$ , these vectors. The jacobian of the transformation is the absolute value of the determinant of the matrix  $A$  defined by

$$A_{i,j} = \begin{cases} \frac{1}{\sqrt{N}} \cos(\vec{q}_j \cdot \vec{r}_i) & \text{if } 1 \leq j \leq N/2 \\ \frac{1}{\sqrt{N}} \sin(\vec{q}_{j-N/2} \cdot \vec{r}_i) & \text{if } N/2 + 1 \leq j \leq N \end{cases} \quad (5.2)$$

In matrix form, we can write this matrix

$$A = \frac{1}{\sqrt{N}} \begin{pmatrix} \cos \vec{q}_1 \cdot \vec{r}_1 & \dots & \cos \vec{q}_{N/2} \cdot \vec{r}_1 & \sin \vec{q}_1 \cdot \vec{r}_1 & \dots & \sin \vec{q}_{N/2} \cdot \vec{r}_1 \\ \cos \vec{q}_1 \cdot \vec{r}_2 & \dots & \cos \vec{q}_{N/2} \cdot \vec{r}_2 & \sin \vec{q}_1 \cdot \vec{r}_2 & \dots & \sin \vec{q}_{N/2} \cdot \vec{r}_2 \\ \vdots & & \vdots & \vdots & & \vdots \end{pmatrix} \quad (5.3)$$

and its transpose

$$A^t = \frac{1}{\sqrt{N}} \begin{pmatrix} \cos \vec{q}_1 \cdot \vec{r}_1 & \cos \vec{q}_1 \cdot \vec{r}_2 & \dots \\ \vdots & \vdots & \\ \cos \vec{q}_{N/2} \cdot \vec{r}_1 & \sin \vec{q}_1 \cdot \vec{r}_1 & \dots \\ \vdots & \vdots & \\ \sin \vec{q}_{N/2} \cdot \vec{r}_1 & \sin \vec{q}_{N/2} \cdot \vec{r}_2 & \dots \end{pmatrix} \quad (5.4)$$

so that

$$\begin{aligned} (AA^t)_{i,j} &= \frac{1}{N} \sum_{n=1}^N [\cos \vec{q}_n \cdot \vec{r}_i \cos \vec{q}_n \cdot \vec{r}_j + \sin \vec{q}_n \cdot \vec{r}_i \sin \vec{q}_n \cdot \vec{r}_j] \\ &= \frac{1}{N} \sum_{n=1}^{N/2} \cos [\vec{q}_n \cdot (\vec{r}_i - \vec{r}_j)] \\ &= \frac{1}{2N} \sum_{\vec{q}} \cos [\vec{q} \cdot (\vec{r}_i - \vec{r}_j)] = \frac{1}{2} \text{Re} \frac{1}{N} \sum_{\vec{q}} e^{i\vec{q} \cdot (\vec{r}_i - \vec{r}_j)} \\ &= \frac{1}{2} \delta_{ij} \quad \Rightarrow \quad \det(AA^t) = \left(\frac{1}{2}\right)^N \end{aligned}$$

Since  $\det A = \det A^t$ , this implies that the jacobian of the transformation is given by

$$|\det A| = \frac{1}{2^{N/2}}$$

Finally,

$$\sum_{\vec{q}} \alpha_{\vec{q}} |x_{\vec{q}}|^2 = 2 \sum_{\vec{q}}' \alpha_{\vec{q}} |x_{\vec{q}}|^2 = 2 \sum_{\vec{q}}' \alpha_{\vec{q}} [\text{Re}(x_{\vec{q}})^2 + \text{Im}(x_{\vec{q}})^2]$$

which implies

$$e^{-\frac{\beta}{2} \sum_{\vec{q}} \alpha_{\vec{q}} |x_{\vec{q}}|^2} = e^{-\beta \sum_{\vec{q}}' \alpha_{\vec{q}} \text{Re}(x_{\vec{q}})^2} e^{-\beta \sum_{\vec{q}}' \alpha_{\vec{q}} \text{Im}(x_{\vec{q}})^2}.$$

This completes the proof of the proposition.

