Short-time dynamics of a metamagnetic model

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We studied a layered metamagnetic Ising model with competing ferromagnetic and antiferromagnetic interactions on a square lattice. The model is formed of ferromagnetic chains coupled by an antiferromagnetic interaction. Using Monte Carlo simulations we have determined the phase diagram of the model, which exhibits a tricritical point. By exploring the short-time scaling dynamics, we have found the dynamic and static critical exponents along the continuous transition line between the antiferromagnetic and paramagnetic phases.

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I. INTRODUCTION

The study of the critical properties of physical systems continues to be a topic of current interest in equilibrium statistical physics [1]. Among the various methods of analysis that are employed to determine phase diagrams and critical exponents, the most important are high- and low-temperature series expansion [2], real space renormalization group [3], ϵ expansion [4], and numerical simulations, such as the Monte Carlo method [5]. However, when we wish to study the nonequilibrium behavior of physical systems, we have only a few techniques at our disposal. In all cases, we need to consider the gain and loss master equation, which is an equation for the time evolution of the state probabilities [6]. In this formalism it is necessary to establish the transition rates among the states, and this defines a dynamical model. An exact solution for the state probability of an interacting particle system is not possible. The linear Ising model is an exception to this general rule, because we know the exact values of the one-point and two-point correlation functions [7]. In order to decouple the hierarchy of equations of motion we can use approximate methods, such as, for instance, the site approximation or the dynamical pair approximation [8,9]. Another way to find the critical properties of nonequilibrium systems is to include momentum-space renormalization group arguments into the master equation formalism. Janssen, Schaub, and Schmittmann [10] showed, through the ϵ expansion, that the usual universal behavior observed at large time scales, very near equilibrium, can also be inferred at the early initial stages of the evolution of the system, which is in a state far from equilibrium. In recent years, some numerical simulations have been applied to spin systems to test the idea of universality in the short-time regime [11,12].

In this work we consider a layered metamagnetic Ising model on a square lattice, with competing ferromagnetic and antiferromagnetic couplings. Using Monte Carlo simulations for the equilibrium states of the model, we were able to find the phase transition between the ordered antiferromagnetic and disordered paramagnetic states. We showed that the phase diagram of the model displays discontinuous and continuous transition lines, which are separated by a tricritical point. Next, we directed our simulations to exploring the short-time dynamics of the model. From an initial state, chosen to be the ground state of the model, we left the system to evolve in time at its critical point, which is given by the values of temperature and magnetic field on the continuous phase boundary. We calculated the static and dynamic critical exponents of the model from the short-time scaling relations. In the next section, we present the model and the scaling relations used in our short-time calculations. In Sec. III, we give our Monte Carlo simulations, the phase diagram, and the values of the critical exponents. Finally, in Sec. IV, we present our conclusions.

II. MODEL

We have considered an Ising spin system on a square lattice, formed by two alternating sublattices 1 and 2. The exchange interaction between first neighboring spins on the same sublattice is of the ferromagnetic type, while the coupling between neighboring spins belonging to different sublattices is of the antiferromagnetic type. The Hamiltonian of the model in the presence of an applied field is

$$\mathcal{H}=-\sum_{i,j}\sigma_{i,j}(J_1\sigma_{i+1,j}-J_2\sigma_{i,j+1}+H), \qquad (1)$$

where $\sigma_{i,j}=\pm 1$ are the spin variables, H is the external magnetic field, and J_1 and J_2 are the ferromagnetic and antiferromagnetic exchange interactions, respectively. The phase diagram and the critical properties of this model were presented by Kincaid and Cohen [13] in an interesting review concerning its mean-field properties. They showed that the phase diagram of the metamagnetic model, in the plane of temperature versus magnetic field, displays a variety of critical points, depending on the ratio between the ferromagnetic and antiferromagnetic exchange couplings. If the value of this ratio is higher than a critical value, the phase diagram exhibits a tricritical point connecting a continuous transition line to a discontinuous one. Both lines describe transitions between an ordered antiferromagnetic phase and a disordered paramagnetic phase. On the other hand, if this ratio is smaller than the same critical value, the tricritical point splits into a critical and a double critical end points. However, this latter result is not supported by experiments [14] and numerical simulations [15]. Only the tricritical point appears in the phase diagram. In recent work [16] we found the phase diagram of this model. We employed the master equation ap-

