Comment on "Multiple-histogram Monte Carlo study of the Ising antiferromagnet on a stacked triangular lattice"

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

A. Mailhot
Institut National de la Recherche Scientifique (EAU), 2800 rue Einstein, C.P. 7500, Ste.-Foy, Québec, Canada G1V 4C7
(Received 5 July 1994; revised manuscript received 1 December 1994)

Histogram analysis of Monte Carlo simulation results of the Ising antiferromagnet on a stacked triangular lattice is reported. Finite-size scaling estimates for critical exponents indicate XY universality. This conclusion supports earlier predictions based on symmetry arguments and is in contrast with the possibility raised by Bunker *et al.* [Phys. Rev. B **48**, 15 861 (1993)] of a new universality class.

Controversy regarding the critical behavior of frustrated spin systems continues.[1] The difficulty in resolving such issues is due partly to the disparity in results, and in their interpretation, among the wide variety of theoretical and numerical approaches available. Even Monte Carlo (MC) simulations performed by two different groups can give results which lead to two different conclusions. Sets of critical exponents associated with different universality classes may differ by only a relatively small amount, especially in the case of the XY and Heisenberg models on the stacked triangular lattice (STL).[2–5] In this paper, finite-size scaling of extensive histogram MC data in the Ising case is shown to yield critical exponents which strongly suggest XY universality. This result supports the symmetry arguments made some 10 years ago by Berker *et al.*[6] and is in contrast with the possibility of a new universality class recently suggested for this system.[7]

The finite-size scaling of histogram MC data can yield highly accurate critical exponents for unfrustrated models.[8,9] For a system of size $L \times L \times L$, exponent ratios determine the scaling with L of both the extrema of thermodynamic functions (except the order parameter) near the critical temperature, T_N, and also these functions evaluated *at* T_N. The latter procedure appears to be both more accurate (especially in the case of the susceptibility) and less computer-time expensive with use of the cumulant-crossing method to obtain reliable estimates of critical temperatures.[8] With the former procedure, histograms must be made at temperatures close to where the extrema occur, which can vary significantly with L. The multiple-histogram technique is useful in this case, but with more computational expense.

Frustrated systems are expected to exhibit more fluctuations due to the proximity of nearly degenerate states.[1] Although much progress has been made in recent years to overcome critical slowing down, these techniques appear largely ineffective on frustrated systems. Special attention must then be given to ensure that MC runs are sufficiently long and that L is sufficiently large for the system to exhibit its true critical behavior.[10]

This paper serves to complement and extend our results on the STL Ising antiferromagnet which focused on the effects of next-nearest-neighbor basal-plane coupling[11] and a magnetic field.[12] With these limited data [i.e., only 1×10^6 MCS (Monte Carlo steps) were used for averaging at each L=12–30], the exponents were estimated by the scaling of extrema of thermodynamic functions also for the near-neighbor model. Given the rather large uncertainties in these results, only *consistency* with XY universality could be claimed.

In contrast, Bunker *et al.*[7] employed the multiple histogram technique to estimate exponents from the scaling of extrema and, although their results are not too far from those of XY universality, the differences were significant enough to raise the possibility that the STL Ising antiferromagnet belongs to a new universality class. Their histograms were generated at L=6–30, with averaging performed using approximately 1×10^6 MCS for the smaller lattices and only 2.2×10^5 MCS at L=30.

We report here the results of extensive MC simulations performed on the STL Ising model with antiferromagnetic near-neighbor exchange coupling in the basal plane, $J_\perp = 1$, and ferromagnetic coupling along the c axis, $J_\parallel = -1$. The Metropolis MC algorithm was used to generate histograms on lattices with L=12–33 using runs with from 5×10^5 MCS for the smaller lattices to 1.2×10^6 MCS for the larger lattices, after discarding the initial 1×10^5–2×10^5 MCS for thermalization. Averaging was then made using from 6 runs for the smaller L to 15 runs at L=30. Averaging was made over 13 runs at L=33. For the largest lattice, this gives a reasonable 15.6×10^6 MCS for averaging. Errors estimated *approximately* by taking the standard deviation of the many runs for each L give some indication of the quality of the data. All histograms were generated at our previous estimate of the critical temperature, $T_N \simeq 2.93$.[11]

Results of applying the cumulant-crossing method[8] to estimate the critical temperature 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

