Tricritical relaxation in an Ising-Glauber model with competing interactions*

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The tricritical relaxation in a three-dimensional kinetic Ising-Glauber model has been studied using a Monte Carlo method. For $T < T_t$ all relaxation functions ϕ_{AB} decay as $\exp(-t/\tau_{AB})$ with a single relaxation time $\tau_{AB} = \tau \sim (T_t - T)^{-\Delta_t}$ and $\Delta_t \approx \gamma_t = 1$ in agreement with the conventional theory of slowing down.

The static properties of magnetic models that exhibit tricritical points are well understood,[1,2] however, nothing is known about the dynamics of these systems near T_t either experimentally or theoretically. Although the dynamics of several other models have been studied[3-6] the reliability of the results has not yet been ascertained. In fact, experimental data[7] from light scattering by ^{3}He-^{4}He mixtures seem to disagree with the mode-coupling theory.[3,4] All of these investigations of tricritical dynamics[3-7] are concerned with systems with certain conservation laws for energy, mass, or momentum. The kinetic Ising-Glauber model (which is appropriate for tricritical magnetic systems) possesses no conserved quantities and therefore belongs to a different dynamic class. No tricritical theory or experiment in the sense of, e.g., Refs. 3, 4, and 6 are available, moreover, previous studies[8-13] of *critical* dynamics have shown that conventional theories of critical slowing down fail for a kinetic Ising model.

We have therefore carried out a Monte Carlo simulation of a kinetic Ising-Glauber model (with competing interactions) which is known[1] to possess a tricritical point

$$\mathcal{H} = J \sum_{\substack{\text{nn} \\ \text{pairs}}} \sigma_i \sigma_j - \frac{J}{2} \sum_{\substack{\text{nnn} \\ \text{pairs}}} \sigma_i \sigma_k + \mu H \sum_i \sigma_i , \tag{1}$$

where $J > 0$ and the spins $\sigma_i, \sigma_j, \sigma_k = \pm 1$ are arrayed on a $20 \times 20 \times 20$ simple cubic lattice with periodic boundary conditions. Previous Monte Carlo studies of the static properties of this model have shown that a tricritical point occurs for $kT_t/J = 6.10 \pm 0.05$ and $\mu H_t/kT_t = 0.90 \pm 0.01$. These data also show that for $\epsilon_t = |1 - T/T_t| \geq 10^{-2}$ no effects of finite size are observable for a system of this size. In contrast to the studies of two-dimensional critical dynamics,[9-11,13] this investigation will produce results which can be compared with an ϵ-expansion renormalization-group treatment.

We have investigated the kinetics of this model by analyzing the equilibrium relaxation functions

$$\phi_{AB}(t) = \frac{\langle A(0)B(t)\rangle - \langle A\rangle\langle B\rangle}{\langle A(0)B(0)\rangle - \langle A\rangle\langle B\rangle} , \tag{2}$$

where A and B stand for staggered magnetization m (order parameter), magnetization M, and energy E, respectively. Approaching the tricritical point for $T < T_t$ along the path $h = \mu H/kT = 0.9$ (which lies wholly within the tricritical region), we expect a divergence in the relaxation time τ^t_{AB}:

$$\tau^t_{AB} = \int_0^\infty \phi_{AB}(t)\, dt = C_{AB} \epsilon_t^{-\Delta^t_{AB}} , \tag{3}$$

where $\epsilon_t = |1 - T/T_t|$. From conventional theory[14,15] we would expect all the relaxation exponents Δ^t_{AB} to be identical[13-15] and equal to the static susceptibility exponent γ_t. Near a simple critical point in three dimensions the latter condition is not valid since $\Delta_{AB} > \gamma$.

A Markov chain of states was generated using the usual Monte Carlo (MC) procedure.[11,16] The initial 3000 MC steps/spin were dropped in order that quasiequilibrium be achieved. Averages over the next 5000 to 10 000 MC steps/spin were then taken for determining the relaxation functions. The error analysis was made according to the prescription described by Ref. 16, replacing expectation values $\langle A\rangle$ by time averages $\langle A\rangle_{\text{av}}$. If this is done in a straightforward manner, however, the relaxation functions [Eq. (2)] will turn out to be systematically smaller than the true relaxation function $\phi_{AB}(t)$. In fact, the estimate for ϕ_{AB} actually becomes negative (in the case of a simple exponential relaxation) at a time

$$t^* = \tau_{AB}[\ln(t_0/\tau_{AB}) - \ln 2] , \tag{4}$$

where t^* is smaller than the time interval t_0 used for the averaging.

