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Configuration space analysis for fully frustrated vector spins

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Résumé. — Des spins vectoriels classiques, sur les sites d'un réseau cubique simple tridimensionnel, avec une distribution périodique complètement frustrée d'interaction d'échange, peuvent posséder une intéressante variété de configurations de base. En particulier, pour des spins d'Heisenberg, la variété a la dimension 5, avec deux paramètres de dégénérescence continus, en plus des angles de rotation globale. Une analyse d'espace de configurations, incluant l'étude statistique des recouvrements pour les paires et les triangles, a été mise en œuvre pour ce modèle test.

Abstract. — Classical vector spins, on the sites of a three-dimensional simple cubic lattice, interacting *via* a periodic fully frustrated array of exchange interactions, may exhibit an interesting manifold of ground state configurations. In particular, for Heisenberg spins, the manifold has dimension 5, with two continuous degeneracy parameters, in addition to global rotation angles. A configuration space analysis, including pair and triangle overlap statistics, has been performed for this test model.

Ever since the properties of frustration and disorder were recognized as the two basic ingredients of the physics of spin glasses [1], there has been a new interest in the separate investigation of frustration without disorder. In particular, during the last decade, a number of analytical and numerical results have been obtained for fully frustrated systems, i.e. lattices with nearestneighbour interactions such that each elementary plaquette is frustrated [2]. Because they can be realized periodically, these systems are potentially amenable to exact treatment. Experimental motivations, ranging from magnetism to order-disorder transitions in f.c.c. lattices or to planar arrays of Josephson junctions under applied field, have also contributed to foster activity in this area.

The focus of this paper is the study of fully frustrated simple cubic lattices with vector spins. A few words will suffice to explain the lines of thought which converge here. Some years ago [3], it was recognized that the simple cubic lattice with Ising spins was perhaps the simplest fully frustrated system for which an unusual phase transition occurred, and extensive numerical investigations were carried out recently [4]. Moving from Ising spins to vector spins [5] with m components ($m = 2$, planar spins ; $m = 3$, Heisenberg spins), we found results concerning the lowest energy configurations which, while in agreement with the earlier theoretical predictions [3], revealed an unexpectedly rich ground state degeneracy. Numerically, starting from random initial configurations of Heisenberg spins and making gradient energy descents, never twice was the same ground state encountered. From this surprise finding arose the idea of applying to this ensemble of ground state configurations the same set of tools which have been recently used for the analysis of configuration spaces of spin glasses [1, 6], and in various combinatorial optimization problems [7, 8], namely pair overlap statistics and search for ultrametricity.

In brief, our main motivation here is to test some new tools for configuration space analysis on a (potentially) exactly solvable model, with global continuous symmetry.

It was shown in reference [3] that the ground states for vector spins on a periodic fully frustrated simple cubic lattice are themselves periodic with a translation period equal to twice the lattice parameter. It is therefore sufficient to find the minimal energy configurations for eight unit-magnitude spins sitting on the corners of one cube. Figure 1 displays our choice of notations for the spin sites and our choice of locations for the negative bonds. Positive and negative bonds are assumed to be of equal absolute magnitude (taken as unity heretofore). Some physical properties, like the ground state energy, are gauge-invariant, i.e. invariant under local transformations which reverse the signs of the bonds adjacent to one site. Such gauge-invariant properties will hold for any bond configuration, periodic or not, compatible with full frustration. Other physical quantities, like total magnetization, are not gauge invariant, and thus are specific of a particular bond configuration.

Another useful result of reference [3] is that the local field has equal magnitude on each site, in any ground state configuration. More precisely, $\mathbf{h} = 2\sqrt{3}\,\mathbf{S}_i$. As a consequence, the ground state energy per spin is $E = -\sqrt{3}$. This is valid for classical vector spins with any number of components ($m \geqslant 2$).

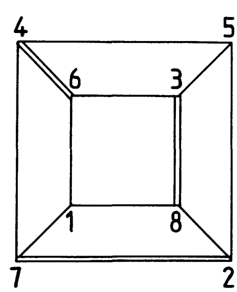

Fig. 1. — Fully frustrated cube : single and double lines represent positive and negative bonds respectively. The numbering of the corner sites is the natural one for this problem.