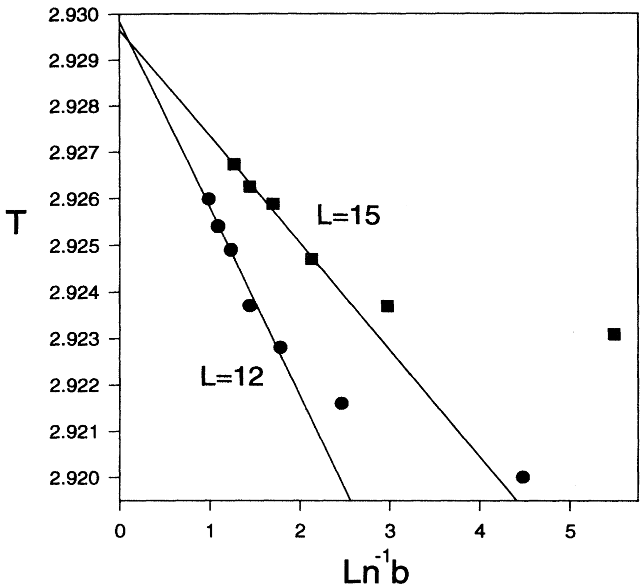

FIG. 1. Results of applying the cumulant-crossing method (see text) to estimate the critical temperature, where $b = L'/L$.

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,[8] i.e., for $Ln^{-1}(L'/L) \lesssim 2.2$. From these results, the critical temperature is estimated to be $T_N = 2.9298(10)$. This value compares well with our previous estimate but differs significantly from that of Bunker *et al.*, $T_N = 2.920(5)$.

Finite-size scaling results at T_N for the specific heat C, spin order parameter M, susceptibility (as defined in Kawamura's work[3,8]) χ, and the first logarithmic derivative of the order parameter $V_1 = \partial[Ln(M)]/\partial K$ (where $K = T^{-1}$)[9] are shown in Figs. 2–5. Except in the case

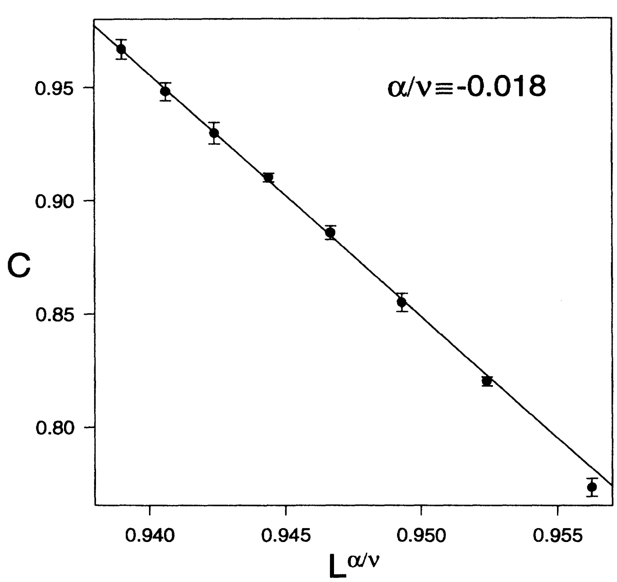

FIG. 2. Finite-size scaling of the specific heat data. Data at L=12 and L=15 is excluded from the fit. Error bars are estimated from the standard deviation found in the MC runs.

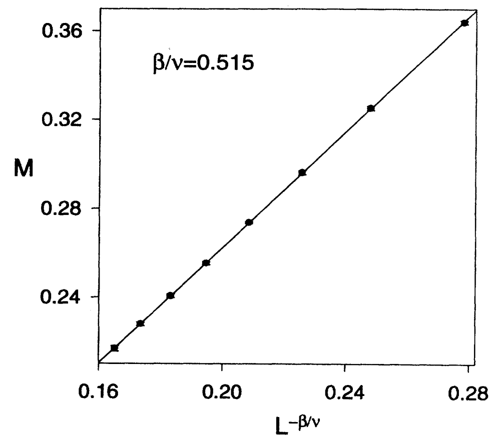

FIG. 3. Finite-size scaling of the order parameter. Data at L=12 and 15 are excluded from the fit. Error bars are estimated from the standard deviation found in the MC runs.

