Numerical evidence of Janssen-Oerding's prediction in a three-dimensional spin model far from equilibrium

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In 1994, Jansen and Oerding predicted an interesting anomalous tricritical dynamic behavior in three-dimensional models via renormalization group theory. However, we highlight the lack of literature about the computational verification of this universal behavior. Here, we use some tricks to capture the log corrections and the parameters predicted by these authors using the three-dimensional Blume-Capel model. We quantify the crossover phenomena by computing the critical exponents near the tricritical point. In addition, we also perform a more detailed study of the dynamic localization of the phase diagram via power-law optimization.

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I. INTRODUCTION

The Blume-Capel (BC) model [1] is a spin-1 model whose Hamiltonian is

$$\mathcal{H} = -J\sum_{\langle i,j\rangle}\sigma_i\sigma_j + D\sum_{i=1}^{N}\sigma_i^2 - H\sum_{i=1}^{N}\sigma_j. \tag{1}$$

Here, $D \geqslant 0$ is the anisotropy term, $\sigma_j = 0, \pm 1$, H is the external field that couples with each spin, and $\langle i, j\rangle$ denotes that sum is taken only over the nearest neighbors in a d-dimensional lattice.

Such a model in two and three dimensions presents a critical line and a first-order transition phase line, and such lines have an intersection point known as a tricritical point (TP). It is called that because for $H > 0$ and $H < 0$, one has two other first-order lines in addition to one from $H = 0$, and all these three lines culminate in that point. If the equilibrium studies of this model are fascinating, their dynamic aspects are even more so, mainly when studied at TP.

Janssen, Schaub, and Schmittmann [2], considering systems without conserved quantities, model A in the terminology of Halperin *et al.* [3], proposed a dynamic scaling relation that includes the dependence on the initial trace of the system for the moments of the magnetization, $m^{(k)}(t, \tau, L, m_0) = b^{-\frac{k\beta}{\nu}} m^{(k)}(b^{-z}t, b^{\frac{1}{\nu}}\tau, b^{-1}L, b^{x_0}m_0)$, where $m^{(k)}$ denotes the kth moment of the magnetization per spin. In this case the average considers the different time evolutions of the system and the different initial conditions since with the same m_0 (initial magnetization) we can have several different spin configurations. Here, t is the time evolution, 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 system.

This approach predicts an initial anomalous slip of magnetization (first moment) on the relaxation of a spin model that, initially at high temperatures ($m_0 \ll 1$), is suddenly placed at its critical temperature. A power law with an exponent $\theta = (x_0 - \beta/\nu)/z > 0$ describes such behavior, which depends on universal exponents: the dynamic one z and the static exponents β and ν, with these last ones being related to the equilibrium of the system. An anomalous dimension x_0 related to initial magnetization completes its dependence.

Zheng and many collaborators (for a review, see Ref. [4]) numerically explored such a scaling relation via Monte Carlo (MC) simulations under many aspects. In the sequence, many other authors enriched the method by proposing new amounts, refinements, and other models, including also ones without a defined Hamiltonian, and even models with a long-range interaction (see, for example, Refs. [5–11]).

However, the method goes beyond and such an approach can be extended, for example, to quantum systems [12–14], to nonequilibrium phenomena in polypeptides [15], and in time-dependent simulations of perfect and imperfect surfaces of the three-dimensional Ising model [16]. Some authors explored the short-time dynamics relaxation in the context of deterministic Hamiltonian dynamics (see, for example, Ref. [17]).

