Effective theory of the phase transition in Heisenberg stacked triangular antiferromagnets

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The nature of the phase transition for the Heisenberg stacked triangular antiferromagnet (STA) is a controversial subject at present. The renormalization group (RG) 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. These predictions are in disagreement with recent Monte Carlo (MC) simulations. In this paper, we test the validity of the local rigidity imposed on the STA used in the NLS model using extensive MC simulations. The obtained critical exponents are quite different from those of the original STA (without local rigidity), indicating that the local rigidity changes the nature of the transition. These exponents are neither of mean-field tricriticality nor of $O(4)$ universality class. It means that some transformations used to build up the NLS model may alter the original STA.

I. INTRODUCTION

The effects of the frustration on the phase transitions in spin systems have been extensively investigated during the last decade.[1] Among the most studied models are periodically canted spin systems known as helimagnets. In these systems, the nature of the phase transition is still a controversial subject. The simplest model of the helimagnet is the stacked triangular antiferromagnets (STA) with Heisenberg spins interacting via nearest-neighbor (NN) bonds. Recent extensive Monte Carlo (MC) simulations which are more precise than early MC works[2] have shown that the transition in STA's 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] Theoretically, a renormalization group (RG) technique in a $4-\epsilon$ pertubative expansion,[7] has suggested a new universality class for that transition. This suggestion has been challenged by Azaria *et al.*[8–10] who used a RG technique for a nonlinear σ (NLS) model with a $2+\epsilon$ expansion. They 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 perplexing since the RG technique with $2+\epsilon$ and $4-\epsilon$ expansions usually yields the same result in three dimensions for nonfrustrated systems.

Since none of the scenarios predicted by Azaria *et al.* was verified by the above-mentioned independent MC simulations of the Heisenberg STA,[3–5] we investigate in this paper the origin of the disagreement between the $2+\epsilon$ and the MC results. To this end, we study, using the histogram MC simulation technique,[11,12] the STA with local rigidity used in the NLS model.[8–10] The local rigidity imposed on the STA means that local fluctuations are neglected.

In Sec. II we describe the model and method. Results are shown and discussed in Sec. III. Concluding remarks are given in Sec. IV.

II. MODEL AND METHOD

We consider the STA. The triangular planes are XY planes coupled with each other along the Z direction. The Hamiltonian is given by

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

where $\mathbf{S}_i$ denotes the classical Heisenberg spin of unit length occupying the ith lattice site, J (>0) is the antiferromagnetic interaction between $\mathbf{S}_i$ and its six NN spins in the same XY plane as well as its two NN spins in the adjacent planes. The sum runs over all NN pairs. The ground state (g.s.) is characterized by a planar spin configuration where the three spins on each triangle form a 120° structure with either positive or negative chirality (see Fig. 1). The g.s. degeneracy is thus twofold, in addition to the continuous degeneracy due to the global rotation.

All previous MC simulations[3–5] performed on the Hamiltonian (1) give the same critical exponents within statistical errors: $\nu = 0.59\pm0.01$, $\beta = 0.28\pm0.02$, $\gamma = 1.25\pm0.03$, and $\alpha = 0.40\pm0.01$.

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] It is in this condition that a field theory has been formulated to study the nature of the phase transition in the STA. The result is that the transition, if not first order or mean-field tricritical, is of the $O(4)$ universality class. Since the MC results did not confirm any of these scenarios, it is desirable to check the validity of the successive transformations used to build up the NLS model.[8–10]

In this paper, we check the validity of the local rigidity imposed on the spin configuration of each triangle in the STA. The argument used to explain this rigidity is that the local fluctuations are massive; thus they do not become critical and can be neglected in studying criticality. While this argument was successfully applied to the colinear antiferromagnet where massive modes do not couple with the massless mode, the application of the local rigidity in noncolinear spin systems is not obvious. This has motivated the present work. Using extensive MC simulations, we study in the present paper the effect of local rigidity on the critical behavior of the STA.

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 systems of linear size L=12, 18, 24, 30, and 36, with periodic boundary conditions. In general, we discarded $1\text{–}2\times 10^6$ MC steps per spin for equilibrating and calculated the energy histogram as well as other physical quantities over 2×10^6 MC steps.

