# Chapter 3

# Ground state of classical, frustrated Heisenberg models

As stated before, the competition between exchange integrals does not lead to ground state degeneracy as systematically as for the AF Ising model on non bipartite lattices. In particular, on a Bravais lattice, it is always possible to minimize the energy with a helical state, and this usually only gives rise to a finite degeneracy obtained by applying the symmetry operators of the point group to the pitch of the helix. Although there is no general theorem to back this claim, it is believed that, even on non-Bravais lattices, the energy can be minimized by helical configurations on sublattices.

Infinite degeneracy is known to occur however in a number of cases. There is no known systematics, but a number of trends have emerged. It is convenient in view of the thermal properties to be discussed later to distinguish between cases where all ground states are periodic and cases where they are not.

## 3.1 Periodic ground states

### 3.1.1 Helical ground state on Bravais lattices

Let's consider a Bravais lattice, i.e. a lattice with one site per unit cell, and classical spins of unit length. The energy of a configuration can be written:

$$E = \frac{1}{2}\sum_i \sum_{\vec{R}_n} J_{\vec{R}_n} \vec{S}_{\vec{R}_i} \cdot \vec{S}_{\vec{R}_i+\vec{R}_n}$$

There is a factor $\frac{1}{2}$ because each bond appears twice in the sum. The problem is to find the minimum under the constraint $||\vec{S}_{\vec{R}_i}||^2 = 1$ for all sites.

Let's first perform Fourier transforms of the spins and of the coupling constants:

$$\vec{S}_{\vec{k}} = \frac{1}{\sqrt{N}} \sum_i \vec{S}_i e^{-i\vec{k}\cdot\vec{R}_i} \Longrightarrow \vec{S}_i = \frac{1}{\sqrt{N}} \sum_{\vec{k}} \vec{S}_{\vec{k}} e^{i\vec{k}\cdot\vec{R}_i}$$
$$J_{\vec{k}} = \sum_{\vec{R}_n} J_{\vec{R}_n} e^{-i\vec{k}\cdot\vec{R}_n} \Longrightarrow J_{\vec{R}_n} = \frac{1}{N} \sum_{\vec{k}} J_{\vec{k}} e^{i\vec{k}\cdot\vec{R}_n}$$

In terms of these Fourier transforms, the energy takes the form:

$$E = \frac{1}{2} \sum_{\vec{R}_i} \sum_{\vec{R}_n} \frac{1}{N^2} \sum_{\vec{k}_1 \vec{k}_2 \vec{k}_3} J_{\vec{k}_1} \vec{S}_{\vec{k}_2} \cdot \vec{S}_{\vec{k}_3} e^{i(\vec{k}_1\cdot\vec{R}_n + \vec{k}_2\cdot\vec{R}_i + \vec{k}_3\cdot(\vec{R}_i+\vec{R}_n))}$$

The sums over $\vec{R}_i$ and $\vec{R}_n$ impose $\vec{k}_2 = -\vec{k}_3 = \vec{k}_1$, and the energy can be rewritten as:

$$E = \frac{1}{2} \sum_{\vec{k}} J_{\vec{k}}\ \vec{S}_{\vec{k}} \cdot \vec{S}_{-\vec{k}}$$

It is not possible to minimize this problem directly because the contraints on the length of the spins do not lead to a simple condition in Fourier space. However one can solve the problem by proceeding in two steps:

- Solve the problem under the weaker constraint $\sum_i ||\vec{S}_i||^2 = N$.

- Check if one can find a solution that satisfies the stronger constraint $||\vec{S}_i||^2 = 1$ for all sites.

