Journal of Applied Physics

Phase transition in a system of interacting triads

Cite as: Journal of Applied Physics **76**, 6350 (1994); https://doi.org/10.1063/1.358263
Published Online: 04 June 1998

H. T. Diep, and D. Loison

Phase transition in a system of interacting triads

H. T. Diep and D. Loison
Groupe de Physique Statistique, Université de Cergy-Pontoise 49, Avenue des Genottes, B.P. 8428, 95806 Cergy-Pontoise Cedex, France

The present work is motivated by the controversy on the nature of the phase transition on the Heisenberg stacked triangular antiferromagnet (STA). In particular, the renormalization group with $4-\epsilon$ expansion suggests a new universality class, while the renormalization group with $2+\epsilon$ expansion using a nonlinear σ (NLS) model shows that the transition, if not mean-field tricritical or first order, is of the known $O(4)$ universality class. In order to verify this conjecture, we study here an equivalent system obtained from the STA by imposing the local rigidity as has been used in the NLS model. The results show that none of the scenarios predicted by the NLS model is found. The critical exponent $\nu=0.48\pm0.05$ is quite different from the original STA without local rigidity, indicating that the local rigidity changes the nature of the transition. It is also different from that of $O(4)$. It means that successive transformations used to buildup the NLS model from the original STA may lead to the $O(4)$ universality class.

I. INTRODUCTION

Phase transitions in frustrated spin systems have been extensively investigated during the last decade.[1] In particular, the nature of the phase transition in the stacked triangular antiferromagnets (STA) with Heisenberg spins interacting via nearest-neighbor (nn) bonds has been widely studied. This system belongs to a general family of periodically canted spin systems known as helimagnets. Recent extensive Monte Carlo (MC) simulations which are more precise than early MC works[2] have shown that the transition in STA is of second order with the critical exponents quite different from those of known universality classes.[3–5] The body-centered tetragonal helimagnet has also shown almost the same critical exponents.[6] Using a renormalization group (RG) technique in a $4-\epsilon$ perturbative expansion, Kawamura[7] has suggested a new universality class for that transition. However, by using a RG technique for a nonlinear σ (NLS) model with a $2+\epsilon$ expansion, Azaria *et al.*[8–10] showed that the transition, if not of first order or mean-field tricritical, is of second order with the known $O(4)$ universality class. This situation is embarrassing since the RG technique with $2+\epsilon$ and $4-\epsilon$ expansions usually yields the same result in three dimensions for nonfrustrated systems. Furthermore, it is clear that none of the scenarios predicted by Azaria *et al.* was verified by the above-mentioned independent MC simulations of the Heisenberg STA.[3–5]

The purpose of this paper is to find out the reason of the disagreement between the $2+\epsilon$ and the MC results. To this end, we study by the histogram MC simulation technique,[11,12] the approximated system used in the NLS model[8–10] and to compare the MC results with those performed on the original STA.[3–5] The approximated system, as seen in Sec. II, is in fact, obtained from the STA by neglecting local fluctuations while keeping the symmetry of the original Hamiltonian.

Section II is devoted to the description of our model and method. Results are shown and discussed in Sec. III. Concluding remarks are given in Sec. IV.

II. MODEL AND METHOD

Let us consider the STA with nn interaction. The ground state (GS) is characterized by a planar spin configuration where the three spins on each triangle form a 120° structure with either left or right chirality. Thus, the GS degeneracy is twofold in addition to the global rotation. The Hamiltonian is given by

$$H=J\sum_{ij} \mathbf{S}_i.\mathbf{S}_j \tag{1}$$

where S_i denotes the classical Heisenberg spin of unit length at the ith site, $J(>0)$ is the interaction between two nn spins, and the sum runs over all nn pairs. The Hamiltonian (1) has been used in previous MC simulations[3–5] which all give the same critical exponents within statistical errors: $\nu=0.59\pm0.01$, $\beta=0.28\pm0.02$, $\gamma=1.25\pm0.03$, and $\alpha=0.40\pm0.01$.

