Global persistence exponent of the double-exchange model

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We obtained the global persistence exponent θ_g for a continuous spin model on the simple cubic lattice with double-exchange interaction by using two different methods. First, we estimated the exponent θ_g by following the time evolution of probability P(t) that the order parameter of the model does not change its sign up to time $t[P(t) \sim t^{-\theta_g}]$. Afterwards, that exponent was estimated through the scaling collapse of the universal function $L^{\theta_g z} P(t)$ for different lattice sizes. Our results for both approaches are in very good agreement with each other.

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During the past few years, a great number of experimental and theoretical works have been published about manganites with perovskite structure, $A_{1-x}B_x$ MnO₃, where A is a rare earth such as La, Nd, and Pr, B is a divalent element such as Sr, Ca, Ba, and Pb, and x is the concentration of B. Such attention is due to the rediscovery of colossal magnetoresistence (CMR) [1–4], an extremely large change in the resistivity when a magnetic field is applied near the Curie temperature. Besides, these manganese oxides possess metalinsulator (MI) transitions, as well as a rich variety of physical properties and possible technological applications, for instance magnetic sensors and memory technology.

In these compounds, the MI transition associated with the ferromagnetic spin alignment has been widely explained by the double-exchange (DE) mechanism [5-10], in which the transfer of an itinerant e_g electron between the neighboring Mn ions through the O^{2-°}ion results in a ferromagnetic interaction. Anderson and Hasegawa [6] showed that the transference element is proportional to $\cos(\phi/2)$, where ϕ is the angle between the ionic neighboring spins. This result was recently confirmed for layered manganites [11]. Although this theory has also succeeded in explaining qualitatively CMR, some authors have argued that alone it cannot 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 [12], a strong electron-phonon interaction [13], or coexisting phases [14]. One might therefore think that double exchange alone cannot explain CMR in manganites [13], 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 state (for x ≈ 0.3) in doped manganites, furnishing the basis for describing manganites with colossal magnetoresistence.

The Hamiltonian of a classical spin model with doubleexchange interactions is given by [15]

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sqrt{1 + \mathbf{S}_i \cdot \mathbf{S}_j},\tag{1}$$

where $\langle i, j \rangle$ indicates that the sum runs over all nearestneighbor pairs of lattice site, *J* is the ferromagnetic coupling constant, and the spin $\mathbf{S}_i = (S_i^x, S_j^y, S_k^z)$ is a three-dimensional vector of unit length.

The critical properties of the DE models have been intensively studied by using Monte Carlo (MC) simulations. In the equilibrium [15-18], the estimates for the static critical exponents indicate that this model belongs to the universality class of the classical Heisenberg model [19]. Several experimental works about the critical properties of the doped perovskite manganites also support this assertion [20-22]. Very recently the dynamic critical behavior of the DE model was studied by using the short-time Monte Carlo simulations, and estimates for the static critical exponents ν and β and the dynamic critical exponents z and θ were derived [23]. That approach is based on the results of Janssen *et al.* [24], which showed that universality and scaling behavior are already present in systems since their early stages of the time evolution after quenching them from high temperatures to the critical one. By using renormalization-group techniques, they obtained for the kth moment of the magnetization, extended to systems of finite size [25], the following scaling relation:

$$M^{(k)}(t,\varepsilon,L,m_0) = b^{-k\beta/\nu} M^{(k)}(b^{-z}t,b^{1/\nu}\varepsilon,b^{-1}L,b^{x_0}m_0), \quad (2)$$

where *t* is time, *b* is an arbitrary spatial rescaling factor, $\varepsilon = (T-T_c)/T_c$ is the reduced temperature, and *L* is the linear size of the lattice. The exponents β and ν are the equilibrium critical exponents associated with the order parameter and the correlation length, and *z* is the dynamical exponent ($\tau \sim \xi^{z}$, where τ is the time correlation). For a large lattice size *L* and small initial magnetization m_0 at the critical temperature (ε =0), the magnetization is governed by a new dynamic exponent θ ,

$$M(t) \sim m_0 t^{\theta},\tag{3}$$

if we choose the scaling factor $b=t^{1/z}$ in Eq. (2). This new critical index, independent of the previously known exponents, characterizes the so-called "critical initial slip," the anomalous increase of the magnetization when the system is quenched to the critical temperature T_c . In the sequence, an-