Since

$$\begin{aligned} \sum_i \vec{S}_i^2 &= \frac{1}{N} \sum_{\vec{k}_1 \vec{k}_2} \sum_i e^{i(\vec{k}_1+\vec{k}_2)\cdot\vec{R}_i} \vec{S}_{\vec{k}_1} \cdot \vec{S}_{\vec{k}_1} \\ &= \sum_{\vec{k}} \vec{S}_{\vec{k}} \cdot \vec{S}_{-\vec{k}} \end{aligned}$$

the weaker constraint takes the simple form

$$\sum_{\vec{k}} \vec{S}_{\vec{k}} \cdot \vec{S}_{-\vec{k}} = N$$

in terms of the Fourier components of the spins. One must thus minimise

$$E = \frac{1}{2} \sum_{\vec{k}} J_{\vec{k}} \vec{S}_{\vec{k}} \cdot \vec{S}_{-\vec{k}}$$

under the constraint $\sum_{\vec{k}} \vec{S}_{\vec{k}} \cdot \vec{S}_{-\vec{k}} = N$.

Let's assume that $J_{\vec{k}}$ is minimal for $\vec{k} = \vec{k}_0$. The minimum of the energy is obtained iff $\vec{S}_{\vec{k}} = \vec{0},\ \vec{k} \neq \vec{k}_0,\ -\vec{k}_0$ and $\vec{S}_{\vec{k}_0} \cdot \vec{S}_{-\vec{k}_0} + \vec{S}_{-\vec{k}_0} \cdot \vec{S}_{\vec{k}_0} = N$.

In real space, the spins are then given by

$$\vec{S}_i = \frac{1}{\sqrt{N}} \left( \vec{S}_{\vec{k}_0} e^{i\vec{k}_0 \cdot \vec{R}} + \vec{S}_{-\vec{k}_0} e^{-i\vec{k}_0 \cdot \vec{R}} \right)$$

Can one find $\vec{S}_{\vec{k}_0}$ and $\vec{S}_{-\vec{k}_0}$ such that:

- $\vec{S}_{\vec{k}_0} \cdot \vec{S}_{-\vec{k}_0} = \frac{N}{2}$

but also such that the local constraints:

- $\vec{S}_i$ réel
- $||\vec{S}_i||^2 = 1$

are satisfied for all $i$? Yes! For example let's consider:

$$\vec{S}_{\vec{k}_0} = \begin{pmatrix} \frac{\sqrt{N}}{2} \\ -i\frac{\sqrt{N}}{2} \\ 0 \end{pmatrix} \qquad \vec{S}_{-\vec{k}_0} = \begin{pmatrix} \frac{\sqrt{N}}{2} \\ i\frac{\sqrt{N}}{2} \\ 0 \end{pmatrix}.$$

This choice leads to:

$$\vec{S}_i = \begin{pmatrix} \cos\left(\vec{k}_0 \cdot \vec{R}\right) \\ \sin\left(\vec{k}_0 \cdot \vec{R}\right) \\ 0 \end{pmatrix}$$

One gets a helical structure of pitch vector $\vec{k}_0$.

To summarize, one can minimize the classical energy with a helical structure whose wave vector is given by the minimum of $J_{\vec{k}}$.

Example: $J_1 - J_2$ model on the square lattice

$$E = J_1 \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{<<i,j>>} \vec{S}_i \cdot \vec{S}_j = \sum_{\vec{k}} J_{\vec{k}} \vec{S}_{\vec{k}} \cdot \vec{S}_{-\vec{k}}$$

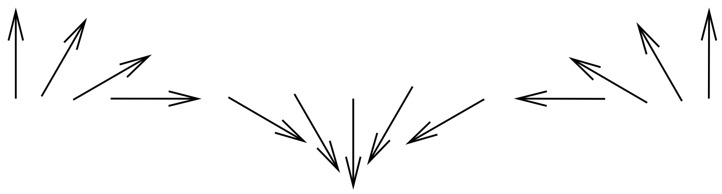


Figure 3.1: Example of a 1D helix of wave vector $\vec{k}_0 = \frac{2\pi}{12a}$.