Following Azaria *et al.*[10] we take the continuum limit at each triangle by putting the three spins at its center. In doing so for all triangles, we generate a new superlattice [see Fig. 1(a)]. In the NLS model, the local rigidity was assumed, i.e., the sum of the three spins on each triangle is set to zero.[8–10,13] The resulting model is a system of triads each of which is defined by the three orthogonal unit vectors $\mathbf{e}_i(x)(i=1,2,3)$ which replace the spins at the center of the xth triangle in Fig. 1(a). The original spins at the xth triangle are obtained by a linear combination of $\mathbf{e}_i(x)(i=1,2,3)$. The system of triads is shown in Fig. 1(b). Note that the third vectors $\mathbf{e}_3(x)$ which are perpendicular to the figure sheet are not shown for clarity. Since there is no more frustration by geometry, one can take indifferently ferromagnetic or antiferromagnetic interaction between nn triads with the following Hamiltonian

$$H_t=-\sum_{xy}\sum_{i=1,2,3} K_i(x,y)\mathbf{e}_i(x).\mathbf{e}_i(y), \tag{2}$$

where $K_i(x,y)$ is the interaction between the two ith unit vectors sitting at the nn, xth, and yth, triads. The original STA is now transformed into a triad system which is defined on a simple cubic lattice. Strictly speaking, the STA corre-

 0021-8979/94/76(10)/6350/3/$6.00

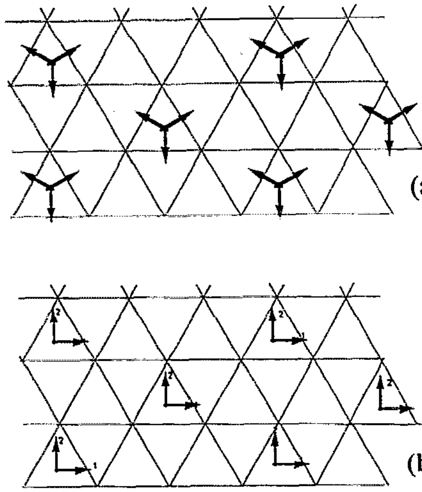

FIG. 1. (a) The continuum limit of the ground state of the STA is taken by putting the spins on each triangle at its center (b) system of triads which is equivalent to the Heisenberg STA with local rigidity. The third unit vectors perpendicular to the figure sheet are not shown.

sponds to the case where the interactions between one of the unit vectors, say $e_3(x)$, are zero.[10] We will consider in this paper not only this case but also the symmetric case where all $K_i(x,y)$ are equal. Since the interactions in (1) are site independent, all interactions for the triad system are also site independent, i.e., $K_i(x,y)=K_i$.

Before showing our results, let us emphasize that the model considered in this paper is equivalent to the Heisenberg model on the STA *only within the so-called local rigidity condition.*

The method used here is the histogram MC technique which has been recently developed by Ferrenberg and Swendsen to study phase transitions.[11,12] The reader is referred to these papers for details. In our simulations, we use a simple cubic lattice of linear size $L=10,12,14,16,18,20$ sites with periodic boundary conditions. In general, we discarded 500 000 MC steps per triad for equilibrating and calculated the energy histogram as well as other physical quantities over 1–2 M MC steps. We first estimate roughly the transition temperature T_0 at each size and calculate at T_0 the energy histogram as well as the following quantities:

$$\langle C\rangle=\frac{(\langle E^2\rangle-\langle E\rangle^2)}{Nk_BT^2}, \quad (3)$$

$$\langle \chi\rangle=\frac{N(\langle O^2\rangle-\langle O\rangle^2)}{k_BT}, \quad (4)$$

$$\langle (O)'\rangle=\langle OE\rangle-\langle O\rangle\langle E\rangle, \quad (5)$$

$$\langle (O^2)'\rangle=\langle O^2E\rangle-\langle O\rangle^2\langle E\rangle, \quad (6)$$

$$\langle (\ln O)'\rangle=\frac{\langle OE\rangle}{\langle O\rangle}-\langle E\rangle, \quad (7)$$

$$\langle (\ln O^2)'\rangle=\frac{\langle O^2E\rangle}{\langle O^2\rangle}-\langle E\rangle, \quad (8)$$

