Weak first-order transition in the quasi-one-dimensional frustrated XY antiferromagnet

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

A. Mailhot
INRS-EAU, 2800 rue Einstein, C.P. 7500, Ste.-Foy, Québec, Canada G1V 4C7
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Abstract

The results of finite-size scaling analysis of histogram Monte-Carlo simulations on the stacked triangular XY antiferromagnet with anisotropic near-neighbor exchange interactions are presented. With ferromagnetic interplane coupling ten times stronger than the antiferromagnetic intraplane interaction ($J_\parallel/J_\perp = -10$), a weak first-order transition is revealed. These results represent the first simulational corroboration of a wide variety of renormalization-group calculations made over the past twenty years. As such, they shed light on recent controversy regarding the critical behavior in this and similar frustrated systems and have particular relevance to recently reported data on CsCuCl$_3$.

75.40.Mg, 75.40.Cx, 75.10.Hk

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Although the earliest, as well as the most recent, efforts using $4-\epsilon$ renormalization-group (RG) techniques to study the critical behavior in simple frustrated antiferromagnets (AF) indicated that these systems undergo a fluctuation-induced first order transition, a plethora of other recent studies have resulted in a wide variety of scenarios. The recent interest in this field has been inspired by the proposal of Kawamura of new chiral universality classes in the XY and Heisenberg cases based on his study of the $4-\epsilon$ RG expansion as well as Monte Carlo (MC) simulations [1]. This suggestion is in contrast with results from a $2+\epsilon$ RG expansion of the nonlinear sigma model ($NL\sigma$) from which either an $O(4)$ (in the Heisenberg case), tricritical, or first-order, transition is expected [2]. It is important to note that most of the critical exponents estimated by Kawamura are not so different from those expected at a mean-field tricritical transition. Although all subsequent MC work has been in support of Kawamura’s chiral universality for the Heisenberg system [3], nearly two years ago the present authors published the results of extensive MC simulations which gave strong support to the idea of tricriticality in the XY case [4]. In that work (hereafter referred to as I), a simple hexagonal lattice was considered with AF exchange interactions in the triangular plane $J_{\perp} = 1$, giving rise to frustration, and ferromagnetic coupling along the $c$-axis, $J_{\parallel} = -1$. This model thus represents isotropic near-neighbor couplings. It was also studied with the addition of an in-plane magnetic field $H$, where a weak first order transition was revealed to an unfrustrated 3-state Potts phase at small values of $H$ [5] (hereafter referred to as II). We report here MC simulation results for the XY model using $J_{\perp} = 1$ and $J_{\parallel} = -10$, which represents somewhat quasi-one-dimensional exchange anisotropy. Finite-size scaling of these new data show strong evidence of a first-order transition at the ordering temperature but with a tendency toward tricritical behavior at a slightly higher temperature. These results are consistent with very recent specific heat data on $CsCuCl_3$ [6].

Relevant work published prior to 1995 is discussed in I, Ref. [7], and references therein. It is useful to review here the more recent results pertaining to the present study, beginning with those based on standard RG theory. Higher-order expansions in $4-\epsilon$ have reaffirmed re-
sults from the earlier studies in support of a first-order transition in both XY and Heisenberg cases [8]. In contrast, a partial resummation based on the 1/N expansion has been shown to yield a continuous transition for both models [9]. The delicate nature of this model is further revealed by the very recent proposal of yet another new fixed point based on RG calculations [10]. Detailed re-examinations of the NLσ model have also given rise to a variety of scenarios. Azaria et al. [11] have demonstrated the existence of an additional length scale which may be relevant for the interpretation of MC results on finite-size systems. In another study, this model has been shown to yield a variety of possibilities, including a two-step process (first proposed by Chubukov [12]) where a first order transition to a “nematic” phase is followed by a continuous transition to a chiral state as the temperature is lowered [13]. Although these results may be of relevance to the present work (see below), it should be emphasized that the validity of the NLσ model of frustrated systems has been questioned [14] as, indeed, has the standard Ginsburg-Landau-Wilson approach [2,11]. Other recent theoretical work includes the observation of a two-step transition process in a frustrated two-dimensional model by MC simulations [15], criticality controlled by a Lifshitz point in helimagnets [16], as well as the possibility to investigate chirality using polarized neutrons [17].

