Phase diagram of *XY* antiferromagnetic stacked triangular lattices

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The phase transition in antiferromagnetic stacked triangular lattices with classical XY spins interacting via antiferromagnetic nearest- and next-nearest-neighbor bonds, J_1 and J_2, is studied by means of extensive histogram Monte Carlo simulations. When $J_2=0$, the transition is of second order with critical exponents slightly different from those given by other authors. It is shown that in a range of J_2, the transition is of first order. The general phase diagram in the (J_2,T) space (T, temperature) is shown and discussed. [S0163-1829(96)03530-8]

I. INTRODUCTION

Various properties of frustrated spin systems have been extensively investigated during the last 15 years.[1] In particular, the nature of the phase transition in these systems has been and is still a subject of controversy. Established theories failed to give correct critical properties of frustrated systems. An example is the much studied stacked triangular antiferromagnet (STA). In the case of the Ising model on the STA with nearest-neighbor (NN) interaction, some recent papers show that the transition is of XY universality class[2] in contradiction with the suggestion of a new universality class[3] or with the tricriticality proposed earlier.[4] In the case of Heisenberg spins on the STA, the controversy was even more embarassing.[5–7] Monte Carlo (MC) simulations[8,9,5,10,11] showed that the transition is of second order with critical exponents different from those of known universality classes. Using a renormalization group (RG) technique in a $4-\epsilon$ perturbative expansion,[12] Kawamura has suggested a new universality class for that transition. However, the RG technique for a nonlinear σ (NLS) model with a $2+\epsilon$ expansion showed that the transition, if not of first order or mean-field tricritical, is of second order with the known O(4) universality class.[13–15] Moreover, a recent paper by Antonenko and Sokolov[16] by a RG technique in three dimensions (3D) with a resummation technique shows that the transition in 3D is clearly of first order for both the XY and Heisenberg cases. The scenarios of Azaria *et al.* as well as the prediction of Antonenko and Sokolov are in contradiction with both the suggestion by Kawamura[12] and recent MC results for the Heisenberg case.[9,5,10,11]

For the XY case, Kawamura has also suggested a new universality class from MC and RG calculations.[12,9] The critical exponents of the transition obtained by Kawamura from standard MC simulations are $\nu=0.54\pm0.02$, $\beta=0.253\pm0.01$, $\gamma=1.13\pm0.05$, and $\alpha=0.34\pm0.06$.[9] However, for the XY spins on the bct lattice, the transition was found to be weakly of first order.[17] Furthermore, recent MC results[18] using the histogram technique[19,20] showed that $\nu=0.50\pm0.01$, $\beta=0.24\pm0.02$, $\gamma=1.03\pm0.04$, and $\alpha=0.46\pm0.10$ suggesting that the transition is mean-field tricritical ($\nu=0.5$, $\beta=0.25$, $\gamma=1$, and $\alpha=0.5$). Antonenko and Sokolov[16] on the other hand conclude in favor of a first-order transition.

Given these disagreements and in view of the controversy on the nature of the transition in the Ising and Heisenberg cases, it would be desirable to clarify the situation in the XY case.

The purpose of this paper is to study by the MC histogram technique[19,20] the phase transition of the XY STA with antiferromagnetic NN and next-nearest-neighbor (NNN) interactions, J_1 and J_2, respectively.

When $J_2=0$, we find that the transition has an aspect of second order, in agreement with earlier MC results. We obtain by the highly accurate histogram method the following exponents $\nu=0.48\pm0.02$, $\beta=0.25\pm0.02$, $\gamma=1.15\pm0.05$, and $\alpha=0.46\pm0.10$ which are, except ν, only slightly different from those obtained by Kawamura given above. Our results are also similar to those given by Plumer *et al.*[18] except a marked difference in the value of γ. We will discuss this point later.

Furthermore, we find in this work the existence of a first-order transition at a finite temperature in the interval of J_2 where collinear spin configuration exists. This is clearly seen by using the histogram method.

