Short-time dynamics of a family of *XY* noncollinear magnets

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Critical scaling and universality in the short-time dynamics for antiferromagnetic models on a three-dimensional stacked triangular lattice are investigated using Monte Carlo simulation. We have determined the critical point by searching for the best power law for the order parameter as a function of time and measured the critical exponents. Our results indicate that it is possible to distinguish weak first-order from second-order phase transitions and confirm that *XY* antiferromagnetic systems undergo a (weak) first-order phase transition accompanied by pseudocritical scaling.

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I. INTRODUCTION

Frustrated systems [1,2] are characterized by competing interactions which may arise due to either disorder or geometry. The behavior of such systems is often unpredictable but the basic concepts of frustrated systems may provide insights into the physics of complex systems and have practical uses in areas ranging from microelectronics to drug delivery [3–5]. Magnetic systems provide simple examples of frustration where exotic cooperative phases such as the "spin glass," "spin liquid," and "spin ice" are found. During the past twenty-five years a great deal of research effort has been put into investigating the nature of phase transitions in Heisenberg and *XY* frustrated systems in three dimensions [6–11]. Particular attention has been devoted to Heisenberg and *XY* stacked triangular antiferromagnets that are commonly referred to as STA models. These models represent the simplest situation of frustration induced by the geometry of the lattice leading to a critical behavior distinct from that encountered in the usual ferromagnetic case. Indeed, in a triangular lattice, the competition due to antiferromagnetic interactions between nearest neighbor spins leads to a ground state with a planar spin configuration. In each elementary triangular cell the spins form a 120° structure with the vector sum of the three spins equal to zero:

$$\mathbf{S}_A + \mathbf{S}_B + \mathbf{S}_C = \mathbf{0}, \tag{1}$$

where the subscripts *A*, *B*, *C* label the sites at the corner of the elementary triangles shown in Fig. 1. As a consequence the order parameter is no longer a simple vector but a matrix, a fact that has led to the idea that these (noncollinear) frustrated magnets could belong to a new "chiral" universality class [12].

The *XY* STA model has been used to describe a great number of stacked triangular materials including $CsCuCl_3$, $CsNiCl_3$, $CsMnI_3$, and $CsCuCl_3$ as well as the *XY* helimagnets Ho, Dy, and Tb. The experimental results indicate that these materials exhibit second-order phase transitions with the exception of $CsCuCl_3$ where the transition [13] is found to be weakly first order. The measured critical exponents exhibit scaling laws but vary from material to material which contradicts the basic idea of a unique set of critical exponents for all materials described by the same model. In some experiments and also in some numerical simulations, the critical exponent η, also called the anomalous dimension, is negative. This is forbidden if the theory which describes the transition is a unitary Landau Ginzburg Wilson (LGW) model [14]. Theoretical investigations using a perturbative renormalization group (RG) calculation up to high order predict the existence of a fixed point and, thus, the possibility of a second-order phase transition [11,15]. The varying critical exponents in this study are associated with a spiral-like RG flow to a chiral, *focus* fixed point [16]. Nonperturbative RG (NPRG) methods predict a weak first-order phase transition and attribute the appearance of scaling by a slowing down of the RG flow in the whole region of the coupling constant space [9,10]. The first numerical investigation of these STA models using Monte Carlo methods indicated a second-order phase transition with a set of critical exponents possibly associated with a new chiral universality class [12]. Some subsequent numerical investigations have been performed on a modified version of the STA model [17], the STAR model, with the R representing a rigid constraint. In this model, the 120° structure of the ground state is *locally* imposed at *all* temperatures. As a consequence the fluctuations of the spins *within* a triangular cell are suppressed while the fluctuations

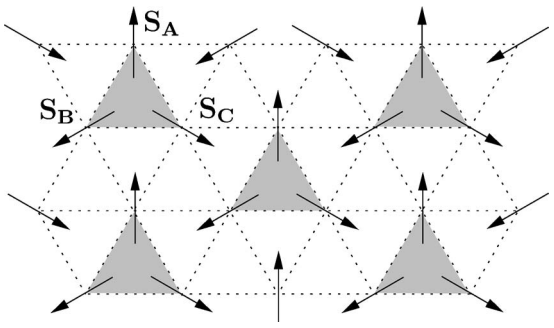

FIG. 1. Ground state of the STA system. The shaded triangles represent elementary plaquettes.

