Frustrated systems 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. 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. 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 neighbour 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 is equal to zero:

\[ S_A + S_B + S_C = 0 \]  

where the subscripts \( A, B, C \) label the sites at the corner of the elementary triangles shown in figure 1. As a consequence the order parameter is no longer a simple vector but a matrix, a fact that has lead to the idea that these (noncollinear) frustrated magnets could belong to a new “chiral” universality class.

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 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 \( \eta \), 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. 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. The varying critical exponents in this study are associated with a spiral-like RG flow to a chiral, focus fixed point. Non-perturbative RG methods (NPRG) 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.

The first numerical investigation of these STA models using Monte Carlo methods indicated a second order phase transition with set of critical exponents possibly associated with a new chiral universality class. Some subsequent numerical investigations have been performed on a modified version of the STA model, 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 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 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.\(^{19,20}\)

\[
H(r) = -\sum_{(ij)} J_{ij} S_i S_j + r \sum_{\text{plaquettes}} (S_A + S_B + S_C)^2
\]

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 figure 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 ’pseudo-critical’ 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 systems sizes \( L = 96, 138 \). Even larger sizes would be needed in the case of the Heisenberg model.\(^{21,22}\) 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 Kagome 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.\(^{21,22}\) Universality and scaling have been observed in systems far from equilibrium. The initial state can be a high \( T \) state which is rapidly quenched to the critical temperature or it can be a completely ordered state heated up to this temperature. Janssen et. al.\(^{23}\) showed that if a

![Figure 2: The \( m_{2z} \) component of the order parameter \( m_{2z} \) as a function of time for \( r = 4 \) and \( L = 72 \) with (a) an ordered initial state and (b) a disordered initial state for various temperatures. The solid line is obtained by quadratic interpolation and a least square fit to the expected power law behavior.](image-url)
system is prepared at high $T$ 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 small microscopic time

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

At the critical point ($\tau = 0$), this form predicts that $m(t)$ increases as $m_0 t^\theta$ where $\theta = (x_0 - \beta/\nu)/z$ is a new critical exponent and the other exponents $\beta, \nu, z$ are the usual critical exponents. Higher moments of the order parameter behave similarly. The critical temperature $T_c$ is located by starting from an initial value of $m_0$ at high $T$ and then quenching to a lower $T \sim T_c$. A log-log plot of $m(t)$ versus time should be linear and the slope yields $\theta$. An ordered state can also be used as an initial state to estimate $T_c$ and in this case the slope yields $\beta/\nu z$. For a 2nd order transition these values of $T_c$ should agree and the exponents should be universal. The derivative $\partial_t \ln m(t, \tau)|_{\tau=0}$ should also exhibit power law behavior with the exponent $1/\nu z$. The advantage of this approach is that critical slowing down is not an issue since the measurements are carried out at short times. Averages are performed over different realizations of the initial values of $m_0$ and thus time averages are replaced by sample averages and the full power of parallelized codes can be used.

The ground state of the model has the spins on the corners of each elementary triangle arranged at $120^\circ$ to one another. There are three sublattices as indicated in figure 1 and the order parameter can be chosen as

$$m_0 = S_A - 0.5S_B - 0.5S_C$$  \hspace{1cm} (4)

We consider both a low temperature and high temperature initial state and then we follow the order parameter as a function of Monte Carlo time steps at some intermediate fixed temperature using the Metropolis algorithm. The results for each initial state are averaged over $10^3 - 20 \times 10^3$ trials depending on the linear size $L$.

Figure 2 shows the behavior for a lattice of linear size $L = 72$ and $r = 4$ for several different temperatures starting from (a) the ordered state and (b) the disordered state. For the ordered state shown in figure 1 only one component of $m_0$ is non zero and we label this component as $m_{0z}$. For the ordered initial state it has its maximum value and for all disordered initial states it has the initial value 0.01. We follow the time dependence of $m_{0z}$ as a function of time $t$ for three temperatures and we use an interpolation scheme to determine the temperature $T_c$ which yields the best power law behavior in the time range $[100, 1000]$. As shown by the solid curve in the figures. 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. The error-
bars on $T_c$ are determined by the number of intermediate temperatures used in the interpolation scheme. We have performed the same calculations for sizes $L = 60, 72, 90$ and the values of $T_c$ are shown in figure 3 plotted versus $L$. The values of $T_c$ are independent of $L$ in this time interval and the system displays hysteresis with the difference in the values of $T_c$ corresponding to the ordered and disordered initial states yielding a value of $\Delta T_c = 0.023(1)$. We have carried out the same procedure for smaller values of $r$. Figures 4(a), 4(b) show the behavior of $T_c$ 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. 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 $\beta$ given in the last column. The values of $\beta$ increase as $r$ decreases in agreement with our previous study using equilibrium methods.22 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.2

In summary, 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 non-universal. 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 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 a even weaker first order transition for STA Heisenberg materials.

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