Histogram Monte Carlo study of the next-nearest-neighbor Ising antiferromagnet on a stacked triangular lattice

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Critical properties of the Ising model on a stacked triangular lattice, with antiferromagnetic first- and second-neighbor in-plane interactions, are studied by extensive histogram Monte Carlo simulations. The results, in conjunction with the recently determined phase diagram, strongly suggest that the transition from the period-3 ordered state to the paramagnetic phase remains in the XY universality class. This conclusion is in contrast with a previous suggestion of mean-field tricritical behavior.

I. INTRODUCTION

There is little consensus in the recent literature regarding critical phenomena associated with the simple stacked triangular antiferromagnet.[1] In the cases of Heisenberg and XY spin models, noncolinear magnetic ordering gives rise to nontrivial symmetry considerations and this has led to contrasting proposals on the nature of the temperature-driven phase transition from the period-3 state to the paramagnetic phase: The suggestion by Kawamura[2] of new universality classes is not included in the scenario of nonuniversality put forth by Azaria, Delamotte, and Jolicoeur,[3] where first-order, mean-field tricritical or O(4) criticality can occur depending details of the model (also see Refs. 4–7). Even the Ising model on this frustrated lattice has a highly degenerate ground state[8,9] and unusual temperature- and magnetic-field-induced phase transitions.[10] The conclusion from symmetry arguments is that the paramagnetic transition belongs to the standard XY universality class,[11] consistent with preliminary Monte Carlo results.[12] More recently, this simple picture has been challenged by Heinonen and Petschek[13] (hereafter referred to as HP) who made the remarkable proposal that this transition is mean-field tricritical, as inspired by their Monte Carlo analysis of critical exponents, the structure factor, and the observation that a sufficiently large value of third-neighbor in-plane interaction J_3 induces a strong first-order transition to a different type of order. (Such an idea has also found support from recent experimental results.[14]) It thus appears that, independently and for completely different reasons, the suggestion of tricriticality associated with the stacked triangular antiferromagnet was made by both HP (for the Ising model) and Azaria, Delamotte, and Jolicoeur (for the Heisenberg model). It is the purpose of this work to reexamine the scenario proposed by HP through means of more extensive (and more accurate) conventional and histogram Monte Carlo simulations of the Ising model with antiferromagnetic first- and second-neighbor in-plane interactions ($J_1, J_2 > 0$).

A number of studies have been made of the effects of farther-neighbor interactions on the triangular antiferromagnet.[15–17] At a critical value $J_2 > 0$, the period-3 state (C3) is destabilized in favor of magnetic order with a periodicity of 2 (C2). Of particular interest to the present work are the results of recent Monte Carlo determinations of J_2-T (temperature) phase diagrams for Ising[18] as well as XY and Heisenberg[19] models. The paramagnetic transition temperature T_N decreases sharply with increasing J_2 until the critical value, after which T_N increases sharply. With $J_1 = 1$, the critical values of J_2 were found to be approximately 0.10 for the Ising model and 0.125 for XY and Heisenberg models. For each model, the transition line to the C3 state was found to be continuous, within the accuracy of these conventional simulations, whereas the C2 transition is always first order. In the case of Heisenberg and XY models, a continuous transition to an incommensurate (IC) order is observed at larger values of J_2 (e.g., $J_2 \approx 1.1$ in the Heisenberg case).

A simple mean-field argument explains the principal features of these phase diagrams and also reveals a connection with the results of HP. For systems governed by the Hamiltonian

$$\mathcal{H} = \frac{1}{2}\sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