in the relative orientation of the disconnected triangular cells, or plaquettes, can still occur. Note that the STA and STAR models have the same symmetries and the "microscopic" changes performed are supposed to be irrelevant to the critical behavior *if* it is universal. In fact, it was found that the STAR model exhibits a strong first-order phase transition, thus raising doubts about the second order character of the phase transition occurring in all *XY* STA models. Finally, recent numerical studies of the STA model and its LGW formulation by Itakura [18] also indicate a first-order phase transition for the STA *XY* model itself.

In order to examine this effect of local rigidity in more detail, we introduced a generalized model in which we can continuously tune the local rigidity from the STA to the STAR limits [19,20],

$$H(r) = -\sum_{\langle ij \rangle} J_{ij}\, \mathbf{S}_i \cdot \mathbf{S}_j + r \sum_{plaquettes.} (\mathbf{S}_A + \mathbf{S}_B + \mathbf{S}_C)^2. \quad (2)$$

The interactions J_{ij} are antiferromagnetic within the triangular layers and ferromagnetic between layers and have the same magnitude $J=1$. The subscripts A,B,C label the three sublattices on the corners of each elementary triangle and the plaquettes refer to disconnected triangles as shown in Fig. 1. The parameter r imposes a constraint on the short wavelength fluctuations of the order parameter. Continuous changes in r from zero to infinity correspond to a continuous change from the STA to the STAR model. In our previous work with systems of linear sizes $L<60$ we found two different types of behavior: for $r<1.0$ the system exhibits a "pseudocritical" behavior whereas, for $r>1.0$, a first-order phase transition occurs. The critical exponents obtained in the $r<1.0$ range appear to vary with the rigidity parameter r. This nonuniversal behavior is inconsistent with true critical behavior at a continuous phase transition for systems having the same symmetry of the order parameter. We concluded that the critical exponents are really pseudocritical exponents and the observed scaling is "pseudoscaling." The estimated values of critical exponents are within the range of the experimentally observed critical exponents for ABX_3 compounds and Tb. In the range $r>1.0$ we were able to estimate the value of latent heat for several values of r. We extrapolated the values of the latent heat to $r=0$ and we found a small but nonzero latent heat for the *XY* STA model, which indicated a very weak first-order phase transition. This behavior was confirmed by studying the energy probability distribution using much larger system sizes $L=96,138$. Even larger sizes would be needed in the case of the Heisenberg model [18]. At negative values of r, the plaquettes are aligned ferromagnetically but interact antiferromagnetically and the symmetry of the order parameter is the same as at positive r. A special case occurs at $r=-1/2$ where we simply have a system of stacked Kagomé layers. Additional degeneracies are expected in this case.

The standard *equilibrium* Monte Carlo approach requires extremely large lattice sizes L and long runs to properly sample statistically independent configurations. Hence, reaching a definite conclusion about the nature of the phase transition that occurs in STA models requires a different approach. This need is even more important for the Heisenberg STA, which, from a numerical or theoretical point of view, is expected to be closer to a second order behavior than the *XY* STA. For this reason we use an approach based on short-time critical dynamics [21,22].

II. SHORT-TIME CRITICAL DYNAMICS

Universality and scaling are generally expected at a second-order phase transition when a system is in equilibrium. In Monte Carlo simulations, equilibrium is reached after a large number of Monte Carlo steps (MCS) or in the long-time regime. However, it was realized some years ago that a universal scaling behavior can also occur within a macroscopic short-time regime of the dynamic evolution of the system [23]. The dynamic process considered can start from a high temperature, disordered state rapidly quenched to the critical temperature or it can start from a completely ordered state heated up to this temperature. Janssen *et al.* [23] showed using a renormalization group method that if a system is prepared at high temperature with an initial value of the order parameter m_0 and then quenched to the critical temperature, the time-dependent order parameter $m(t)$ obeys the following scaling form after a macroscopic small time:

$$m(t,\tau,L,m_0) = b^{-\beta/\nu} m(t/b^z, b^{1/\nu}\tau, L/b, b^{x_0} m_0), \quad (3)$$