In order to impose local rigidity on the triangles, we first partition the lattice into interacting triangles which *do not have common corners.* This is done as follows: In each XY plane (see Fig. 1) one chooses on the first row one "supertriangle" out of every three triangles. Thus, two nearest supertriangles which do not share a common corner on a row are separated by a head-up and a head-down triangle. This is done for all odd-numbered rows in all XY planes. The spins of the system are then assigned on the supertriangles. Note that each spin belongs to only one supertriangle. Finally, we obtain a system of interacting supertriangles. Local rigidity means that the three spins in each supertriangle form a 120° structure. Except in the g.s., the 120° structure of a supertriangle is not geometrically the same, in spin space, as those of the neighboring supertriangles at finite temperatures T. Thus, local rigidity means that there are no local fluctuations within a supertriangle, but fluctuations between supertriangles are allowed.

The MC updating procedure for the state of the supertriangles is made as follows: At a supertriangle, we take a new random orientation for one of its three spins (two degrees of freedom); we next choose a second spin so as to form with the first spin a 120° angle (one degree of freedom), the orientation of the third spin being that which makes a 120° structure with the first two spins (no free choice). The interaction energy between the spins of this supertriangle with the spins of the neighboring supertriangles is calculated. If it is lower than the energy of the old state, then the new state of the supertriangle is accepted. Otherwise, it is accepted only with a probability, according to the standard Metropolis algorithm. We next move to another supertriangle for updating.

To use the histogram technique, we first estimate roughly the "transition" temperature T_0 at each lattice size and calculate at T_0 the energy histogram as well as the following quantities:

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

$$\langle \chi\rangle = \frac{N(\langle O^2\rangle - \langle O\rangle^2)}{k_BT} , \tag{3}$$

$$\langle (O)'\rangle = \langle OE\rangle - \langle O\rangle\langle E\rangle , \tag{4}$$

$$\langle (O^2)'\rangle = \langle O^2E\rangle - \langle O\rangle^2\langle E\rangle , \tag{5}$$

$$\langle (\ln O)'\rangle = \frac{\langle OE\rangle}{\langle O\rangle} - \langle E\rangle , \tag{6}$$

$$\langle (\ln O^2)'\rangle = \frac{\langle O^2E\rangle}{\langle O^2\rangle} - \langle E\rangle , \tag{7}$$

$$\langle V\rangle = 1 - \frac{\langle E^4\rangle}{3\langle E^2\rangle^2} , \tag{8}$$

$$\langle U\rangle = 1 - \frac{\langle O^4\rangle}{3\langle O^2\rangle^2} \tag{9}$$

$$\langle (U)'\rangle = \langle UE\rangle - \langle U\rangle\langle E\rangle , \tag{10}$$

where E denotes 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, $\langle\cdots\rangle$ 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]

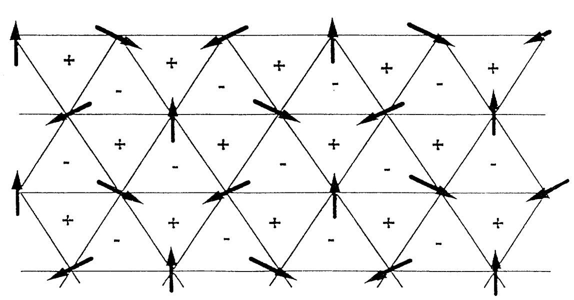

FIG. 1. A g.s. configuration of the STA (120° structure) shown in an XY plane. The chirality of each triangle is indicated by + or −. The other g.s. configuration with opposite chirality is obtained by reversing all spins.

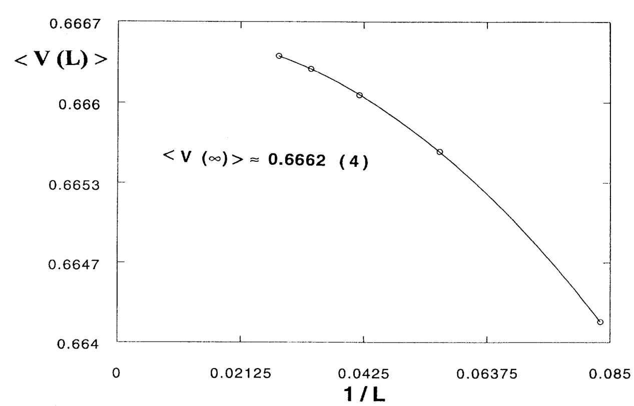

FIG. 2. The energy cumulant $\langle V\rangle$ as a function of $1/L$.