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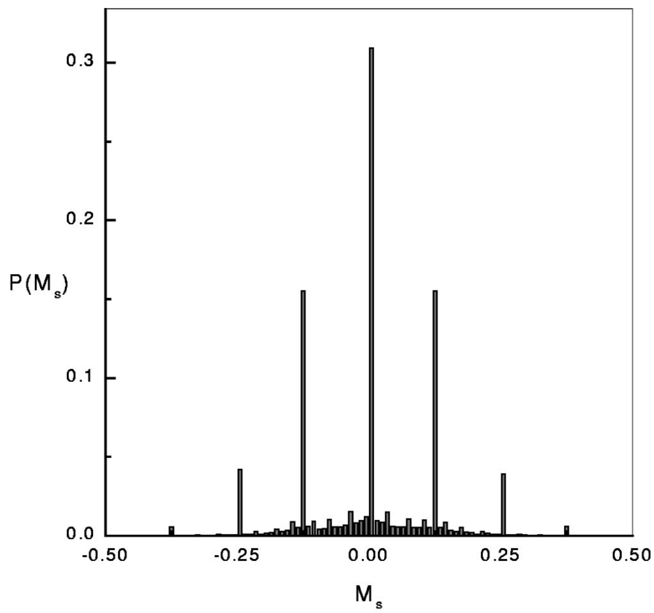

FIG. 1. Distribution probability for the values of the staggered magnetization, at the discontinous phase transition. $T=0.6$, $H=2.04$, and $L=16$. T is in units of J/k_B and H in units of J.

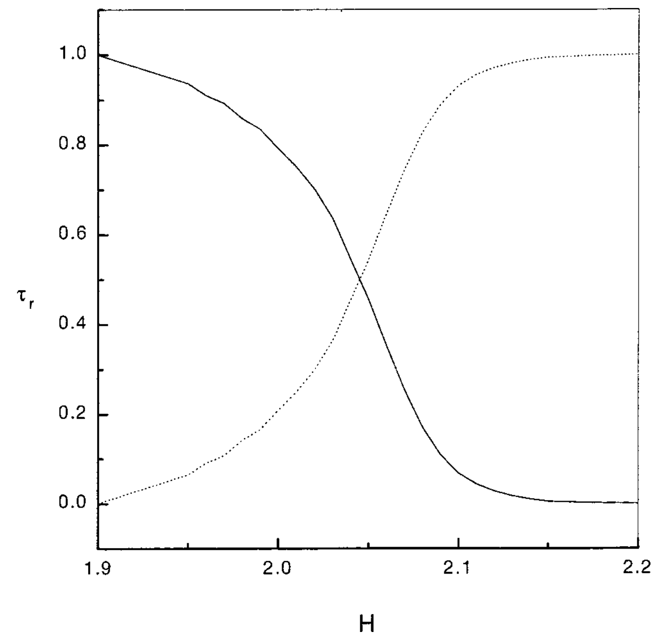

FIG. 2. Residence time as a function of the magnetic field H, for the temperature $T=0.6$ and $L=16$. The continuous line gives the residence time for the antiferromagnetic states, while the dotted line is the residence time for the paramagnetic states. The residence time τ_r is dimensionless.

proach and used the dynamical pair approximation to break the chain of the equation of motion for the pair probabilities. Although the pair approximation includes only nearest-neighbor correlations, it gives only a tricritical point for any value of the ratio between the ferromagnetic and antiferromagnetic couplings, in accordance with the experimental and simulation results.

Now we present the equations that govern the relaxation of the spin system from an initial state that is completely ordered. In this spin model the order parameter is the staggered magnetization. We choose a point on the continuous transition line of the phase diagram where the critical values of temperature and magnetic field are T_c and H_c, respectively. For a fixed value of the field (H_c), considering a value of temperature very near this critical point, and taking the value $M_0=1$ for the order parameter at time $t=0$, we can write the following scaling form [17] for the kth moment of the order parameter:

$$M^{(k)}(t,\tau,L)=b^{-k\beta/\nu}M^{(k)}(b^{-z}t,b^{1/\nu}\tau,b^{-1}L), \tag{2}$$