So the calculation of the partition function reduces to the calculation of gaussian integrals:

$$\int d\text{Re}(x_{\vec{q}}) e^{-\beta \alpha_{\vec{q}} \text{Re}(x_{\vec{q}})^2} = \left( \frac{\pi}{\beta \alpha_{\vec{q}}} \right)^{1/2}$$

The integral on the imaginary part gives the same result, and the integral over the  $y_i$  coordinates can be evaluated in the same way, leading to

$$Z = e^{-\beta E_0} 2^N \prod_{\vec{q}}' \left( \frac{\pi}{\beta \alpha_{\vec{q}}} \right) \left( \frac{\pi}{\beta \beta_{\vec{q}}} \right)$$

The logarithm of the free energy is thus given by

$$\ln Z = -\beta E_0 + N \ln(2\pi) + N \ln k_B T - \frac{1}{2} \sum_{\vec{q}} \ln \alpha_{\vec{q}} - \frac{1}{2} \sum_{\vec{q}} \ln \beta_{\vec{q}}$$

and the free energy by

$$F = E_0 - N k_B T \ln(2\pi) - N k_B T \ln k_B T + \frac{1}{2} k_B T \sum_{\vec{q}} \ln \alpha_{\vec{q}} + \frac{1}{2} k_B T \sum_{\vec{q}} \ln \beta_{\vec{q}}$$

or

$$F = E_0 - N k_B T \ln(2\pi) + \frac{1}{2} k_B T \sum_{\vec{q}} \left( \ln \frac{\alpha_{\vec{q}}}{k_B T} + \ln \frac{\beta_{\vec{q}}}{k_B T} \right)$$

In frustrated magnets, if the ground state is infinitely degenerate,  $E_0$  is the same for all ground states, but *not* the  $\alpha_{\vec{q}}$  and  $\beta_{\vec{q}}$  in general. This leads us to the fundamental result of this chapter: Thermal fluctuations lift the degeneracy in favour of the state that minimizes  $\sum_{\vec{q}} (\ln \alpha_{\vec{q}} + \ln \beta_{\vec{q}})$ .

#### 5.1.4 Order by disorder

Let us use the results of the previous sections to discuss two cases of order by disorder for the  $J_1 - J_2$  model on the square lattice.

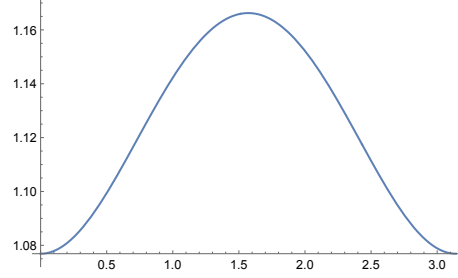


Figure 5.3: Integral of  $\ln \beta_{\vec{q}}$  as a function of  $\theta$  for  $J_2 = J_1 = 1$ .

### Selection of the helical states for $J_2 > J_1/2$

For  $J_2 > J_1/2$ , there is a one parameter family of ground states defined by the angle  $\theta$  between the two sublattices.  $\alpha_{\vec{q}}$  is independent of  $\theta$ , but not  $\beta_{\vec{q}}$ . It turns out that  $\sum_{\vec{q}} \ln \beta_{\vec{q}}$  is minimal for  $\theta = 0$  and  $\theta = \pi$  (see Fig.5.3). These two states correspond to the two helices with pitch vectors  $(0, \pi)$  and  $(\pi, 0)$  respectively. This result is an example of a general trend: Thermal fluctuations tend to favour the most collinear configurations.

The presence of two helical states is expected to lead to an Ising transition at finite temperature, a prediction that has been verified by classical Monte Carlo simulations. One can actually simply define an Ising variable on the dual lattice by

$$\sigma_i = \text{sign}[(\vec{S}_{1i} - \vec{S}_{3i}) \cdot (\vec{S}_{2i} - \vec{S}_{4i})]$$

where the spins  $\vec{S}_{1i}, \vec{S}_{2i}, \vec{S}_{3i}, \vec{S}_{4i}$  are the four spins around the plaquette  $i$  going clockwise from top left to bottom left. This Ising variables is equal to +1 in the helical state of pitch vector  $(0, \pi)$  and to -1 in the helical state of pitch vector  $(\pi, 0)$  (see Fig. 5.4).

