The short-time behavior of a classical ferromagnet with double-exchange interaction

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We investigate the critical dynamics of a classical ferromagnet on the simple cubic lattice with double-exchange interaction. Estimates for the dynamic critical exponents \( z \) and \( \theta \) are obtained using short-time Monte Carlo simulations. We also estimate the static critical exponents \( \nu \) and \( \beta \) studying the behavior of the samples at an early time. Our results are in good agreement with available estimates and support the assertion that this model and the classical Heisenberg model belong to the same universality class.

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I. INTRODUCTION

In the last decade many works have been devoted to the study of the perovskite manganites, \( A_{1-x}B_xMnO_3 \), where \( A \) and \( B \) are rare-earth and alkaline-earth ions, respectively, and \( x \) is the concentration of \( B \). The perovskite manganites are metal oxides that exhibit some remarkable properties. The most noticeable of them is colossal magnetoresistance (CMR), an extremely large change in the resistivity when a magnetic field is applied in the vicinity of the critical temperature. Usually these materials have been studied in the context of the double-exchange theory (DE). In one of these works, Anderson and Hasegawa showed that the transfer element is proportional to \( \cos(\theta/2) \), where \( \theta \) is the angle between the ionic neighbouring spins. This result was recently confirmed for layered manganites. Nevertheless, although this theory has succeeded in explaining qualitatively CMR, some authors have argued that it cannot alone provide a complete description of this phenomenon. They suggest that, in addition to the double exchange, a complete understanding of these materials should include strong electron correlations, a strong electron-phonon interaction, or coexisting phases. One might therefore think that double-exchange alone cannot explain CMR in manganites, but this remains an open question. What we know is that in the study of the manganites the double-exchange theory plays an important role, both in the study of CMR and in explaining the presence of a ferromagnetic phase (for \( x \approx 0.3 \)) in doped manganites, furnishing the basis for describing manganites with colossal magnetoresistance.

The mechanism of the double-exchange consists of a strong intrasite exchange between localized ions (core spin \( S^c \)) and non-localized electrons (\( E_g \) orbitals). Based on this hypothesis Zener succeeded in explaining in 1951 the occurrence of the metal ferromagnetic phase in manganites. Due to a strong intrasite exchange interaction the spin of the electron always aligns parallel to the spin of the ion. When an electron hops from site \( i \) to site \( j \) its spin must also change from being parallel to \( S^c_i \) to being parallel to \( S^c_j \), but with an energy loss proportional to the cosine of half the angle between the core spins.

In Ref. [10], the critical behavior of a classical ferromagnet with double-exchange interaction was studied and estimates for the static critical exponents \( \nu \) and \( \beta \), and the critical temperature \( T_c \) were derived. These simulations indicate that this model belongs to the universality class of the classical Heisenberg model.

In this paper, we perform short-time Monte Carlo simulations to explore the critical dynamics of a classical ferromagnet with double-exchange interaction. We evaluate the dynamic exponents \( z \), \( \theta \) and the static exponents \( \nu \) and \( \beta \). Our estimates for static indices are in good agreement with previous results available in the literature for the same model. In addition, the result for the dynamic exponent \( z \) compare well with previous estimates for the classical Heisenberg model. In summary, present results confirm that both models belong to the same universality class.

The article is organized as follows. In the next Section we define the model. In Section III we give a brief description of short-time Monte Carlo technique and present our results; in Section IV we summarize and conclude.

II. THE MODEL

We use the short-time Monte Carlo simulations to investigate the dynamical critical behavior of a classical spin model with double-exchange interaction. We consider a simple cubic lattice \( L \times L \times L \) with periodic boundary conditions. The Hamiltonian for such system is given as:

\[
H = -J \sum_{\langle ij \rangle} S_i \cdot S_j + \sum_i h_i S_i,
\]

where \( J \) is the exchange integral, \( \langle ij \rangle \) denotes a sum over nearest neighbor sites, \( h_i \) is the magnetic field, and \( S_i \) is the spin at site \( i \).

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\[ \mathcal{H} = -\sum_{<i,j>} J \sqrt{1 + S_i \cdot S_j}, \] (1)

where \( <i,j> \) indicates that the sum runs over all nearest-neighbor pairs of lattice site, \( J \) is the ferromagnetic coupling constant and the spin \( S_i = (S_i^x, S_i^y, S_i^z) \) is a three-dimensional unit of length.

We used lattice sizes \( L = 20, 25, 30, 40 \) and 60 and performed short-time simulations at the critical temperature \( T_c = 0.74515 \), in units of \( J/k_B \), where \( k_B \) is the Boltzmann’s constant.