where $\tau=(T-T_c)/T_c$ is the reduced temperature, b is the spatial rescaling factor, and L is the lattice size. The exponents β and ν are the well known equilibrium exponents, and z is the dynamical critical exponent. This scaling relation for the order parameter is similar to the one used in long-time regime studies. Here, it is used to investigate the macroscopic short-time regime, as in the work of Jaster *et al.* [17] For $k=1$, we have the proper staggered magnetization, and, choosing the scaling factor to be $b=t^{1/z}$, we obtain

$$M(t,\tau)=t^{-\beta/\nu z}M(1,t^{1/\nu z}\tau), \tag{3}$$

where it is assumed that the linear dimension L is very large. At the critical point $\tau=0$, the staggered magnetization displays the following power-law behavior:

$$M(t)\sim t^{-c_1}, \tag{4}$$

where $c_1=\beta/\nu z$. Taking the derivative of Eq. (2) with respect to τ and choosing the same scaling factor as before, we can write the following relation at the critical point:

$$DM(t)\sim t^{c_2}, \tag{5}$$

where $c_2=1/\nu z$, and $DM(t)$ is the logarithmic derivative of $M(t,\tau)$ with respect to τ, at the critical point where $\tau=0$. As the staggered magnetization is different from zero in the initial stages of the evolution, we can also define a time dependent second-order cumulant. It is given by

$$U(t)=\frac{M^{(2)}}{(M)^2}-1\sim t^{c_3}, \tag{6}$$

where $c_3=d/z$, and d is the spatial dimensionality of the spin system. Therefore, by measuring the three independent exponents c_1, c_2, and c_3, we can obtain the static (β,ν) and the dynamical (z) critical exponents. This procedure is easier to implement than the usual one, where we need to prepare the system to have, at the initial time, a very small value of the magnetization and of the correlation length.

III. SIMULATIONS

Before we consider the application of short-time dynamics, as briefly explained in the last section, we first need to determine the critical parameters of the model. In order to attain this goal, we performed Monte Carlo simulations in this model. We considered a two-dimensional lattice, with linear length ranging from $L=16$ to $L=128$. We have taken, for the transition probability rate among states, the following one-spin-flip Glauber prescription [7]:

