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1997 J. Phys.: Condens. Matter 9 L165

(http://iopscience.iop.org/0953-8984/9/11/002)

J. Phys.: Condens. Matter **9** (1997) L165–L170. Printed in the UK PII: S0953-8984(97)81462-2

LETTER TO THE EDITOR

Evidence for a weak first-order transition in the quasi-one-dimensional frustrated *XY*-antiferromagnet

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Received 21 January 1997

Abstract. The results of a finite-size scaling analysis of histogram Monte Carlo simulations on the stacked triangular XY-antiferromagnet with anisotropic near-neighbour 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 behaviour in this and similar frustrated systems, and have particular relevance to recently reported data on $CsCuCl_3$.

Although the earliest, as well as the most recent, efforts using $4-\epsilon$ renormalization-group (RG) techniques to study the critical behaviour 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 (NLσ) 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-neighbour couplings. It was also studied with the addition of an in-plane magnetic field H, where a weak first-order transition to an unfrustrated three-state Potts phase at small values of H [5] (hereafter referred to as II) was revealed. 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 shows evidence of a first-order transition *at* the ordering temperature but with a tendency toward tricritical behaviour at a slightly higher temperature. These results are consistent with very recent specific heat data on $CsCuCl_3$ [6].

0953-8984/97/110165+06$19.50

Table 1. The dependences of the exponents x on the assumed critical temperature, fitting function (see the text), and excluded data. Errors indicate only the robustness of the fit.

	F_1			F_2		
$L =$	15–33	18–33	21–33	15–33	18–33	21–33
$T = 4.673$						
χ'	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)
$T = 4.695$						
χ'	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)

Relevant work published prior to 1995 is discussed in I, reference [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 results 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]. We also note that the recent histogram MC simulations of Boubcheur *et al* [15] on the XY-model corroborate some of the results given in I. MC simulations have also been used to identify a first-order transition in a related frustrated XY-system [16].

In addition to some recent review articles which summarize experimental estimates of critical exponents [17], several new results on specific materials have appeared [18, 20, 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 $CsCuCl_3$ [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 1×10^6 MC steps per spin (MCS) for the smaller lattices and 2.5×10^6 MCS for the larger lattices, after discarding the initial 2×10^5–7×10^5 MCS for thermalization. Averaging was then performed over 6 (smaller L) to 16 (larger L) runs, giving 4×10^7 MCS for the calculation of averages with the larger lattices. Errors were then

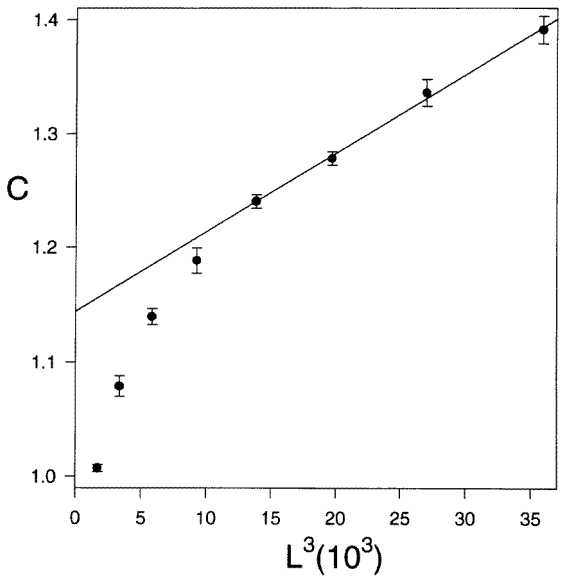

Figure 1. The finite-size scaling at $T = 4.673$ of the specific heat data for $L = 12$–33. Data for $L = 12$–21 are excluded from the fit. The error bars are estimated from the standard deviation found in the MC runs.

estimated by taking the standard deviation of results among the runs. From an estimation of the order-parameter correlation time (following I) at $T = 4.69$, it can be concluded that averaging was made using approximately 500 independent configurations per run for the largest lattice.

A rough determination of the transition temperature was first made by examination of various thermodynamic quantities in short-run temperature sweeps at $L = 24$. From these results, the estimate $T_c \simeq 4.6$ was made. Histograms were then generated at $T_0 = 4.55, 4.59, 4.65, 4.69$ and 4.71 in an effort to determine T_c more accurately. Two methods were used. At smaller lattice sizes ($L = 12$–27), finite-size scaling of extrema in the susceptibility χ', as well as the logarithmic derivative of the order parameter V_1 (see reference [3] for definitions), were made for both spin and chiral order parameters. Scaling performed on the assumption of tricriticality ($\nu = \frac{1}{2}$) gives a reasonably good straight-line fit and yields the estimate $T_c \simeq 4.67$. The corresponding results for chiral order were nearly identical. Our data do not have sufficient precision for the simultaneous determination of both T_c and ν.