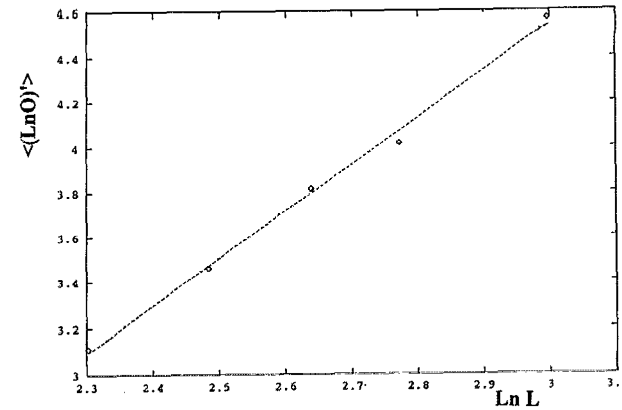

FIG. 2. $\langle (\ln O)'\rangle$ vs $\ln L$. The slope is $1/\nu=2.08$.

$$\langle V\rangle=1-\frac{\langle E^4\rangle}{3\langle E^2\rangle^2}, \quad (9)$$

$$\langle U\rangle=1-\frac{\langle O^4\rangle}{3\langle O^2\rangle^2}, \quad (10)$$

$$\langle (U)'\rangle=\langle UE\rangle-\langle U\rangle\langle E\rangle, \quad (11)$$

where E is the internal energy of the system, T the temperature, O the order parameter, C the specific heat per site, χ the magnetic susceptibility per site, U the fourth-order cumulant, V the fourth-order energy cumulant, $\langle ...\rangle$ means the thermal average, and the prime denotes the derivative with respect to $\beta=1/(k_BT)$. Using the energy histogram at T_0, one can calculate physical quantities at neighboring temperatures, and thus the transition temperature at each size is known with precision.[11,12]

III. RESULT

Let us show the results for the two following cases.

A. $K_1=K_2=K$, $K_3=0$

The system in this case is equivalent to the STA with local rigidity. The transition is found of second order. Using the finite size scaling for the maxima of $\langle C\rangle$, $\langle \chi\rangle$, $\langle (\ln O)'\rangle$, etc.[11,12] we obtained the critical temperature for the infinite system which is $T_c(\infty)=1.5325\pm0.0020$. The exponent ν can be obtained from the inverse of the slope of $\langle (\ln O)'\rangle$ [and $\langle (\ln O^2)'\rangle$] versus $\ln L$. This is shown in Fig. 2 where $\nu=0.48\pm0.05$. The critical exponents γ and β are obtained by plotting $\ln\langle O\rangle$ and $(\ln\langle\chi\rangle)$ vs $\ln L$, respectively (not shown here). They are $\beta=0.22\pm0.04$ and $\gamma=1.15\pm0.07$. These exponents are completely different from those of the original STA (without local rigidity) (see values of exponents given in the preceding section). They are also different from those of the $O(4)$ universality class which are $\nu=0.74$, $\beta=0.39$, $\gamma=1.47$.

There are two things we learn from these results: (i) the local rigidity changes the nature of the phase transition; (ii) when one starts with the local rigidity, one does not find the scenarios predicted by the NLS model in $2+\epsilon$ expansion.[10] It means that the subsequent approximations used in the theoretical calculation,[10] for instance, the continuum limit performed at some steps, may alter the nature of the transition

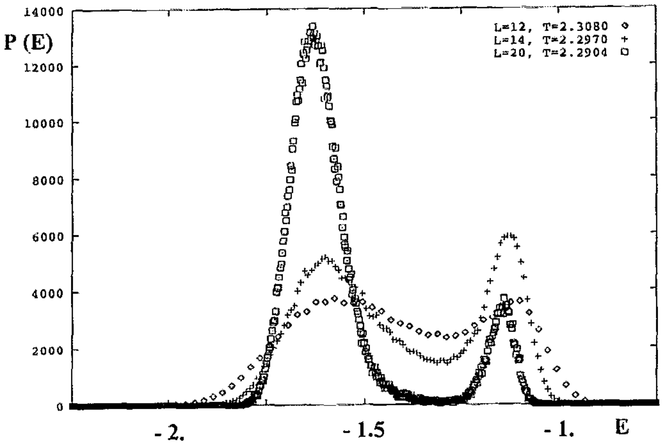

FIG. 3. Energy histogram $P(E)$ for $L=12$ at $T=2.3080$ (diamonds), for $L=14$ at $T=2.2970$ (crosses), and for $L=20$ at $T=2.2904$ (squares). Bimodal distribution characteristic of first-order transition is seen. E is internal energy per unit vector $\mathbf{e}_i(x)(i=1,2,3)$

found by MC simulation for the discrete lattice system. We believe that the continuum limit used in the NLS model excludes possible topological defects which can change the transition nature.

