Short-time dynamic exponents of an Ising model with competing interactions

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In this work the two-dimensional Ising model with nearest- and next-nearest-neighbor interactions is revisited. We obtain the dynamic critical exponents $z$ and $\theta$ from short-time Monte Carlo simulations. The dynamic critical exponent $z$ was obtained from the time behavior of the ratio

$$F_2 = \langle M^2 \rangle_{m_0=0}/\langle M \rangle^2_{m_0=1} \sim t^{d/z},$$

where $M(t)$ is the order parameter at instant $t$, $d$ is the dimension of the system and $\langle \cdots \rangle$ is the average of the quantity $\langle \cdots \rangle$ over different samples. We have also obtained the static critical exponents $\beta$ and $\nu$ by investigating the time behavior of the magnetization.

Keywords: Dynamic critical exponents, Monte Carlo simulation, non-universality

I. INTRODUCTION

The two-dimensional Ising model with nearest- and next-nearest-neighbor interactions $J_1$ and $J_2$, respectively, presents non-universal critical behavior for $-J_2/J_1 > 1/2$. The existence of a non-universal critical line for $-J_2/J_1 > 1/2$ was suggested for the first time by van Leeuwen in 1975, who investigated the fixed point structure and critical surface of two-dimensional Ising models. Subsequently, in 1977, Krinsky and Mukamel conjectured that the critical behavior of the model should belong to the universality class of the two-component vector model. Also in 1977, Nightingale worked on finite size calculations of the model and showed that the exponents vary continuously with the coupling ratio between nearest- and next-nearest-neighbor interactions.

The model is defined by the Hamiltonian

$$H = -J_1 \sum_{\langle i,j \rangle} S_i S_j - J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i S_j,$$

where $S_i = \pm 1$ are Ising spin variables and the notation $\langle i,j \rangle$ and $\langle\langle i,j \rangle\rangle$ denotes that each sum runs over nearest- and next-nearest-neighbors, respectively. At $T = 0$ the ordering is ferromagnetic for $-J_2/J_1 < 1/2$, whereas it is super-antiferromagnetic (SAF) for $-J_2/J_1 > 1/2$. In the SAF phase, a row (column) of up spins alternates with a row (column) of down spins, as depicted in Fig. 1. From both numerical and analytical approaches, it was shown that in the plane of the reduced temperature $kT/J$ against the competition parameter $-J_2/J_1$, the phase diagram presents ferromagnetic, paramagnetic and super-antiferromagnetic phases. The critical line between the ferromagnetic and paramagnetic phases belongs to the universality class of the two-dimensional Ising model, whereas the critical exponents along the critical line separating the SAF ordered phase from the paramagnetic phase are found to be non-universal. Static critical exponents on the SAF-Paramagnetic critical line were obtained by Monte Carlo simulations, high temperature series expansion, renormalization group calculations, finite-size scaling, cluster variation and coherent-anomaly methods. It was observed that such critical exponents vary as a function of the coupling ratio $-J_2/J_1$, thus confirming non-universality in this model.

Today it is well known that, far from equilibrium, the short-time relaxation of the order parameter follows a universal scale form $M(t) \sim m_0 t^\theta$, where $M(t)$ is the order parameter at instant $t$ (measured in Monte Carlo Steps per Spin - MCS), $m_0 = M(0)$ is a (small) initial order parameter value and $\theta$ is a dynamic critical exponent associated to the anomalous increasing of the magnetization after the quenching of the system. Short-time Monte Carlo simulations of the model performed in a recent paper by Ye et al. showed that the dynamic critical exponent $\theta$ is also non-universal along the SAF-Paramagnetic transition line, once it depends on the ratio $-J_2/J_1$.

To our knowledge, for this model there are no previous attempts to obtain the dynamic critical exponent $z$, which is defined as $\tau \sim \xi^z$, where $\tau$ and $\xi$ are time and spatial correlation lengths, respectively. Therefore, in this work we obtain the dynamic critical exponent $z$ of the model from the time evolution of the ratio

$$F_2 = \langle M(t)^2 \rangle_{m_0=0}/\langle M(t) \rangle^2_{m_0=1} \sim t^{d/z},$$

where $M(t)$ is the order parameter at instant $t$, $d$ is the dimension of the system and $\langle \cdots \rangle$ is the average of the quantity $\langle \cdots \rangle$ over different samples with initial order parameter value $m_0$. This ratio has proven to be useful in
determining the exponent $z$, according to recent results obtained for the 2D Ising model, $q = 3$ and $q = 4$ states Potts models [18] and at the tricritical point of the Blume-Capel model [19]. In this technique curves of $\ln(F_2)$ against $\ln(t)$ lay on the same straight line for different lattice sizes, without any re-scaling in time, resulting in more precise estimates for $z$.

