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Tricritical behavior of the frustrated XY antiferromagnet

M. L. Plumer and A. Mailhot*
Centre de Recherche en Physique du Solide et Département de Physique, Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1

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Extensive histogram Monte Carlo simulations of the XY antiferromagnet on a stacked triangular lattice reveal exponent estimates that strongly favor a scenario of mean-field tricritical behavior for the spin-order transition. The corresponding chiral-order transition occurs at the same temperature but appears to be decoupled from the spin order. These results are relevant to a wide class of frustrated systems with planar-type order and serve to resolve a long-standing controversy regarding their criticality.

The nature of phase transitions in frustrated systems that can be mapped onto spin models has been studied extensively over the past twenty years by means of renormalization-group (RG) methods and Monte Carlo (MC) simulations.[1] The triangular antiferromagnet serves as the simplest example of geometry-induced frustration, which in this case gives rise to the noncolinear 120° spin structure. This type of magnetic order can also be described as a helically polarized spin density. The appropriate Landau-Ginzburg-Wilson Hamiltonian is usually taken as

$$\mathscr{H}=r\mathbf{S}\cdot\mathbf{S}^*+(\nabla\cdot\mathbf{S})(\nabla\cdot\mathbf{S}^*)+U_1(\mathbf{S}\cdot\mathbf{S}^*)^2+U_2|\mathbf{S}\cdot\mathbf{S}|^2,$$

where $\mathbf{S}$ is a complex vector and there are *two* fourth-order terms as a consequence of frustration. One reason for the plethora of studies of this Hamiltonian is that in addition to describing helical spin systems, it is also relevant to the dipole phase of superfluid ^{3}He, Josephson-junction arrays in a transverse magnetic field, as well as the fully frustrated bipartite lattice (see Refs. 1 and 2 for references). Although some of the earlier RG studies suggested a continuous transition within standard universality classes, others found evidence for a first-order transition.[2] In view of these results, the tricritical behavior suggested by the histogram MC simulations of the XY stacked triangular antiferromagnet (STAF) reported here may not be too surprising.

Interest in the criticality of frustrated spin systems has recently been enhanced due to the suggestion by Kawamura of "chiral" universality classes associated with the XY and Heisenberg STAF's.[3,4] This claim is partially supported by arguments which demonstrate that the symmetry of the order parameter V in the XY case involves a discrete twofold chiral degeneracy as well as that of the two-dimensional rotation group, so that $V=Z_2\times S_1$.[3–5] If this is indeed the relevant symmetry, and if the transition is neither first order nor tricritical, then the universality class should be different from the standard ones. The strongest support for the existence of these universality classes comes from Kawamura's MC simulations. These were of the conventional type using rather large lattices $L\times L\times L$ with $L=18-60$ but with a possibly modest number of Monte Carlo steps per site (MCS), 6–20 runs with 2×10^4 MCS each. Critical exponents were estimated by the conventional "data collapsing" method, which necessitates a simultaneous estimation of the critical temperature. In the Heisenberg case, the reported values are $\alpha=0.24(8)$, $\beta=0.30(2)$, $\gamma=1.17(7)$, and $\nu=0.59(2)$. These results have recently been corroborated by three different groups using the more accurate finite-size scaling based on histogram MC data.[6–8] In the XY case, the exponent values reported by Kawamura are $\alpha=0.34(6)$, $\beta=0.253(10)$, $\gamma=1.13(5)$, and $\nu=0.54(2)$. Both of these sets of exponents are quite different from those of any standard class in three-dimensions (3D). However, they are somewhat suggestive of mean-field tricriticality (apart from the values for α), where $\alpha=\frac{1}{2}$, $\beta=\frac{1}{4}$, $\gamma=1$ and $\nu=\frac{1}{2}$. Note that it is only Kawamura's estimate for β in the XY case which coincides with these values within error.

Unique sets of exponents were also found for the chirality order, which Kawamura suggests occurs at the same critical temperature. The coincidence, or not, of the two critical temperatures has received much attention in corresponding 2D frustrated systems.[5,9] Most authors appear to support the notion that they are the same.