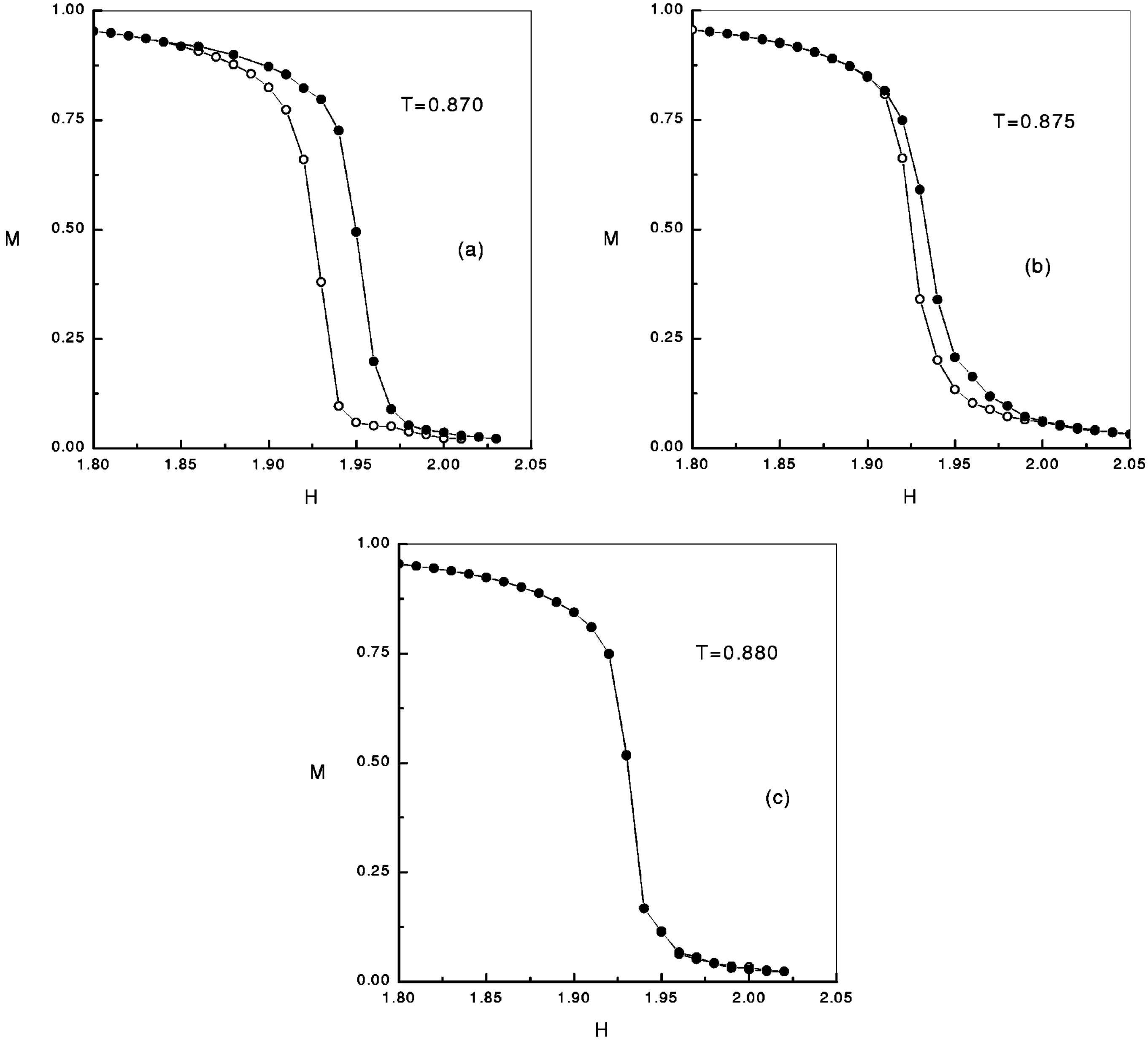

FIG. 3. Staggered magnetization versus magnetic field for three selected values of temperature near the tricritical point. Open circles are for increasing values of the field and closed circles are for decreasing values of the field. The lattice size is $L=128$. (a) $T=0.870$, (b) $T=0.875$, and (c) $T=0.880$.

$$w_{i,j}(\sigma)=\frac{1}{2}\left[1-\sigma_{i,j}\tanh\left(\frac{1}{k_BT}[J_1(\sigma_{i-1,j}+\sigma_{i+1,j})-J_2(\sigma_{i,j-1}+\sigma_{i,j+1})+H]\right)\right], \tag{7}$$

where k_B is the Boltzmann constant and T is the absolute temperature of the heat bath. In the actual simulation, we choose $J_1=J_2=J$. For a fixed pair of values of T and H, we have considered 10^5 Monte Carlo steps (MCS) to calculate the mean values of the sublattice magnetizations m_1 and m_2, from which we obtain the magnetization $m=(m_1+m_2)/2$ and the staggered magnetization $M=(m_1-m_2)/2$, which is the order parameter. We have also determined the fourth-order cumulant of the staggered magnetization, in order to better locate the critical point. Thermalization was achieved, after we discarded the initial 10^4 MCS. For the continuous transition the critical point was determined, as usual, by the point where all the fourth-order cumulants cross themselves. In general, we applied this procedure by fixing the value of T and changing the value of H for every lattice size L. We also checked the results by fixing H and changing T. In the case of the discontinuous transition, we determined the staggered magnetization curve as a function of the field, for a fixed value of temperature. This procedure is not an efficient one, because it is difficult to distinguish a continuous from a discontinuous curve, especially near the tricritical point, but it gives an idea of the range of values of the field where the transition is of first order. With the purpose of improving the determination of the transition field, we have also constructed a histogram of the probability distribution of the staggered magnetization. For example, we show in Fig. 1 a

