Short-time dynamics for the spin-$\frac{3}{2}$ Blume-Capel model

B. C. S. Grandi and W. Figueiredo*
Departamento de Física, Universidade Federal de Santa Catarina, 88040-900 Florianópolis, SC, Brazil
(Received 30 July 2004; published 16 November 2004)

We employed Monte Carlo simulations and short-time dynamic scaling to determine the static and dynamic critical exponents for the generalized two-dimensional Blume-Capel model of spin-$\frac{3}{2}$. We showed that the critical behavior at the second-order phase-transition line between the paramagnetic and ferromagnetic phases is in the same universality class of the two-dimensional Ising model. However, at the double critical end point, which is present in the phase diagram of the model, the critical exponent β, associated to the order parameter, is different from that of the Ising model.

DOI: 10.1103/PhysRevE.70.056109 PACS number(s): 64.60.Ht, 64.60.Fr, 02.70.Uu

I. INTRODUCTION

Besides the usual critical phenomena, certain physical systems display other very interesting multicritical behavior. These studies have been carried out both theoretically and experimentally in the past few years. Recently, Plascak and Landau [1] determined the phase diagram of the generalized Blume-Capel model of spin-$\frac{3}{2}$, in two dimensions. They paid particular attention to the behavior at the double critical end point (DCE) of this model. For a nonzero value of the crystal field Δ, the model presents four possible ferromagnetic ordered phases: two symmetrical phases where the spins are predominantly in the states $\pm\frac{3}{2}$ (F_{+3} and F_{-3} phases), and two other symmetrical phases, with the spins in the states $\pm\frac{1}{2}$ (F_{+1} and F_{-1} phases). In a T-Δ plane, there is a line of four coexistent ordered phases, $F_{\pm3}$ and $F_{\pm1}$, extending from $T=0$ and $\Delta=dJ$ (d is the spatial dimension and J is the exchange interaction) up to the double critical end point (where two critical phases coexist: $F_{+3}\equiv F_{+1}$ and $F_{-3}\equiv F_{-1}$), for $T=T_d$ and $\Delta=\Delta_d$.

In Ref. [1], Monte Carlo simulations with the histogram reweighting and finite-size scaling techniques have been used to locate the first-order transition line and the precise position of the double critical end point. Then, from the dependence of the double critical end point temperature on L (the linear dimension of the square lattice), they found the values for the critical exponent ν of the DCE. They concluded that the critical behavior at this multicritical point belongs to the same universality class of the corresponding two-dimensional Ising model.

In this work, we revisited this problem with the idea to determine other critical exponents associated with the DCE, besides the exponent ν found by these authors. We employed in our analysis Monte Carlo simulations along with the short-time dynamics. As is well known, Janssen, Schaub, and Schmittmann [2], through renormalization-group arguments, showed that the universal scaling behavior, observed in the long-time relaxation behavior of the dynamic evolution of the systems, is already present at the short times just after the start of the relaxation. Since then, numerical simulations have been used to investigate the short-time critical dynamics of several spin systems [3–7]. Once we know the location of the critical point of the system, we are able to determine its critical properties. For this end, we need to prepare the system in a state in which the spatial and temporal correlation lengths are near zero, and to put it at its critical point. Thus by using the apropriate scaling relations for the moments of the order parameter, we can determine the critical exponents.

In this study, we prepared our system with a zero correlation length at zero temperature, because this is the simplest way to determine the critical expoents, and it was already used with success in different spin problems [8,9]. Then, this method was used to find the critical exponents along the second-order transition line for different values of the crystal field of the generalized Blume-Capel model, and at the double critical end point of the model. In the next section, we present the model and the finite-size scaling relations used for the short-time dynamics. In Sec. III, we show our Monte Carlo simulations and the calculation of the related critical exponents and, finally, in Sec. IV, we present our conclusions.

II. THE MODEL AND SHORT-TIME EQUATIONS

We consider a generalized Blume-Capel model, in two dimensions, of spins $\sigma=\frac{3}{2}$, whose states are $\sigma_i=\pm\frac{3}{2},\pm\frac{1}{2}$. The Hamiltonian of the model can be written as

$$\mathcal{H} = -J\sum_{(i,j)}\sigma_i\sigma_j + \Delta\sum_{i=1}^{N}\sigma_i^2 - H\sum_{i=1}^{N}\sigma_i, \qquad (1)$$

where $J>0$ is the ferromagnetic exchange interaction, Δ is the crystal-field anisotropy, H is a uniform external field, and N is the total number of spins. The phase diagram of this model was studied in detail by Plascak and Landau [1], through Monte Carlo simulations. At the $H=0$ plane, they found the second-order λ-transition line and the first-order coexistence line that ends at a double critical end point. At this point, two critical phases coexist.