The consequences of this theory, at criticality, are described as a transition between two power laws:

$$m(t) = \begin{cases} m_0 t^{\theta} & \text{for} \quad t_0 < t < m_0^{-z/x_0}, \\ t^{-\lambda} & \text{for} \quad t \gg m_0^{-z/x_0}, \end{cases} \tag{2}$$

where $\lambda = z^{-1}\beta/\nu$ and $m(t)$ is the magnetization per spin, which corresponds to the first moment $m^{(1)}(t)$. One way to check the second tail $m(t) \sim t^{-\lambda}$ of this behavior is to prepare systems from a wholly ordered initial system ($m_0 = 1$). In the two-dimensional Blume-Capel model, time-dependent MC (TDMC) simulations show exactly such behavior of its critical points ($D \geqslant 0$). However, for the TP, such simulations show that θ is negative as theoretically predicted by Janssen and Oerding [18] and via time-dependent MC simulations by da Silva *et al.* [19]. This previous work showed that the magnitude of this exponent is more than double the ones found for the critical ones (Ising-like points).

Grasberger [20] and Jaster *et al.* [21] initially studied the tridimensional kinetic spin-1 Ising model (Blume-Capel model for $D = 0$) using TDMC simulations to obtain the exponents of the model for the critical point of this model. However, what happens when $D > 0$? Does the behavior described by Eq. (2) remain valid for critical and tricritical points? Can TDMC simulations show the crossover effects between the critical line (CL) and tricritical point (TP)?

This paper will explore the critical behavior of the three-dimensional Blume-Capel model compared with the results from its version in two dimensions via TDMC. We will show solid numerical evidence of the log corrections for the TP in its three-dimensional version theoretically predicted by Janssen and Oerding [18]. We complete our study estimating critical and tricritical parameters with a refinement of the power laws. The computation of critical exponents along the critical line captures the crossover effects at proximities of the tricritical point.

II. RESULTS

We start our study by computing the coefficient of determination that here measures the "quality" of the power law [22],

$$r = \frac{\sum_{t=t_{\min}}^{t_{\max}} (\overline{\ln m} - a - b \ln t)^2}{\sum_{t=t_{\min}}^{t_{\max}} [\overline{\ln m} - \ln m(t)]^2}, \quad (3)$$

with $\overline{\ln m} = \frac{1}{(t_{\max}-t_{\min})} \sum_{t=t_{\min}}^{t_{\max}} \ln m(t)$. After a previous study of size systems, one used systems with a linear dimension $L = 40$ ($N = L^3 = 6.4 \times 10^4$ spins). Here, $m(t) = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i \rangle = \frac{1}{N_{run} N} \sum_{j=1}^{N_{run}} \sum_{i=1}^{N} \sigma_{i,j}(t)$ with $\sigma_{i,j}(t)$ denoting the ith spin state at the jth run, at time t. We obtained such an amount by performing averages over $N_{\text{run}} = 300$ different runs (time evolutions). We also used $t_{\min} = 10$ and $t_{\max} = 100$ MC steps for our estimates.

We vary $k_B T/J$ from 1.218 until 1.618, from $D/J = 2.645$ until 3.040 with values spaced at $\Delta = 2.5 \times 10^{-3}$ for both parameters. This diagram (Fig. 1) shows a suggestive narrow region (blue) that includes the critical line since it contains the points with the highest coefficients of determination, i.e., candidates to the critical points. The region becomes narrower as it approaches the TP [see, for example, $D/J = 2.844\,79(30)$ and $k_B T/J = 1.4182(55)$ [23]] for the tricritical coupling ratio, which is a "foreshadowing" of the crossover effects. After this point, it becomes even narrower, and this is only an "echo" of the critical region since one expects only a first-order transition for $D/J \geqslant 2.8502$ [24] and in this case, out of the Fig. 1 since this first-order transition point corresponds to temperature $k_B T/J = 0.221(1)$.

In addition, it is essential to mention that if we perform a severe restriction to the coefficient of determination, $0.9998 < r < 1$, one does not observe points after $D/J > 2.844\,79$ (TP), as observed in the inset plot in Fig. 1. This corroborates the fact that these extra blue points found in the original figure were, as previously mentioned, only a "reverberation" of the critical region and that the method of the coefficient of determination is reliable indeed.