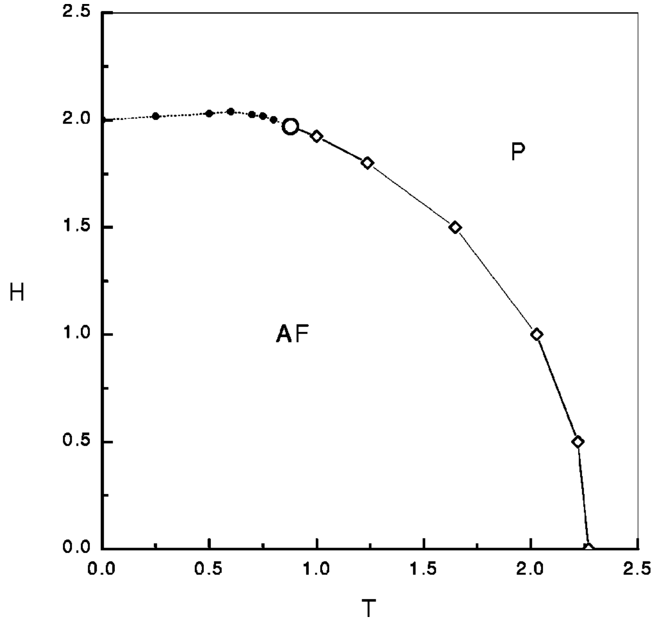

FIG. 4. Phase diagram in the plane magnetic field H versus temperature T. Continuous phase transitions are represented by the open diamonds, while the discontinuous transitions are given by the closed circles. The open circle indicates the tricritical point. AF and P are the antiferromagnetic and paramagnetic phases, respectively. T is in units of J/k_B and H in units of J. The lines serve to guide the eyes.

typical histogram for $T=0.6$, $H=2.04$, and $L=16$. As we can see, the height of the peak at $M=0$ is approximately equal to the sum of heights of the two nearest peaks. This means that the system exhibits two different states with almost the same probability. In this case we used 20×10^6 MCS to obtain the histogram, in order to give an opportunity to the system to visit its most probable states many times. For better location of the transition field, we also found the residence time for the antiferromagnetic and paramagnetic states, as exhibited in Fig. 2. During the observation time, we computed the time spent around the most probable states as a function of the field for a fixed value of temperature. We expect that the crossing point of the two curves in Fig. 2 gives the desired transition field. However, near the tricritical point, the determination of the transition field using this procedure is also difficult. This happens because critical slowing down is also present even on the magnetization curve for this first-order transition. In this work the location of the tricritical point was achieved through the disappearance of hysteresis [18]. For a fixed value of temperature, we drew the staggered magnetization curves for increasing and decreasing values of the magnetic field. In Figs. 3, we show these curves for a system of size $L=128$, and for three values of temperature near the tricritical point. Our estimate for the tricritical temperature is $T_t=0.878\pm0.002$. Finally, in Fig. 4, we exhibit the complete phase diagram of the model showing the continuous and discontinuous transition lines separating the antiferromagnetic and paramagnetic phases. The tricritical point, which is indicated by an open circle, joins these two lines.

Now we present the results we obtained for the critical exponents along the continuous transition line through the formalism of short-time scaling critical dynamics. We have

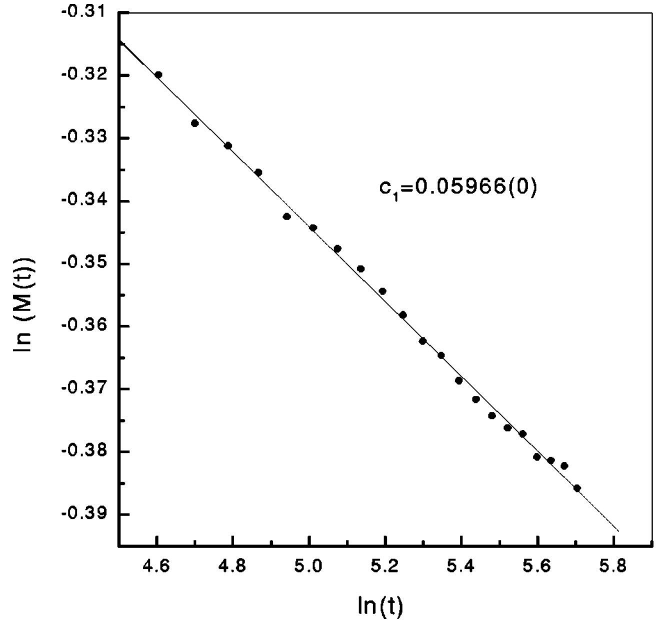

FIG. 5. Plot of $\ln[M(t)]$ versus $\ln(t)$ at $T_c=1.647$ and $H_c=1.50$. The straight line gives the best fit to the data points.