where t is the time, $\tau=(T-T_c)/T_c$ is the reduced temperature, L is the linear size of the system, and b is a generic scaling factor. In Eq. (3) β,ν,z are the usual critical exponents while x_0, the scaling dimension of m_0, is a new exponent associated with the short-time dynamics. The scaling behavior described by Eq. (3) is only observed in an intermediate time range which is large compared to microscopic times but still much smaller than the macroscopic time scales needed to reach the new equilibrium state. Hence follows the name short-time dynamics. Note that, at the critical point ($\tau=0$), the scaling form predicts that $m(t)$ increases as $m_0\, t^\theta$ where $\theta=(x_0-\beta/\nu)/z$ is a new critical exponent. Higher moments of the order parameter behave similarly.

The existence of the short-time dynamic scaling (3) has been confirmed in a large number of systems through Monte Carlo simulations (see for instance Ref. [24] and references therein). Beyond its intrinsic interest the short-time dynamics method has also provided a very efficient way to identify the *static* critical exponents as well as the critical temperature. Indeed, since the initial nonequilibrium state has short ranged spatial correlations, one might expect that the time evolution of the order parameter in this intermediate time region will be independent of the lattice size L provided it is not too small. Also, since the correlation time is small, this approach is free of critical slowing down. An important application of the short-time dynamics for our purpose is the possibility to distinguish a (weak) first-order from a second-order transition. This comes from the observation [22,25] that for a first-order phase transition occurring at a critical temperature T_c there exist two metastable states: a disordered one at $T>T_c$ and an ordered one at $T<T_c$. These states disappear at the temperatures T_{c1} and T_{c2}, respectively. For a second-order phase transition the short-time dynamic behavior exhibits a genuine scaling starting from both the ordered

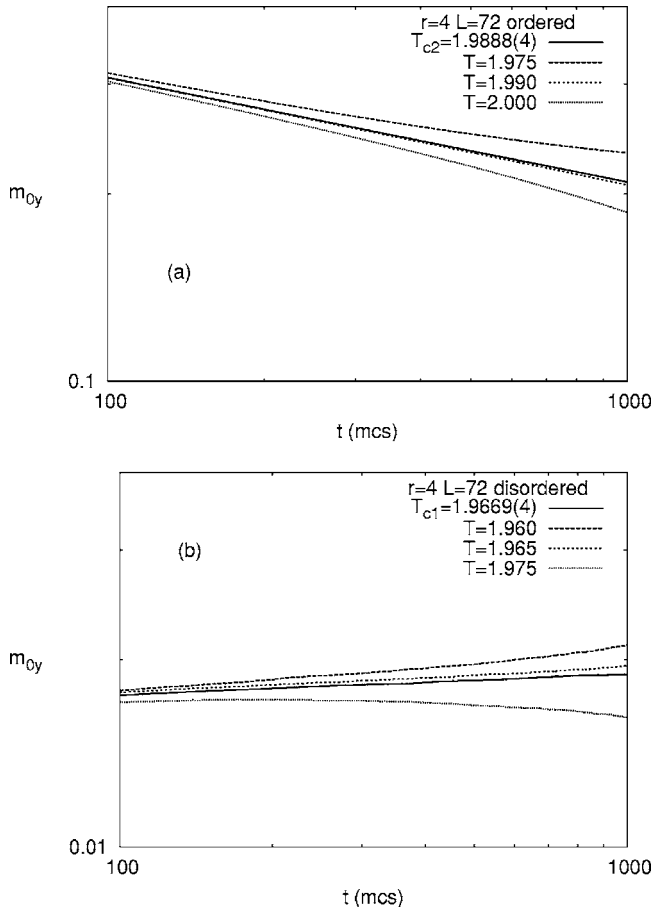

FIG. 2. The y component of the order parameter $\mathbf{m}_0$ as a function of time (MCS) for $r=4$ and $L=72$ with (a) an ordered initial state and (b) a disordered initial state for various temperatures T in units of J. The solid line is obtained by quadratic interpolation and a least squares fit to the expected power law behavior.

and disordered phase with $T_{c1}=T_{c2}=T_c$. For a weak first-order transition one observes only a pseudoscaling behavior at the (pseudocritical) temperatures T_{c1} and T_{c2} with the condition: $T_{c1}<T_c<T_{c2}$. Thus the difference between the pseudocritical temperatures T_{c1} and T_{c2} provides a quantitative measurement of the strength of the first-order transition. The important point is that, whereas it is difficult to determine T_{c1} and T_{c2} in equilibrium, it appears to be relatively easy to determine them in the context of a short-time dynamic analysis. This procedure has already been used with success to study the behavior of the two-dimensional Potts model [22]. We apply it in the context of frustrated magnets.