For this reason, we also applied the cumulant-crossing method to estimate the critical temperatures corresponding to both spin and chiral orderings. The results also revealed 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. However, it may be observed from these data that the inverse critical temperature β_c associated with the spin order appears to be near 0.214 ($T_c \simeq 4.673$) whereas it is closer to 0.213 ($T_c \simeq 4.695$) for the chiral order. It is not possible to claim that there are two distinct transitions from these data alone.

Finite-size scaling of thermodynamic functions was performed at the two temperatures $T = 4.673$ and $T = 4.695$. The analysis is complicated by the relatively large finite-size and fluctuation effects associated with exchange anisotropy. In an effort to allow for

the possibility that the smaller lattices used in this simulation were not sufficiently large to accommodate the true critical behaviour, scaling of thermodynamic quantities 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 thermodynamic quantity under consideration [19]. 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 temperature, $T = 4.673$. 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 dependences of the exponent estimates on the assumed fitting function, as well as excluded data, are presented in table 1 for χ' ($x = \gamma/\nu$), 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 was 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.

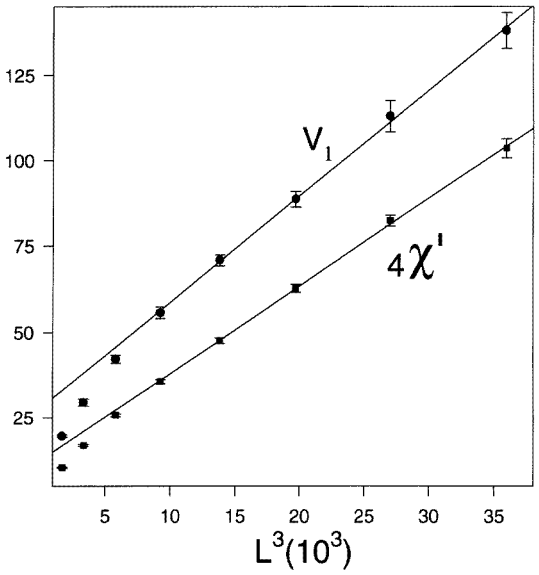

Figure 2. The finite-size scaling at $T = 4.673$ of the spin susceptibility χ' as well as the logarithmic derivative of the order parameter V_1 (see the text). Data for $L = 12$–18 are excluded from the fit.

Confirmation that finite-size scaling at $T = 4.673$ indicates a first-order transition is demonstrated by figures 1 and 2 where good asymptotic straight-line fits are found with the assumption that $x = 3$ for C, χ', and V_1 for both spin orders. Corresponding plots involving the chiral order yield equally good results. *The data presented in this manner*

are convincing in view of the discussion in reference [19], and in particular, of the similar scaling found in II for the transition to the three-state Potts phase. (Note that the asymptotic exponent estimates discussed above are close enough to 3 that such plots appear to yield near-perfect fits.) Although it is known from rigorous symmetry arguments that the three-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 [19]. Similar conclusions can be drawn regarding the present model.

That the transition here is indeed only very weakly first order is also evident from the observation of a single peak in both the energy and order-parameter histograms. That only one peak in $P(E)$ is discernible is fully consistent with the predicted shape of the energy distribution as calculated using our data for the specific heat of figure 1 and the work of Peczak and Landau [19]. Our estimate for the energy cumulant (see I and II), $U^* = 0.666\,6631(3)$, is also consistent with this conclusion. We further note that the assumption of tricritical exponents yields scaling, with a notiecable (but small) reduction in 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 behaviour (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 of 0.3(3), 0.6(7), and 0.9(12) were found using using $L = 18$–33, 21–33, and 24–33, respectively. Corresponding results for χ', V_1, and M are presented in table 1. Scaling on the assumption of tricritical exponents yields a similar quality of asymptotic straight-line fit to the data as presented in figures 1 and 2, 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 forward in I. In that work, it was noted that the proximity of the three-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 particular 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 NLσ model in reference [13] also indicates the importance of cubic contributions to the Hamiltonian.

Perhaps the recent theoretical work of Azaria *et al* [11] is the most relevant. Their conclusion that true critical behaviour 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.

Conclusions regarding the critical behaviour 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 [6]. These specific heat data indicate an unusually large exponent $\alpha \simeq 0.35$, suggestive of tricritical behaviour, except very close to the transition, where first-order behaviour is observed. This interpretation is entirely consistent with the analysis of our MC data at the two temperatures $T = 4.695$ and $T = 4.673$. A similar scenario has also been put forward based on experimental data

available for several rare-earth helimagnets [20].

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. Universality suggests that the transition in the isotropic case is also weakly first order. This work serves to strengthen the conclusions of several older, and also the most recent, $4-\epsilon$ RG analyses as well as new studies based on the NLσ model. In addition, a clearer picture is emerging (proximity of the three-state Potts phase) that explains the difficulty in treating this long-standing problem theoretically, experimentally, and numerically.

We thank E Sorensen for suggesting this work, U Schotte for discussions on $CsCuCl_3$, and the Service de l'Informatique for the partial use of 10 RISC 6000 Workstations. This work was supported by the NSERC of Canada and FCAR du Québec.

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