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

II. MODEL AND METHOD

We consider a system composed of the triangular lattices stacked along the z axis. The Hamiltonian is given by

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

where $\mathbf{S}_i$ is an XY spin of unit length occupying the ith lattice site and the sum runs over NN and NNN pairs in the xy planes (perpendicular to the stacking direction z) and over NN pairs in the z direction. All interactions are antiferromagnetic (>0) with $J_{ij}=J_1$ for the NN in-plane interaction and $J_{ij}=J_2$ for the NNN in-plane interaction. For simplicity, the NN interaction along the stacking direction is assumed to be $J_{ij}=J_1$. Hereafter, the energy and temperature will be measured in units of J_1.

For XY spins (also for Heisenberg spins), the classical ground state (g.s.) can be determined by minimizing the

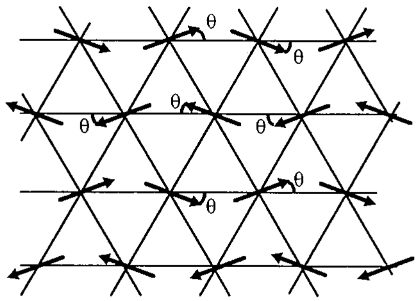

FIG. 1. Ground state configuration for $0.125<a<1$. θ is arbitrary (see text).

energy.[21] It is given as follows: for $0<J_2<0.125J_1$, the classical g.s. is the 120° structure, for $0.125J_1<J_2<J_1$ the classical g.s. degeneracy is continuous, the collinear configurations (one line up, one line down) are particular g.s. configurations in this range of parameters (see Fig. 1). For $J_2>J_1$, the g.s. is incommensurate with threefold degeneracy: spins on each line are parallel and two neighboring spin lines form an angle θ given by $\cos\theta=-(1+a)/2a$ where $a=J_2/J_1$.

We use in this work the histogram MC technique which has been recently developed by Ferrenberg and Swendsen.[19,20] The reader is referred to these papers for details. We have used the systems of $N=L^3$ spins where $L=12$, 18, 24, 30, 36, and 42, with periodic boundary conditions. In addition to these sizes, we used also $L=14$, 28, and 50 in the collinear phase. In general, we discarded 1–2 million MC steps per spin for equilibrating the system and calculated the energy histogram as well as other physical quantities over the next 2 million MC steps. We first estimate as precisely as possible ''transition'' temperature T_0 at each size and calculate at T_0 the energy histogram $P(E)$ (E is the system energy) as well as the following quantities:

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

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

$$\langle(O)'\rangle=\langle OE\rangle-\langle O\rangle\langle E\rangle, \quad (4)$$

$$\langle(O^2)'\rangle=\langle O^2E\rangle-\langle O\rangle^2\langle E\rangle, \quad (5)$$

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

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

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

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

$$\langle(U)'\rangle=\langle UE\rangle-\langle U\rangle\langle E\rangle, \quad (10)$$

