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Magnetic-field-induced first-order transition in the frustrated XY model on a stacked triangular lattice

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The results of extensive Monte Carlo simulations of magnetic-field-induced transitions in the XY model on a stacked triangular lattice with antiferromagnetic intraplane and ferromagnetic interplane interactions are discussed. A low-field transition from the paramagnetic to a three-state (Potts) phase is found to be very weakly first order with behavior suggesting tricriticality at zero field. In addition to clarifying some long-standing ambiguity concerning the nature of this Potts-like transition, the present work also serves to further our understanding of the critical behavior at T_N, about which there has been much controversy.

The possibility of unusual critical behavior associated with geometrically frustrated antiferromagnets has given rise to a wide variety of speculation.[1] In the cases of Heisenberg and XY models on the stacked triangular lattice, Kawamura[2] has argued, by means of symmetry analysis and a $4-\epsilon$ renormalization-group expansion, in favor of a new chiral universality class with unusual critical exponents as determined by Monte Carlo simulations. A field-theoretic $2+\epsilon$ expansion by Azaria, Delamotte, and Jolicoeur,[3] however, has inspired the suggestion that such systems exhibit nonuniversality where first-order, mean-field tricritical, or O(4) criticality can occur depending on unspecified details of the model (also see Ref. 4). Two very recent Monte Carlo simulations on the Heisenberg model have yielded different results dependent upon details of the analysis. Bhattacharya *et al.*[5] maintain that this system exhibits O(4) universality whereas the results our own work[6] are inconclusive, possibly consistent with a pseudocritical region.[7] Two similar numerical studies of the Ising model, although yielding substantially the same results, have led to the speculation of yet another universality class by one group,[8] in contrast with our interpretation[9] that the previous suggestion of standard XY universality[10] is confirmed. It is also of interest to note that the Monte Carlo results which led to the proposal of a different universality class associated with the frustrated pyrochlore antiferromagnet[11] have been reinterpreted in support of a first-order transition.[12] It is becoming increasingly clear that the results of direct numerical simulations of frustrated spin systems can be difficult to interpret. The present work represents an attempt to reveal the critical behavior of the XY model on a stacked triangular lattice by application of a magnetic field H. The analysis of these Monte Carlo simulation results is guided by expected behavior based on symmetry arguments of a less controversial nature and lend support to the proposal of tricriticality (or an extremely weak first-order transition) for this system.

This work was inspired by the extensive study of Lee *et al.*[13] who examined the XY antiferromagnet on a triangular lattice (unstacked) in an applied magnetic field. At $H=0$, the transition exhibits Kosterlitz-Thouless behavior, but the field breaks rotational symmetry and transitions involving true long-range spin order occur. For $H>0$, but not too large, a colinear phase is stabilized with the *symmetry* of the three-state Potts model. The real three-state Potts model exhibits a continuous transition in two dimensions (2D) and, after numerous numerical simulations over the past 20 years, it appears to be generally accepted that the transition is weakly first order for the 3D lattice.[14,15] For the so-called continuous three-state Potts model, an effective Landau-Ginsburg-Wilson (LGW) Hamiltonian is constructed which contains a term cubic in the order parameter.[16] Within mean-field theory, such models yield a first-order transition, independent of space dimensionality. The transition in 2D is thus driven to be continuous by critical fluctuations, with known critical exponents verified by the work of Lee *et al.* Some analyses of renormalization-group and series expansions for the 3D case indicate a transition which may be continuous, but most studies favor the first-order scenario.[14,17] The conclusion of an earlier Landau-type analysis, which partially included effects of fluctuations, is that models of this type may exhibit either a continuous or first-order transition depending on relative parameter values.[18] Although contrary results would have been surprising, it was not *a priori* certain that the transition to the three-state ordered phase considered here would be first order. We find convincing evidence that the transition is indeed weakly first order. This study represents a detailed Monte Carlo simulation of a model equivalent to the continuous three-state Potts Hamiltonian in 3D.