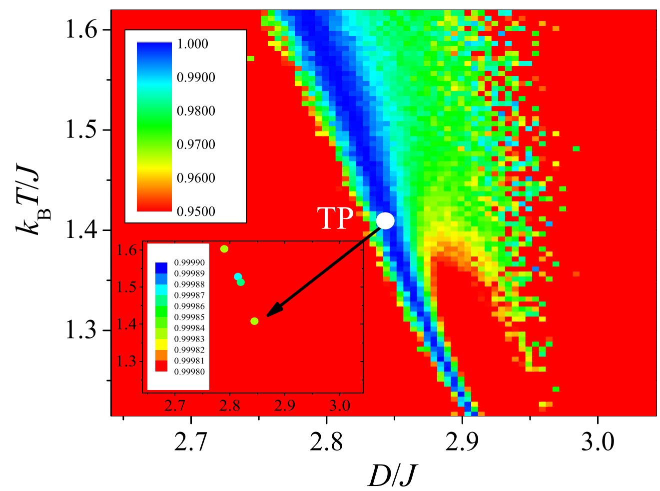

FIG. 1. Coefficient of determination for different parameters $k_B T/J$ and D/J. Until the point $k_B T/J \approx 1.418$ and $D/J \approx 2.845$ (TP according to literature estimates), the narrow blue region contains the critical line. The inset plot shows the reminiscent points over a significantly restricted situation, $0.9998 < r < 1$, showing that the optimization does not find other points after the TP point in this situation.

Nevertheless, are the optimal points indeed the critical line points? By using the critical points presented in Butera and Pernici [24] obtained via low- and high-temperature expansions (see Table 5 in Ref. [24]), we can check if our critical points are precisely well estimated.

We fixed some values of D/J picked up from this same table. For each input D/J, we obtained the optimal corresponding value $k_B T/J$, which corresponds to the maximal r value [see Fig. 2(a)]. With these points in hand, we compared with the critical line obtained by Butera and Pernici [24] as described in Fig. 2(b), who used equilibrium numerical methods. We observed an excellent match with such a results method, showing that we can obtain the critical values of the three-dimensional Blume-Capel model using time-dependent MC simulations with the refinement method based on the coefficient of determination.

What about the crossover effects? How is the sensitivity of these exponents as they approach the tricritical point? For that, we look at different time evolutions. First, to calculate the exponent θ, we should study the system with varying values of m_0 by performing an extrapolation $m_0 \to 0$.

We used a more accessible alternative proposed by Tome and Oliveira [25] by calculating

$$C(t) = \frac{1}{N^2} \left\langle \left(\sum_{i=1}^{N} \sigma_i(t) \right) \left(\sum_{i=1}^{N} \sigma_i(0) \right) \right\rangle = \frac{1}{N^2 N_{\text{run}}} \sum_{i=1}^{N} \sum_{k=1}^{N} \sum_{j=1}^{N_{\text{run}}} \sigma_{i,j}(t) \sigma_{k,j}(0). \quad (4)$$

Such an estimate considers $\sigma_{i,j}(0)$ randomly drawn (0, -1, or $+1$, with probability 1/3), such that $m(0) = \frac{1}{N_{\text{run}} N} \sum_{i=1}^{N} \sum_{j=1}^{N_{\text{run}}} \sigma_{i,j}(0) \approx 0$, which yields $C(t) \sim t^{\theta}$ when N_{run} is large enough.