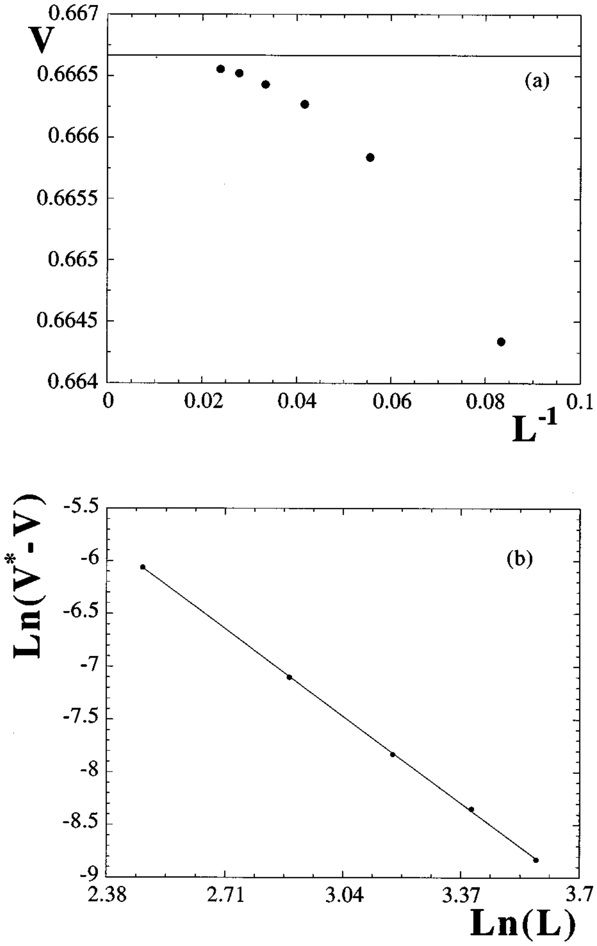

FIG. 2. (a) The fourth-order energy cumulant vs L^{-1} calculated at the critical temperature $T=1.4580$ (see text). The horizontal line is V^*, the value of V extrapolated at infinite size which is 0.666 63(3). (b) ln-ln plot of V^*-V vs L. The slope is 2.52. See text for comments.

where T is 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 $\beta=1/(k_BT)$. Note that the order parameter O is defined in this work as

$$\langle O\rangle=\left\langle\sum_i\left|O_i\right|\right\rangle/N, \quad (11)$$

where O_i ($i=1,2,3$) is the ith sublattice magnetization. This definition is equivalent to the ''noncollinear staggered magnetization'' obtained by making a rotation of $+120°$ ($-120°$) for the second (third) magnetization before summing over the three sublattice magnetizations. Using $P(E)$ calculated at T_0, one can calculate physical quantities at neighboring temperatures, and thus the ''real transition'' temperature at each size is known with precision.[19,20]

III. RESULTS

Let us show first the case where $J_2=0$. The transition is clearly of second order. The energy cumulant V tends to

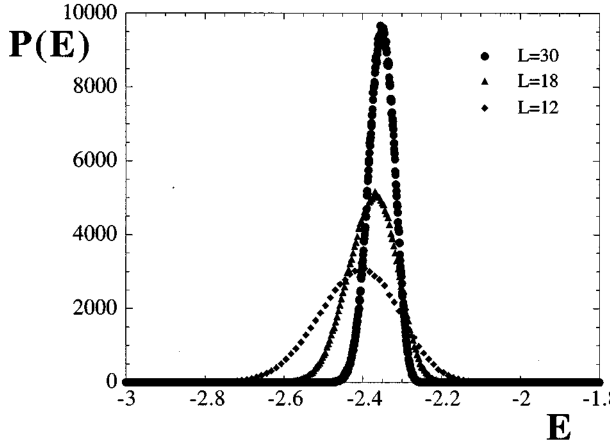

FIG. 3. Energy histogram $P(E)$, E being energy per spin, for different linear lattice sizes $L=12$ (diamonds), 18 (triangles), and 30 (circles), at $T_c(\infty)=1.4580$.

2/3 at the transition for increasing size as it should be in a second-order transition. We show in Fig. 2(a) V as a function of L^{-1}. The extrapolated value at infinite size $V^*=0.666\,63(3)$ is indeed very close to 2/3. Using this value, we plot in Fig. 2(b) $\ln(V^*-V)$ versus $\ln L$. As expected, the points lie on a straight line with a slope equal to 2.52. This slope, which is not 3, means that V is not volume dependent, hence the transition is not of first order. We have varied the simulation temperature T_0 to detect bimodal energy distribution, but we did not find it so. This indicates again that the transition is not of first order. Note however that for extremely weak first-order transitions, simulations at finite sizes cannot give a definite answer. Figure 3 shows $P(E)$ for various sizes at $T=1.4580$ the extrapolated value of the critical temperature at the infinite size (see below).

Using the finite-size scaling for the maxima of $\langle C\rangle$, $\langle\chi\rangle$, $\langle(\ln O)'\rangle$, etc.,[19,20] we obtained the critical temperature for the infinite system which is $T_c(\infty)=1.4580\pm0.0005$ which is the same as that obtained by Kawamura[9] and slightly smaller than that given by Plumer *et al.* which is 1.4584(6).[18] 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. 4 where $\nu=0.48\pm0.02$. The critical exponents γ and β are obtained by plotting $\ln\langle O\rangle_{\max}$ and $\ln\langle\chi\rangle_{\max}$ versus $\ln L$, respectively. They are $\beta=0.250\pm0.02$ (not shown) and $\gamma=1.15\pm0.05$ (see Fig. 5).