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FIG. 1. Time evolution of the global persistence probability P(t) for a lattice size L=60 and $m_0=0.00125$. The error bars were calculated over five sets of 5000 samples.

other new independent dynamic critical exponent was found by Majumdar *et al.* [26] to describe the behavior of the global persistence probability P(t) that the order parameter has not changed its sign up to time *t*. At criticality, P(t) is expected to decay algebraically as

$$P(t) \sim t^{-\theta_g},\tag{4}$$

where θ_g is the global persistence exponent. Since then, the study of the persistence behavior has attracted an enormous amount of interest, playing an important role in the study of systems far from equilibrium [26–38].

Since the time evolution of the order parameter is in general a non-Markovian process, the new critical exponent θ_g is independent of the usual exponents. However, as argued by Majumdar *et al.* [26], if the global order parameter is described by a Markovian process, θ_g is not a new independent exponent, being related to other critical exponents by the equation



FIG. 2. Dynamical exponent θ_g as a function of the initial magnetization m_0 for cubic lattices with L=60. Each point represents an average over five sets of 5000 samples.

TABLE I. The global persistence exponent θ_g from the power law behavior for different initial magnetizations m_0 and even lattice sizes.

L	$m_0 = 0.005$	$m_0 = 0.0025$	$m_0 = 0.00125$	Extrapolated value
20	0.315(14)	0.326(8)	0.337(12)	0.342(4)
30	0.315(5)	0.322(12)	0.335(9)	0.339(5)
40	0.315(9)	0.321(31)	0.336(28)	0.339(7)
50	0.319(10)	0.325(11)	0.336(14)	0.338(6)
60	0.313(7)	0.315(14)	0.333(10)	0.336(9)

$$\theta_g = \alpha_g = -\theta + \frac{d}{z^2} - \frac{\beta}{\nu z}.$$
 (5)

The global persistence probability P(t) can be defined as

$$P(t) = 1 - \sum_{t'=1}^{t} \rho(t'), \tag{6}$$

where $\rho(t')$ is the fraction of the samples that have changed their state for the first time at the instant t'.

In this paper, we performed short-time Monte Carlo simulations to explore the scaling behavior of the global persistence probability P(t), for a classical ferromagnet with double-exchange interaction. The dynamical exponent θ_g that governs the behavior of P(t) at criticality is obtained by using two different approaches: the straight application of the power law behavior [see Eq. (4)] and by means of timeseries data collapse. To our knowledge, this is the first time that this exponent is calculated for a three-dimensional model and continuous spin variables.

In our simulations, we considered $L \times L \times L$ (L=20, 25, 30, 35, 40, 50, and 60) simple cubic lattices with periodic boundary conditions. Simulations were done at critical temperature [15] $T_c=0.74515$, in units of J/k_B , where k_B is Boltzmann's constant. The update we used is local and follows the METROPOLIS algorithm, i.e., at each site of the lattice



FIG. 3. Scaling collapse of the scaled persistence probability vs scaled time for L_1 =50 and L_2 =60. The curves were obtained from five independent bins of 5000 samples.

TABLE II. The global persistence exponent θ_g for the best collapse for the double-exchange model.

$L_2 \mapsto L_1$	$ heta_g$
60⇒50	0.335(9)
$60 \mapsto 40$	0.333(13)
60 → 30	0.329(14)
50 → 35	0.337(11)
40 → 25	0.330(12)
$40 \mapsto 20$	0.332(12)

(during the simulation) a trial orientation of the spin is randomly chosen and accepted or rejected according to the probability $e^{-\beta(E'-E)}$, where E'(E) is the new (old) energy of the spin system, $\beta = J/k_BT_c$, and k_B is the Boltzmann constant. The estimates were obtained from five independent bins with 5000 samples each for *t* up to 500 Monte Carlo sweeps.