B. $K_1=K_2=K_3=K$

In this case, we find a strong first-order transition. This is unexpected since the symmetry of the Hamiltonian is invariant with respect to the previous case. We show in Fig. 3 the energy histogram $P(E)$ performed for several lattice sizes at the transition temperature of each size. The bimodal distribution characteristic of a first-order transition is seen. The two maxima, which are separated by a continuum for small sizes, show a real discontinuity between them for $L=20$. Note that for $L=20$ the two maxima do not have the same height because the temperature at which the simulation was performed is not precisely the transition temperature. Another signature of the first order is the fact that the energy cumulant $\langle V \rangle$ does not tend to 2/3 at the transition for increasing size as it should be in a second-order transition. Instead, it decreases with increasing size to reach the value of 0.628 for $L=20$. The maxima of $\langle C \rangle$ and $\langle \chi \rangle$ vary as L^3, providing another evidence of the first-order character. Details will be shown elsewhere.

At this stage, it is interesting to note that there should be a critical value of K_3 between 0 and 1 where the transition undergoes a crossover from second to first order. The determination of this tricritical point is left for a future study.

IV. CONCLUSION

Here we have studied a system of interacting triads which is equivalent to the STA if one neglects local fluctuations by imposing a local rigidity on all triangles. In the case which is equivalent to the Heisenberg STA ($K_1=K_2=K$, $K_3=0$), we do not find the same critical exponents as those found for the STA. It means that the local rigidity changes the nature of the transition. The obtained critical exponents are, in addition, different from those of $O(4)$ found in the NLS calculation. We think that during the successive transformations of the initial STA to build the NLS model,[10] some ingredients may have been lost, though the system symmetry is preserved. In the case where $K_1=K_2=K_3=K$, we find that the transition is unexpectedly of first order, though the symmetry of the system does not change with respect to the case where $K_1=K_2=K$, $K_3=0$. We hope that this work will stimulate further theoretical investigations on the nature of phase transition in helimagnets.

ACKNOWLEDGMENTS

The authors wish to thank P. Azaria and B. Delamotte for suggesting this problem and for helpful discussion.

[1] *Magnetic Systems with Competing Interactions*, edited by H. T. Diep (World Scientific, Singapore, in press).

[2] H. Kawamura, J. Appl. Phys. **63**, 3086 (1988); J. Phys. Soc. Jpn. **58**, 584 (1989).

[3] H. Kawamura, J. Phys. Soc. Jpn. **61**, 1299 (1992); and in *Recent Advances in Magnetism of Transition Metal Compounds*, edited by A. Kotani and Suzuki (World Scientific, Singapore, 1992).

[4] D. Loison and H. T. Diep, Phys. Rev. B (in press).

[5] T. Bhattacharya, A. Billoire, R. Lacaze, and Th. Jolicoeur, J. Phys. I France **4**, 181 (1994).

[6] H. T. Diep, Phys. Rev. B **39**, 397 (1989).

[7] H. Kawamura, Phys. Rev. B **38**, 4916 (1988).

[8] P. Azaria, B. Delamotte, and Th. Jolicoeur, Phys. Rev. Lett. **64**, 3175 (1990).

[9] P. Azaria, B. Delamotte, and Th. Jolicoeur, J. Appl. Phys. **69**, 6170 (1990).

[10] P. Azaria, B. Delamotte, F. Delduc, and Th. Jolicoeur, Nucl. Phys. B **408**, 485 (1993).

[11] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **61**, 2635 (1988).

[12] A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. **63**, 1195 (1989).

[13] T. Dombre and N. Read, Phys. Rev. B **39**, 6797 (1989).