We study the Hamiltonian

$$\mathcal{H} = J_\parallel \sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_\perp \sum_{\langle kl\rangle} \mathbf{S}_k \cdot \mathbf{S}_l - H \sum_i S_{xi} \quad (1)$$

where the spins lie in the basal plane, $J_\parallel$ is the interplane interaction, $J_\perp > 0$ indicates the antiferromagnetic coupling which is frustrated for the triangular geometry,

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$\langle i,j \rangle$ and $\langle k,l \rangle$ represent near-neighbor sums along the hexagonal c axis and in the basal plane, respectively, and the field is applied in the basal plane direction x. The magnetic order realized by this model can be conveniently described in terms of a spin density expressed as a low-order Fourier expansion[1]

$$\mathbf{s}(\mathbf{r}) = \mathbf{m} + \mathbf{S}e^{i\mathbf{Q}\cdot\mathbf{r}} + \mathbf{S}^{*}e^{-i\mathbf{Q}\cdot\mathbf{r}}, \qquad (2)$$

where $\mathbf{m}$ is the uniform component induced by the magnetic field, $\mathbf{Q}$ is the wave vector, and the complex polarization vector can be written in terms of real vectors, $\mathbf{S} = \mathbf{S}_a + i\mathbf{S}_b$. The 120° spin structure known to occur at zero field below the Néel temperature T_N is described by a period-3 basal-plane modulation, along with a helical polarization for $\mathbf{S}$. At $H = 0$, the critical behavior is independent of the sign of the interaction $J_{\|}$. For $J_{\|} < 0$ there is no interplane modulation, but for $J_{\|} > 0$ a period-2 structure is stabilized. This difference gives rise to a term cubic in $\mathbf{S}$ in a Landau-type free energy, or LGW Hamiltonian, *only* for the case $J_{\|} < 0$: $F_3 \sim (\mathbf{m}\cdot\mathbf{S})\mathbf{S}\cdot\mathbf{S}$+c.c. For a linearly polarized spin density, one can write $\mathbf{S} = \mathbf{S}_r e^{i\phi}$, where $\mathbf{S}_r \| \mathbf{m}$ is real, to get a contribution $F_3 \sim mS_r^3\cos(3\phi)$. The three (Potts) states arise from the three inequivalent choices of the phase angle $\phi = n\pi/3$, where n is an integer. Higher-order terms in the free energy can stabilize $\phi = (2n+1)\pi/6$ depending on field and temperature values.[19] In this case the cubic term is zero.

In order to determine the magnetic-field temperature phase diagram, standard Monte Carlo simulations were performed on the Hamiltonian (1) with $J_{\|} = -1$ and $J_{\perp} = 1$ for lattices $L\times L\times L$ with L=12–24. Runs of 1–2$\times 10^4$ Monte Carlo steps (MCS) per spin were made, with the initial 4–8$\times 10^3$ MCS discarded for thermalization. Boundary lines were estimated as in our previous work.[20] Not surprisingly, the result shown in Fig. 1 is similar to the 2D case studied by Lee *et al.* In particular, in addition to the paramagnetic phase 1, there are two ordered phases, 6 and 9, with a linear polarization of the spin density and an elliptical phase 7 (phases are numbered following a previous convention).[21] At $H = 0$, the expected 120° spin configuration was observed, with the Néel temperature $T_N \simeq 1.45$ in agreement with Kawamura[2] and Ref. 20. These phases have the same symmetry as determined in the 2D case. Phase 6 with $\mathbf{S}\|\mathbf{H}$ is the three-state Potts phase discussed by Lee *et al.*

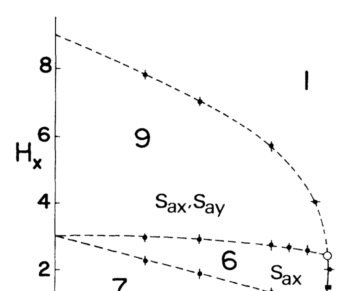

FIG. 1. Phase diagram determined by standard Monte Carlo simulations (points with error bars). Indicated are the paramagnetic phase 1, phases 6 and 9 having colinear order, and phase 7 with an elliptical (chiral) spin structure. Squares at $H = 0.7$ and 1.5 indicate boundary points determined by highly accurate histogram analyses. Solid and dashed lines are guides to the eye and indicate first- and second-order transitions, respectively.

A molecular-field treatment of this model,[22] which yields results independent of dimension, gives a phase diagram where the linear state 6 is absent and two critical lines which merge at T_N. This is somewhat puzzling since the cubic term responsible for the stability of phase 6 occurs in the expansion of the free energy, in powers of $\mathbf{s}(\mathbf{r})$, which can be derived within this mean-field theory. Such an expansion gives an expression for F($\mathbf{m}$,$\mathbf{S}$), which is identical in structure to what is obtained for a phenomenological Landau-type free energy (also mean field).[19,20] The only difference is that in the latter case each of the (six) fourth-order terms have an independent coefficient B_i (since each term is an independent invariant), whereas in the molecular-field treatment all these coefficients are equal. We find that by making just one of the B_i different from the others, a phase diagram with the correct structure (Fig. 1) is found, where the 1-6 boundary is first order as expected.[23] Molecular-field theory appears to somewhat accidentally exclude phase 6. This model also yields the result that the 1-9 phase boundary represents a line of continuous transitions since the phase angle ϕ approaches the value $\pi/6$ at this boundary line, and so the cubic term is not relevant.