In contrast with the suggestion of chiral universality, the conclusion of a study of the nonlinear σ model in $2+\epsilon$ dimensions by Azaria *et al.*[10] is that the criticality of such frustrated systems, at least in the Heisenberg case, is nonuniversal. Depending on unspecified system parameters, one can have either standard O(4) criticality, a first-order transition, or mean-field tricritical behavior. It is natural to extend these arguments to the XY case and speculate either a first-order or tricritical transition.[11,12] We note that the nature of the chiral transition was not addressed by these authors.

This already confusing situation was recently further exacerbated by the results of Zumbach's local-potential-approximation treatment of the RG.[13] This work emphasizes the possibility of "almost second-order phase transitions" for frustrated systems, where there can be a set of effective critical exponents (also see Refs. 3 and 14). At least in the Heisenberg case, the distinction between this possibility and that of a chiral universality class may never be satisfactorily resolved by MC simulations.

Although many recently reported experimental results have been interpreted in a way that supports chiral universality,[15] Azaria *et al.* have argued that earlier data are fully consistent with their scenario.

The finite-size scaling of thermodynamic functions evaluated from histogram MC data has demonstrated the ability to

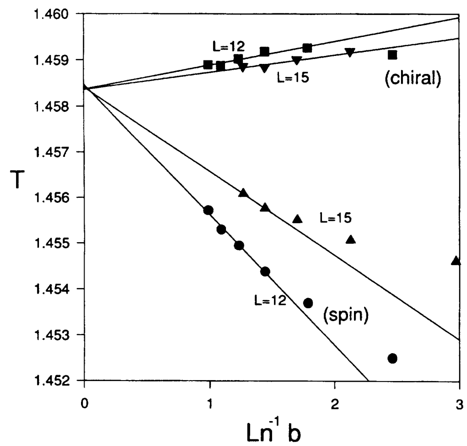

FIG. 1. Results of applying the cumulant-crossing method (see text) to estimate the critical temperatures associated with the spin and chiral orderings where $b=L'/L$.

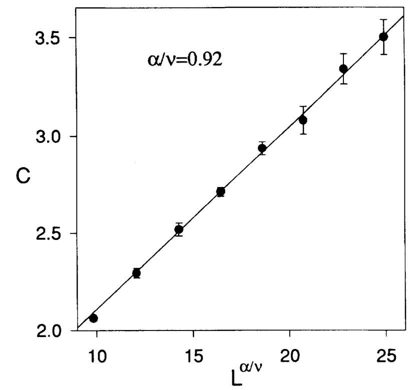

FIG. 2. Finite-size scaling of the specific-heat data for $L=12-33$. Data at L=12 are excluded from the fit. Error bars are estimated from the standard deviation found in the MC runs.

yield highly accurate critical-exponent estimates for unfrustrated systems.[16,17] In addition, this procedure when combined with the cumulant crossing method gives an independent and accurate estimate of critical temperatures.[16] This latter feature is particularly useful for frustrated systems in view of the possibility that spin and chiral degrees of freedom order at different, but nearby, temperatures.

It is hoped that the results of MC simulations presented here will provide convincing evidence that the *XY* STAF exhibits mean-field tricritical behavior.

Near-neighbor antiferromagnetic exchange coupling in the basal plane, $J_\perp=1$, and ferromagnetic coupling along the c axis, $J_\parallel=-1$, were used.[18] The Metropolis MC algorithm was employed in combination with the histogram technique on lattices with $L=12$–33 and runs using 1×10^6 MCS for the smaller lattices and 1.2×10^6 MCS for the larger lattices, after discarding the initial $2\times10^5-5\times10^5$ MCS for thermalization. Averaging was then made over 6 (smaller L) to 17 (larger L) runs. For the largest lattices, this gives a respectable 20.4×10^6 MCS for averaging. The advantage of performing many runs is that errors can be estimated (approximately) by taking the standard deviation. The present work represents one of the very few reports of finite-size scaling of MC data which includes error bars. All histograms were generated at Kawamura's estimate of the critical temperature, $T_c=1.458$.