III. NUMERICAL SIMULATION

The ground state of the generalized model considered in this paper has the spins on the corners of each elementary triangle arranged at 120° to one another. There are three sublattices as indicated in Fig. 1 and the order parameter can be chosen as

$$\mathbf{m}_0 = \mathbf{S}_A - 0.5\mathbf{S}_B - 0.5\mathbf{S}_C. \tag{4}$$

In order to study the short-time behavior, we consider a zero temperature initial state where $\mathbf{m}_0$ has its maximum value

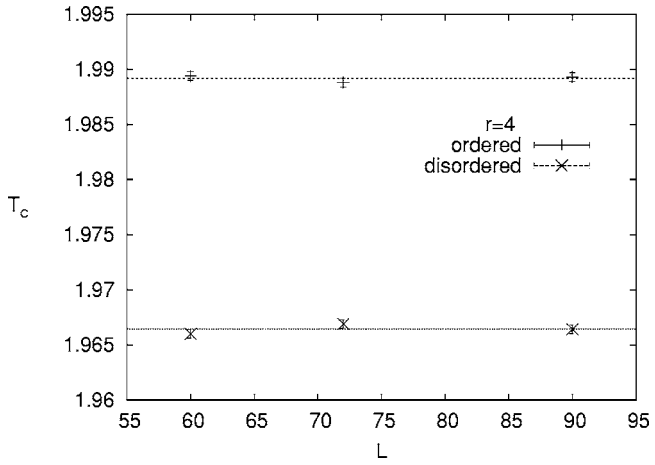

FIG. 3. The $r=4$ pseudocritical temperatures (in units of J) for both disordered (T_{c1}) and ordered (T_{c2}) initial states plotted as a function of L. The lines indicate the average T_c in each case and predict a $\Delta T_c=0.023(1)$.

which we take to be in the y direction and label as m_{0y}. We also prepare the system in a high temperature disordered initial state with $m_{0y}=0.01$. We then rapidly quench the system to a number of temperatures close to the values of the critical temperature obtained previously [19,20] using equilibrium methods and we follow the order parameter m_{0y} as a function of Monte Carlo time steps (MCTS) using the Metropolis algorithm. The results for each initial state are averaged over $10^3-20\times10^3$ trials depending on the linear size L. We follow the time dependence of m_{0y} as a function of time t for three fixed temperatures and we use an interpolation scheme to determine the temperature T_c which yields the best power law behavior in the time range $[100,1000]$. This intermediate time range was found to give the best power law behavior which only emerges after a time period which is long in microscopic terms [21]. The error bars on T_c are determined by the number of intermediate temperatures used in the interpolation scheme. This procedure is carried out for both low temperature and high temperature initial states. For a disordered initial state, a log-log plot of $m_{0y}(t)$versus time should be linear and the slope yields θ. For an ordered state the slope yields $\beta/\nu z$. The derivative $\partial_\tau \ln m(t,\tau)|_{\tau=0}$ should also exhibit power law behavior with the exponent $1/\nu z$. For a second-order phase transition these values of T_c should agree and the exponents should be universal while for a first-order phase transition distinct critical temperatures exist. Averages are performed over different realizations of the initial values of m_{0y} and thus time averages are replaced by sample averages and the full power of parallelized codes can be used.