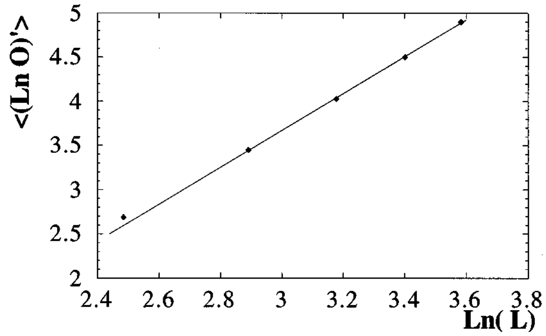

FIG. 4. $\langle(\ln O)'\rangle$ vs $\ln L$. The slope of the curve is equal to $1/\nu=2.08$. $\langle(\ln O^2)'\rangle$ vs $\ln L$ (not shown) gives the same slope.

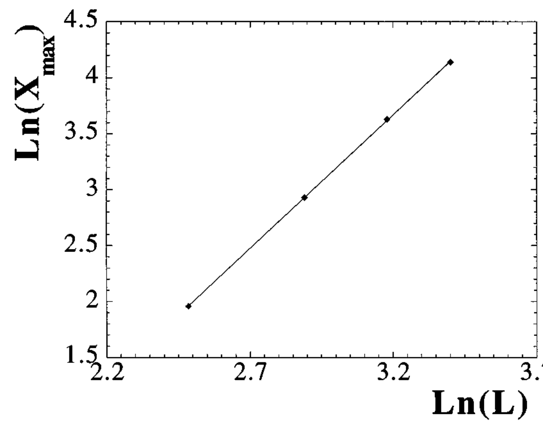

FIG. 5. Maximum of susceptibility χ as a function of L in a ln-ln scale. The slope yields $\gamma/\nu=2.413$.

The critical exponents obtained here are similar to those given by Kawamura[9] except ν. They are also very close to those given by Plumer *et al.*[18] except γ. While Kawamura suggested a new universality class for this transition, Plumer *et al.* argued that it would be mean-field tricritical since their values of ν and γ are close to 0.5 and 1, markedly different from the values given by Kawamura (see the Introduction). Our results show that, while ν is close to 0.5, the value of γ is not that of mean-field tricriticality. The difference between our value of γ and that of Plumer *et al.* comes certainly from simultaneously the estimate of ν and $T_c(\infty)$. In addition, the highly accurate MC results do not indicate a first-order transition in disagreement with the prediction of Antonenko and Sokolov.[16]

The phase diagram in the (T,a) is shown in Fig. 6 where the result using the mean-field theory[22,23] is also displayed. A comparison will be made below. Now, the transition from the collinear ordered phase to the paramagnetic state is of first order. Figure 7 shows the energy distribution at the transition temperature for $a=0.12$. The double peaks observed here even for a very small L indicate the first-order character.

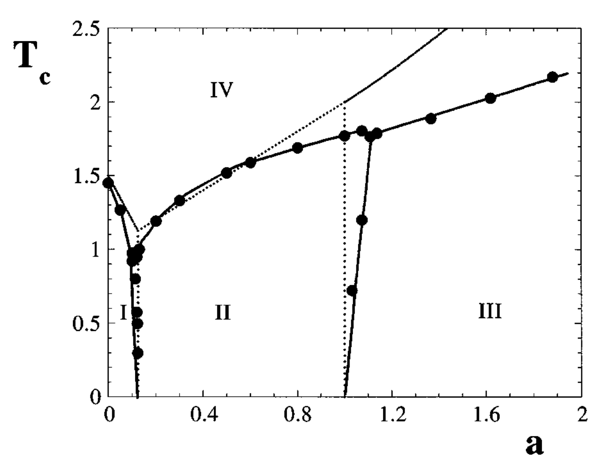

FIG. 6. Phase diagram in the plane (a,T) by Monte Carlo simulations (solid circles). Solid lines are guide to the eye. Phases I, II, III, and IV denote the 120° state, the collinear state, the incommensurate state, and the paramagnetic phase, respectively. The mean-field result is shown by dotted lines. See text for comments.