In this work we also reobtain the dynamic exponent $\theta$ along the non-universal critical line using the time correlation of the order parameter [20]

$$\langle M(0)M(t) \rangle \sim t^{\theta}, \quad (3)$$

and compare our results with those obtained in ref. [17], where the exponent $\theta$ was obtained from the scale form $M(t) \sim m_0 t^{\theta}$. The advantage in the use of Eq. (3) is that one does not need to fix precisely the initial order parameter value $m_0$. The only requirement is that $\langle m_0 \rangle = 0$. Contrarily, the scale form $M(t) \sim m_0 t^{\theta}$ demands sharply prepared initial states with a precise value of $m_0$, besides a delicate limit $m_0 \to 0$.

We have also calculated the static critical exponents $\beta$ and $\nu$ of the model. Such exponents are obtained indirectly because, from numerical simulations, we are able to obtain only the ratios of exponents $\beta/\nu z$, $1/\nu z$ and $\lambda = (d - 2\beta/\nu)/z$, as discussed in Ref. [21]. In order to obtain the former ratio ($\beta/\nu z$), we have used the scale relation [21]

$$M(t) \sim t^{-\beta/\nu z}, \quad (4)$$

according to which the order parameter $m_0 = M(0) = 1$ decays in the short-time evolution of the system. On the other hand, the ratio $1/\nu z$ was obtained from the scale relation [21]

$$\partial_\kappa \ln M(t, \kappa)|_{\kappa=0} \sim t^{1/\nu z}, \quad (5)$$

which is obtained by differentiating the quantity $\ln M(t, \kappa)$ in relation to $\kappa$ at the critical point, where $\kappa = (T - T_c)/T_c$ and $T_c$ is the critical temperature.

From the scaling relation [21]

$$M^2(t) \sim t^\lambda, \quad (6)$$

we have also calculated the exponent

$$\lambda = \left(d - \frac{2\beta}{\nu} \right) \frac{1}{z}. \quad (7)$$

The exponent $\nu$ is given by

$$\nu = \frac{1}{(1/\nu z)(z)}, \quad (8)$$

whereas the exponent $\beta$ is given by

$$\beta = \left( \frac{\beta}{\nu z} \right) \left( \frac{1}{\nu z} \right)^{-1}. \quad (9)$$

Finally, from the exponents $z$, $\nu$ and $\lambda$, the critical static exponent $\beta$ may also be obtained from

$$\beta = \frac{\nu}{2} (d - z \lambda). \quad (10)$$

The layout of this paper is as follows: In section II we define the order parameter of the model and we give details about the numerical simulations performed. In section III we present the results obtained for both dynamic and static critical exponents. Finally, in section IV we briefly discuss the main results of this work.

II. SHORT-TIME MONTE CARLO SIMULATIONS

Simulations were performed in two-dimensional lattices with periodic boundary conditions. The spin states were updated using one-spin-flip heat-bath algorithm. For each value of the competition parameter $-J_2/J_1 > 1/2$ considered, we used the corresponding critical temperature given in ref. [17].
FIG. 1: Example of one possible super-antiferromagnetic (SAF) ordering. In this example, rows of up spins alternate with rows of down spins. The other possible configuration of this ordered state corresponds to columns of up spins alternating with columns of down spins.

Once the simulations were performed along the line between the SAF and Paramagnetic phases, the order parameter $M$ considered in this work is that corresponding to the SAF ordering. The SAF phase may be seen as two interpenetrating sublattices, each sublattice been formed by alternating rows, as the example depicted in Fig. 1: One sublattice (say, sublattice A) corresponds to rows $++\ldots +$, whereas the other sublattice (say, B) corresponds to rows $--\ldots -$. By inverting the signs of all spins in each sublattice, one obtains another configuration in which sublattice A is formed by down spins and sublattice B corresponds to up spins. Thus, this ground state is twofold. We call attention of the reader to the existence of another twofold SAF ordering, which consists of columns of up spins alternating with columns of down spins. Thus, the SAF ground state is fourfold, what implies that the transition line SAF-Para is of kind $4 \rightarrow 1$. Following Zittartz [22], this phase transition is candidate to exhibit non-universal behavior.