Figure 2 shows the behavior for a lattice of linear size $L=72$ and $r=4$ starting from (a) the ordered state and (b) the disordered state and then quenched to three different temperatures. The solid curve in each case is obtained using an interpolation scheme at each time to find the temperature which yields the best scaling behavior. All temperatures are measured in units of J. For the ordered initial state we find that a value $T_{c2}=1.9888(4)$ yields the best scaling whereas for the disordered initial state we find $T_{c1}=1.9669(4)$. The

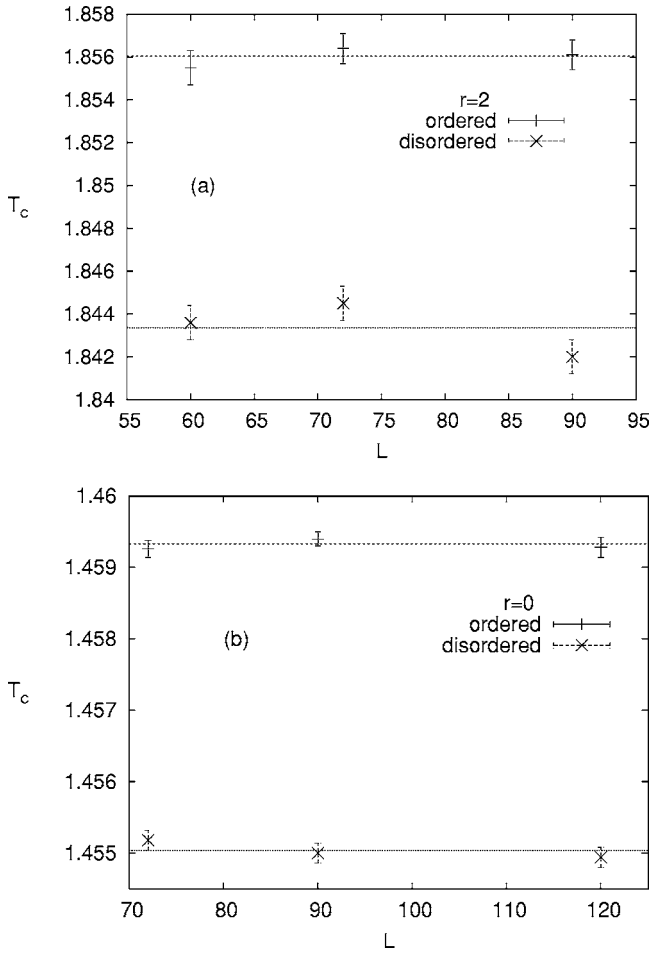

FIG. 4. The pseudocritical temperatures (in units of J) for both disordered (T_{c1}) and ordered (T_{c2}) initial states plotted as a function of L for (a) $r=2$ and (b) $r=0$. The lines indicate the average T_c in each case and predict a $\Delta T_c=0.013(1)$ ($r=2$) and $\Delta T_c=0.0043(1)$ ($r=0$).

fact that these values of T_c are different is consistent with our previous results [19,20] which indicated a latent heat for $r=2$. We have performed the same calculations for sizes $L=60,72,90$ and the values of T_{c1},T_{c2} are shown in Fig. 3 plotted vs L. The values of T_{c1},T_{c2} are different and are independent of L in this time interval. The system displays hysteresis with the average difference in the two values of T_c yielding $\Delta T_c=0.023(1)$. The same procedure has been followed for smaller values of r. Figures 4(a) and 4(b) show the behavior of T_{c1},T_{c2} for $r=2$ and $r=0$, respectively. In both cases the results indicate a weak first-order transition and the values of the critical temperatures obtained here using the present approach straddle those obtained using equilibrium methods [20]. Table I summarizes the results for the differences in T_c as determined from the ordered and disordered initial states as well as estimates for the various critical exponents obtained from the best power law dependence on t. The values of the exponents vary with the constraint parameter r which indicates nonuniversal behavior. Using our measured values of $\beta/\nu z$ and $1/\nu z$ we estimate the values of β given in the last column. The values of β increase as r decreases in agreement with our previous study using equilibrium methods [19,20]. The value of $\beta=0.27(1)$ for $r=0$ is slightly larger than that predicted by previous numerical studies but is consistent with the value obtained in experiments on STA XY antiferromagnets [9].