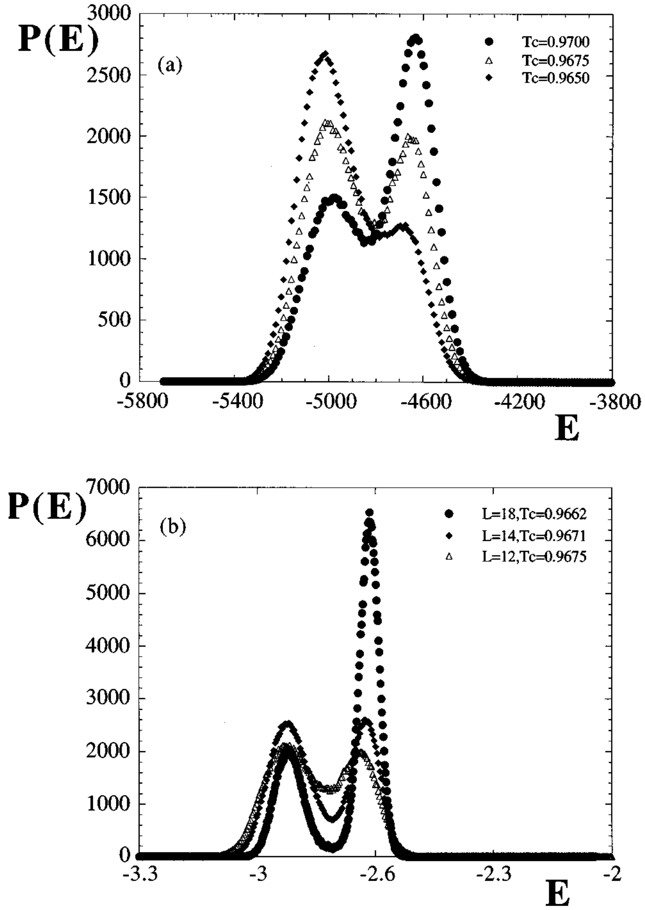

FIG. 7. (a) Energy distribution at three temperatures in the transition region in the case $a=0.120$ and $L=12$. The double peaks are observed for these temperatures, indicating that the transition is of first order with a wide transition region. (b) With increasing sizes, the dip between the double peaks goes to zero, indicating that the energy is discontinuous at the transition.

With increasing sizes, these two peaks are separated by a region of zero probability [Fig. 7(b)], indicating a discontinuity of the energy at the transition. The same thing is found for $a=1$. However, the first-order character at the middle of the line ($a=0.5$, for example) is much more difficult to determine. The first-order character is seen only at a very large size. Figure 8 shows the results from standard MC runs for $L=30$ and $L=50$. As seen, the discontinuity is seen only at $L=50$. The first-order nature is confirmed by histogram MC simulations shown in Fig. 9 where the double peaks are observed. It is interesting at this stage to note that the correlation length at a first-order transition, though finite, may be rather long compared with the lattice size used in simulations. Therefore, care should be taken to make sure that the continuous aspect of the transition is not due to a finite size effect. Otherwise, critical exponents determined from the assumption of a second-order transition are only effective exponents which may not correspond to known universality classes. To be sure that the second-order character observed in the case of $J_2=0$ does not come from small sizes, we have done standard simulation for $L=60$. The results confirm the second order aspect in all physical quantities as shown earlier.

