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Phase transitions in non-collinear ordering without frustration

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Abstract

We study a Heisenberg and *XY* model on a cubic lattice with a cubic exchange coupling having a non-collinear ground state not due to frustration. This model has attractive properties: complex breakdown of symmetry, temperature dependence of the angles between the spins and phase transitions between ordered phases. © 1999 Published by Elsevier Science B.V. All rights reserved.

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1. Introduction

Competing interactions in frustrated vector spin systems can create a non collinear ground state (GS). Phase transitions between this GS and the paramagnetic phase at high temperatures have been extensively investigated during the last decade [1]. In particular the nature of the behavior of systems like triangular antiferromagnets or helimagnets where the GS is planar have been considered but remain controversial [2,3]. For helimagnets problems appear because of the use of periodic boundary conditions in Monte Carlo (MC) simulations [4,5]. Indeed in this case the turn angle Q between the spins varies as function of the temperature [6]. Thus we cannot obtain commensurability between Q and the lattice size at all temperatures. To resolve this problem one could use different types of boundary conditions [7] but then it is difficult to obtain reliable values for the critical exponents due to the existence of surface contributions. For the same reason few attentions has been paid to transitions between non-collinear and collinear phases which appear in many frustrated systems.

To overcome this difficulty we introduce in this study a new model which has the symmetries (thus the transitions associated) of frustrated models but where the turn angle Q is automatically commensurable with the lattice size L and L a multiple of two. The Hamiltonian is $H=\sum_{(ij)}[J_1\boldsymbol{S}_i\cdot\boldsymbol{S}_j+J_3(\boldsymbol{S}_i\cdot\boldsymbol{S}_j)^3]$ and for certain ratio J_3/J_1 the GS is non-collinear and phase transitions between non-collinear and collinear phases could occur. We have shown that this cubic term does not add symmetry [8], contrary to an addition of a square term which generates a local Ising symmetry. We note that a cubic term is present in experimental systems [9]. This new model is interesting because the non-collinear GS does not come from frustration between links but is inherent

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to each link. It is a good candidate to explore through numerical simulations some properties of frustrated systems which are impossible to study otherwise. Moreover, in the conclusion we will show that our model can be very useful to test some theoretical predictions on various breakdown of symmetries accessible with difficulties with only a linear term in the Hamiltonian.

In the next section we present the model and details of the Monte Carlo simulations. The following section (3) is devoted to the phase diagram in the case of XY spins and the Section 4 to the Heisenberg case. Section 5 contains the conclusion.

2. Model and simulation

We take an Hamiltonian of the form

$$H = \sum_{\langle ij \rangle} \left[J_1 \boldsymbol{S}_i \cdot \boldsymbol{S}_j + J_3 \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_j \right)^3 \right] + \sum_{\langle\langle ij \rangle\rangle} \left[J_{NNN} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \right] \quad (1)$$

where $\boldsymbol{S}_i$ is a N component classical vector of unit length, J_1 and J_{NNN} are ferromagnetic coupling constants ($J_1 < 0$ and $J_{NNN} < 0$), J_3 an antiferromagnetic coupling constant ($J_3 > 0$), $\langle ij \rangle$ the nearest neighbors and $\langle\langle ij \rangle\rangle$ the next-nearest neighbors. The J_{NNN} interaction is introduced to stabilize the GS in the case b) (see below) and for this article, this last interaction is chosen to be equal to one: $J_{NNN} = -1$. The term $(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)^3$ is also odd like $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$ and does not spoil the symmetry contrary to a square term which introduces a local Ising symmetry [10]. The GS of two spins depends on the ratio $\eta = -J_3/J_1$:

(a) $\eta \le 1/3$, the GS is ferromagnetic (Fig. 1a).
(b) $1/3 \le \eta \le 4/3$, the GS is canted (Fig. 1b). The angle Q between the spins is given by

$$\cos(Q) = \frac{1}{\sqrt{3\eta}} \quad (2)$$

(c) $\eta \ge 4/3$, the GS is antiferromagnetic (Fig. 1c).

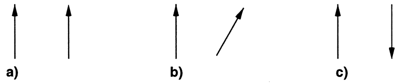

Fig. 1. (a) $\eta \le 1/3$ the GS is ferromagnetic. (b) $1/3 \le \eta \le 1$ the GS is canted. (c) $\eta \ge 1$ the GS is antiferromagnetic.