Further simplification occurs by noticing that the simple cubic lattice is a bipartite lattice which has a natural decomposition into two sublattices. This will allow us to concentrate on one sublattice (sites 1, 2, 3, 4 in Fig. 1). Indeed, the orientations of the spins on the second sublattice are determined by the local field equations :

$$\begin{aligned}\sqrt{3} \cdot \mathbf{S}_5 &= \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4 \\ \sqrt{3} \cdot \mathbf{S}_6 &= \mathbf{S}_1 + \mathbf{S}_3 - \mathbf{S}_4 \\ \sqrt{3} \cdot \mathbf{S}_7 &= \mathbf{S}_1 - \mathbf{S}_2 + \mathbf{S}_4 \\ \sqrt{3} \cdot \mathbf{S}_8 &= \mathbf{S}_1 + \mathbf{S}_2 - \mathbf{S}_3 .\end{aligned} \tag{1}$$

Writing that the modulus of every spin, on the left hand side, is of unit magnitude gives four relations. Actually only three of them are independent and they provide the three necessary and sufficient constraints which the spins $\mathbf{S}_1, \mathbf{S}_2, \mathbf{S}_3, \mathbf{S}_4$ must satisfy in order to define a ground state configuration :

$$\begin{aligned}\mathbf{S}_2 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_4 + \mathbf{S}_2 \cdot \mathbf{S}_4 &= 0 \\ - \mathbf{S}_1 \cdot \mathbf{S}_3 + \mathbf{S}_3 \cdot \mathbf{S}_4 + \mathbf{S}_1 \cdot \mathbf{S}_4 &= 0 \\ \mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_2 \cdot \mathbf{S}_4 - \mathbf{S}_1 \cdot \mathbf{S}_4 &= 0 .\end{aligned} \tag{2}$$

The total number of variables in the problem is equal to $4(m - 1)$, i.e. the number of spins on one sublattice of the cube, times the number of angular variables per spin. Since there are three constraints, the number of free parameters, that is the dimension of the manifold of ground state configurations, is $4m - 7$.

It is purposeful to consider that all configurations which are equivalent under global rotations make only one solution [1]. Since the dimension of SO(m) is $m(m - 1)/2$, the effective dimension of the manifold of solutions is equal to $\mathrm{Max}(4m - 7 - m(m - 1)/2, 0)$. Indeed [5], there is a finite number of solutions, namely 12, for planar spins ($m = 2$). For Heisenberg spins ($m = 3$), the effective dimension of the manifold of solutions is 2, meaning that there are continuous ways of distorting a ground state configuration without changing its energy. Unless otherwise stated, the following will be concerned with Heisenberg spins.

We have found that the manifold of solutions is connected, namely that it is possible to go continuously from any ground state configuration to any other. In some sense, in the huge space of all possible spin configurations, there is a unique ground state valley. Escape in the third spin dimension allows any planar solution to be connected with any other planar solution.

Strong empirical evidence came from numerical computations of the modulus $M = |\mathbf{M}|$ of the magnetization (total magnetization divided by the number of spins), which, despite its lack of gauge invariance, is a useful Morse function [9] on the manifold of solutions. Indeed, two configurations with different M cannot be equivalent under rotation. Figure 2 shows the spectrum of values of $\tilde{M} = 8M$ obtained by sampling the configuration space with many random starts followed by energy descents. By definition, for ground state configurations, one has :

$$8\mathbf{M} = \mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4 + \mathbf{S}_5 + \mathbf{S}_6 + \mathbf{S}_7 + \mathbf{S}_8 \tag{3}$$

which can be rewritten as :

$$8\mathbf{M} = (1 + \sqrt{3})(\mathbf{S}_1 + \mathbf{S}_5) = (1 + 1/\sqrt{3})(\sqrt{3} \cdot \mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4) . \tag{4}$$

As a consequence, M is bounded by :