The correlation time τ for the spin order parameter was estimated[19] to be about 620 MCS at $L=24$ and $T=1.458$. With the assumption $\tau\sim L^2$, it can thus be expected that averaging was performed using roughly 500 independent configurations[20] in a single run for our largest lattice size. Although τ decreases sharply away from T_c, it remains rather large. At $T=1.440$, for example, τ was found to be approximately 200 MCS. This result implies that averaging was made using not more than about eight independent configurations in a single run for Kawamura's simulations at this temperature with $L=60$.

Results of applying the cumulant-crossing method[16] to estimate the critical temperatures associated with both spin and chiral orderings are presented in Fig. 1. The points represent the temperatures at which the order-parameter cumulant $U_m(T)$ at L' crosses the cumulant at $L=12$ or $L=15$. There is considerable scatter in the data and care must be taken to use only results with L sufficiently large to be in the asymptotic region where a linear extrapolation is justified.[16] In the case of the spin order, this appears to be for $\ln^{-1}(L'/L)\leq1.5$ but somewhat larger in the case of chiral order. As with the Heisenberg model, finite-size effects appear much less pronounced for the chiral degrees of freedom.[8] These results suggest that the two types of order occur at the same temperature, $T_c=1.4584(6)$. The possibility that there are two *very* close but distinct ordering temperatures can never be ruled out based on finite-size simulations.[21]

The possibility that the transition is weakly first order was also examined. No evidence for a double-peak structure was found in the energy histograms, consistent with a continuous transition. In addition, the fourth-order energy cumulant U evaluated at T_c yielded a result extrapolated to $L\to\infty$ of $U^*=0.666\,652(20)$, consistent with a value $\frac{2}{3}$ expected for a continuous transition.[22] A somewhat smaller value occurs in the case of a weak first-order transition.[18] We note, however, that other continuous transitions which occur in this model under the influence of an applied magnetic field have values of U^* closer to $\frac{2}{3}$ than found in the present case.[18] Finally, the assumption of volume-dependent scaling of various thermodynamic quantities did not yield a straight-line fit, even for the data at large L.

Finite-size scaling results at T_c for the specific heat C, spin order parameter M, susceptibility (as defined in Kawamura's work[4,8,16]) χ, and the first logarithmic derivative of the order parameter $V_1=\partial[\ln(M)]/\partial K$ (where $K=T^{-1}$)[17] are shown in Figs. 2–4. Exponent ratios were estimated by performing ln-ln plots and also by assuming a scaling dependence $F=aL^x$ for a function of interest (plus a constant term in the case of the specific heat). Except for the specific heat where errors are very large, the two methods gave essentially the same results only if the smaller lattices $L=12$ and $L=15$ were excluded. In order to estimate errors due to the uncertainty in T_c, identical scaling was also performed at $T=1.4579$ and $T=1.4590$. The resulting exponent ratios, along with those associated with chiral order, are presented in Table I. All results correspond to fits performed on data for $L=18-33$, except in the case of the specific heat where $L=15$ data were also included to reduce the error [otherwise,

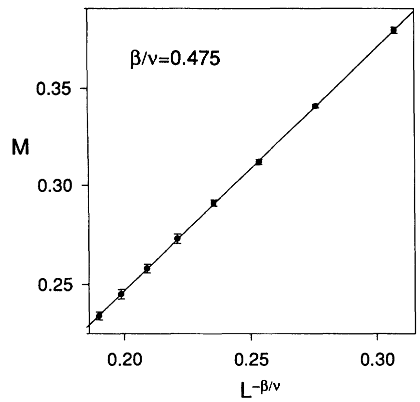

FIG. 3. Finite-size scaling of the order parameter. Data at $L=12$ and 15 are excluded from the fit. Error bars are estimated from the standard deviation found in the MC runs.

the result is $\alpha=0.47(20)$]. The given errors represent the robustness of the fitting procedure and do not account for error bars on the figures. Results for the exponents ν and ν_κ estimated from the *second* logarithmic derivative V_2 (Refs. 8 and 17) are 0.51(1) and 0.55(1), respectively.

For ease of comparison, the results of Kawamura's work are also included in Table I. Note that in order to obtain best-fit exponents by the data-collapsing method, Kawamura used two different values of T_c: 1.458 for spin order and 1.459 for chiral order (within the range of our estimate for T_c). Within errors, however, he concludes that the two transitions were the same.