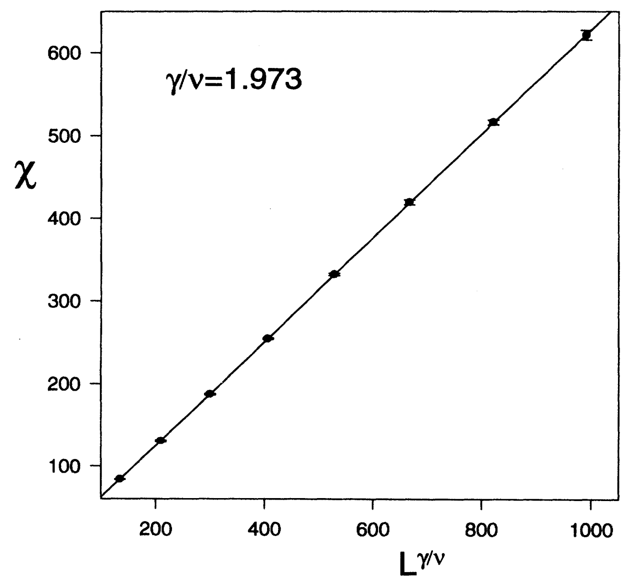

FIG. 4. Finite-size scaling of the susceptibility χ, as in Fig. 3.

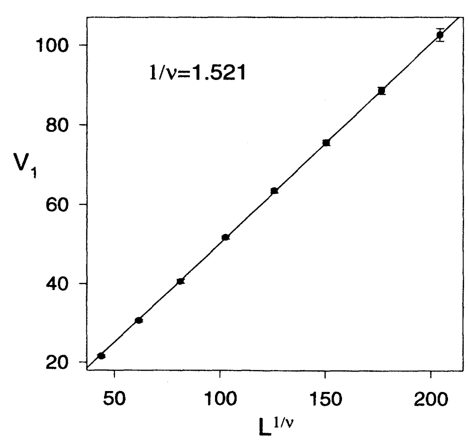

FIG. 5. Finite-size scaling of the logarithmic derivative of the order parameter V_1 (see text), as in Fig. 3.

TABLE I. Comparison of estimates for critical exponents of the unfrustrated XY model and those for the stacked triangular (STL) Ising antiferromagnet.

	α	β	γ	ν
XY: RG $(4-\epsilon)$[a]	−0.013(15)	0.349(4)	1.315(7)	0.671(5)
XY: HT Series[b]	−0.01(2)	0.345(10)	1.323(15)	0.670(7)
XY: HT Series[c]	−0.01(3)	0.348(15)	1.315(9)	0.67(1)
XY: Histogram MC[d]	−0.010(6)	0.347(3)	1.316(5)	0.670(2)
XY: Histogram MC[e]	+0.014(20)	0.331(10)	1.324(1)	0.662(7)
STL Ising: This work[f]	+0.012(30)	0.341(4)	1.31(3)	0.662(9)
STL Ising: Bunker *et al.*[g]	−0.05(3)	0.311(4)	1.43(3)	0.685(3)

[a]Renormalization group from Ref. 13 and scaling relations.
[b]High-temperature series from Ref. 14 and scaling relations.
[c]High-temperature series from Ref. 15 and scaling relations.
[d]From Ref. 16 and scaling relations.
[e]From Ref. 17 and scaling relations.
[f]With α determined from scaling relations.
[g]From Ref. 7 with α determined from scaling relations.

of the specific heat, exponent ratios were estimated by assuming a scaling dependence $F = aL^x$ for a function of interest. Scatter in the data was too large to extract a reliable estimate for α/ν and Fig. 2 shows the scaling results with an assumption of XY universality. A good straight-line fit is obtained using data from the five largest lattices. Estimates for the other exponent ratios were made using either all the data, with the L=12 data excluded, with L=12–15 data excluded, etc. Only the estimates for $1/\nu$ displayed a significant variation when data for the smaller lattices were not included in the fitting procedure. These were made using V_1, with the results 1.531(6), 1.526(5), 1.521(5), and 1.515(5), respectively (quoted uncertainties represent the robustness of the fitting procedure and does not include the effects of the error bars). Corresponding results using the second logarithmic derivative[8] V_2 are 1.536(6), 1.532(5), 1.527(5), and 1.521(4). The sets of values represent fits from 8 (first numbers) to only 5 (last numbers) data points. Although caution must therefore be used in weighing the significance of these latter estimates, the sets of values suggest that $1/\nu \simeq 1.51(2)$ is a reasonable extrapolation for the thermodynamic limit.

Scaling of estimated maxima of the function V_1 was also performed. The result of using our data for L=12–30 is $1/\nu \simeq 1.46$, exactly the value found by Bunker *et al.* With only results L=21–30 included, the estimate $1/\nu \simeq 1.44$ was obtained. Since simulations were all performed at only one temperature (T=2.93), the uncertainty associated with these scaling results is large. For example, the maxima in V_1 at L=30 was found at $T = 2.952$, quite far from the simulation temperature. In principle, larger values for the maxima in V_1 would be obtained if the simulations were performed at temperatures closer to where they occur. This would lead to an increase in the value of $1/\nu$. Similar conclusions may be relevant in the case of the results at L=30 of Bunker *et al.*

The final values quoted for β/ν and γ/ν correspond to fits made with the two smallest lattices excluded. In order to estimate errors due to the uncertainty in T_N, identical scaling was also performed at $T = 2.9288$ and $T = 2.9308$. Uncertainties arising from the error bars indicated on the figures were always found to be smaller. The resulting exponents (using $\nu \simeq 1/1.51 = 0.662$) and error estimates are presented in Table I, along with a variety of exponent estimates for the standard XY model, as well as those of Bunker *et al.* Our results are well within the range of values found for the XY model.