The criticality of the 1-6 transition boundary was studied at two points using the Ferrenberg-Swendsen histogram method[24] of analyzing Monte Carlo data. This technique is well suited for the study of transitions which may be very weakly first order, particularly when used to determine the internal-energy cumulant[11,25]

$$U(T) = 1 - \tfrac{1}{3}\langle E^4\rangle/\langle E^2\rangle^2. \qquad (3)$$

This quantity exhibits a minima near T_N, which achieves the value $U^* = \frac{2}{3}$ in the limit $L \to \infty$ for continuous phase transitions. In the case of a first-order transition, $U^* < \frac{2}{3}$ is expected. The histogram method may also be used to determine precisely the location of extrema near T_N which occur in other thermodynamic functions. These are expected to demonstrate simple asymptotic volume dependence in the case of first-order transitions or have an L dependence governed by critical-exponent ratios in the case of continuous transitions. In addition to U, results are given here for the specific heat (C) and staggered susceptibility (χ) as well as the logarithmic derivative of the order parameter (V), which is equivalent to[26]

$$V(T) = \langle ME\rangle/\langle M\rangle - \langle E\rangle, \qquad (4)$$

where the relevant order parameter M is defined as in Ref. 20. Simulations were performed at $H = 0.7$ and $H = 1.5$ on lattices with L=12–33. Thermodynamic averages were made using 1×10^6 MCS for the smaller lattices and up to 2.6×10^6 MCS for the larger lattices, after discarding the initial $2\text{–}3 \times 10^5$ MCS for thermalization. If necessary, several runs at different T were made to ensure that the extrema of the desired function occurred close to at least one simulation temperature. The estimated critical temperatures are 1.488(2) and 1.522(2) for $H = 0.7$ and 1.5, respectively.

Asymptotic scaling of the extrema with volume for the case $H = 0.7$ demonstrated in Figs. 2–4 is consistent with a first-order transition.[7] An indication that it is only weakly first order is revealed by noting that the estimate $U^* = 0.66660(3)$ from Fig. 2 is more than an order of magnitude closer to $\frac{2}{3}$ than the value determined for the five-state Potts model in 2D,[25] 0.66612, considered to be one of the weakest first-order transitions known. It is also of interest to note that the value $U^* = 0.6460(2)$ was determined by Fukugita *et al.*[15] for the discrete three-state Potts model on a cubic lattice, also known to be only weakly first order.[27] Independent estimates for the latent heat, $E_{T_N^+} - E_{T_N^-}$, can be made from our results for U^* as well as the slope of the specific-heat data in Fig. 3, by comparison with analytic expressions given in Ref. 25 and the fact that $E_{T_N^+} \simeq E_{T_N^-}$. Both of these methods yield the same estimate (an indication of the accuracy of these data), 0.017, which is very small (cf. 0.059 for the 2D five-state Potts model and 0.222 for the 3D, three-state Potts model[28]). Similar first-order behavior was found in the data at $H = 1.5$. Evidence that the 1-6 transition becomes more strongly first order as H increases is given by the estimates $U^* = 0.66643(3)$ and $E_{T_N^+} - E_{T_N^-} \simeq 0.032$ at this higher-field value. Histogram data were also taken at H=0.7 for the 6-7 transition, which has a critical temperature estimated to be 1.425(4). In a manner similar to our analysis of a continuous transition on the stacked triangular lattice,[9] scaling consistent with the Ising universality class is evident. This is the expected result as this transition involves only the order parameter S_{by}. Details of these results, along with histogram analyses of the other two transition lines, will be presented elsewhere.[23] Preliminary results for the 1-9 transition indicate this transition is continuous, as it is within the phenomenological Landau-type model discussed above.