The order parameter $M$ is defined as $M = (M^A - M^B)/2$, where

$$M^A = \frac{1}{N^2} \sum_{x=1}^{N} \sum_{y=1}^{N} S_{2x-1,y},$$

$$M^B = \frac{1}{N^2} \sum_{x=1}^{N} \sum_{y=1}^{N} S_{2x,y}.$$  \hspace{1cm} (11)

$$M^B = \frac{1}{N^2} \sum_{x=1}^{N} \sum_{y=1}^{N} S_{2x,y}.$$ \hspace{1cm} (12)

In order to deal with square sublattices, we used lattices of $2N = 144$ rows and $N = 72$ columns. In the absence of a magnetic field, the symmetry $M^A = -M^B$ is expected. Thus, when preparing initial states for numerical simulations we have taken this expected symmetry into account, i.e., we prepared initial $t = 0$ configurations such that $M^A(0) = -M^B(0)$. For the exponent $z$, one sees from Eq. (2) that two independent runs are necessary in order to obtain the ratio $F_2$: One of them starts with $m_0 = M(0) = 1$ and the other run starts with $m_0 = M(0) = 0$. For $m_0 = 1$, we just set $S_{x,y} = 1$ in sublattice A and $S_{x,y} = -1$ in sublattice B. On the other hand, for $m_0 = 0$, we set $S_{x,y} = 1$ in sublattice A and $S_{x,y} = -1$ in sublattice B, inverting randomly the sign of half of the spin variables in each sublattice. The ratios of exponents $\beta/\nu z$ and $1/\nu z$ are obtained from Monte Carlo simulations with initially ordered states, i.e., initial states with $m_0 = 1$. For the exponents $\theta$ and $\lambda$, we must have for the initial order parameter $\langle m_0 \rangle = 0$. In order to obtain such an initial state, we give a probability $p = 0.5$ for every spin in sublattice A to point up. Thus, we calculate $M^A(0)$ and impose $M_B(0) = -M^A(0)$. The spin configuration in sublattice B is chosen in order to satisfy such imposition. Finally, the time interval used for the runs performed in this work was $[1,150]$, and the final results for the dynamic critical exponents were extracted from a time interval $[t_1, t_2]$ \hspace{1cm} (1 \leq t_1 < t_2 \leq 150) which maximizes the goodness of fit $q$. For example, suppose that from two time intervals $[t_1, t_2]$ and $[t_1', t_2']$ one obtains $q = 0.99$ and $q = 0.4$, respectively. The critical exponent obtained from the time interval $[t_1, t_2]$ is assumed to be correct.

The error bars of the exponents $\theta$, $z$, $\beta/\nu z$ and $\lambda$, showed in the following section, are the standard deviation from the mean value obtained from five independent runs with different initial seeds for the random numbers generator. For the quantity $\beta/\nu$ and for the exponents $\beta$ and $\nu$, which are obtained indirectly, the error bars were evaluated from usual error propagation.
FIG. 2: Non-universal behavior of the dynamic critical exponent $\theta$, as a function of the ratio between nearest- and next-nearest-neighbor interactions $-J_2/J_1$. In the graph, the high of each X corresponds to the error bars found in Ref. [17]. The points with error bars shown explicitly are the results obtained in this work from the time correlation of the order parameter.

FIG. 3: Dynamic critical exponent $z$, as a function of the ratio between nearest- and next-nearest-neighbor interactions $-J_2/J_1$.