This problem will occur in all numerical calculations (e.g., Monte Carlo, molecular dynamics)

of time-dependent quantities. We have attempted to eliminate this error by using $\langle A(t)B(t+t_1)\rangle_{av}$ instead of $\langle A\rangle_{av}\langle B\rangle_{av}$ where $t_1 \gg \tau_{AB}$. This procedure leads to increased error bars in the estimates but eliminates the systematic error.

The Monte Carlo data were taken at several temperatures near T_t ($0.013 \leq |1 - T/T_t| \leq 0.1$); $kT_t/J = 6.12 \pm 0.02$. In the antiferromagnetic region ϕ_{MM} is obtained with better precision than the other relaxation functions since $\langle M\rangle$ is small compared to $\langle m\rangle$ and $\langle E\rangle$. For all temperatures ϕ_{MM} is well described by a simple exponential decay with time. A log-log plot of the relaxation time τ_{MM} describing this decay is shown versus relative temperature distance $\epsilon_t = |1 - T/T_t|$ in Fig. 1. For comparison an average relaxation time $\bar{\tau}_{AB}$, as determined from all other relaxation functions, is shown along with $\langle m\rangle^{1/\beta_t}$. The exponent Δ^t_{MM} [see Eq. (3)] for the magnetization-magnetization relaxation is found to be $\Delta^t_{MM} = 0.98 \pm 0.10$. In Fig. 2 we show the temperature variation of the characteristic relaxation times associated with the other relaxation functions. (Error bars are shown only for τ_{mm}; however, errors for the other τ_{AB} are comparable.) The scatter in these data is considerably larger than for τ_{MM} owing to the necessary subtractions in Eq. (2). Nonetheless, the data are all consistent with a single exponent having the classical value $\Delta_{AB} = \Delta = 1$. Since $\gamma_t = 1$, this agrees with the results of conventional theory of slowing down[14] which predicts that $\Delta = \gamma$. (This result also is identical to the behavior predicted by mean-field theory.[15])

In addition to having the same relaxation exponents, the self- and cross-correlations all appear

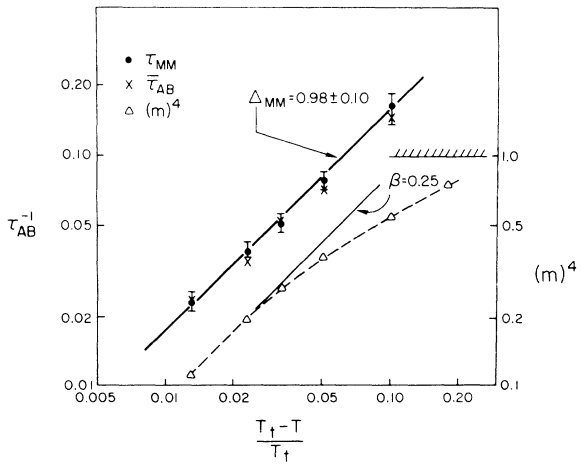

FIG. 1. Inverse relaxation time τ^{-1}_{MM} of the magnetization autocorrelation vs $\epsilon_t = |1 - T/T_t|$. Solid line corresponds to conventional relaxation behavior with $\Delta_t = \gamma_t$.

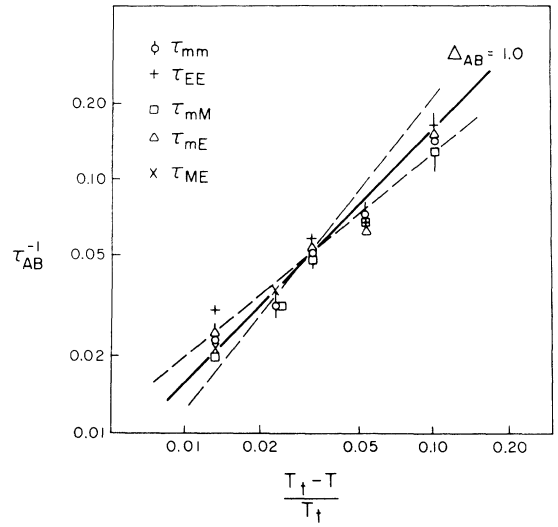

FIG. 2. Inverse relaxation times τ^{-1}_{AB} of auto- and cross-correlations of the order parameter, energy, and magnetization. All data are plotted on the *same* scale. Solid line corresponds to conventional relaxation behavior [see Eq. (3)] with all C_{AB} and τ_{AB} identical and $\Delta \equiv \Delta_{AB} = \gamma_t = 1$.

