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First-order transition in antiferromagnetic stacked triangular lattices with vector spins

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In this article, we show by Monte Carlo simulations that the phase transition is definitely of first order in the antiferromagnetic stacked triangular lattices with both classical XY and Heisenberg spins in a range of the antiferromagnetic next-nearest neighbor interaction J_2. The phase diagram in the $(J_2/J_1, T)$ space (J_1: nearest-neighbor interaction,T: temperature) is shown and discussed.

I. INTRODUCTION

The nature of the phase transition in the stacked triangular lattices with classical vector spins interacting with each other via nearest-neighbor (nn) antiferromagnetic interaction J_1 has been extensively studied during the last few years.[1-4] Even so, it remains an open question at present: for example, in the case of Heisenberg spins, while there is an agreement between various authors about the values of the critical exponents, Kawamura[1,2] has conjectured a new class of universality in contradiction to Azaria, Delamotte, and Jolicoeur,[3,4] who predicted that if the phase transition is not of first order, then it is of second order with either mean-field tricritical exponents or the known $O(4)$ ones. Generally speaking, the stacked antiferromagnetic triangular lattices (SAFTL) belong to the family of helimagnetic structures and an important number of experimental investigations has been done to study the nature of the helimagnetic-paramagnetic transition.[5-10] Though most of the experimental data seem to give the critical exponents in agreement with those predicted theoretically,[1-4] some of them do not exclude the possibility of a weakly first-order transition,[9] and in the Holmium case, there is no such agreement.[10] Monte Carlo (MC) simulations of a helical structure on a body-centered tetragonal lattice show, in the case of Heisenberg spins, a continuous transition with critical exponents similar to those obtained for the SAFTL.[11] However, these simulations suggested a first-order transition for the case of XY spins.

In this work, we study the nature of the phase transition in the SAFTL with XY and Heisenberg spins, taking into account J_1 and J_2, the nn and next-nearest-neighbor (nnn) interactions, respectively. Our purpose is to study the behavior of the transition in the phase space near the controversy point: If the scenario of tricriticality predicted by Azaria, Delamotte, and Jolicoeur[3] in the Heisenberg case, where only nn interaction is taken into account, is correct, then there should exist in the neighborhood of this point a first-order transition. We find in this work the existence of a first-order transition in the vicinity of the critical value $J_2=0.125J_1$. At this value, a collinear spin configuration coexists with the 120° structure in the classical ground state (GS).

Section II is devoted to the description of the GS structure and the MC method. Results for the Heisenberg case are shown and discussed in Sec. III. A preliminary phase diagram is shown in the phase space $(J_2/J_1,T)$, where T is the temperature. Results for the XY case are also briefly shown. Concluding remarks are given in Sec. IV.

II. MODEL AND METHOD

We consider the SAFTL with vector spins. The triangular lattices are the xy planes and these triangular lattices are stacked along the z axis. The Hamiltonian is given by

$$H=\Sigma_{ij}J_{ij}S_iS_j, \tag{1}$$

where Si (Sj) is a vector spin of unit length occupying the lattice site i (j) and the sum runs over nn and nnn in the xy planes and nn in the z direction. We assume J_1 the antiferromagnetic nn interaction (>0) and J_2 the antiferromagnetic nnn interaction (>0) in the xy planes, and $J_3=J_1$ the nn interaction along the z direction. Hereafter, the energy and temperature will be measured in the unit of J_1.

For vector spins, the classical GS can be determined by minimizing the energy after a Fourier transform.[12] It is given as follows: for $0<J_2<0.125J_1$, the classical GS is the 120° structure, for $0.125J_1<J_2<J_1$, the classical GS degeneracy is continuous; the collinear configurations (one line up one line down) are three particular GS configurations in this range of parameters. For $J_2>J_1$, the CGS is incommensurate with threefold degeneracy: one of the nn spins make an angle α given by: $\cos\alpha=-(1+a)/2a$ where $a=J_2/J_1$.