Finite-size scaling of our data (as in Figs. 2–5) was also made with the *assumption* of exponent ratios as estimated by Bunker *et al.* Except perhaps for the susceptibility, there is no visible distinction in the quality of the two sets of straight-line fits. This result emphasizes the need for high-quality statistics in order to obtain reliable exponents. Although a corresponding comparison by Bunker *et al.* using the "data collapsing" method (Figs. 16 and 17 of that work) seems to favor their exponent estimates over those of XY universality, we note that the transition temperature was not used as a fitting parameter as is usual in such plots.[3]

In conclusion, these results clearly indicate that the Ising antiferromagnet on a stacked triangular lattice exhibits a phase transition which belongs to the standard XY universality class. This is in agreement with the symmetry arguments of Berker *et al.*[6] and not with the possibility of a new universality class recently suggested by Bunker *et al.*[7] As noted by these latter authors, their conclusions are contingent upon the absence of large systematic errors. We believe that the critical exponents estimated by Bunker *et al.* are different from ours due to one or more of the following factors. They were made using lattices that were too small; there were insufficient statistics at the larger lattice sizes; the critical temperature was not accurately estimated. The scaling of extrema of thermodynamic functions, rather than at the critical point, may also reduce the accuracy of exponent estimates. These conclusions serve as a general reminder that special care must be taken in the numerical simulation of frustrated spin systems.

This work was supported by NSERC of Canada and FCAR du Québec.

[1] *Magnetic Systems with Competing Interactions*, edited by H.T. Diep (World Scientific, Singapore, 1994).
[2] M.L. Plumer and A. Mailhot, Phys. Rev. B **50**, 16 113 (1994).
[3] H. Kawamura, J. Phys. Soc. Jpn. **54**, 3220 (1985); **55**, 2095 (1986); **55**, 2157 (1986); **56**, 474 (1987); Phys. Rev. B **38**, 4916 (1988); **42**, 2610(E) (1990); J. Phys. Soc. Jpn. **61**, 1299 (1992).
[4] T. Bhattacharya, A. Billoire, R. Lacaze, and Th. Jolicoeur, J. Phys. I (France) **4**, 122 (1994); D. Loison and H.T. Diep, Phys. Rev. B **50**, 16 453 (1994); A. Mailhot, M.L. Plumer, and A. Caillé, *ibid.* **50**, 6854 (1994).
[5] P. Azaria, B. Delamotte, and Th. Jolicoeur, Phys. Rev. Lett. **64**, 3175 (1990); P. Azaria, B. Delamotte, F. Delduc, and Th. Jolicoeur, Nucl. Phys. **B408**, 485 (1993).
[6] A.N. Berker *et al.*, J. Appl. Phys. **55**, 2416 (1984); D. Blankschtein *et al.*, Phys. Rev. B **29**, 5250 (1984).
[7] A. Bunker, B.D. Gaulin, and C. Kallin, Phys. Rev. B **48**, 15 861 (1993).
[8] P. Peczak, A.M. Ferrenberg, and D.P. Landau, Phys. Rev. B **43**, 6087 (1991).
[9] 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).
[10] M.L. Plumer, A. Mailhot, and A. Caillé, Phys. Rev. B **48**, 3840 (1993); **49**, 15 133 (1994); A. Mailhot and M.L. Plumer, *ibid.* **48**, 9881 (1993).
[11] M.L. Plumer *et al.*, Phys. Rev. B **47**, 14 312 (1993).
[12] M.L. Plumer and A. Mailhot (unpublished).
[13] J.C. Le Guillou and J. Zinn-Justin, J. Phys. Lett. (Paris) **46**, L137 (1985).
[14] M. Ferer, M.A. Moore, and W. Wortis, Phys. Rev. B **8**, 5205 (1973).
[15] P. Butera, M. Comi, and A.J. Guttmann, Phys. Rev. B **48**, 13 987 (1993).
[16] W. Janke, Phys. Lett. A **148**, 306 (1990).
[17] A. P. Gottlob and M. Hasenbusch, Physica A **201**, 593 (1993).