with

$$\begin{aligned}
J_{\vec{k}} &= J_1\left(e^{i\vec{k}\vec{x}} + e^{-i\vec{k}\vec{x}} + e^{i\vec{k}\vec{y}} + e^{-i\vec{k}\vec{y}}\right) \\
&+ J_2\left(e^{i\vec{k}(\vec{x}+\vec{y})} + e^{i\vec{k}(\vec{x}-\vec{y})} + e^{-i\vec{k}(\vec{x}+\vec{y})} + e^{i\vec{k}(-\vec{x}+\vec{y})}\right) \\
&= 2J_1\left(\cos(k_x) + \cos(k_y)\right) + 2J_2\left(\cos(k_x + k_y) + \cos(k_x - k_y)\right) \\
&= 2J_1\left(\cos(k_x) + \cos(k_y)\right) + 4J_2\cos(k_x)\cos(k_y)
\end{aligned}$$

The minimization leads to:

$$\frac{\partial J}{\partial k_x} = -2J_1\sin(k_x) - 4J_2\sin(k_x)\cos(k_y) = 0$$
$$\frac{\partial J}{\partial k_y} = -2J_1\sin(k_y) - 4J_2\sin(k_y)\cos(k_x) = 0$$

These equations are satisfied by ($k_x = 0$ or $\pi$, $k_y = 0$ or $\pi$) or if

$$\cos k_x = \cos k_y = \frac{-J_1}{2J_2}$$

which is only possible if $\frac{J_1}{2J_2} < 1 \rightarrow \frac{J_1}{2} < J_2$. Let's now compare the value of $J_{\vec{k}}$ for the various solutions:

$k_x = k_y = 0 \rightarrow J_{\vec{k}} = 4J_1 + 4J_2$

$k_x = 0, k_y = \pi \rightarrow J_{\vec{k}} = -4J_2$

$k_x = k_y = \pi \rightarrow J_{\vec{k}} = -4J_1 + 4J_2$

$\cos k_x = \cos k_x = \frac{-J_1}{2J_2}$

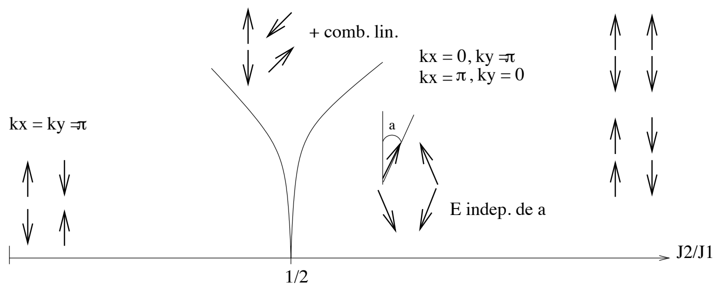
$$\begin{aligned} \rightarrow J_{\vec{k}} &= 2J_1\left(\frac{-2J_1}{2J_2}\right) + 4J_2\frac{J_1^2}{4J_2^2} \\ &= \frac{-2J_1^2}{J_2} + \frac{J_1^2}{J_2} = -\frac{J_1^2}{J_2} \end{aligned}$$

But if $J_1 < 2J_2$, $-4J_2 < \frac{-J_1^2}{J_2}$. The ground state is thus reached for $k_x = 0, k_y = \pi$ or $k_x = \pi, k_y = 0$.

For $\frac{J_2}{J_1} = \frac{1}{2}$, the minimum $J_{\vec{k}} = -2J_1$ is reached for

$$k_x = \pi, k_y \text{ arbitrary} \quad \text{or} \quad k_y = \pi, k_x \text{ arbitrary}$$

Finally, for $J_1 < 2J_2$, one can make a linear combination of two helices. This leads to a continuous family of degenerate classical ground states (see next section).




### 3.1.2 Linear combination of helices

Very often, there are only a few ground states. They are given by the helical states that correspond to the different values of $\vec{k}$ that minimize $J_{\vec{k}}$ and that are related by operations of the point group symmetry. However, even in that case, it is sometimes possible to generate an infinite number of ground states. Indeed, if two pitch vectors are such that their difference is half a vector of the reciprocal lattice, one can make arbitrary linear combinations with an appropriate choice of relative phase.