$$0 \leqslant 8M \leqslant 2(1 + \sqrt{3}) . \tag{5}$$

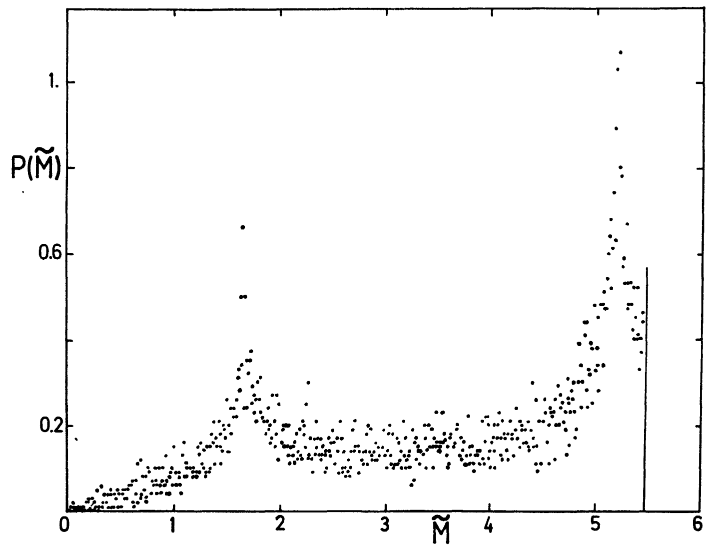

Fig. 2. — Normalized probability distribution of the magnetization modulus of the cube $\tilde{M} = 8\,M$ (see text). The vertical line indicates the upper bound $\tilde{M} = 5.464...$ The two Van Hove singularities occur at $\tilde{M}_1 = 1.655...$ and $\tilde{M}_2 = 5.207...$ which correspond to planar configurations.

For planar spins, there are 6 solutions with :

$$8\,M_1 = \sqrt{2}(1 + \sqrt{3})\,(1 - \sqrt{(2/3)})^{1/2}$$

and 6 solutions with :

$$8\,M_2 = \sqrt{2}(1 + \sqrt{3})\,(1 + \sqrt{(2/3)})^{1/2}\,.$$

However, for Heisenberg spins, all values of the interval defined by (5) are accessible. There is no gap in the spectrum, and the extremal configurations correspond to $\mathbf{S}_2$, $\mathbf{S}_3$, $\mathbf{S}_4$ forming an orthonormal frame and $\mathbf{S}_1$ pointing along the (1, 1, 1) direction (maximal M) or in the opposite direction (minimal M).

The spectrum of figure 2 exhibits characteristic singularities [10], analogous to those of a phonon spectrum in dimension two : a discontinuity at the upper edge, a linear behaviour at the lower edge, two logarithmic Van Hove singularities in between.

Figure 2 is at least consistent with our assertion on the connexity of the manifold of solutions. Since the analytical proof of the connexity is straightforward but tedious, we prefer to emphasize the overlap analysis.

The overlap of two spin configurations, α and β, is defined quite naturally by their scalar product in configuration space :

$$q_{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N} \mathbf{S}_i^{\alpha} \cdot \mathbf{S}_i^{\beta}\,. \tag{6}$$

To eliminate the degeneracy due to global rotation, one defines the overlap of two solutions as the maximal overlap up to mutual rotations. Such a definition has already been used to analyse Heisenberg spin glasses [11]. For two ground state configurations, α and β, of vector spins on a fully frustrated simple cubic lattice, expression (6) reduces to

$$q_{\alpha\beta} = \frac{1}{4}(\mathbf{S}_1^\alpha \cdot \mathbf{S}_1^\beta + \mathbf{S}_2^\alpha \cdot \mathbf{S}_2^\beta + \mathbf{S}_3^\alpha \cdot \mathbf{S}_3^\beta + \mathbf{S}_4^\alpha \cdot \mathbf{S}_4^\beta) . \tag{7}$$

This expression is valid for any spin dimension m.

For Heisenberg spins, we have obtained numerically the pair overlap distribution $P(q)$, that is the probability that two ground state configurations taken at random have a maximal overlap equal to q :

$$P(q) = \iint \delta(q - q_{\alpha\beta})\, \mathrm{d}\mu_\alpha\, \mathrm{d}\mu_\beta \tag{8}$$

where μ is a convenient measure on the manifold of solutions (our choice for μ measures attractor basin sizes). Our data are plötted in figure 3 and they show that $P(q)$ is indeed a non trivial function. Let us stress that $P(q)$ is gauge-invariant, and therefore somehow more fundamental than the magnetization spectrum of figure 2. Generically, one expects the upper edge singularity to behave as :

$$P(q) \sim (1 - q)^{(\delta - 2)/2} \tag{9}$$

where δ is the effective dimension of the manifold of solutions ($\delta = 2$, for Heisenberg spins), whereas for the lower edge singularity one expects :

$$P(q) \sim q^{2\delta - 1} . \tag{10}$$

Indeed the numerical data of figure 3 are consistent with a jump at $q = 1$, and $P(q) \sim q^3$ for q