### Selection of the collinear helices for $J_2 = J_1/2$

For  $J_2 = J_1/2$ , all helical states defined by pitch vectors  $\vec{Q}$  of the form  $(k_x, \pi)$  and  $(\pi, k_y)$ , i.e. on the boundary of the first Brillouin zone, are ground states of the Heisenberg model. Since  $J_{\vec{Q}}$  is the same for all the ground states,  $\alpha_{\vec{q}} = J_{\vec{q}} - J_{\vec{Q}}$  is independent of  $\vec{Q}$ , and the selection is again due to  $\beta_{\vec{q}} = (J_{\vec{q}+\vec{Q}} + J_{\vec{q}-\vec{Q}})/2 - J_{\vec{Q}}$ . It turns out that  $\sum_{\vec{q}} \ln \beta_{\vec{q}}$  is minimal for three pitch vectors:  $(0, \pi)$ ,  $(\pi, 0)$  and  $(\pi, \pi)$ . Interestingly enough, the collinear states are again selected by thermal fluctuations.

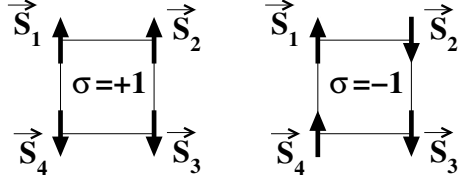


Figure 5.4: Definition of the Ising variable for the  $J_1$ – $J_2$  model on the square lattice  $\sigma = \text{sign}[(\vec{S}_1 - \vec{S}_3) \cdot (\vec{S}_2 - \vec{S}_4)]$  for the two helical states stabilized by thermal fluctuations when  $J_2 > J_1/2$ .

Note that the degeneracy between the helical states  $(0, \pi)$  and  $(\pi, 0)$  and the Néel state  $(\pi, \pi)$  is not protected by symmetry since the states are different, and treating fluctuations beyond the harmonic level is expected to lift the degeneracy, in agreement with Monte Carlo simulations, which found that the Néel state is actually favoured over the helical states  $(0, \pi)$  and  $(\pi, 0)$ .

## 5.2 Models with non-coplanar ground states

What about more complicated systems with an infinite number of non-coplanar ground states? Let us look at the kagome antiferromagnet. For that system, the degeneracy is very high, and the ground state manifold includes many non-coplanar configurations. It also contains an infinite number of coplanar configurations. Indeed, the energy is minimized if the sum of the spins on each triangle is equal to zero. For coplanar configurations, up to a global rotation, each spin has 3 possibilities, and the degeneracy in this submanifold is the same as for the 3-state Potts model, which is known to have a residual entropy. Let us study fluctuations around these states.

In all these states, the angles between a spin and its neighbours are all equal to  $\frac{2\pi}{3}$ . So the expansion of the energy is independent of the state. Up to second order, it is given by:

$$E = \frac{J}{2} \sum_{i,j} [(3\delta_{ij} - M_{ij}) x_i x_j - 2M_{ij} y_i y_j] \quad (5.5)$$

with

$$M_{ij} = \begin{cases} 1 & \text{if } i = j \\ \frac{1}{2} & \text{if } |i - j| = 1 \\ 0 & \text{otherwise} \end{cases} \quad (5.6)$$

The fact that it is independent of the state leads to the first important result: Harmonic fluctuations do not select among the coplanar states.

To go further, we need to take into account the fact that there are 3 sublattices. If we define the Fourier transform of the matrix  $M$  by

$$(M(\vec{q}))_{\alpha\beta} = \sum_{\vec{R}_i} e^{-i\vec{q}(\vec{R}_i + \vec{r}_\alpha - \vec{R}_j - \vec{r}_\beta)} M_{\vec{R}_i + \vec{r}_\alpha, \vec{R}_j + \vec{r}_\beta} \quad (5.7)$$

where  $\vec{R}_i$  is the position of the unit cell, and  $\vec{r}_\alpha$  is the position inside the unit cell, one finds:

$$M(\vec{q}) = \begin{pmatrix} 1 & \cos(q_x) & \cos(q_y) \\ \cos(q_x) & 1 & \cos(q_x - q_y) \\ \cos(q_y) & \cos(q_x - q_y) & 1 \end{pmatrix} \quad (5.8)$$