III. RESULTS

A. Dynamic critical exponents

In this subsection we present the results obtained for the dynamic critical exponents $\theta$ and $z$. In Fig. 2 it is shown the dynamic exponent $\theta$ in function of the ratio $-J_2/J_1$, obtained from Eq. (3). Non-universality is observed, since $\theta$ clearly depends on the ratio $-J_2/J_1$. This result is in accordance with that obtained in Ref. [17]. In Fig. 3 we present the dynamic exponent $z$ as a function of $-J_2/J_1$, obtained from the ratio given in Eq. (2). From Fig. 3 one can not affirm if the exponent $z$ is universal or not, once the variation of $z$ with the coupling parameter $-J_2/J_1$ is not so pronounced as observed for the exponent $\theta$. Furthermore, since the major variation (or fluctuation) of $z$ occurs close to the disorder point ($-J_2/J_1 = 0.5$), such fluctuation may result from a crossover effect.

From both Fig. 2 and Fig. 3 we observe that, as the coupling parameter $-J_2/J_1$ increases, the exponents $\theta$ and $z$ tend towards their known Ising values $0.19 \cdots$ and $2.15 \cdots$, respectively.
In this subsection we show, as a function of the ratio \(-J_2/J_1\), the ratio of the exponents $\frac{\beta}{\nu z}$, $\frac{\beta}{\nu}$ and $\lambda = \frac{(d-2\beta/\nu)}{z}$, and the static critical exponents $\beta$ and $\nu$. In Figs. 4, 5, and 6 as a function of the coupling parameter, we show the ratios $\beta/\nu z$, $\beta/\nu$ and $\lambda$. We observe that the behavior of these quantities as the coupling parameter $-J_2/J_1$ varies is quite similar to that observed for the exponent $z$. So, we are not able to affirm anything about non-universality of these quantities. Particularly, from Fig. 5 we observe that the ratio $\beta/\nu$ does not reach its known exact Ising value $\beta/\nu = 1/8$ for large enough values of $-J_2/J_1$. We confirmed this result by Finite Size Scaling calculations combined with conformal invariance [23].

The static critical exponent $\nu$, obtained from Eq. (8), is shown in Fig. 7 as a function of the coupling parameter $-J_2/J_1$. The non-universal behavior observed for this exponent was already found before using Monte Carlo [24] and transfer-matrix [9] methods. In Fig. 7 we observe that the exponent $\nu$ tends towards the known exact two-dimensional Ising value $\nu = 1$ as $-J_2/J_1$ increases.

The non-universal behavior of the static critical exponent $\beta$, evaluated from both Eqs. (9) and (10), is shown in Fig. 8 as a function of the ratio $-J_2/J_1$. We observe the good agreement for the numerical values obtained for the exponent $\beta$ from Eqs. (9) and (10). In the second case, we note bigger error bars. This is due to the fact that the
FIG. 6: Exponent \( \lambda = (d - 2\beta/\nu)/z \), as a function of the ratio between nearest- and next-nearest-neighbor interactions \(-J_2/J_1\).

FIG. 7: Non-universal behavior of the static critical exponent \( \nu \), as a function of the ratio between nearest- and next-nearest-neighbor interactions \(-J_2/J_1\).

evaluation of the exponent \( \beta \) from Eq. (10) involves more exponents previously obtained, and so the error propagation implies the bigger error bars observed.
FIG. 8: Non-universal behavior of the static critical exponent $\beta$, obtained from Eqns. (9) (full circles) and (10) (triangles up), as a function of the ratio between nearest- and next-nearest-neighbor interactions $-J_2/J_1$. 
IV. SUMMARY AND DISCUSSION

In this work we study the dynamic critical exponents of the two-dimensional Ising model with competing nearest- and next-nearest-neighbors interactions. We obtained the dynamic exponent \( z \) along the transition line between the SAF and Paramagnetic phases by using a method recently proposed based on the mixing of initial conditions [18]. To our knowledge, this work is the first attempt to obtain the exponent \( z \) for this model. We have also calculated the dynamic critical exponent \( \theta \) using the time correlation scale form of the order parameter [20] and our results are in good agreement with those obtained in ref. [17]. Non-universality was also observed for the static critical exponents \( \beta \) and \( \nu \). In particular, as the ratio \(-J_2/J_1\) increases, we observed that the dynamic critical exponents tend towards their known Ising values. However, the ratio \( \beta/\nu \) does not tends towards its known exact Ising value \( \beta/\nu = 1/8 \) as the coupling ratio \(-J_2/J_1\) increases. We have confirmed this result by means of Finite Size Scaling caculations combined with conformal invariance [23].

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