From the results in Table I, it can be seen that β, γ, β_κ, and γ_κ are the most sensitive to the choice of T_c. Variation in the exponents due to the error bars on the figures was about the same. With these considerations, our best estimate of the exponents and their associated errors at $T_c=1.4584(6)$ are given by $\alpha=0.46(10)$, $\beta=0.24(2)$, $\gamma=1.03(4)$, and $\nu=0.50(1)$ for spin order, and $\beta_\kappa=0.38(2)$, $\gamma_\kappa=0.90(9)$, and $\nu_\kappa=0.55(1)$ for chiral order. These results for the spin order strongly suggest that the transition is mean-field tricritical.

A possible interpretation for this behavior can be found in our recent results of applying an in-plane magnetic field.[18]

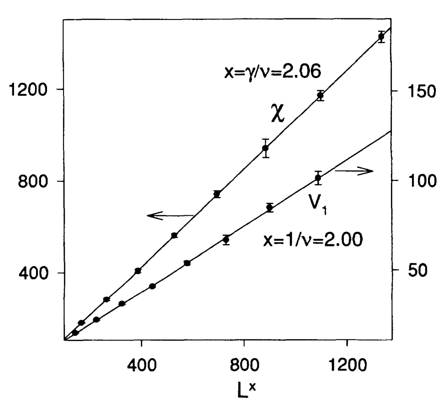

FIG. 4. Finite-size scaling of the susceptibility χ as well as the logarithmic derivative of the order parameter V_1 (see text), as in Fig. 2.

TABLE I. Variation of exponents with assumed critical temperature, along with Kawamura's results.

T_c	1.4579	1.4584	1.4590	Kawamura
α	0.47(8)	0.46(10)	0.39(13)	0.34(6)
β	0.23(1)	0.24(1)	0.26(1)	0.25(1)
γ	1.07(2)	1.03(2)	0.99(2)	1.13(5)
ν	0.51(1)	0.50(1)	0.50(1)	0.54(2)
β_κ	0.36(1)	0.38(1)	0.40(1)	0.45(2)
γ_κ	0.96(2)	0.90(2)	0.81(2)	0.77(5)
ν_κ	0.56(1)	0.55(1)	0.54(1)	0.55(2)

This work reveals that T_c is a multicritical point, with one phase having the symmetry of the three-state Potts model and consequently a weak first order transition. The effect of the field is to generate a term third order in **S** in the free energy, of the form $\sim mS^3$, where m is the $q=0$ Fourier component of the spin density induced by the field. Since the system is frustrated in the triangular plane, one might expect that short-range order along the c axis is already well developed at temperatures near T_c, in the present case corresponding to the spin component m. At zero applied field, coupling between this short-range order and S could generate a third-order term which influences the critical behavior. For other types of systems, there may be similar coupling to other Fourier components.[23]

It is also noteworthy that even though our simulations on the XY model were made with about a factor of 10 more MCS than in the Heisenberg system,[8] larger fluctuations were observed in the present case for the spin order. This can be observed by comparing the cumulant-crossing data of Fig. 1 with the corresponding results of Ref. 8. Larger fluctuations are expected if the transition is at or near a tricritical point.

Our results for the chiral order are more difficult to interpret. The values for the exponents are not too different from those of Kawamura (when the errors are accounted for), and do not correspond to any known universality class (also see Ref. 9). The estimates for ν_κ are in agreement but are significantly different from our value of ν for the spin order. This may indicate that the chiral order has a distinct correlation length and that its criticality is decoupled from the spin order,[9,11] as it is in the 2D TAF.[5]

In conclusion, these results of extensive histogram MC simulations of the stacked triangular XY antiferromagnet strongly support the scenario of tricritical behavior associated with the spin order, in agreement with Azaria *et al.* and in contrast with the proposal of XY-chiral universality by Kawamura. (Recent MC simulations do support, however, the existence of a Heisenberg-chiral universality class.[6–8]) This resolves a long-standing controversy in the literature, and is relevant to a wide class of frustrated systems. Further work is necessary to fully understand the nature of the chiral ordering transition which appears to be decoupled from the spin order.