We have performed extensive MC simulations. The sample sizes used in our simulations are $L\times L\times L$ with $L=12$, 18, 24, 30, and 36. Periodic boundary conditions have been used (in the incommensurate phase, $J_2>J_1$, care has been taken to choose only compatible angles). In each run, from 10 000 to 20 000 MC steps per spin have been discarded for equilibrating and 10 000 to 20 000 MC steps per spin have been used for averaging. We have used various methods to determine the nature of the transition, such as the hysteresis measurements, the procedure proposed by Creutz, Jacob, and Rebbi[13] and the finite-size scaling for the first-order transition suggested by Landau, Challa, and Binder.[14] The details will be shown elsewhere.[15] Hereafter, we show only one typical example for each of the Heisenberg and XY cases.

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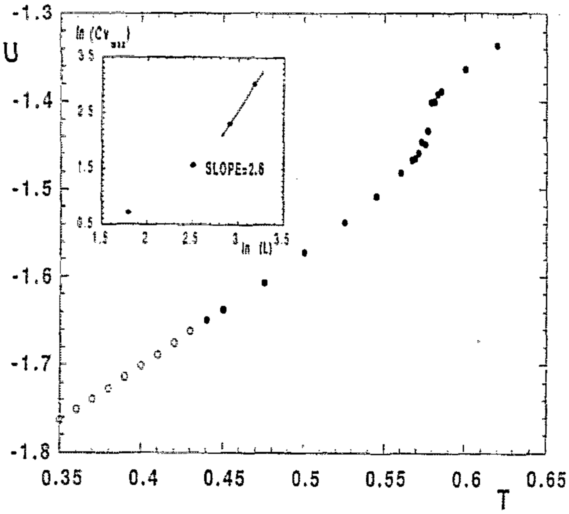

FIG. 1. The Heisenberg case: Internal energy per spin U vs temperature T for $J_2=0.120J_1$. The low T phase is indicated by void circles and the high T one up to paramagnetic phase by solid circles. The low T transition is characterized by a slight (but sudden) change in the slope of U (not easily seen in this scale). The high T transition is of first order. The inset shows $\ln(C_{v\max})$ vs $\ln(L)$.

III. RESULTS

We show first the results for the Heisenberg case. For J_2, small and not close to $0.125J_1$, there is a transition from the 120° structure to the paramagnetic state at a finite temperature. However, when J_2 is larger than about $0.115J_1$, there are two transitions: the low-temperature one is between the 120° structure and a collinear spin configuration and the high-temperature one between the latter and the paramagnetic phase. Figure 1 displays the typical example of the phase transition at $J_2=0.120J_1$. The high-temperature transition is clearly of first order with a "discontinuity" in the internal energy U, while the low-temperature one shows only a slight, but sudden, change in the slope of U (not easy to see in the scale of Fig.1), which gives a discontinuity in the specific heat (not shown here). Though the low-temperature transition has the appearance of a second-order transition, the symmetries of the two phases (120° and colinear) are not compatible; therefore, we do not exclude the possibility of an extremely weak first-order transition. The data of other physical quantities confirm the first-order character of the high-temperature transition. We show in the inset of Fig. 1 the finite size scaling of the maximum of the specific heat, $C_v$max, as a function of L, in a ln-ln scale. The slope for largest sizes studied is 2.6, which shows that for larger sizes, $C_v$max is proportional the system volume. This indicates that the transition is of first order.[14] Figure 2 displays the phase diagram in the phase space $(J_2/J_1,T)$ where the void circles show the first-order transitions. No attempt has been made to determine the critical exponents along the solid curve connecting the squares which show second-order transitions. As said earlier, the nature of the line between the 120° phase and the collinear phase is somewhat uncertain.