prepared the system to be in a completely ordered state, and it was left to evolve in time at the chosen critical values of temperature and field. We have considered up to 500 MCS to evaluate the exponents, and our results represent averages over 2000 samples of linear length $L=256$. For instance, we exhibit in Fig. 5, for $T_c=1.647$ and $H_c=1.50$, the log-log plot of staggered magnetization versus time. We also show the best fit to our data points. From the slope of this curve we found that $c_1=0.059\,66(0)$. In Fig. 6, we exhibit the log-log plot of the logarithmic derivative of the staggered magnetization with respect to the reduced temperature at the critical point, versus time. From the slope of the curve, which fits the

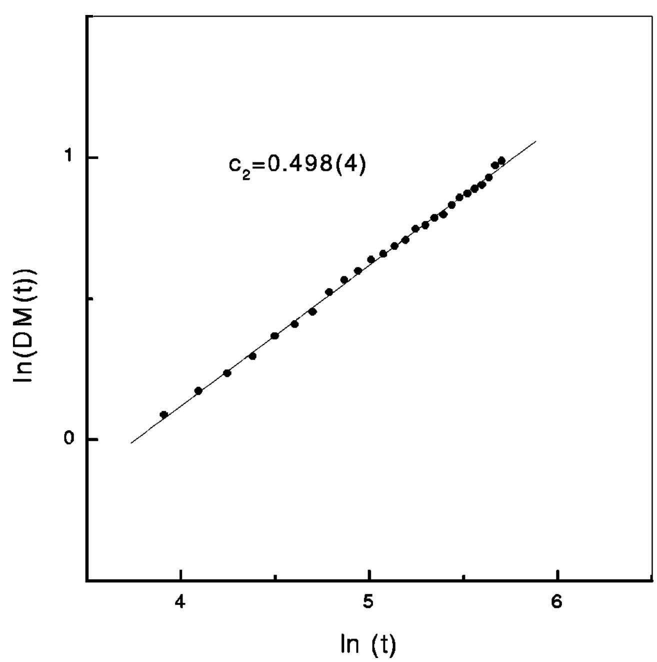

FIG. 6. Plot of $\ln[DM(t)]$ versus $\ln(t)$ at $T_c=1.647$ and $H_c=1.50$. The straight line gives the best fit to the data points.

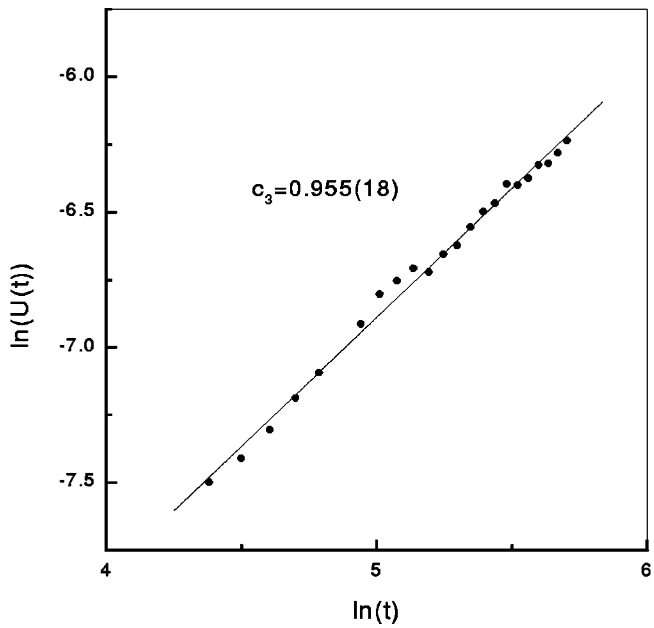

FIG. 7. Plot of $\ln[U(t)]$ versus $\ln(t)$ at $T_c=1.647$ and $H_c=1.50$. The straight line gives the best fit to the data points.

data points, we found $c_2=0.498(4)$. Finally, in Fig. 7, we show the log-log plot of the second-order cumulant versus time, and the best fit to the data points. The slope of the curve in this figure gives $c_3=0.955(18)$. With these values, we can find the critical exponents β, ν, and z. For this particular critical point of the transition line, we have found the following values: $\beta=0.120(6)$, $\nu=0.96(3)$, and $z=2.09(4)$. For other critical points on the continuous transition line we also found values for these exponents by employing the same procedure as above. For instance, we can see in Fig. 8 the values of the exponents ν and z plotted against the ratio between the critical values of the field and