In addition to some recent review articles which summarize experimental estimates of critical exponents [18], several new results on specific materials have appeared [19,21,6]. Although many of these data support the existence of chiral universality, most do so only marginally and some data clearly suggest O(4) criticality or a first order transition. Of particular relevance to the present work are the results on CsCuCl3 [6], discussed in more detail below.

As in I and II, the standard Metropolis MC algorithm was used in this work, along with analysis based on the histogram technique, on \( L \times L \times L \) lattices with \( L=12-33 \). However, because the exchange anisotropy causes a lower Metropolis acceptance rate, longer runs (typically by about a factor of two) were employed here, with thermodynamic averages per run calculated using \( 1 \times 10^6 \) MC steps per spin (MCS) for the smaller lattices and
2.5 \times 10^6 \text{ MCS} \text{ for the larger lattices, after discarding the initial } 2 \times 10^5 - 7 \times 10^5 \text{ MCS}
for thermalization. \text{ Averaging was then made over 6 (smaller L) to 16 (larger L) runs, giving } 4 \times 10^7 \text{ MCS for the calculation of averages with the larger lattices. Errors were then estimated by taking the standard deviation of results among the runs.}

A rough determination of the transition temperature was first made by examination
of various thermodynamic quantities in short-run temperature sweeps at \( L = 24 \). \text{ From}
these results, the estimate \( T_c \approx 4.6 \) was made. \text{ Histograms were then generated at } T_0 = 4.55, 4.59, 4.65, 4.69 \text{ and 4.71 in an effort to determine } T_c \text{ more accurately. Two methods}
were used. \text{ At smaller lattice sizes } (L = 12 - 27), \text{ finite-size scaling of extrema in the}
susceptibility \( \chi' \), as well as the logarithmic derivative of the order parameter \( V_1 \) (see Ref. \( \text{[3]} \) for definitions), \text{ were made for both spin and chiral order parameters. Scaling made with}
the assumption of tricriticality (\( \nu = \frac{1}{2} \)) gives a reasonably good straight-line fit and yields
the estimate \( T_c \approx 4.67 \). \text{ The corresponding results for chiral order were nearly identical. Scaling with the assumption of a first-order transition did not yield a good straight-line fit. An accurate determination of the temperature at which extrema occur requires data from}
many histograms generated at different temperatures \( T_0 \). \text{ Our data do not have sufficient}
precision for the simultaneous determination of both } T_c \text{ and } \nu.\text{ For this reason, we also applied the cumulant-crossing method to estimate the critical temperatures corresponding to both spin and chiral orderings. The results shown in Fig. 1 also reveal the effects of relatively large fluctuations and are not amenable to further finite-size scaling analysis (as performed in I) in an effort to better estimate } T_c. \text{ However, it may be observed from these data that the inverse critical temperature } \beta_c \text{ associated with the spin order appears to be near 0.214 (} T_c \approx 4.673 \text{) whereas it is closer to 0.213 (} T_c \approx 4.695 \text{) for the chiral order. It is not possible to claim that there are two distinct transitions by these data alone.}

Finite-size scaling of thermodynamic functions was performed at the two temperatures
\( T=4.673 \) and \( T=4.695 \). \text{ The analysis is complicated by the relatively large finite-size and}
fluctuation effects associated with exchange anisotropy. In an effort to allow for the possi-
bility that the smaller lattices used in this simulation were not sufficiently large to accomo-
date the true critical behavior, scaling of thermodynamic quatities with the functional form
\( F_1 = a + bL^x \) was considered in addition to the usual assumption \( F_2 = bL^x \). (Of course, only the form \( F_1 \) was used for the specific heat). Differences between the estimated critical exponents using these two fitting functions varied considerably. This is believed to be a reflection of the different relative strengths of finite-size effects depending on the thermody-
namic quantity under consideration \[20\]. In some cases, strong effects were also found if the smaller values of \( L \) were not included in the fit.