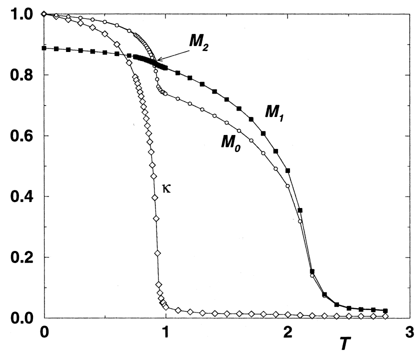

Fig. 2. Magnetization and chirality for XY spins. M_0 is calculated with two sub-lattices and a rotation of Q, M_2 using the norm of the two sub-lattices magnetizations and M_1 corresponds to the ferromagnetic case. κ is the chirality.

We use in this work the standard Metropolis algorithm. We have tried also a cluster algorithm for this model [8], however it is not efficient for the canted-collinear transition because the latter happens at lower temperature where the cluster sizes become too big. Simulations have been done for L from 6 to 36 where L must be a multiple of 2 in order to use periodic boundary conditions. Some hundred thousand MC steps for equilibration were carried out and up to seven million steps were used for the largest sizes to obtain reliable averages.

We use the histogram MC technique developed by Ferrenberg and Swendsen [11,12]. From a simulation done at T_0, this technique allows to obtain thermodynamic quantities at T close to T_0.

3. Phase diagram for XY spins

We first study our model defined by (1) with XY spins. We have performed many simulations in varying the value of J_3/J_1 for cubic lattices. Here we concentrate on the case $J_3/J_1 = 1$ in Figs. 2 and 3. The ground state is depicted in Fig. 1b, with an angle $Q = 54.7°$. The parameter M_0 is obtained by dividing the lattice in two sublattices with only collinear spins, then calculating the magnetization of each sublattice and adding them doing a rotation of an angle Q. M_2 is obtained by averaging the norm of the two sublattices. If Q is temperature-independent we should obtain the same result, otherwise M_2 would be larger than M_0. We calculate the order

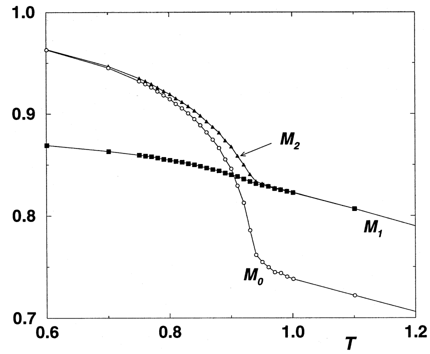

Fig. 3. Magnification of Fig. 2. For $0.7 < T < 0.95$ the stable state is neither M_1 nor M_0.

parameter for parallel spins M_1 which is the sum of all the spins. The last quantity calculated is the chirality. Indeed when the GS is non-collinear for XY spins there is a Z_2 (Ising) symmetry which is broken and the chirality κ is the order parameter defined by the sum over all links of $\boldsymbol{S}_i \times \boldsymbol{S}_j$. κ in Fig. 2 goes to zero before magnetizations. Moreover M_2 is bigger than M_0 thus Q is temperature dependent and, for high temperatures, M_2 coalesces with M_1 therefore the state is collinear. We can conclude from these figures that two transitions occur: one from the canted state to the collinear state at $T \sim 0.9$ and one from the collinear state to a paramagnetic state at $T \sim 2.2$. Moreover the transition canted-collinear is continuous without an abrupt change of state. We see in Fig. 4 the value of Q calculated with the help of M_2 and M_1 by the relation $\cos(Q) = 2\, M_1/M_2 - 1$ where we have assumed that each sublattice has the same magnetization. Q changes

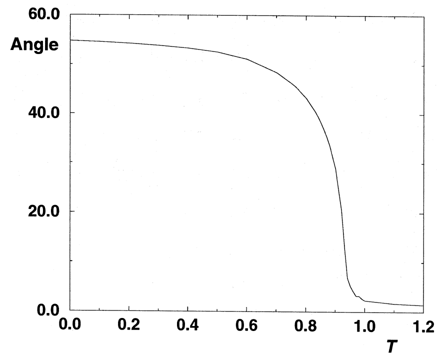

Fig. 4. Angle as function of the temperature calculated from M_0 and M_1. The tail different of 0 for $T > 0.9$ comes from the method of calculation.

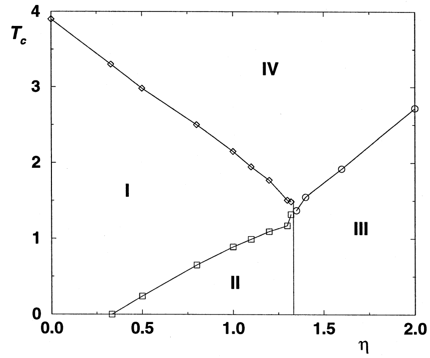

Fig. 5. Phase diagram for XY spins. $\eta = -J_3 / J_1$. I = parallel, II = canted, III = antiparallel, IV = paramagnetic.

smoothly with the temperature. We think that this picture is not restricted to our model but is more general and in particular prevents from a clear interpretation of the results in the helimagnetic case with XY spins [4] where the variation of the angle associated to the periodic conditions must have a strong influence on the critical behavior [2,5].