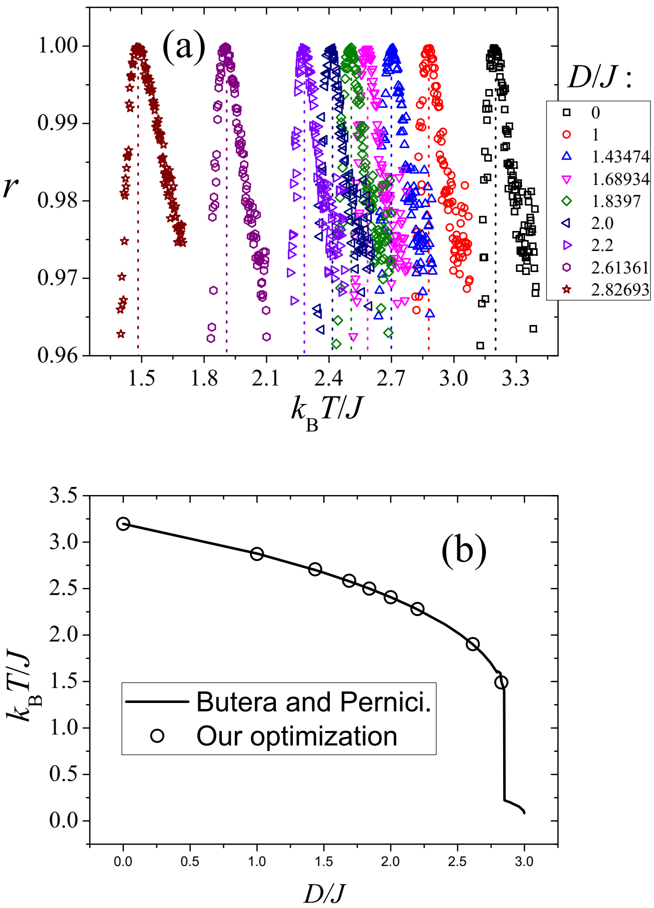

FIG. 2. (a) Curves $r \times (k_B T)/J$ for some values of D/J. (b) The points obtained with the optimization in (a) compared with the curve obtained by Butera and Pernici [24].

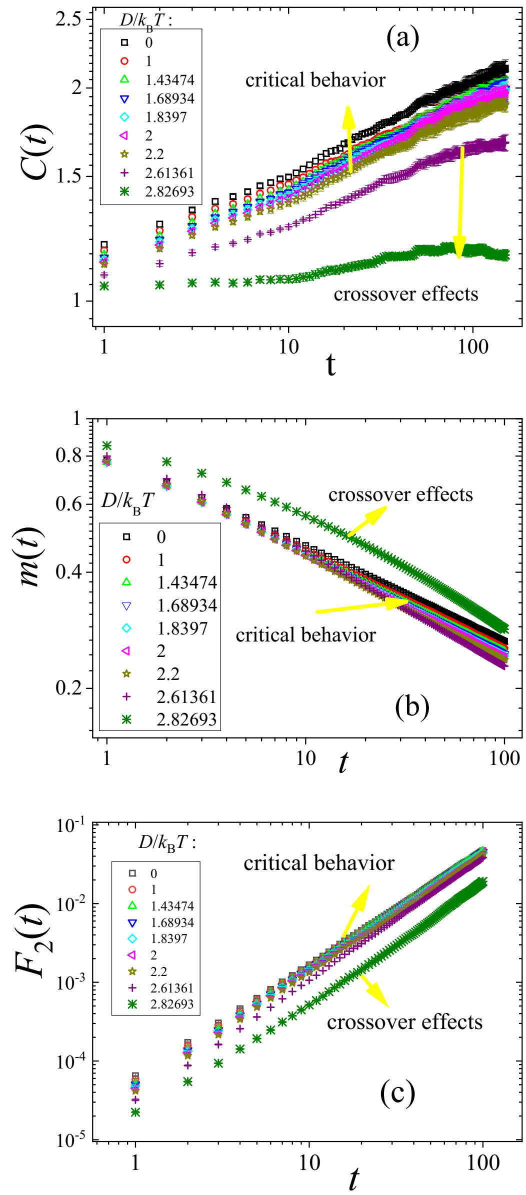

FIG. 3. (a) Time evolution of $C(t)$. (b) Time evolution of $m(t)$ for $m_0 = 1$. (c) $F_2(t) \times t$. The used points are the same ones that we refined in Fig. 2.