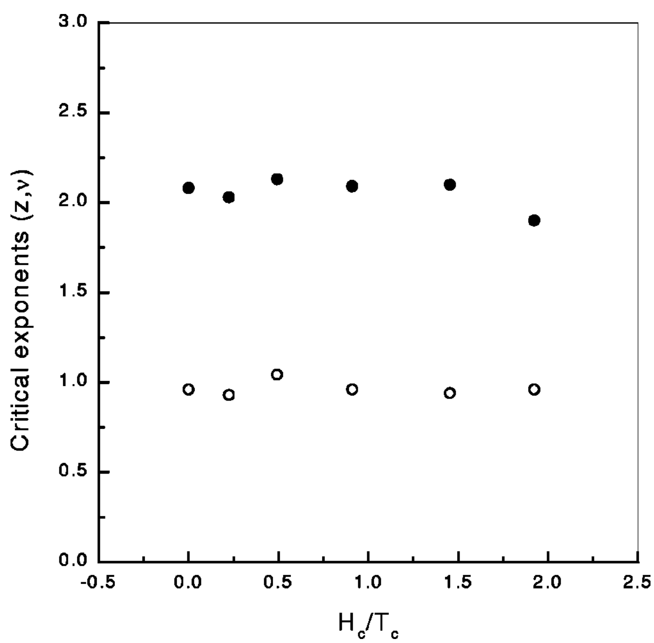

FIG. 8. Critical exponents z (closed circles) and ν (open circles) plotted against the ratio between the critical values of the field and temperature (H_c/T_c) along the continuous phase boundary.

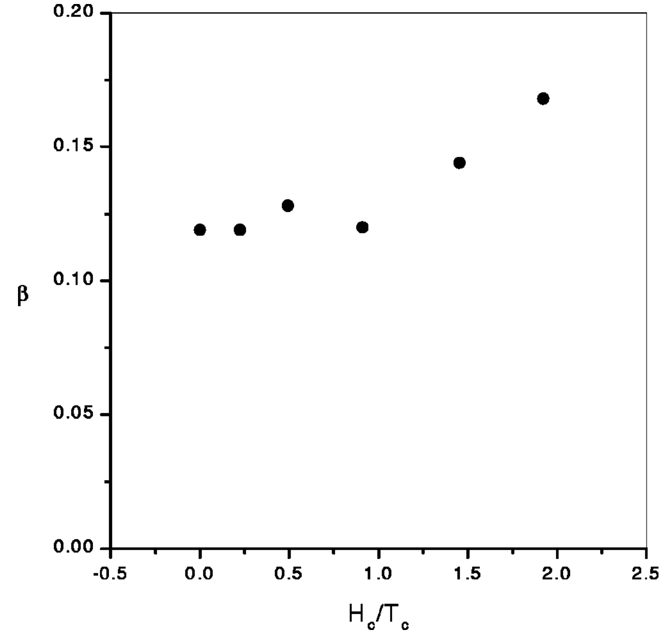

FIG. 9. Critical exponent β plotted against the ratio between the critical values of the field and temperature (H_c/T_c) along the continuous phase boundary.

temperature. We see that these exponents are well behaved for all values of the ratio H_c/T_c, up to the vicinity of the tricritical point, where this ratio assumes the value $H_t/T_t=2.20$. However, as we can observe in Fig. 9, the values of the exponent β are influenced by the presence of the tricritical point. For values of the ratio H_c/T_c less than 1.0, the β exponent is the same as in the two-dimensional Ising model, as predicted by universality arguments. However, for values of the ratio H_c/T_c larger than 1, we clearly observe the crossover between critical and tricritical behavior.

IV. CONCLUSIONS

We have studied a two-sublattice layered metamagnetic model on a square lattice, with competing ferromagnetic and antiferromagnetic couplings. Using the Monte Carlo method, we have determined the phase diagram of the model, which exhibits continuous and discontinuous phase transitions between the antiferromagnetic and paramagnetic phases. Through the short-time scaling critical dynamics, we have found the static and dynamic critical exponents along the continuous transition line of the model. The values of the exponents ν and z are almost independent of temperature and magnetic field along the critical line up to near the tricritical point. On the other hand, the value of the exponent β is affected by the presence of the tricritical point, showing a crossover between critical and tricritical behavior. To the best of our knowledge this is the first time that short-time dynamics has been applied to a model system in the presence of an external magnetic field.

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