the Fourier transform of the exchange interaction $J(\mathbf{Q})$ determines the wave vector which characterizes the spin modulation of the first ordered state to stabilize as the temperature is lowered. (This result is independent of the number of spin components.) In the case of ferromagnetic interactions along the c axis ($J_0 < 0$), $Q_{\parallel} = 0$ and the modulation occurs entirely in the basal plane. We consider here $J(\mathbf{Q}_{\perp})$ with up to third-neighbor in-plane interactions included.[20] Wave vectors which maximize this function give the desired result, shown in Fig. 1. With $J_3 = 0$, the C2 phase is stabilized for $\frac{1}{8} \leq J_2 \leq 1$ and the IC state is realized for $J_2 \geq 1$. As found by HP, the C2 state also occurs with $J_2 = 0$ and a ferromagnetic third-neighbor interaction. Their critical value $J_3 \sim -0.08$ can be compared with the present mean-field result $J_3 = -\frac{1}{9} \simeq -0.111$. The scenario put forth by these authors calls for interactions between primary C3 and secondary C2 fluctuations to drive the transition first order (to the C3 phase) at very small values $J_3 < 0$. Thus $J_3 \simeq 0$ would be a tricritical point (not to be confused with the multicritical point where C3, C2, and paramagnetic phases meet). In view of the phase diagram Fig. 1 and the results of Ref. 18, such behavior should also be revealed by considering the effects of small J_2 (as done in the present study). Finally, note that the dramatic depression in T_N at the multicritical point observed in the Monte Carlo results of Ref. 18 is seen from Fig. 1 to likely be a result of large critical fluctuations since the IC and C2 phases are degenerate at this value of J_2. The relatively weak dependence of T_N on $J_3 < 0$ observed by HP is consistent with this explanation.

Although the conventional Monte Carlo simulations of Ref. 18 suggest that the transition with $0 \leq J_2 < 0.1$ remains continuous, the implementation of more sensitive finite-size scaling techniques may be required to detect a very weak first-order transition, as might be expected near a tricritical point. The Ferrenberg-Swendsen histogram Monte Carlo method[21–23] has proven useful for

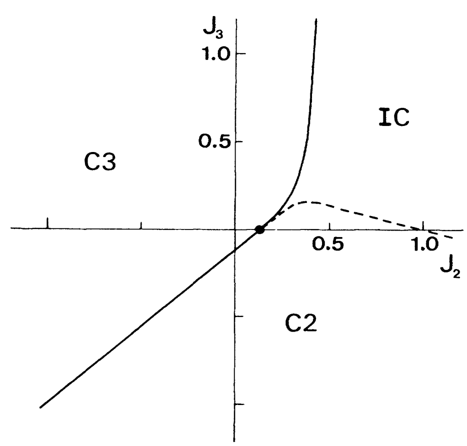

FIG. 1. Phase diagram determined by maximizing $J(\mathbf{Q}_{\perp})$ with up to third-neighbor in-plane interactions (with antiferromagnetic first-neighbor coupling $J_1 = 1$) where C2 and C3 represent commensurate phases of periodicity 2 and 3, respectively, and IC denotes the incommensurate phase. Solid and dashed lines indicate first- and second-order transitions, respectively.

this purpose, especially when used to determine the limiting value of the (internal) energy cumulant[24]

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

This quantity has a minimum at a phase transition, with the property $U(T_N) \to U^* = \frac{2}{3}$ in the infinite-lattice limit. The histogram method allows for the possibility of the precise determination of extrema exhibited by other thermodynamic functions at T_N. The scaling behavior with system size of these quantities can yield accurate estimates of critical exponents in the case of a continuous transition or reveal simple volume dependence if the transition is first order. The utility of this type of Monte Carlo method for the present purposes is very nicely described by Reimers, Greedan, and Björgvinsson.[25] Recently, Bunker, Gaulin, and Kallin[26] made such a histogram analysis of the present model in the case of nearest-neighbor in-plane interactions only. They found critical exponents consistent with XY universality, in contrast with HP. Our work corroborates and extends their results.

Guided by the results of Ref. 18, we test the proposals of HP by performing Monte Carlo simulations at three values of J_2: 0, 0.08, and 0.25. Conventional Monte Carlo analysis at $J_2 = 0$ reveals that the critical region is rather narrow in temperature, thus providing an expalanation for the erroneous exponent estimates given by HP. Extensive histogram simulations at $J_2 = 0.08$ provide convincing evidence that the transition remains continuous and of XY universality. The results at $J_2 = 0.25$ serve as an example of scaling behavior in the case of a first-order transition to the C2 state.

II. $J_2 = 0$

Conventional Monte Carlo simulations were performed for the case of nearest-neighbor in-plane interactions only. Runs of 2×10^4–10^5 Monte Carlo steps (MCS's) per spin were made with the initial 4×10^3–2×10^4 MCS's discarded for thermalization. In the case of smaller runs, quantites were averaged over four independent simulations using random initial-spin configurations. Periodic boundary conditions on lattices $L \times L \times L$ with $L = 12$–30 were used. Finite-size scaling of only the critical exponent β was considered, using the C3 order parameter $M \sim t^{\beta}$ [$t = (T_N - T)/T_N$)] defined in terms of a Fourier component as in Ref. 27. The extrapolation technique of Landau[28] was used on results close to the transition temperature, known from HP to be near $2.9J_1$, to estimate their values for $L \to \infty$. The results are presented in Fig. 2, where $L = 12$ data were excluded in the fit for the highest four temperatures. T_N was then adjusted to yield the best linear fit of the extrapolated data for $\ln(M_{\infty})$ vs $\ln(t)$ plots.