For this experiment, one used $N_{\text{run}} = 30\,000$ runs, and we measured the slopes in the interval [30,150] MC steps. The exponent λ was obtained by performing simulations starting with $m_0 = 1$ of $m(t)$. In this case, one used $N_{\text{run}} = 300$ runs since simulations with $m_0 = 1$ require many fewer runs. In order to obtain the exponent z, one simulates $m^{(2)}(t) = \frac{1}{N_{\text{run}} N^2} \sum_{j=1}^{N_{\text{run}}} (\sum_{i=1}^{N} \sigma_{i,j}(t))^2$ by starting with $m_0 = 0$, and thus one considers the ratio [26]

$$F_2(t) = \frac{m^{(2)}(t)_{m_0=0}}{[m(t)_{m_0=1}]^2}, \tag{5}$$

which behaves as $F_2(t) \sim t^{d/z}$. For $m^{(2)}(t)_{m_0=0}$, only $N_{\text{run}} = 1000$ runs are enough for good estimates. For estimates of λ and z, we performed fits in the interval [10,100] MC steps.

Figures 3(a)–3(c) show the time evolutions of $C(t)$, $m(t)$ for $m_0 = 1$, and $F_2(t)$, respectively, for $D/J = 0,\ 1, 1.434\,74$, $1.689\,34$, 1.8397, 2, 2.2, $2.613\,61$, and $2.826\,93$, corresponding to the critical temperatures given respectively by $k_B T/J = 3.196\,22$, $2.877\,369$, 2.7, $2.579\,14$, 2.5, $2.407\,314$, $2.275\,495$, 1.9, and 1.5. It is interesting to observe those power laws present changes when they approach the tricritical point: $D/J = 2.844\,79 k_B T/J = 1.4182$. These crossover effects, visually observed in these plots, can also be numerically checked.

To do that, let us check the exponents shown in Table I analyzing their universality. One has only values for $D = 0$ in the literature. For example, θ calculated by Jaster *et al.* [21] by directly analyzing the initial slip of the magnetization $m(t) = m_0 t^{\theta}$, performing $m_0 \to 0$ yields $\theta = 0.108(2)$, which is in agreement with our estimate. Similarly, these same authors obtained $z = 2.042(6)$ that agrees with our estimate with two uncertainty bars. By using MC simulations [27] and ε expansion [28] similar estimates are found, $z = 2.0245(15)$, and $z = 2.0235(8)$, respectively.

Finally, these authors obtained $\beta/\nu = 0.517(2)$ which agrees with our estimates. It is essential to mention that we obtained larger error bars, considering five different bins, corresponding to five different exponents, that, when averaged,

TABLE I. Exponents of the Blume-Capel model along the critical line obtained with TDMC simulations. The bold results highlight the crossover effects.

$\frac{D}{J}$	0	1	1.43474	1.68934	1.8397	2.0	2.2	2.61361	2.82693
λ	0.2492(14)	0.2536(11)	0.2565(15)	0.2585(13)	0.26164(74)	0.2651(13)	0.26873(82)	**0.2984(10)**	**0.3035(64)**
z	2.068(14)	2.051(14)	2.037(13)	2.022(12)	2.029(18)	2.005(26)	2.006(19)	**1.928(12)**	**1.8865(66)**
θ	0.111(16)	0.091(16)	0.114(11)	0.112(14)	0.112(13)	0.110(15)	0.1080(68)	**0.081(15)**	**0.003(11)**
β/ν	0.5153(45)	0.5201(46)	0.5225(45)	0.5227(39)	0.5309(49)	0.5315(74)	0.5391(54)	**0.5753(41)**	**0.573(23)**

yield our final estimate with respective uncertainty. It is important to mention that if we consider a unique time series with uncertainties of the points and only then, calculating an exponent whose uncertainty comes from the linear fit, we obtain smaller error bars. Here, we opted by using the more conservative method (first) with larger error bars.