Indeed, suppose that two vectors $\vec{k}_0$ and $\vec{k}_1$ ($\vec{k}_1 \neq \vec{k}_0, -\vec{k}_0$) minimize $J(\vec{k})$. Then the general solution of the problem with the weak constraint is given by

$$\vec{S}_{\vec{R}} = \frac{1}{\sqrt{N}}(\vec{S}_{\vec{k}_0}e^{i\vec{k}_0.\vec{R}} + \vec{S}_{-\vec{k}_0}e^{-i\vec{k}_0.\vec{R}} + \vec{S}_{\vec{k}_1}e^{i\vec{k}_1.\vec{R}} + \vec{S}_{-\vec{k}_1}e^{-i\vec{k}_1.\vec{R}})$$

For this solution to be acceptable however, it must satisfy the strong constraint of unit length at each site. Let's assume that the helices are coplanar, and let's denote by $u$ and $v$ the amplitude of the $\vec{k}_0$ and $\vec{k}_1$ components:

$$\vec{S}_{\vec{R}} = \begin{pmatrix} u\cos(\vec{k}_0\vec{R}+\phi_0)+v\cos(\vec{k}_1\vec{R}+\phi_1) \\ u\sin(\vec{k}_0\vec{R}+\phi_0)+v\sin(\vec{k}_1\vec{R}+\phi_1) \\ 0 \end{pmatrix} \tag{3.1}$$

The condition of unit length at site $\vec{R}$ reads:

$$\vec{S}^2_{\vec{R}} = u^2+v^2+2uv\cos((\vec{k}_0-\vec{k}_1)\cdot\vec{R}+\phi_0-\phi_1) = 1$$

This will be true if $u^2+v^2=1$ and $(\vec{k}_0-\vec{k}_1)\cdot\vec{R}+\phi_0-\phi_1 = \frac{\pi}{2}[\pi]$. For this to hold for any $\vec{R}$, $(\vec{k}_0-\vec{k}_1)\cdot\vec{R}$ must be independent of $\vec{R}$ modulo $\pi$. This will be true if $\vec{k}_0-\vec{k}_1 = \vec{K}/2$ where $\vec{K}$ is a vector of the reciprocal lattice because, in that case,

$$(\vec{k}_0-\vec{k}_1)\cdot\vec{R} = 0\ [\pi]$$

Then, if one chooses $\phi_0-\phi_1=\frac{\pi}{2}$, the condition is fulfilled.

Example: $J_1-J_2$ model on the square lattice when $J_2 > J_1/2$.

### 3.1.3 Infinite number of helices

It can also happen that the number of pitch vectors that minimize $J_{\vec{k}}$ is infinite. This is accidental in the sense that modifications of the coupling constants will in general lift this degeneracy. This has been shown however to be relevant for the physics of some spinels.

**Simplest example:** $J_1-J_2$ model on the square lattice with $J_2=J_1/2$. For that ratio, $(k_x,\pi)$ and $(\pi,k_y)$ are all possible pitch vectors. This leads to lines of pitch vectors.

**2D example:** $J_1-J_2$ model on the honeycomb lattice with $J_2/J_1 > \frac{1}{6}$. In that case, although there are two sites per unit cell, the Luttinger-Tisza approach allows one to find helical ground states, and in this parameter range there is a line of pitch vectors.

**3D example:** $J_1 - J_2$ model on diamond lattice with $J_2/J_1 > \frac{1}{8}$. The diamond lattice can be seen as the dual lattice of the pyrochlore lattice. This case is very similar to the honeycomb lattice. The Luttinger-Tisza approach leads to a 2D surface of pitch vectors.

## 3.2 Non periodic ground states

This discussion is far from exhausting the possibilities to reach an infinite degeneracy. We saw for the Ising model that the ground state degeneracy can be extensive, with local modifications that imply the presence of non-periodic ground states. This is also possible for Heisenberg spins. By analogy with the Ising case, this can be expected if one constructs the lattice from units that have a degenerate ground state provided the constraints from inter-units coupling are not numerous enough to fix the ground state, in the spirit of geometrical frustration in general.