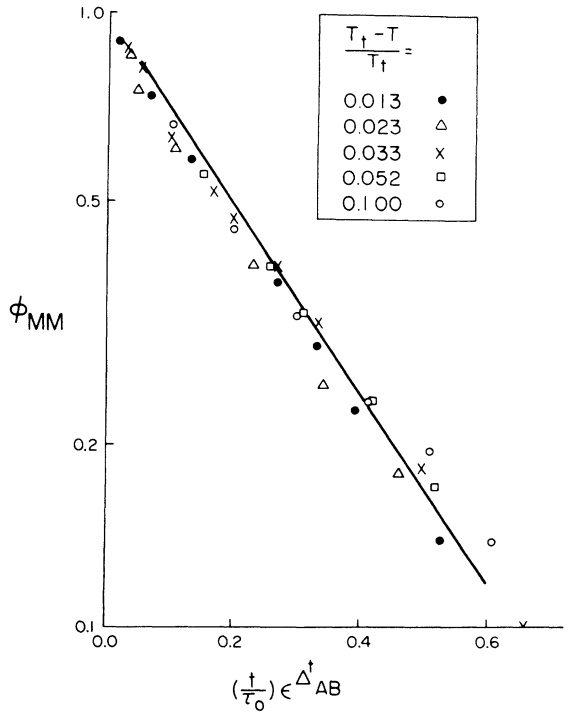

FIG. 3. Magnetization relaxation function vs scaled time (using $\Delta^t_{MM} = 1.0$). Solid line has slope =1.5 corresponding to $C = 1.55$ as determined from Fig. 2 [see Eq. (6)].

to have the same amplitudes C_{AB} [see Eq. (3)], in contrast to the differences found near an ordinary critical point (see Ref. 11 and references contained therein). The latter property can be understood if one writes the relaxation function for ordinary critical behavior as a sum of the exponentials[13]

$$\phi_{AB} = \sum_i \alpha_{AB}^{(i)} e^{-\lambda_i t}, \tag{5}$$

where the eigenvalues λ_i are independent of the particular type of correlation function $\langle AB \rangle$, while the coefficients $\alpha_{AB}^{(i)}$ are not. Integration according to Eq. (3), in general, therefore gives different amplitudes $C_{AB} = \tau_{AB} |\epsilon|^{\Delta}$ for different correlations. In the case of a simple exponential decay the relaxation time is simply the inverse of the eigenvalue $\tau = \lambda^{-1}$, independent of the choice of A and B. This is in agreement with our MC calculations giving good evidence for the consistency of our results (Figs. 1 and 2). (Even though the error bars are relatively large, there is no obvious systematic deviation seen in the data points.)

The existence of a single classical relaxation behavior

$$\phi_{AB} \sim e^{-t/\tau}, \quad \tau = C\epsilon_t^{-1} \tag{6}$$

is also clearly indicated by the simple logarithmic plot of ϕ vs $(t/\tau_0)\epsilon$ shown in Fig. 3. (τ_0 is a scale factor establishing 1 MC step/spin in actual time units.) We first note that all the points fall essentially on a single curve. This curve is well-represented by a straight line thus confirming simple exponential relaxation. We cannot, of course, exclude the possibility that for $\epsilon_t < 0.01$ a different relaxation with $\Delta > \gamma$ dominates the decay for large t. As $\phi_{AB}(t)$ changes by one order of magnitude, however, there is no indication of any deviation from the $\Delta = \gamma$ behavior over the times studied (even at $\epsilon_t \approx 0.01$). We therefore used a simple exponential fit to the data evaluating τ_{AB}, rather than using some phenomenological extrapolation[11] for carrying out the integration indicated in Eq. (3).

In conclusion, we note that the passing from $d = 4$ (four dimensions) to $d = 3$ seems to have a similar effect on both the dynamic as well as static behavior[1] in that in both cases the properties change over from nonclassical to classical (mean-field-like). Logarithmic corrections have been predicted[17] in the static critical properties in $d = 4$ and tricritical properties in $d = 3$. A renormalization-group study[18] of critical dynamics in $d = 4$ revealed logarithmic corrections, and by analogy to the static case we would expect similar corrections in the $d = 3$ tricritical dynamics. No such corrections were observed (even for ϕ_{MM}) indicating that if they exist the amplitudes must be reasonably small. The limited accuracy available even for relatively large values of t_0 makes the observation of such corrections extremely difficult.

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