Our estimates for each exponent were obtained from five independent bins. The dynamic evolution of the spins is local and updated by the Metropolis algorithm. For \( 20 \geq L \geq 40 \) the estimate for the exponent \( \theta \) was performed using 10000 independent samples, while for the exponents \( z, \nu \) and \( \beta \) we used 50000 samples. For \( L = 60 \) all the estimates were performed using 2000 samples. In order to maximize the quality of the linear fitting, each exponent is determined in the time interval \([200, 500]\), except for the exponent \( z \) which was measured in the interval \([30, 250]\).

### III. SHORT-TIME SCALING RELATIONS AND RESULTS

Following the works of Janssen, Schaub and Schmittmann\(^{14a}\) and Huse\(^{14b}\), the study of the critical properties of statistical systems became in some sense simpler, because they allow to circumvent the well-known problem of the critical slowing down, characteristic of the long-time regime. They discovered using renormalization group techniques and numerical calculations, respectively, that there is universality and scaling behavior even at the early stage of the time evolution of dynamical systems without conserved quantities (model \( A \) in the terminology of Halperin \textit{et al}\(^{15}\)).

In this new universal regime, in addition to the familiar set of static critical exponents and the dynamic critical exponent \( z \), a new dynamic critical exponent \( \theta \) is found. This new critical index, independent of the previously known exponents, characterizes the so-called \textit{critical initial slip}, the anomalous increase of the magnetization when the system is quenched to the critical temperature \( T_c \).

Several works on phase transitions and critical phenomena using this technique have been published\(^{16,17}\). The results corroborate the prediction of universality and scaling behavior in the short-time regime and the static critical exponents so obtained are in good agreement with well-known values calculated in the equilibrium. In addition, this approach has permitted obtaining more precise estimates for the dynamic critical exponent \( z \).

The dynamic scaling relation obtained by Janssen \textit{et al} for the \( k \)-th moment of the magnetization, extended to systems of finite size\(^{18,19}\), is written as

\[ M^{(k)}(t, \tau, L, m_0) = b^{-k\beta/\nu} M^{(k)}(b^{-z}t, b^{1/\nu}\tau, b^{-1}L, b^{x_0}m_0), \] (2)

where \( t \) is time, \( b \) is an arbitrary spatial rescaling factor, \( \tau = (T - T_c)/T_c \) is the reduced temperature and \( L \) is the linear size of the lattice. The exponents \( \beta \) and \( \nu \) are the equilibrium critical exponents associated with the order parameter and the correlation length, and \( z \) is the dynamic exponent characterizing time correlations in equilibrium. For a large lattice size \( L \) and small initial magnetization \( m_0 \) at the critical temperature \((\tau = 0)\), the magnetization is governed by a new dynamic exponent \( \theta \),

\[ M(t) \sim m_0 t^\theta \] (3)

if we choose the scaling factor \( b = t^{1/z} \).

In addition, a new critical exponent \( x_0 \), which represents the anomalous dimension of the initial magnetization \( m_0 \), is introduced to describe the dependence of the scaling behavior on the initial conditions. This exponent is related to \( \theta \) as \( x_0 = \theta z + \beta/\nu \). In the following section we evaluate the critical exponents \( \theta, z, \nu \) and \( \beta \) using scaling relations obtained from Eq. (2).

#### A. The dynamic exponent \( \theta \)

Usually the dynamic critical exponent \( \theta \) is calculated using Eq. (3) or through the autocorrelation

\[ A(t) \sim t^{\theta - d/2}, \] (4)

where \( d \) is the dimension of the system.

In the first case, careful preparation of the initial configurations \((m_0 \ll 1)\) is essential, as well as the delicate limit \( m_0 \rightarrow 0 \). In the autocorrelation case, one must to know in advance the exponent \( z \), which is an order of magnitude greater than \( \theta \), so that a small relative error in \( z \) induces a large error in \( \theta \).

In the present work we find the dynamic critical exponent \( \theta \) using the time correlation of the magnetization\(^{20}\)

\[ C(t) = \langle M(0)M(t) \rangle \sim t^\theta. \] (5)

Here, the averaging is over a set of random initial configurations. The time correlation allows the direct calculation of the dynamic exponent \( \theta \), without the need of a careful preparation of the initial state nor of the limiting procedure, the only requirement being that \( \langle M_0 \rangle = 0 \).

In Fig. 1 we show the time dependence of the time correlation \( C(t) \) in double-log scale for the system with \( L = 60 \). Table 1 shows our estimates for the critical exponent \( \theta \) along with \( d/z, 1/\nu z \) and \( \beta/\nu z \).

These results show that for \( L \geq 25 \) the finite size effects are less than the statistical errors. Therefore, we conclude that the values for an infinite lattice are within the errorbars of our results for \( L = 60 \).
the time for the lattices $L$ which collapses curves for two lattices of different sizes.