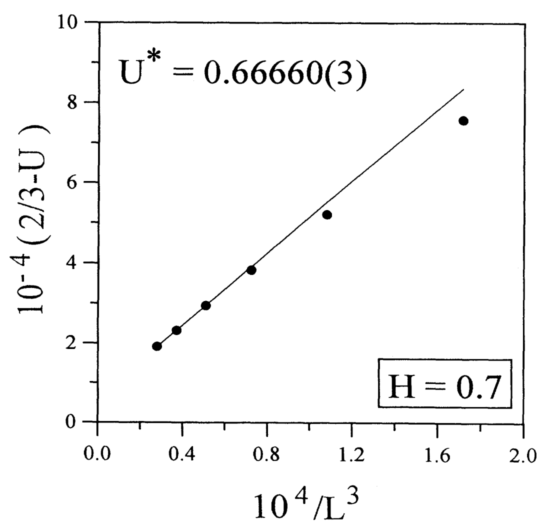

FIG. 2. Scaling of the energy-cumulant minima with volume for the 1-6 transition at $H = 0.7$. Data for $L = 12$ and 15 have been omitted to allow for an expanded scale, emphasizing the larger L results. The straight line represents a fit to the four largest lattice sizes.

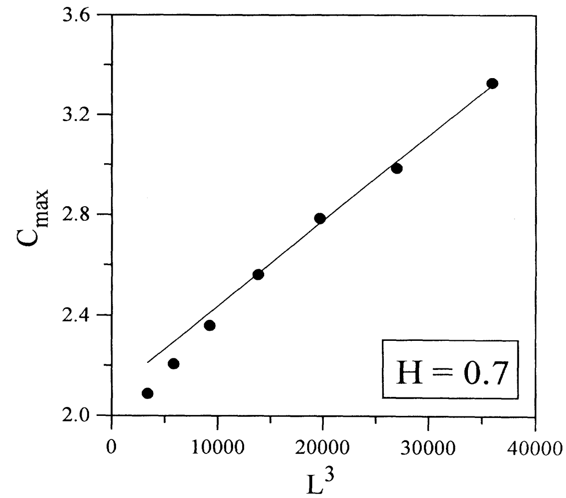

FIG. 3. Scaling behavior of the specific-heat maxima with volume as in Fig. 2.

The corresponding phase diagram for the case of antiferromagnetic interplane coupling has only one linear state with **S**⊥**H** and two critical lines emanating from T_N, which are transitions of XY (S_1) and Ising (Z_2) universality.[20] This structure nicely reveals the $Z_2 \times S_1$ symmetry of the order parameter[2] for the transition at T_N. The results of the present study suggest that this picture does not occur in the case of $J_{\parallel} < 0$ (or for $J_{\parallel} > 0$ with an applied field staggered along the c axis).

The Monte Carlo histogram simulations of this work give a clear indication that the present version of the

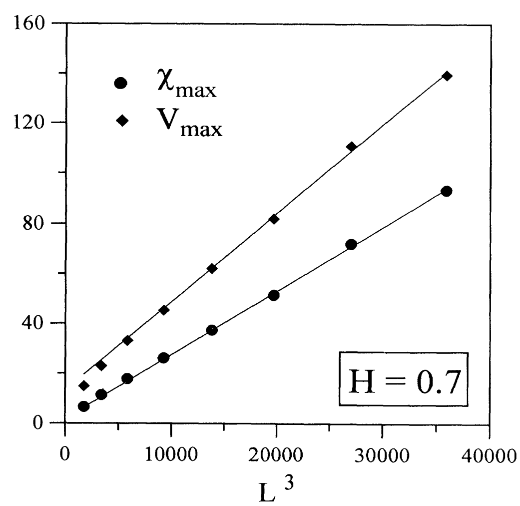

FIG. 4. Scaling behavior of the maxima of the susceptibility χ and logarithmic derivative of the order parameter V as in Fig. 2.

continuous three-state Potts model exhibits a very weak first-order transition in 3D. In addition, our results suggest that this transition becomes more weakly first order as the field is lowered. T_N thus appears to have characteristics in common with a tricritical point, a possibility suggested by Azaria, Delamotte, and Jolicoeur.[3] This scenario is made somewhat ambiguous by the fact that T_N is also a multicritical point where more than one phase meet. The conventional Monte Carlo simulations of Kawamura[2] were used to estimate critical exponents associated with his proposed chiral universality class which are not very different from those expected for mean-field tricriticality (a possibility that was considered in Ref. 2). In view of these results and the recent ambiguity in interpreting Monte Carlo data for the frustrated Heisenberg model,[5,6] as well as the discussion by Peczak and Landau[7] of pseudocritical behavior associated with weakly first-order transitions, our results are consistent with the transition at T_N for the XY model being tricritical or very weakly first order. It appears that only histogram Monte Carlo simulations at T_N which are very extensive (long runs on large lattices) have the possibility to add new information on this problem. As a final point, we note that hexagonal $La_2Co_{1.7}$ appears to be a system described by the present model Hamiltonian.[29]

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