We have constructed the phase diagram for the XY case in Fig. 5. We obtained four phases: parallel (I), canted (II), antiparallel (III) and paramagnetic (IV) as function of η. From a point of view it is disappointing that there is no transition canted-paramagnetic because our first objective was to study this type of transition without the problem of competing interactions. On the other hand this model will allow us to study the phase transition canted-collinear which exists in numerous lattices (helimagnetic or triangular anisotropic for example).

We describe now the various transitions: the parallel-paramagnetic and antiparallel-paramagnetic transitions should be of type of the standard ferromagnetic system because the breakdown of the symmetry is the same and the cubic term is irrelevant [8]. The canted-antiparallel transition must be of first order because there is an abrupt change of symmetries. Last, the canted-parallel transition must be of Ising type because only an Ising symmetry is broken between the two phases.

4. Phase transition for Heisenberg spins

We discuss now the case of Heisenberg spins. The phase diagram is very similar to the XY case.

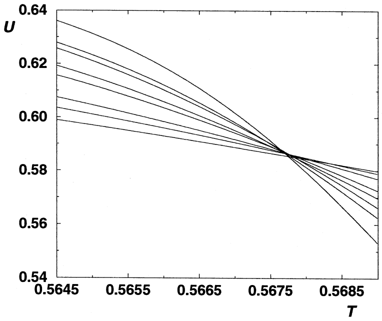

Fig. 6. Binder's parameter U as function of the temperature for various sizes L ($L = 10$, 12, 14, 18, 20, 22, 26, 30) for Heisenberg spins with $\eta = 1$.

However breakdowns of symmetries are more complicated. The transition between the collinear and the paramagnetic phase is of the type $SO(3)/SO(2)$ (symmetry at high temperature/symmetry at low temperature), i.e. of the standard ferromagnetic phase. For the same reason as in the XY case (irrelevance of the cubic term) the transition belongs to this class. The same breakdown appears for the anticollinear-paramagnetic transition, therefore it belongs also to this class. The transition between the canted and the collinear phase is more interesting. The breakdown of the symmetry is $SO(2)/SO(1) = SO(2)$, i.e. similar to the ferromagnetic-paramagnetic transition for the XY spins. Therefore we conclude that the transition must belong to this type. We note that this is one of the first times that this 'reduction' of symmetry is shown in this form. We think that this result applies for the transition canted-collinear in helimagnets, which cannot be studied directly by numerical simulations (see introduction). We will know verify this prediction using finite size scaling relations.

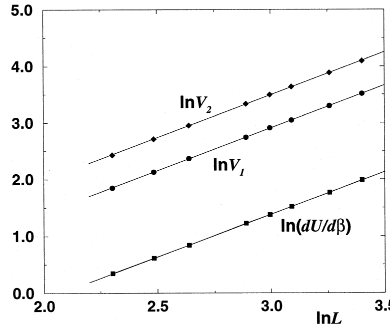

Fig. 8. Values of V_1, V_2, $dU/d\beta$, as function of L in a ln-ln scale at T_c for Heisenberg spins with $\eta = 1$. The value of the slopes gives $1/\nu$ and we obtain $\nu = 0.663(12)$, 0.662(13), 0.668(16) (up to down). The estimated error bars are smaller than the symbols.

We choose for the study of this transition $\eta = 1$. The right order parameter is a 'chirality vector' $\boldsymbol{\kappa}$ defined by the sum over all links of $\boldsymbol{S}_i \times \boldsymbol{S}_j$. To find the critical temperature T_c we use Binder's cumulant defined as

$$U = 1 - \langle \kappa^4 \rangle / \left(3 \langle \kappa^2 \rangle^2 \right). \tag{3}$$

We determine the intersections of the curves $U(T)$. Ideally the value of U for two different lattice sizes L and $L' = bL$ should be the same at the critical temperature [13]. In Fig. 6, U is plotted as function of the temperature for different sizes from $L = 10$ to $L = 30$. Due to the presence of residual corrections

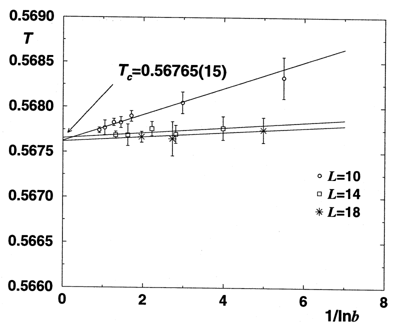

Fig. 7. Estimated T_c plotted vs inverse logarithm of the scale factor $b = L'/L$ for Heisenberg spins with $\eta = 1$. The results for $L = 10, 14, 18$ are shown. The estimated temperature is $T_c = 0.56765(15)$.