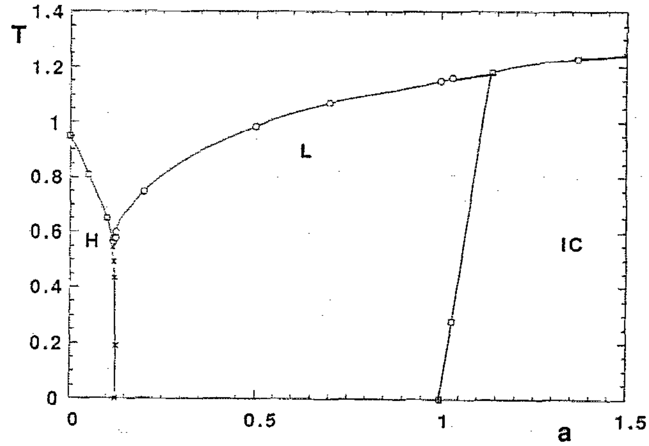

FIG. 2. The Heisenberg case: Preliminary phase diagram in the $(a=J_2/J_1,T)$ space. First-order transitions are shown by void circles. Squares indicate the second-order transitions (see text for comment). L, H, and IC mean collinear, helimagnetic (120° structure), and incommensurate phases, respectively.

The case of XY spins shows behavior very similar to that of the Heisenberg case discussed above. We show a typical example in Fig. 3 where the first-order character of the high-temperature transition is seen with a gap larger than that of the Heisenberg case. The phase diagram also has the same shape as that shown in Fig. 2. The full results together with a detailed analysis will be shown elsewhere.[15]

IV. CONCLUDING REMARKS

The effect of nnn interaction J_2 on the phase transition has been investigated here. The existence of a region of first-order transitions is clearly seen. Due to its close proximity to the controversy point ($J_2=0$), it is possible that the exponents determined there[1,2] are somewhat affected by the first-order region, giving it a tricritical feature.[3] This interpretation may reconcile the previous contradictory

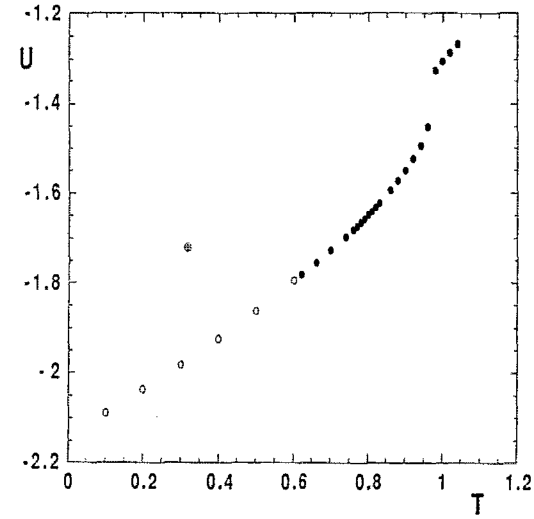

FIG. 3. The same caption as that of Fig. 1 for the XY case.

conclusions.[1,3] This is believed to be true for both the XY and Heisenberg cases. Another interesting finding in this article is the fact that the collinear configurations are preferred at finite temperatures over the infinite number of GS in the range $0.125J_1 < J_2 < J_1$. This phenomenon, which has been called order by disorder, was predicted for vector spin systems by Henley.[16] In addition, one observes that the collinear phase space is extended over the noncollinear ones at finite T. This is seen in Fig. 2, where the curve issued from $J_2 = 0.125J_1$ is canted to the left and that from $J_2 = J_1$ to the right. Therefore, the colinear configurations are preferred at finite T even when they are not ground state. Finally, let us note that the first-order transition between the colinear phase and the paramagnetic phase can be explained as follows: in the colinear phase selected by the phenomenon order by disorder, the degeneracy, apart from the infinite degeneracy due to global rotation, is three, since there are three ways to choose the antiparallel spin pairs in a triangle. This threefold degeneracy is reminiscent of the three-state Potts model in three dimensions. As a consequence, the transition is of first order. Note, however, that unlike the Potts model, there is a possible influence of the continuous degrees of freedom of vector spins (excitations of spin-waves) that can change the nature of the phase transition. This may explain why, away from the critical values of J_2 ($0.125J_1$ and J_1), the first-order character of the transition is weakened (smaller gaps), and in the range $J_2 > J_1$, the transition is of second order. Details will be shown elsewhere.[15]

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