We observe a slight variation of the exponents λ, z, θ, and β/ν up to 2.2. However, after this value, the crossover effects are fairly sensitive for $\frac{D}{J} = 2.613\,61$ and 2.826 93, which corroborates the one visually observed in Fig. 3. Thus one can conclude that the law described by Eq. (2) is suitable to describe the critical points of the Blume-Capel model in three dimensions and crossover effects with $\theta > 0$. It would be suggestive to think that for the tricritical point as in two dimensions, we should find a similar law to Eq. (2) but with $\theta < 0$. However, it does not occur for tricritical points from three-dimensional systems. Janssen and Oerding [18] demonstrated that such a problem demands logarithmic corrections to explain the relaxation dynamics. Nevertheless, the question is as follows: Can we observe this behavior via time-dependent MC simulations? The answer is positive, and we will show how to perform it, which is the most important point of this paper, and it requires a suitable numerical exploration.

The results obtained by Janssen and Oerding [18], using methods of renormalized field theory, suggest (after some simple manipulations) that magnetization, for three dimensions, at the tricritical point, behaves as

$$m(t) = m_0 \frac{\ln(t/t_0)^{-a}}{\{1 + t[\ln(t/t_0)]^{-(1+4a)} m_0^4\}^{1/4}}. \quad (6)$$

According to this theory, a is precisely given by $\frac{3}{40\pi}$. Thus the order parameter (magnetization) must present a crossover between a pure logarithmic behavior for short times followed by a power law with logarithmic corrections:

$$m(t) = \begin{cases} m_0[\ln(t/t_0)]^{-a} & \text{for} \quad t_0 < t \ll m_0^{-4}, \\ \left(\frac{t}{\ln(t/t_0)}\right)^{-\frac{1}{4}} & \text{for} \quad t \gg m_0^{-4}. \end{cases} \quad (7)$$

Here, t_0 is the microscopic timescale. Nevertheless, we perform time-dependent MC simulations for the TP of the three-dimensional Blume-Capel model. Thereby, we analyzed the relaxation from $m_0 = 1$, in order to capture the behavior $m(t) \sim (\frac{t}{\ln(t/t_0)})^{-\frac{1}{4}}$. In this case, it is interesting to change t_0 to observe the law for short times as observed in Fig. 4(a). It is most important here to use the correct scale. For that we performed a plot of $\ln[m(t)]$ vs $\ln[\frac{t}{\ln(t/t_0)}]$. We can observe that for lower t_0 values, we observe prolonged linear behavior. Figure 4(b) shows the particular case ($t_0 = 0.1$) used to measure the slope that must be 1/4 according to the prediction obtained by Janssen and Oerding. One finds $\xi = 0.250\,34(53)$ corroborating the prediction. This value was obtained in the time interval 5–100 MC steps with the goodness of fit (Q) equal to 0.72. We obtained the most acceptable value for the interval 10–100 MC steps $\xi = 0.2505(19)$, with $Q = 0.99$. It is important to notice that for $t_{\max} > 100$, the results were unsatisfactory. For example, for 10–200, one obtains $\xi = 0.267\,17(82)$ with $Q = 5.2 \times 10^{-9}$.

For the second part, we performed simulations for small values of m_0. However, obtaining reasonable estimates for small values of m_0 is numerically complicated due to the fluctuations. Thus, we used $m_0 = 0.08$, 0.06, 0.04, and 0.02. We show the time evolutions in Fig. 5(a).

Thus we measured the slopes in the possible regions where one observed a reasonably short duration linear behavior in the plot of $\ln[m(t)] \times \ln[\ln(t)]$, for different values of m_0.