In this case, according to the scaling relation Eq. (8), for $L_1 = 40$ and $L_2 = 25$ we obtained $z = 1.96(2)$, whereas for $L_1 = 60$ and $L_2 = 30$ we obtained $z = 1.96(4)$. A more precise estimate for the dynamic exponent $z$ can be obtained by combining results from samples submitted to different initial conditions ($m_0 = 1$ and $m_0 = 0$). According to the Ref. [24] the function $F_2(t) = M^{(2)}(t)/M(t)$ behaves as $t^{d/z}$ where $d$ is the dimension of the system. This approach proved to be very efficient in estimating the exponent $z$, according to results for the Ising model, the three- and four-state Potts models, the tricritical point of the Blume-Capel model, the Baxter-Wu model and nonequilibrium models like Domany-Kinzel and contact process. In this technique, for different lattice sizes, the double-log curves of $F_2$ versus $t$ fall on a single straight line, without any rescaling of time, resulting in more precise estimates for $z$.

The time evolution of $F_2$ is shown on log scales in Fig. 3 for $L = 60$. In Table III we show the values of $d/z$ for the five lattice sizes. Taking into account the value of this ratio for the lattice $L = 60$ we obtain

$$z = 1.975(4)$$

Our results for $z$ indicate that besides presenting the same static critical exponents double-exchange
FIG. 3: Time Evolution of $F_2$. The error bars, calculated over 5 sets of 2000 samples, are smaller than the symbols.

Heisenberg models have the same dynamic exponent when submitted to the same updating.

C. The static exponents $\nu$ and $\beta$

The static exponent $\nu$ can be obtained by fixing $b^{-z}t = 1$ in Eq. (2) and differentiating $\ln M(t, \tau)$ with respect to $\tau$ in the critical point. Taking into account samples with ordered initial configurations ($m_0 = 1$), we obtain the following power law

$$\partial_\tau \ln M(t, \tau)|_{\tau=0} \sim t^{1/\nu z}.$$  \hspace{1cm} (10)

In numerical simulations we approximate the derivative by a finite difference; our results were obtained using finite differences of $T_{c}\pm\delta$ with $\delta = 0.01$, in units of $J/k_B$. In Fig. 4 the power law increase of Eq. (10) is plotted in double-log scale for $L = 60$.

From the slope of the curve one can estimate the critical exponent $1/\nu z$ (see Table II).

Using the exponent $z$ obtained from $U_4(t, L)$ and the estimate of $1/\nu z$ for $L = 60$, we obtain the static exponent

$$\nu = 0.68(2).$$  \hspace{1cm} (11)

while following the scaling relation $F_2(t)$ the result is

$$\nu = 0.682(8).$$  \hspace{1cm} (12)

Finally we can evaluate the static exponent $\beta$ by the dynamic scaling law for the magnetization

$$M(t) \sim t^{-\beta/\nu z},$$  \hspace{1cm} (13)

obtained from Eq. (2), by considering large systems and setting $b = t^{1/z}$ at the critical temperature $\tau = 0$. In Fig. 5 we show the time evolution of the magnetization in double-log scale for $L = 60$. The estimates of the exponent $\beta/\nu z$ for the five lattice sizes are shown in Table II.

Using the previous result obtained for $1/\nu z$ (Table II), we find

$$\beta = 0.354(5).$$  \hspace{1cm} (14)

Our estimates for the static exponents $\nu$ and $\beta$ are in good agreement with the theoretical results of the Ref. [10] ($\nu = 0.6949(38)$ and $\beta = 0.3535(30)$), Ref. [11] ($\nu = 0.7036(23)$ and $\beta = 0.3616(31)$) and Ref. [28] ($\nu = 0.704(6)$ and $\beta = 0.362(4)$), as well as the experimental results of the Ref. [29] ($\beta = 0.37(4)$) and the Ref. [30] ($\beta = 0.374(6)$).
IV. DISCUSSION AND CONCLUSIONS

In this article we have performed short-time Monte Carlo simulations in order to evaluate the dynamic and static critical exponents of a classical ferromagnet with double-exchange interaction. The exponent $\theta$ was estimated using the time correlation of the magnetization. We found the dynamic exponent $z$ through the collapse of the fourth-order time-dependent Binder cumulant and also, alternatively, using the function $F_2(t)$ which combines simulations performed with different initial conditions. Using scaling relations for the magnetization and its derivative with respect to the temperature at $T_c$, we have obtained the static exponents $\nu$ and $\beta$ which are in good agreement with the values available in literature. Comparison of our results with those for the classical Heisenberg model corroborate the assertion that the models belong to the same universality class.

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