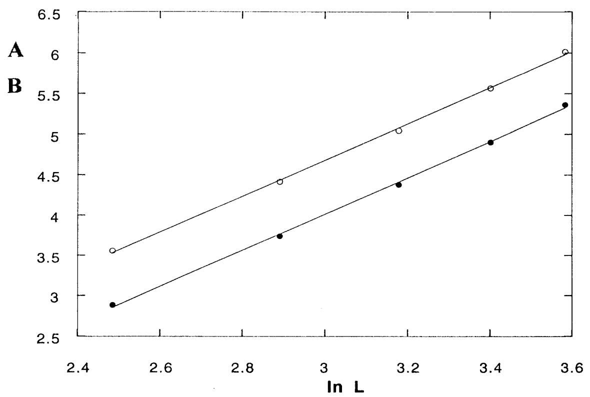

FIG. 3. $A = \langle(\ln O)'\rangle_{\max}$ and $B = \langle(\ln O^2)'\rangle_{\max}$ versus $\ln L$ (upper and lower curves, respectively). The slopes of the two curves are the same and are equal to $1/\nu = 2.08$.

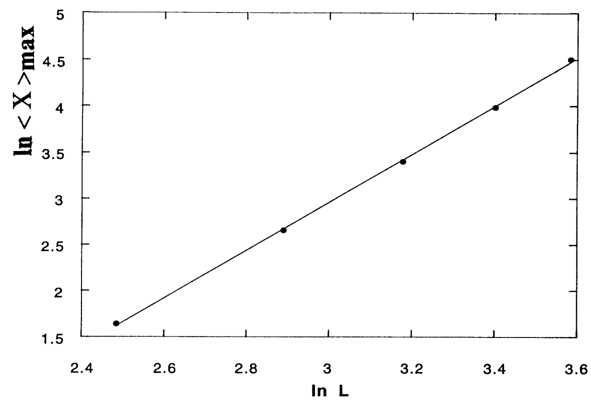

FIG. 4. Maximum of susceptibility $\langle\chi\rangle$ as a function of L in a log-log scale. The slope yields $\gamma/\nu = 2.596$.

III. RESULTS

The transition is found to be of second order. The energy cumulant $\langle V\rangle$ does tend to 2/3 at the transition for increasing size as it should be in a second-order transition. This is shown in Fig. 2.

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 $T_c(\infty) = 1.431 \pm 0.001$. The exponent ν can be obtained from the inverse of the slope of $\langle(\ln O)'\rangle_{\max}$ and $\langle(\ln O^2)'\rangle_{\max}$ versus $\ln L$. This is shown in Fig. 3 where $\nu = 0.44 \pm 0.02$. The critical exponents β and γ are obtained by plotting $\ln\langle O\rangle$ (not shown) and $\ln\langle\chi\rangle_{\max}$ versus $\ln L$, respectively. They are $\beta = 0.19 \pm 0.03$ and $\gamma = 1.16 \pm 0.07$ (see Fig. 4). These exponents are completely different from those of the original STA (without local rigidity) (see values of exponents given in Sec. II). They are also different from those of the $O(4)$ universality class which are $\nu = 0.74$, $\beta = 0.39$, and $\gamma = 1.47$.

Several remarks are in order.

(i) The local rigidity *does change* the critical exponents the phase transition.

(ii) Even when one imposes local rigidity on the STA, one does not find the scenarios predicted by the NLS model in the $2+\epsilon$ expansion.[10]

At this stage, it is interesting to note that a recent MC simulation[14] performed on a system of interacting triads (or model of perpendicular vectors), which is equivalent to the STA when a continuum limit is first taken on the STA and the local rigidity is then imposed,[10] showed also a second-order transition with the same exponents within statistical errors. It means that the model of interacting triads used in the NLS calculation[10] and the model of rigid triangles considered here are equivalent. However, the fact that the present MC results disagree with the NLS results means that the subsequent approximations used in the NLS model,[10] for instance, the continuum limit performed at some later steps, may make the nature of the transition different from that found here by MC simulations for a discrete lattice system.

IV. CONCLUSION

We have studied here the nature of the phase transition in the STA by imposing a local rigidity on all triangles as used in the NLS model. We do not find the same critical exponents as those found for the STA without local rigidity. We conclude that the imposed local rigidity changes the nature of the transition. In addition, the obtained critical exponents are different from those of $O(4)$ found in the NLS calculation. Therefore, we believe 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.

We hope that this work sheds light on the above-mentioned controversy about the nature of phase transition in helimagnets, and will stimulate further theoretical investigations on this problem.

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