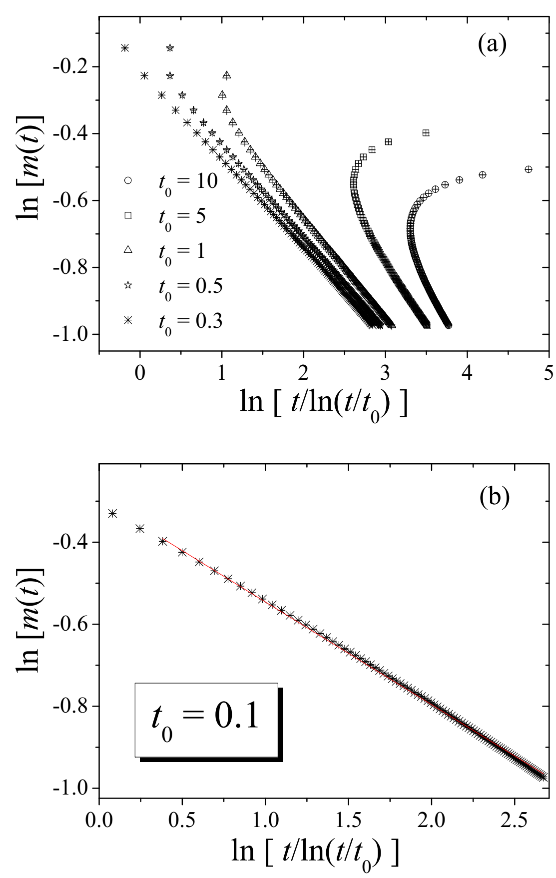

FIG. 4. (a) Time evolution of $m(t)$ at the tricritical point, considering different values of t_0. (b) Time evolution of $m(t)$ for the particular case $t_0 = 0.1$.

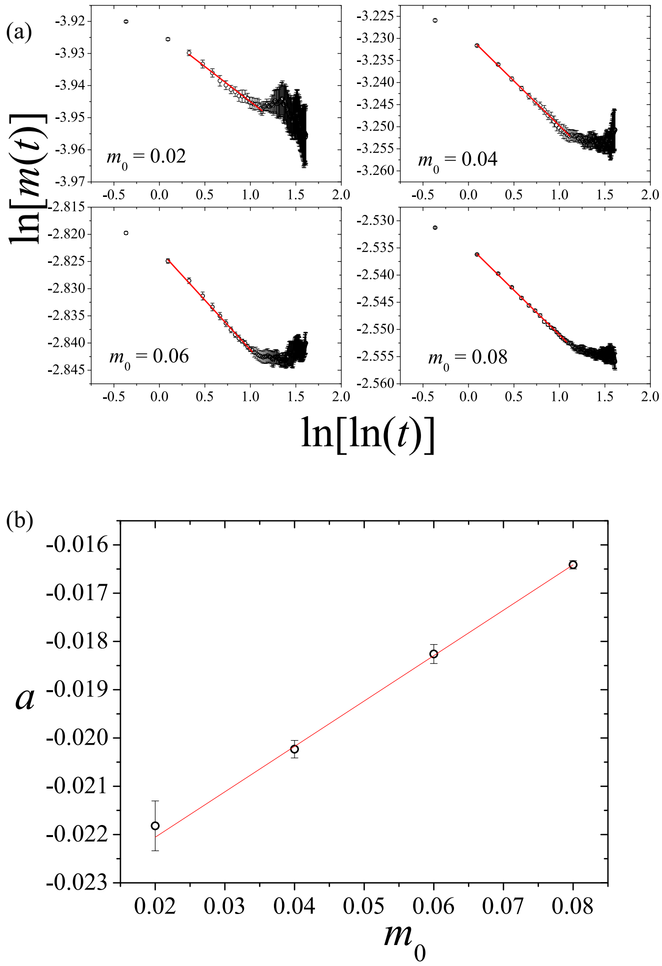

FIG. 5. (a) Time evolutions at the tricritical point for values $m_0 = 0.02$, 0.04, 0.06, and 0.08. (b) Numerical extrapolation of the exponent a.

See the straight lines (in red) as indicated in Fig. 5(a). The slopes supposedly supply the value of the exponent a according to Eq. (7). We also observe a linear behavior of a as a function of m_0 [see Fig. 5(b)]. With this in hand, one can perform an extrapolation for $m_0 \to 0$. Such an extrapolation yields our estimate $a_{\text{estimated}} = 0.023\,93(13)$, in good agreement when compared with the theoretical prediction, $a = \frac{3}{40\pi} \approx 0.023\,873$.