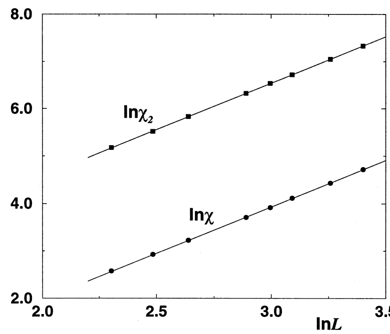

Fig. 9. Values of χ and χ_2 as function of L in a ln-ln scale at T_c for Heisenberg spins with $\eta = 1$. The value of the slope gives γ/ν. We obtain 1.960(20) and 1.966(17) (up to down). The estimated error bars are smaller than the symbols.

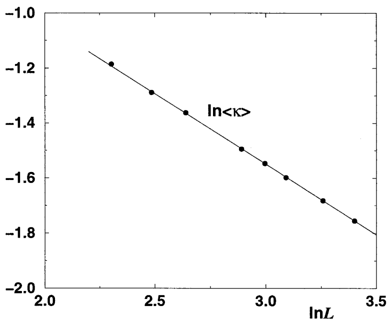

Fig. 10. Values of $\langle \kappa \rangle$ as function of L in a ln-ln scale at T_c for Heisenberg spins with $\eta = 1$. The value of the slopes gives β/ν and we obtain 0.512(10). The estimated error bars are smaller than the symbols.

to finite size scaling, one actually needs to extrapolate the critical temperature T_c for $(\ln b)^{-1} \to 0$. We obtain in Fig. 7:

$$T_c = 0.56765(15) . \quad (4)$$

The estimate for the universal quantity U at T_c (U^*) is

$$U^* = 0.5880(15) . \quad (5)$$

This value agrees with the value found in MC for the standard XY class: $U^* = 0.586(1)$ [14].

With the value of T_c we can find the critical exponents using log-log fit [15,16]. We obtain from $V_1 = \langle \kappa E \rangle / \langle \kappa \rangle - \langle E \rangle$, $V_2 = \langle \kappa^2 E \rangle / \langle \kappa^2 \rangle - \langle E \rangle$ and $dU/d\beta$ an estimate of $1/\nu$ (Fig. 8), from $\chi = N(\langle \kappa^2 \rangle - \langle \kappa \rangle^2)/(k_B T)$ and $\chi_2 = N\langle \kappa^2 \rangle/(k_B T)$ (Fig. 9) of γ/ν, and from $\langle \kappa \rangle$ (Fig. 10) of β/ν. Combining these results we finally obtain:

$$\nu = 0.665(10) , \quad \gamma = 1.306(30) , \quad \beta = 0.340(12) .$$

All our errors are calculated with the help of the Jackknife procedure [17] and include the influence of the uncertainty in estimating T_c. We find again the same result as for the standard XY model: $\nu = 0.670(2)$, $\gamma = 1.316(5)$ [14]. Thus the transition between canted and parallel spins belongs to the standard XY case.

5. Conclusion

We have shown that the transition for $O(N)$ vectors between canted (planar) and collinear $O(N)$ spins is of the standard ferromagnetic $O(N-1)$ class. This is similar to transitions in helimagnetic, Villain and anisotropic triangular lattices.

Our objective now is to study more complicated transitions. Indeed our approach allows to study numerous breakdown of symmetries which are difficult to obtain with Hamiltonians of linear terms only. For such models the non-collinear ordering comes from the competition between different links while, in our model, it is a property of each link. For a triangular lattice the ground state will have a three-dimensional canted phase (not longer planar) and the transition canted-parallel will be of the type $O(N-1)/O(N-3) = O(M)/O(M-2)$ with $M = N-1$. This is similar to the very controversial case of frustrated triangular lattices, with linear term only in Hamiltonian, for the canted-paramagnetic transition [2,3] and would be of great help to test the universality concept. Moreover for more complicated lattices like hexagonal-closed-packet one could also study breakdowns of symmetry like $O(N-1)/O(N-4)$ and therefore test the predictions related to the Stiefel model [18–20]. These studies are in progress.

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