In general, greater fitting-procedure effects were found for the scaling at the lower tem-
perature, \( T = 4.673 \). Exponent estimates were generally larger if the form \( F_1 \) was used and increased (in most cases) if the smaller \( L \) data were excluded. For example, in the case of the specific heat \( C \) (where \( x = \alpha/\nu \)), exponent values 1.3(3), 1.7(5), and 2.5(10) (where errors reflect only the robustness of the fit) were found using only data for \( L=18-33, 21-33, \) and 24-33, respectively. The dependence of exponent estimates on the assumed fitting function, as well as excluded data, are presented in Table I for \( \chi' \) \( (x = \gamma/\nu) \), \( V_1 \) \( (x = 1/\nu) \), and the order parameter \( M \) \( (x = -\beta/\nu) \). (Only results of fitting the form \( F_2 \) to \( M \) are presented due to the large errors found if the form \( F_1 \) is assumed). The results of these fits are very suggestive of a first-order transition. Note that although no discontinuity is observed in \( M(T) \) at \( T_c \), the small exponent value is indicative of a very sharp rise near the transition, as expected if a jump in \( M \) is smoothed-out due to significant finite-size effects.

Confirmation that finite-size scaling at \( T = 4.673 \) indicates a first-order transition is demonstrated by Figs. 2-4 where good asymptotic straight-line fits are found with the assumption that \( x = 3 \) for \( C, \chi' \) and \( V_1 \) for both spin and chiral order. The data presented in this manner are convincing in view of the discussion in Ref. \[20\], and in particular, of the similar scaling found in II for the transition to the 3-state Potts phase. Although it is known from rigorous symmetry arguments that the 3-state Potts transition is indeed first order, this is revealed only at the larger lattice sizes in MC simulations and is indicative of a very small latent heat. The observation of only asymptotic volume dependence at a
weak first order transition has been previously emphasized [20]. Similar conclusions can be
made regarding the present model. That the transition here is indeed only very weakly first
order, is also evident by the observation of a single peak in the energy histograms as well
as our estimate for the energy cumulant (see I and II), $U^* = 0.666\,6631(3)$. In addition,
the assumption of tricritical exponents yields scaling as in Figs. 2-4 with a noticable (but
small) inferior quality based on goodness-of-fit ($R^2$) tests.

In contrast to these results, finite-size scaling at the higher temperature $T = 4.695$ yields
exponents closer to those expected of tricritical behavior (and with diminished effects due
to the smaller lattices), where $\alpha/\nu = 1$, $\beta/\nu = \frac{1}{2}$, $\gamma/\nu = 2$, and $1/\nu = 2$. For the specific
heat, exponent values $0.3(3)$, $0.6(7)$, and $0.9(12)$ were found using $L=18-33$, 21-33,
and 24-33, respectively. Corresponding results for $\chi'$, $V_1$ and $M$ are presented in Table I.
Scaling with the assumption of tricritical exponents yields a similar quality of asymptotic
straight-line fit to the data as presented in Figs. 2-4, whereas the assumption of volume
dependence yields a somewhat (but clearly) inferior fit.