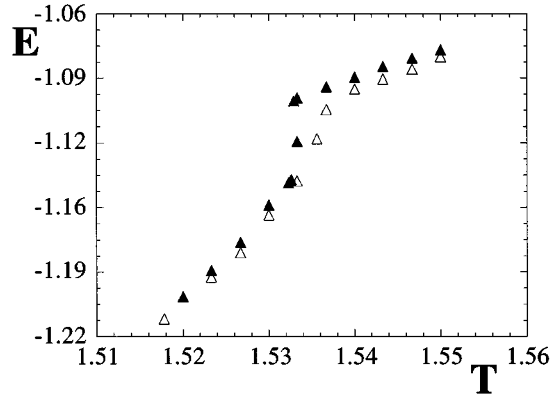

FIG. 8. Finite size effect on the internal energy per spin E for $a=0.5$. The open (solid) triangles are results for $L=30$ (50). See text for comments.

Let us note that in Fig. 6 the critical line issued from $a=0.125$ is canted to the left and that issued from $a=1$ canted to the right, indicating again that the collinear state is favored over the neighboring noncollinear phases at finite temperatures.

Now, let us discuss the mean-field result shown dotted lines in Fig. 6. This result is obtained in each phase by calculating the critical temperature T_c as a function of a (for the method, see Gabay *et al.*[22] and Zhang *et al.*[23] First, although the values of T_c are close to those of MC simulations, the nature of first-order transition cannot be seen by mean field. Second, the lines issued from $a=0.125$ and from $a=1$ are vertical, unlike the MC lines which are canted as discussed above.

IV. CONCLUDING REMARKS

We have calculated by MC simulations the phase diagram of the STA with XY spins. The effect of nnn interaction J_2 is shown to cause the existence of a region of first-order transition. We have also reconsidered the case $J_2=0$. No evidence of a first-order transition was found for this case, in contradiction with the prediction of Antonenko and Sokolov.[16] Our results for the critical exponents are rather

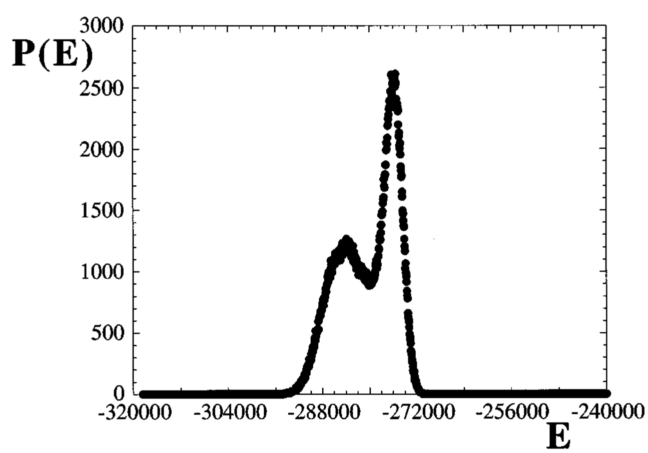

FIG. 9. Bimodal energy distribution at the transition temperature in the case $a=0.5$ and $L=50$. See text for comments.

close to those of Kawamura except ν and to those of Plumer *et al.* except γ as discussed above. It is worthwhile at this stage to discuss the difference between our results and the previous ones. For ν, the two histogram works (the present and that by Plumer *et al.*[18]) give the same exponents except γ. In our opinion, this may be due to the slightly different value of $T_c(\infty)$ used in the two works. The smaller $T_c(\infty)$ is, the larger γ and probably β are. This has been seen in the Ising case.[2] Furthermore, due to the proximity of the first-order line to the controversial point $(J_2=0)$, it is possible that the exponents determined at this point are somewhat affected by the first-order region, giving it some tricritical features. This interpretation may reconcile the previous contradictory conclusions. Another interesting finding in this paper is the fact that the collinear configurations are preferred at finite temperatures over the infinite number of GS in the range $0.125<a<1$. This phenomenon, which has been called order by disorder,[24] was predicted for vector spin systems by Henley.[25] Finally, let us note that the first-order transition between the collinear phase and the paramagnetic phase can be explained as follows: in the collinear phase the degeneracy is three, apart from the infinite degeneracy due to global rotation, 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 which is known to undergo a first-order transition. This may be the origin of the first-order line observed here.

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