It is also interesting to use the decay $m(t) \sim (\frac{t}{\ln(t/t_0)})^{-\frac{1}{4}}$ expected from ordered initial states ($m_0 = 1$) to obtain the tricritical parameters. In this case, we must change the coefficient of determination to

$$r = \frac{\sum_{t=t_{\min}}^{t_{\max}} \left[\overline{\ln m} - a - b\ln\left(\frac{t}{\ln(t/t_0)}\right)\right]^2}{\sum_{t=t_{\min}}^{t_{\max}} [\overline{\ln m} - \ln m(t)]^2}. \tag{8}$$

Based on this amount, obtained in Ref. [23], we performed two experiments: one fixed $D/J = 2.844\,79$ by varying k_BT/J, and alternatively by fixing $k_BT/J = 1.4182$, one varies D/J. Figures 6(a) and 6(b) show both situations, respectively. The optimal values correspond to the maximal r, corroborating the estimates for the TP from literature (see, for example, Refs. [23,24]), showing that our refinement method can be modified to attend the temporal laws at TP, i.e., including the log corrections.

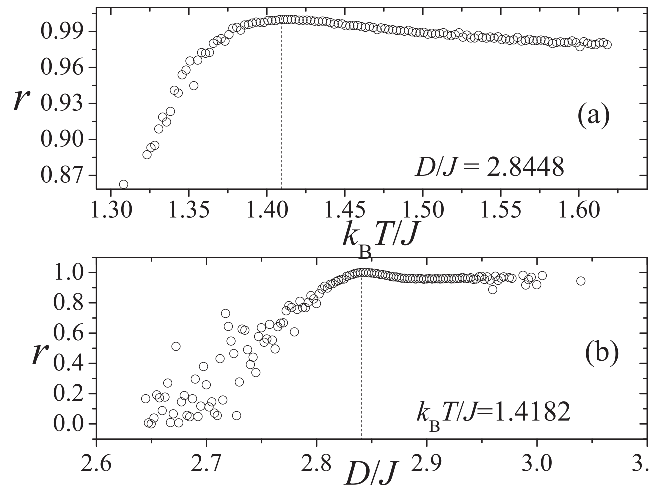

FIG. 6. (a) Coefficient of determination as a function of k_BT/J considering D/J fixed in 2.844 79. (b) Coefficient of determination as a function of D/J fixing $k_BT/J = 1.4182$.

It is interesting to observe that if the magnetization relaxes at TP as a power-law $t^{-1/4}$ with additional logarithmic corrections, starting from $m_0 = 1$, the system seems to predict what happens in the mean-field regime, since in a recent work, we considered that evolution of magnetization in such a regime follows the differential equation [29]

$$\frac{dm}{dt} = -m + \frac{2e^{-\beta D}\sinh(\beta Jzm)}{2e^{-\beta D}\cosh(\beta Jzm) + 1}. \tag{9}$$

From a very simplified point of view, such an equation leads to a crossover between a power-law $m(t) \sim t^{-1/2}$ at the CL to a power-law $m(t) \sim t^{-1/4}$ at the TP. Thus, the "trace" of this exponent 1/4, which must occur for $d \geqslant 4$ [30,31], would already appear in three dimensions but with logarithmic corrections.

III. CONCLUSIONS

In summary, this paper verifies the theoretical predictions which suggest log corrections for the tricritical point [18]. We also obtained the critical exponents for the critical line in three dimensions. One observes the crossover effects using time-dependent Monte Carlo simulations, considering the time evolution of different amounts as the time correlation, the ratio that considers the first and second moment of magnetization with different initial conditions, and the direct time evolution of magnetization. Our predictions suggest that the mean-field behavior has some brief similarities with three-dimensional results suggested by a recent mean-field study developed in Ref. [29] .

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