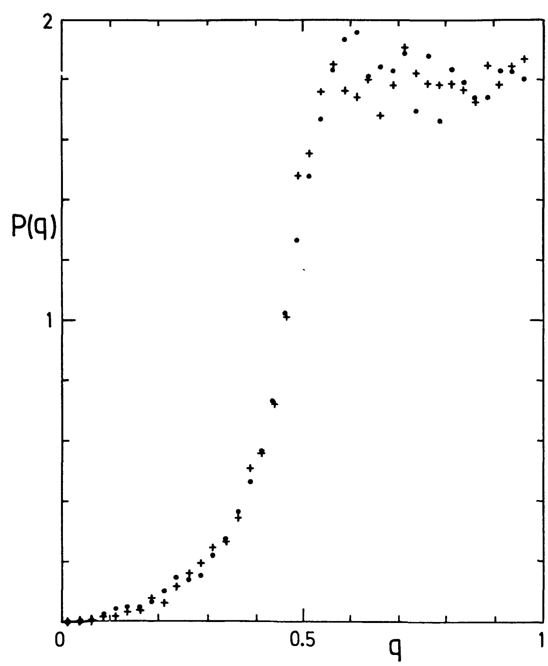

Fig. 3. — Normalized distribution of pair overlaps of configurations obtained with two sets of 200 configurations each (solid circles and crosses).

small. This last prediction stems from the hint that the most dissimilar solutions (with zero overlap) belong to the subset of planar solutions. Note that, for $m = 2$, the function $P(q)$ is a sum of δ-functions :

$$P(q) = \frac{1}{4}\,\delta(q) + \frac{1}{3}\,\delta\left(q - \frac{1}{2\sqrt{2}}\right) + \frac{1}{3}\,\delta\left(q - \frac{\sqrt{3}}{2\sqrt{2}}\right) + \frac{1}{12}\,\delta(q - 1)\,. \tag{11}$$

Finally, we consider the triangle statistics, whose importance was stressed by the discovery of ultrametric structures in the mean field theory of spin glasses [6]. More precisely, we consider the function :

$$C(q_1, q_2) = P(q_1, q_2) - P(q_1)\,P(q_2) \tag{12}$$

with

$$P(q_1, q_2) = \iiint \delta(q_1 - q_{\alpha\beta})\,\delta(q_2 - q_{\alpha\gamma})\,\mathrm{d}\mu_\alpha\,\mathrm{d}\mu_\beta\,\mathrm{d}\mu_\gamma\,. \tag{13}$$

Our numerical data for $C(q_1, q_2)$ are plotted in figure 4. Since $C(q_1, q_2)$ has been advocated as an appropriate signature for the triangle statistics of a given configuration space [6, 7], it is useful to build a repertoire of behaviours corresponding to test models. As such, the data of figure 4 are to be compared with those obtained for spin glasses or travelling salesman problems [7], whose interpretation was in need for terms of comparison. It should be noted that ultrametricity cannot strictly hold here, since an ultrametric set must be totally disconnected and cannot be a continuous manifold.

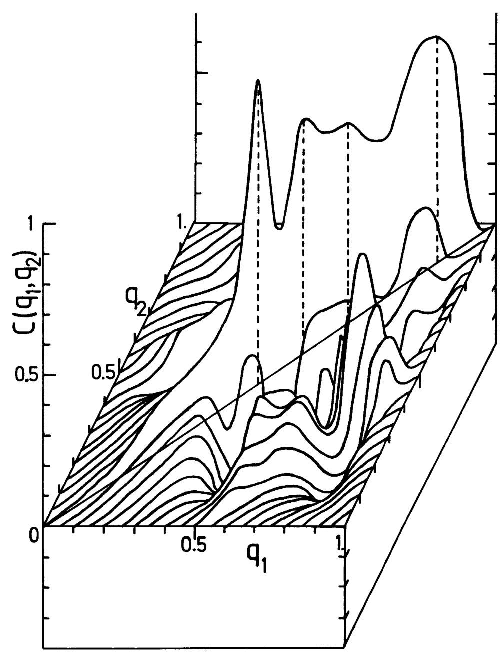

Fig. 4. — Profile of the function $C(q_1, q_2)$ (see Eq. (12)) in the planes parallel to the diagonal plane $q_1 = q_2$, obtained with a set of 200 configurations.

In conclusion, this study has been concerned with the ground state properties which are remarkable enough. Yet, it is natural to wonder whether this large ground state degeneracy survives at finite temperatures, with two additional Goldstone modes, besides the usual spin wave excitations.

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