Initial analysis performed on data for $12 \leq L \leq 24$ and $2.0 \leq T \leq 2.7$ yielded values $T_N \simeq 2.82$ and $\beta \simeq 0.19$, close to those of HP. However, a more detailed study using data at larger L and higher T revealed a different set of results. It was difficult to achieve good linear fits of

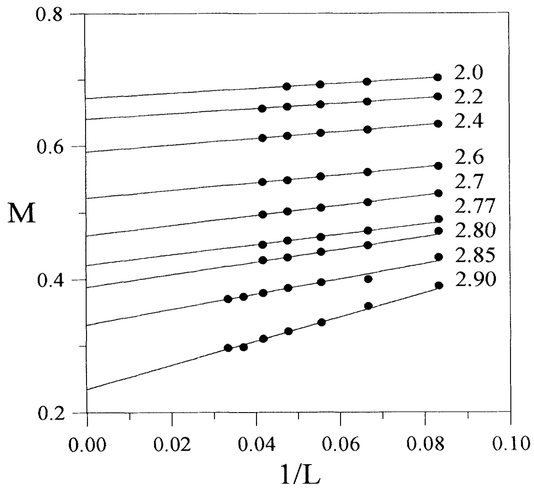

FIG. 2. Finite-size scaling of the order parameter at $J_2 = 0$ and selected temperatures $T = 2.00$–2.90 for lattice sizes $L = 12$–30. L=12 values were excluded from the fit for the four highest temperatures.

all the data between T=2.00 and T=2.90 so that some of the lower-temperature points were excluded. The outcome of this procedure was instructive. Using only the six highest temperatures ($T = 2.60$–2.90) gave the estimates $T_N \simeq 2.92$ and $\beta \simeq 0.30$. Figure 3 shows results with only the four highest temperatures included, which yield the estimates $T_N \simeq 2.93(1)$ and $\beta \simeq 0.33(3)$. The latter values are dramatically different from those of HP but are consistent with more accurate histogram results (see below and Ref. 26) and the expected XY universality. The above analysis strongly suggests that this model exhibits an unusually narrow critical region of temperature. This may be a consequence of the proximity of the C2-order instability and the coupling of these fluctuations to the primary C3 order, as suggested to be important for this model by HP.

Such a system is ideally suited to exhibit the power of the histogram method, where exponents can be extracted from simulations performed *very* close to the transition temperature. Since these simulations were done mainly as a test for later runs at $J_2 = 0.08$ and to corroborate the more detailed study of Ref. 26, only a single histogram was made for each lattice size L=12,15,18,21,24,30 at the temperature T=2.93 with 1.2×10^6 MCS's per spin, where 2×10^5 MCS's were discarded for thermalization. More details are presented in the next section for the case of $J_2 = 0.08$, and in the interest of brevity, we present no data here but state only the results of our analysis. Finite-size scaling of the maxima (or minima) for the specific heat (C), susceptibility (χ), energy cumulant (U), and logarithmic derivative of the order parameter[23]

$$V(T) = \langle ME \rangle / \langle M \rangle - \langle E \rangle \tag{3}$$

yields estimates for α/ν, γ/ν, U^*, and $1/\nu$, respectively. In addition, $M(T_N)$ scales as $L^{-\beta/\nu}$, where T_N can be adjusted to give the best linear fit. The results $\alpha/\nu < 0.2(3)$, $\beta/\nu = 0.50(3)$ (using $T_N = 2.928$), $\gamma/\nu = 2.03(6)$, $1/\nu = 1.46(5)$, and $U^* \simeq 0.666667(5)$ were obtained. (Errors are difficult to assign; those given here are estimated from the robustness of the linear fitting. Evaluation of results from many simulations are necessary to obtain more reliable estimates of statistical errors.) These values compare favorably with renormalization-group results[29] $\alpha/\nu = -0.018$, $\beta/\nu = 0.519$, $\gamma/\nu = 1.96$, and $1/\nu = 1.49$. The quantity $(U^* - U)$ scales as L^{-m}, where in principle $m = \alpha/\nu$. However, only very weak maxima in C and minima in U were observed,[24] consistent with a very small value of α. As noted in Ref. 24, in such cases $(U^* - U)$ may exhibit simple volume dependence. The observed exponent $m \simeq 2.75$ is consistent with this expectation.