The energy can be rewritten

$$E = \frac{J}{2} \sum_q [\vec{y}_{-\vec{q}}^t (3\mathbb{I} - M_{\vec{q}}) \vec{y}_{\vec{q}} + \vec{x}_{-\vec{q}}^t M_q \vec{x}_{\vec{q}}] \quad (5.9)$$

where  $\vec{x}_{\vec{q}} = (x_{\vec{q}}(\vec{r}_1), x_{\vec{q}}(\vec{r}_2), x_{\vec{q}}(\vec{r}_3))^t$  is the vector of the  $x$  components inside a unit cell. The eigenvalues of  $M_{\vec{q}}$  are given by:

$$\lambda_0 = 0, \quad \lambda_{\pm}(\vec{q}) = \frac{3}{2} \left( 1 \pm \sqrt{1 - A_{\vec{q}}} \right) \quad (5.10)$$

with

$$A_{\vec{q}} = \frac{8}{9} [1 - \cos(q_x) \cos(q_y) \cos(q_x - q_y)]. \quad (5.11)$$

There is a branch of zero modes for the  $y$  fluctuations. This is because, for a certain type of displacement perpendicular to the plane, the coefficient of the quadratic term in the expansion vanishes. The consequences of these zero modes are far reaching:

1. When a mode is quadratic, it gives a contribution  $-\frac{1}{2}k_B T \ln T$  to the free energy. Indeed,

$$Z \propto \int_{-\infty}^{+\infty} e^{-\beta A x^2} dx = \beta^{-1/2} \int_{-\infty}^{+\infty} e^{-A u^2} du$$

so that

$$F = -k_B T \ln Z = -\frac{1}{2} k_B T \ln T + \dots$$

This first term is the dominant one at low temperature.

By the same argument, when a mode is quartic, it gives a contribution  $-\frac{1}{4}k_B T \ln T$  to the free energy. Indeed,

$$Z \propto \int_{-\infty}^{+\infty} e^{-\beta A x^4} dx = \beta^{-1/4} \int_{-\infty}^{+\infty} e^{-A u^4} du$$

so that

$$F = -k_B T \ln Z = -\frac{1}{4}k_B T \ln T + \dots$$

Since, at low temperature,

$$-\frac{1}{4}k_B T \ln T < -\frac{1}{2}k_B T \ln T$$

configurations with zero modes are favoured at low temperature.

2. For the Heisenberg model on kagome, one can prove that no non-coplanar state has as many zero modes as coplanar states. This suggests that coplanar states are selected by thermal fluctuations, a conclusion backed by numerical simulations. This implies that the system can be seen as a fluctuating nematic state since, in a coplanar state, there is long range order in the operator  $\vec{S}_i \times \vec{S}_j$ , where sites  $i$  and  $j$  are nearest neighbours.
3. Furthermore, for the kagome model, one can safely assume that the next order for a zero mode is quartic. Indeed:
  - There can be no term  $y^3$  in the expansion. Otherwise one would not be expanding around the ground state.
  - Terms of the form  $xy^2$  give, after a gaussian integration over  $x$ , another contribution  $O(y^4)$  since

$$\int_{-\infty}^{+\infty} e^{-\frac{1}{2}Ax^2+jx} dx = \left(\frac{2\pi}{A}\right)^{1/2} e^{\frac{j^2}{2A}}$$

4. The presence of zero modes has direct consequences for the low temperature specific heat. Indeed, since the specific heat is related to the free energy by

$$C = -T \frac{\partial^2 F}{\partial T^2},$$

the low-temperature contribution of a quadratic mode is  $\frac{1}{2}k_B$ , and that of a quartic mode is  $\frac{1}{4}k_B$ . For the kagome,  $1/3$  of the  $y$  modes

are quartic, i.e.  $1/6$  of the total number of modes. Since there are two modes per site, the specific heat per site is given by

$$\frac{C}{N} = 2 \left( \frac{5}{6} \times \frac{1}{2} k_B + \frac{1}{6} \times \frac{1}{4} k_B \right) = \frac{11}{12} k_B,$$

in excellent agreement with Monte Carlo simulations.