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*Present address: INRS-EAU, 2800 rue Einstein, C.P. 7500, Sainte-Foy, Québec, G1V 4C7 Canada.

[1] *Magnetic Systems with Competing Interactions*, edited by H.T. Diep (World Scientific, Singapore, 1994).
[2] S.A. Antonenko and A.I. Sokolov, Phys. Rev. B **49**, 15 901 (1994).
[3] H. Kawamura, Phys. Rev. B **38**, 4916 (1988); **42**, 2610(E) (1990); J. Phys. Soc. Jpn. **55**, 2157 (1986).
[4] H. Kawamura, J. Phys. Soc. Jpn. **54**, 3220 (1985); **55**, 2095 (1986); **56**, 474 (1987); **61**, 1299 (1992).
[5] D.H. Lee *et al.*, Phys. Rev. Lett. **52**, 433 (1984); Phys. Rev. B **33**, 450 (1986).
[6] T. Bhattacharya, A. Billoire, R. Lacaze, and Th. Jolicoeur, J. Phys. I (France) **4**, 122 (1994).
[7] D. Loison and H.T. Diep (unpublished).
[8] A. Mailhot, M.L. Plumer, and A. Caillé, Phys. Rev. B **50**, 6854 (1994).
[9] M. Gabay *et al.*, Phys. Rev. B **40**, 264 (1989); E. Granto and M.P. Nightingale, *ibid.* **48**, 7438 (1993); G. Ramirez-Santiago and J.V. José, Phys. Rev. Lett. **68**, 1224 (1992); Phys. Rev. B **49** 9567 (1994).
[10] P. Azaria, B. Delamotte, and Th. Jolicoeur, Phys. Rev. Lett. **64**, 3175 (1990); P. Azaria, B. Delamotte, F. Delduc, and Th. Jolicoeur, Nucl. Phys. B **408**, 485 (1993).
[11] The nonlinear σ model does not strictly apply to the *XY* case. P. Azaria (private communication).
[12] H. Kawamura, Phys. Rev. B **47**, 3415 (1993).
[13] G. Zumbach, Phys. Rev. Lett. **71**, 2421 (1993); Nucl. Phys. B **413**, 754 (1994); **413**, 771 (1994).
[14] P. Peczak and D.P. Landau, Phys. Rev. B **39**, 11 932 (1989).
[15] M.L. Plumer, K. Hood, and A. Caillé, Phys. Rev. Lett. **60**, 45 (1988); B.D. Gaulin *et al.*, *ibid.* **62**, 1380 (1989); J. Wang, D.P. Belanger, and B.D. Gaulin, *ibid.* **66**, 3195 (1991); M.L. Plumer and A. Caillé, *ibid.* **68**, 1042 (1992); R. Deutschmann *et al.*, Europhys. Lett. **17**, 637 (1992); D. Beckmann *et al.*, Phys. Rev. Lett. **71**, 2829 (1993); M. Enderle, G. Furtuna, and M. Steiner, J. Phys.: Condens. Matter **6**, L385 (1994).
[16] P. Peczak, A.M. Ferrenberg, and D.P. Landau, Phys. Rev. B **43**, 6087 (1991).
[17] A.M. Ferrenberg and D.P. Landau, Phys. Rev. B **44**, 5081 (1991); C. Holm and W. Janke, *ibid.* **48**, 936 (1993); K. Chen, A.M. Ferrenberg, and D.P. Landau, *ibid.* **48**, 3249 (1993).
[18] M.L. Plumer, A. Mailhot, and A. Caillé, Phys. Rev. B **48**, 3840 (1993); **49**, 15 133 (1994).
[19] S. Tang and D.P. Landau, Phys. Rev. B **36**, 567 (1987).
[20] A. Ferrenberg, D.P. Landau, and K. Binder, J. Stat. Phys. **63**, 867 (1991).
[21] A.V. Chubukov, Phys. Rev. B **44**, 5362 (1991).
[22] M.S.S. Challa, D.P. Landau, and K. Binder, Phys. Rev. B **34**, 1841 (1986).
[23] O. Heinonen and R.G. Petschek, Phys. Rev. B **40**, 9052 (1989); M.L. Plumer *et al.*, *ibid.* **47**, 14 312 (1993).