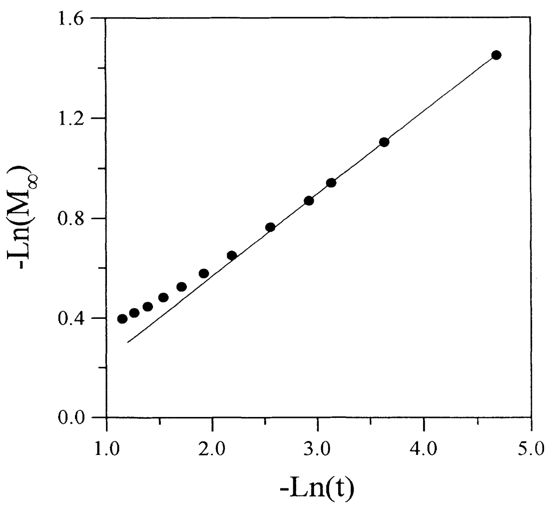

FIG. 3. ln-ln plot of the order-parameter values for $J_2 = 0$ extrapolated to $L \to \infty$ from the results of Fig. 2. Only the four highest temperatures were used in the linear fit, with the results $T_N \simeq 2.93(1)$ and $\beta \simeq 0.33(3)$.

III. $J_2 = 0.08$

Finite-scaling analysis of histogram Monte Carlo simulations for the case of $J_2 = 0.08$ is presented here. A relatively large value of the second-neighbor coupling was desired to enhance the possibility of observing first-order effects, but not too close to the multicritical point at $J_2 \simeq 0.1$, where larger fluctuations might be expected. However, since J_2 is quite small relative to the other energy scale in the model ($J_1 = 1$), longer runs are necessary to fully realize its effects (and achieve the same accuracy as with $J_2 = 0$). With these considerations, it can be expected that the extraction of critical exponents will be less reliable than for the case of $J_2 = 0$.

Simulations were performed using the same parameters as described above for the case $J_2 = 0$, but at two or three different temperatures near the transition estimated from the results of Ref. 18 to be $T_N \simeq 2.2$. This ensured that the histogram was made at a temperature close enough to the extrema of the thermodynamic quantity of interest for the extraction of meaningful results. As a general guide to reliable data, the temperature of

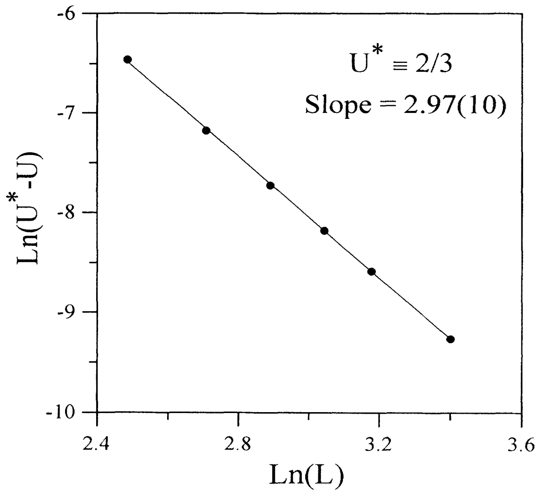

FIG. 4. Scaling of the energy-cumulant minima for $J_2 = 0.08$ with U^* set to $\frac{2}{3}$. The resulting estimate for m is given by the slope.

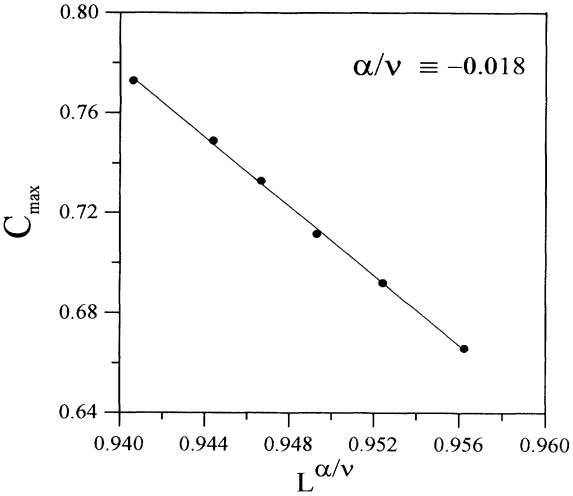

FIG. 6. Scaling behavior of the specific-heat maxima assuming the renormalization-group value of α/ν for the XY universality class.

the extrema should lie within the range determined by half of the maximum of the histogram. If it does not, a new histogram should be generated at a temperature closer to the extrema of the desired function.