In the first method, we used the scaling relation given by Eq. (4) in order to obtain θ_g as a function of m_0 for several values of the initial magnetization. Here, it is necessary to work with a precise and small value of the magnetization, $m_0 \sim 0$. Next, the estimate for θ_g is obtained extrapolating that series to the limit in which $m_0 \rightarrow 0$.

In Fig. 1, we show the decay of the global persistence probability for L=60 and $m_0=0.00125$ in double-log scales. Figure 2 exhibits the behavior of the exponent θ_g for $m_0 = 0.005$, 0.0025, and 0.00125, as well as a linear fit that leads to the value $\theta_g = 0.336(9)$.

In Table I, we present the estimates for θ_g as a function of different initial magnetizations m_0 for other lattice sizes.

Our results obtained through the linear extrapolations for $m_0 \rightarrow 0$ are presented in the last column. The estimates of the exponent θ_g for odd lattice sizes (*L*=25 and 35) were obtained for different values of m_0 . For *L*=25, we used $m_0 = 0.0064, 0.0032$, and 0.0016 and the extrapolated value was $\theta_g = 0.337(5)$, whereas for *L*=35 we used $m_0 = 240/(35^3)$, 120/(35³), and 60/(35³) and the extrapolated value $\theta_g = 0.338(5)$.

In the second method, we used the fact that the dependence of P(t) on the initial magnetization can be cast in the following finite-size scaling relation [26]:

$$P(t) = t^{-\theta_g} f(t/L^z) = L^{-\theta_g z} \tilde{f}(t/L^z), \tag{7}$$

where z is the dynamical exponent. Thus, the quantity $L^{\theta_g z} P(t)$ is a universal function of the scaled time (t/L^z) and the wanted value of θ_g is that which fulfills that condition for different lattices. The best estimate for θ_g is found through the χ^2 test [39].

Unlike the first method used in this paper, in the collapse method the exponent θ_g is obtained without the need for

TABLE III. The exponents θ_g and α_g for several models.

Models	$ heta_g$	α_g
Ising model [28]	0.236(3)	0.212(2)
Three-state Potts model [28]	0.350(8)	0.324(3)
Blume-Capel model [30]	1.080(4)	0.904(21)
DE model [see Eq. (9)]	0.335(9)	0.026(17)

careful preparation of the initial magnetization m_0 nor the limiting procedure. The only requirement is that $\langle m_0 \rangle \sim 0$, where $\langle \cdot \rangle$ is an average done over the samples at t=0. On the other hand, the collapse method demands the dynamical exponent *z* to be known beforehand. In this paper, we used the estimate obtained very recently for this exponent, z = 1.975(10) [23].

In Fig. 3, we show the collapse of the curves obtained for L=50 and 60. The open circles show the collapse of the larger lattice rescaled in time. Our best estimate for θ_g for $L_2=60$ and $L_1=50$ is

$$\theta_g = 0.335(9).$$
 (8)

The estimates for other lattice sizes are shown in Table II. These results are in very good agreement with the estimates obtained directly from the power law predicted in Eq. (4).

Using, for instance, the result of Eq. (8) and the estimates of the exponents θ , z, β , and ν obtained in Ref. [23], both for the largest lattice size (*L*=60), we verify through Eq. (5), the non-Markovian aspect of the phenomenon we are dealing with, since

$$\theta_g = 0.335(9)$$
 and $\alpha_g = -\theta + \frac{d}{z^2} - \frac{\beta}{\nu z} = 0.026(17).$ (9)

Thus, the global persistence exponent in this case is also independent of other critical exponents, but the difference between our estimate for θ_g and the value obtained from Eq. (5) is greater than that observed when discrete spin models were analyzed (see Table III).

In summary, we have performed short-time Monte Carlo simulations in order to investigate the scaling behavior of the persistence probability P(t) for a three-dimensional system with double-exchange interaction. The dynamic critical exponent θ_g that governs the behavior of P(t) at criticality was estimated by using two different approaches: the straight application of the power law behavior $P(t) \sim t^{-\theta_g}$ and the collapse method for the universal function $L^{\theta_g z} P(t)$. The results are consistent with the expected non-Markovian character of the process.

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