Let us consider systems composed of corner sharing units (simplices) of $q$ sites inside which all sites are coupled to each other, with energy:

$$E = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j = \frac{J}{2} \sum_{\alpha} \left| \vec{L}_\alpha \right|^2 - \frac{J}{2} N q \tag{3.2}$$

where the sum over $\alpha$ runs over all simplces, $\vec{L}_\alpha$ is the sum of the spins inside simplex $\alpha$, and $N$ is the number of simplices of the sample. To discuss the degeneracy, it is convenient to use a Maxwell argument that consists in counting the number of degrees of freedom and the number of constraints.

A configuration satisfies the local constraint as soon as $\vec{L}_\alpha = \vec{0}$ for each unit. If we consider spins of length 1 with $n$ components ($n = 1$ for Ising, $n = 2$ for $XY$, $n = 3$ for Heisenberg), each unit imposes $n$ constraints, and the total number of constraints is equal to $K = Nn$.

Now, the number of degrees of freedom is $n-1$ per spin, and the number of spins is $\frac{Nq}{2}$, so that the total number of degrees of freedom is $F = N(n-1)q/2$. Then, the maxwellian dimension of the ground state manifold is given by:

$$D_M = F - K = N\left[(n-1)\frac{q}{2} - n\right] \tag{3.3}$$

$$= \frac{N}{2}\left[n(q-2) - q\right] \tag{3.4}$$

This will be extensive if $n(q-2) - q > 0$. Let's look at some specific situations.

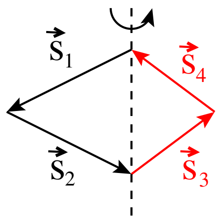



Figure 3.2: Possible spin configurations on a tetrahedron satisfying the constraint that the total spin vanishes. Once two spins, say $\vec{S}_1$ and $\vec{S}_2$, have been chosen, the other two, $\vec{S}_3$ and $\vec{S}_4$, have only one degree of freedom, the angle of the plane in which they lie with respect to that of $\vec{S}_1$ and $\vec{S}_2$.

**Pyrochlore and checkerboard** These systems consist of corner sharing tetrahedra, so $q = 4$. This implies that the maxwellian dimension will grow with the system size if $2n-4>0$, or $\rightarrow n>2$. So for Heisenberg spins ($n = 3$), $D_M = N$.

For the pyrochlore or the checherboard lattice, it is actually easy to visualize how to construct them. This can be done as follows: The condition $\vec{L}_\alpha = \vec{0}$ in a tetrahedron leads to 5 degrees of freedom (2 per spin, i.e. 8, minus 3 constraints). So, when 2 spins have been chosen, there remains one and only one degree of freedom for the remaining 2. A convenient way to visualise this is the following:

Once $\vec{S}_1$ and $\vec{S}_2$ have been chosen, the only freedom for $\vec{S}_3$ and $\vec{S}_4$ is the angle $\phi$ of the plane in which they lie with respect to the plane in which $\vec{S}_1$ and $\vec{S}_2$ lie. So, if one builds the pyrochlore layer by layer (or the checherboard line by line), for all the tetrahedra connecting the last layer to the next one, there is one degree of freedom, and this extra layer is fixed. The process can continue, and there is one degree of freedom per tetrahedron. So, if we fix the spins in one layer, the manifold of ground states has dimension $N$.

**Kagome** For Heisenberg spins ($n = 3$), $D_M = 0$. But we saw in the Introduction that the Heisenberg model on the kagome lattice has an infinite number of ground states. Where is the problem? The constraints are not independent because of closed loops.

More generally, $D_M$ is just a lower bound (provided there are states satisfying the constraints). So this argument based on the Maxwell dimension is useful but it is not the definitive answer: If $D_M$ is macroscopic, there will be a huge degeneracy, but if $D_M = 0$, there may or may not be a macroscopic degeneracy.