Logarithmic scaling plots were made of the various thermodynamic functions as described in the previous section. Convincing evidence that the transition remains continuous is found in results for the energy cumulant, where the value U^*=0.666655(20) was extracted. Figure 4 displays results for $(U^* - U)$, with the assumption $U^* = \frac{2}{3}$; the good linear fit further supports this conclusion. The specific heat (as well as U) again exhibited only very weak temperature maxima, with a small dependence on L, as displayed in Fig. 5. It can be concluded from these data that α/ν is very small. Scaling of the other functions produced the estimates $\beta/\nu = 0.50(3)$ (using $T_N = 2.197$), $\gamma/\nu = 2.07(6)$, $1/\nu = 1.40(5)$, and $m = 3.10(10)$, obtained from all of the data. Using data from only the three largest lattice sizes yielded slightly different results for $\gamma/\nu = 2.00(6)$, $1/\nu = 1.42(5)$, and $m = 3.04(10)$. In an effort to demonstrate further that our data are consistent with XY universality, the scaling plots shown in Figs. 6–9 were made using the renormalization-group exponents. The results are convincing on this point. We note that no visual discrimination could be made between these plots and those made with our extracted exponents.

IV. $J_2 = 0.25$

Finally, a brief summary of histogram results for the case of $J_2 = 0.25$ where a relatively strong first-order

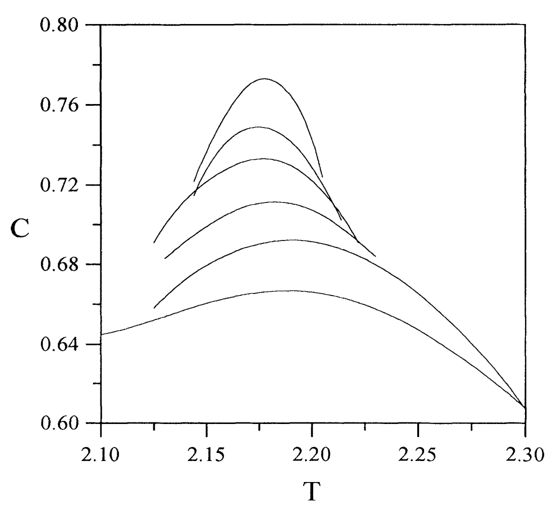

FIG. 5. Temperature behavior of the specific heat showing the weak maxima and small lattice-size dependence for $L = 12$ (lower curve) to $L = 30$ (upper curve).

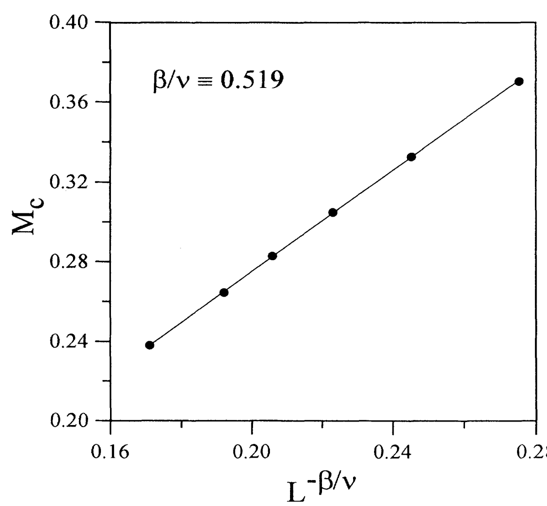

FIG. 7. Scaling behavior of the order parameter at $T_N = 2.195$ assuming the renormalization-group value of β/ν for the XY universality class.