With the assumption that the transition temperature of the present model is close to
4.67 (based on the reasonable premise that the spin (and not chiral) order parameter is
more relevant in determining $T_c$), the MC analysis presented here is strongly supportive of
several of the very recent theories and experimental results associated with phase transitions
in geometrically frustrated systems. The fact that we find a stronger tendency towards a
first-order transition in the present somewhat-quasi-one-dimensional exchange model than
in I is consistent with arguments put forth in I. In that work, it was noted that the proximity
of the 3-state Potts phase could generate an effective cubic term in the Hamiltonian, the
relative importance of which increases with increasing short-range order along the c-axis
chains. Such short-range order is enhanced by a larger value of $J_\parallel$. These effects are of par-
ticular importance in the present system since the three-dimensional ordering temperature
is reduced by frustration allowing short-range order to be well developed by the time $T$ is
reduced to $T_c$. The very recent mean-field treatment of the $NL\sigma$ model in Ref. [13] also
indicates the importance of cubic contributions to the Hamiltonian.
Perhaps the recent theoretical work of Azaria et al. \cite{11} is most relevant. Their conclusion that true critical behavior may be revealed with MC simulations only by using relatively large lattices is fully consistent with the present results and may eventually be proven relevant for the Heisenberg model.

Conclusion regarding the critical behavior in the somewhat-quasi-one-dimensional ($J_\parallel/J_\perp \simeq -5$) compound $CsCuCl_3$ also appear to support the scenario of a very weak first order transition for frustrated $XY$ systems \cite{6}. These specific-heat data indicate an unusually large exponent $\alpha \simeq 0.35$, suggestive of tricritical behavior, except very close to the transition where first-order behavior is observed. A similar scenario has also been put forth based on the analysis of experimental data on several rare-earth helimagnets \cite{21}.

In conclusion, the finite-size scaling analysis presented here is the first evidence from MC simulations that the frustrated hexagonal antiferromagnet exhibits a weak first order phase transition to the paramagnetic state. This work serves to strengthen the conclusions of several older, and also the most recent, of $4 - \epsilon$ RG analyses as well as new studies based on the $NL\sigma$ model. In addition, a clearer picture is emerging (proximity of the 3-state Potts phase) that explains the difficulty in treating this long-standing problem theoretically, experimentally and numerically.

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TABLES

TABLE I. Dependence of exponents $\chi$ on the assumed critical temperature, fitting function (see text) and excluded data. Errors indicate only the robustness of the fit.

\begin{table}[h]
\centering
\begin{tabular}{ccccccc}
\hline
\multicolumn{6}{c}{$T = 4.673$} \\
$L$ = & 15-33 & 18-33 & 21-33 & 15-33 & 18-33 & 21-33 \\
\hline
$\chi'$ & 2.9(1) & 2.7(1) & 2.8(1) & 2.36(4) & 2.38(4) & 2.41(4) \\
$V_1$ & 2.3(1) & 2.5(2) & 2.7(3) & 2.00(5) & 2.02(6) & 2.07(6) \\
$M$ & & & & -0.365(5) & -0.364(8) & -0.347(3) \\
\hline
\multicolumn{6}{c}{$T = 4.695$} \\
$\chi'$ & 2.17(6) & 2.3(1) & 2.2(2) & 2.12(2) & 2.12(2) & 2.13(2) \\
$V_1$ & 1.83(7) & 1.9(1) & 1.9(2) & 1.78(1) & 1.78(2) & 1.79(2) \\
$M$ & & & & -0.48(1) & -0.501(7) & -0.51(1) \\
\hline
\end{tabular}
\end{table}
FIGURES

FIG. 1. (a) Spin order-parameter cumulant crossing as a function of inverse temperature $(\beta = 1/T)$ for the lattice sizes indicated. (b) Corresponding results for chiral order.

FIG. 2. Finite-size scaling at $T = 4.673$ of the specific heat data for $L = 12 - 33$. Data at $L=12-21$ are excluded from the fit. Error bars are estimated from the standard deviation found in the MC runs.

FIG. 3. Finite-size scaling at $T = 4.673$ of the spin susceptibility $\chi'$ as well as the logarithmic derivative of the order parameter $V_1$ (see text). Data at $L=12-18$ are excluded from the fit.

FIG. 4. Thermodynamic functions associated with chiral order, as in Fig. 3.