TABLE I. Results for the difference in critical temperatures ΔT_c and the exponents for various values of the constraint parameter r.

r	ΔT_c	θ	$\beta/\nu z$	$1/\nu z$	β
0	0.0043(1)	0.081(4)	0.218(1)	0.79(2)	0.27(1)
2	0.013(1)	0.045(5)	0.188(2)	0.83(2)	0.23(1)
4	0.023(1)	0.028(5)	0.169(1)	0.82(1)	0.20(1)

IV. CONCLUSION

We have investigated the critical behavior of a family of XY noncollinear magnets on the stacked triangular lattice geometry using the short-time dynamics approach. The critical temperatures obtained using this approach straddle those obtained previously using equilibrium methods and indicate that the transition is accompanied by hysteresis. The critical exponents are found to vary with the constraint parameter r. Since this parameter does not change the symmetry of the model the exponents are nonuniversal. Our results strongly suggest that the phase transition of STA XY antiferromagnets is weakly first order in agreement with the NPRG field theory predictions and with our previous equilibrium Monte Carlo results. The method used here has the advantage that scaling behavior emerges at relatively short times and also for smaller sizes since our values of T_c are almost independent of L. The results indicate that for the STA XY materials, experiments need to be carried out at reduced temperatures $\tau \ll 10^{-3}$ in order to identify the true weak first-order nature of the transition. The present method also provides a way to study the question of an even weaker first-order transition for STA Heisenberg materials.

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[1] G. Toulouse, Commun. Phys. (London) **2**, 115 (1977).
[2] R. Moessner and A. P. Ramirez, Phys. Today **59**(2), 24 (2006).
[3] A. P. Ramirez, Nature (London) **421**, 483 (2003).
[4] P. Schiffer, Nature (London) **420**, 35 (2002).
[5] S.-H. Lee, C. Broholm, W. Ratcliff, G. Gasparovic, Q. Huang, T. H. Kim, and S.-W. Cheong, Nature (London) **418**, 856 (2002).
[6] *Magnetic Systems with Competing Interactions*, edited by H. T. Diep (World Scientific, Singapore, 1994).
[7] M. F. Collins and O. A. Petrenko, Can. J. Phys. **75**, 605 (1997).
[8] H. Kawamura, J. Phys.: Condens. Matter **10**, 4707 (1998).
[9] B. Delamotte, D. Mouhanna, and M. Tissier, Phys. Rev. B **69**, 134413 (2004).
[10] B. Delamotte, D. Mouhanna, and M. Tissier, J. Phys.: Condens. Matter **16**, S883 (2004).
[11] P. Calabrese, P. Parruccini, A. Pelissetto, and E. Vicari, Phys. Rev. B **70**, 174439 (2004).
[12] H. Kawamura, J. Phys. Soc. Jpn. **61**, 1299 (1992).
[13] H. B. Weber, T. Werner, J. Wosnitza, H. v. Löhneysen, and U. Schotte, Phys. Rev. B **54**, 15924 (1996).
[14] J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena*, 3rd ed (Oxford University Press, New York, 1989).
[15] A. Pelissetto, P. Rossi, and E. Vicari, Phys. Rev. B **63**, 140414(R) (2001).
[16] P. Calabrese, P. Parruccini, and A. I. Sokolov, Phys. Rev. B **66**, 180403(R) (2002).
[17] D. Loison and K. D. Schotte, Eur. Phys. J. B **14**, 125 (2000).
[18] M. Itakura, J. Phys. Soc. Jpn. **72**, 74 (2003).
[19] A. Peles, B. W. Southern, B. Delamotte, D. Mouhanna, and M. Tissier, Phys. Rev. B **69**, 220408(R) (2004).
[20] A. Peles, Ph.D. thesis, University of Manitoba, 2004 (unpublished).
[21] B. Zheng, Int. J. Mod. Phys. B **12**, 1419 (1998).
[22] L. Schülke and B. Zheng, Phys. Rev. E **62**, 7482 (2000).
[23] H. K. Janssen, B. Schaub, and B. Schmittmann, Z. Phys. B: Condens. Matter **73**, 539 (1989).
[24] B. Zheng, F. Ren, and H. Ren, Phys. Rev. E **68**, 046120 (2003).
[25] L. A. Fernandez, J. J. Ruiz-Lorenzo, M. P. Lombardo, and A. Tarancon, Phys. Lett. B **277**, 485 (1992).