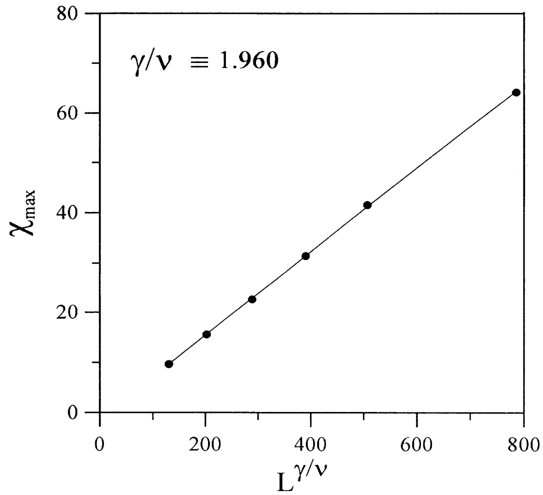

FIG. 8. Scaling behavior of the susceptibility maxima assuming the renormalization-group value of γ/ν for the XY universality class.

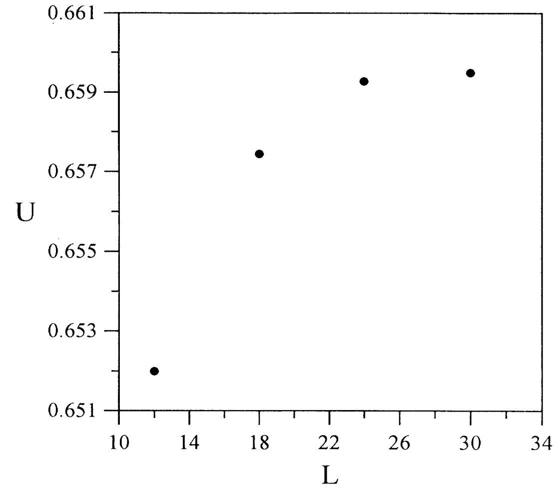

FIG. 10. Scaling of the energy-cumulant minima with L for the case $J_2 = 0.25$. The extrapolated estimate for U^* is 0.6595(3).

transition to the C2 phase is expected.[18] The main purpose of these simulations is to illustrate that the energy cumulant is sensitive to the order of the transition for the present model. Since the ordered state has a periodicity of 2, even values of the lattice size L were used. Simulations were perfomed with L=12,18,24,30 at a range of temperatures guided by considerations as outlined in the previous section, near the known transition point $T_N \simeq 2.66$. Very large fluctuations were found in the results for the χ and V, likely a consequence of metastability effects. Finite-size scaling of these data was not fruitful. Figure 10 displays scaling results for the minima in U, which were used to obtain the saturation value U^*=0.6595(3). This result, along with a reasonably good linear fit of the specific heat maxima vs L^3, confirms the strong first-order nature of this transition and further strengthens the conclusions of the previous section.

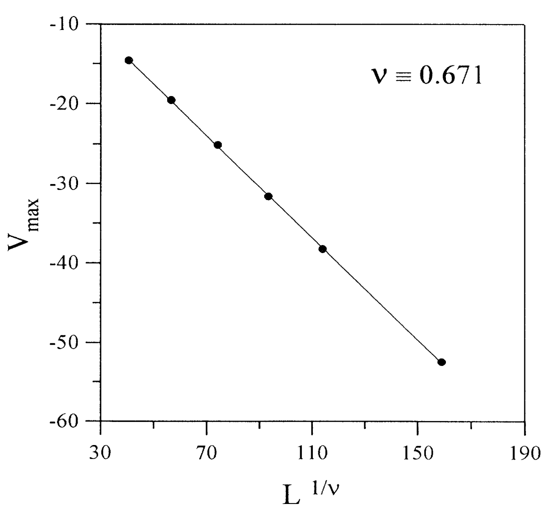

FIG. 9. Scaling behavior of the maxima in the logarithmic derivative of the order parameter (3) assuming the renormalization-group value of $1/\nu$ for the XY universality class.

V. SUMMARY AND CONCLUSIONS

The results presented in this work and in Refs. 18 and 26 strongly suggest that the phase transition associated with the period-3 state of the next-nearest-neighbor Ising antiferromagnet on a stacked triangular lattice exhibits XY universality. In contrast with the proposal by Heinonen and Petschek, no mean-field tricritical behavior is observed. The idea by these authors that the coupling of fluctuations to the nearby period-2 order should be important, however, appears to be responsible for a shrinking of the true critical region and offers an explanation for their erroneous estimates of critical exponents. The histogram Monte Carlo method was found to be ideally suited for the exposition of the real critical behavior in this system. It remains to be tested if these conclusions are relevant in the case of continuous-spin models on this frustrated lattice where there are diverse proposals regarding the criticality.

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