The static and dynamic critical exponents can be determined from the dynamic relaxation equations when the system starts from a completely ordered state, uncorrelated

*Email address: wagner@fisica.ufsc.br

spins, with the order parameter assuming its maximum value. For the system studied, we employed two different definitions for the order parameter, depending on which transition we are looking for. Along the λ line, the order parameter is the total magnetization of the system, which goes to zero at the points of this line. On the other hand, for the double critical end point (DCE), we define the order parameter as being the difference $m(t)=M(t)-M_d$, where $M(t)$ is the total magnetization at time t and M_d is the magnetization at the DCE. Also, this latter order parameter becomes zero at the DCE. We assume that near a point at the λ line, or near the DCE, the kth moment of the corresponding order parameter $m(t)$ scales as [8]

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

where t is the time, τ is the reduced temperature

$$\tau = \frac{T-T_c}{T_c}, \tag{3}$$

L is a linear dimension of the system, and b is a spatial rescaling factor. β and ν are the well known static exponents and z is the dynamic critical exponent. This scaling relation is assumed to be valid in the macroscopic short-time regime. For example, for $k=1$ and for $b=t^{1/z}$, we obtain the scaling law to the order parameter,

$$m(t) = t^{-\beta/\nu z}m(1,t^{1/\nu z}\tau), \tag{4}$$

where it is assumed that L is very large. If $\tau=0$, this scaling relation can be written as

$$m \sim t^{-c_1}, \tag{5}$$

with $c_1=\beta/\nu z$. In Eq. (4), taking the derivative of m with respect to τ and evaluating it at $\tau=0$, we obtain the logarithmic derivative of the order parameter,

$$\left.\frac{\partial \ln m(t,\tau)}{\partial\tau}\right|_{\tau=0} \sim t^{c_2}, \tag{6}$$

where $c_2=1/\nu z$.

Once the order parameter assumes its maximum value at $t=0$, we can also obtain the time-dependent second-order cumulant $U_2(t)$ defined by

$$U_2(t) = \frac{m^{(2)}}{(m)^2} - 1. \tag{7}$$

At the initial times it reduces to

$$U_2(t) \sim t^{c_3}, \tag{8}$$

where $c_3=d/z$; d is the spatial dimension of the system. Therefore, from the short-time dynamic evolution of the order parameter and its second moment, we can obtain the static critical exponents β and ν and the dynamic critical exponent z along the λ line and at the multicritical point DCE.

III. SIMULATIONS AND RESULTS

We have performed Monte Carlo simulations, with periodic boundary conditions, on a square lattice with $N=L^2$ sites, with values of L ranging from $L=8$ up to $L=128$. We have employed the heat bath algorithm to take into account the transition rate between states. We have started the simulations with a completely ordered state, where all spins assume their maximum value, i.e., $\sigma_i=\frac{3}{2}$. We have investigated two different types of critical points. First, we considered the critical behavior along the λ line, where the system passes continuously from an ordered ferromagnetic to a paramagnetic phase. The second case we considered is related to the critical behavior at the double critical end point: at this point, two critical phases coexist, $F_{+3}\equiv F_{+1}$ and $F_{-3}\equiv F_{-1}$. We have seen that for any critical point considered it is sufficient to consider the first 300 Monte Carlo steps (MCS; $1\text{MCS}=L^2$ trials to change the value of the spins in the lattice) to calculate the critical exponents of interest. In order to get a good statistics, we had to consider a large number of independent samples to calculate the $\langle m(t)\rangle$ and its second moment $\langle m^{(2)}(t)\rangle$ at the critical points. With the values of $\langle m(t)\rangle$ and $\langle m^{(2)}(t)\rangle$, we can determine the second-order cumulant, $\langle U_2(t)\rangle$, and the logarithmic derivative of the order parameter with respect to τ, $[\partial \ln m(t,\tau)/\partial\tau]|_{\tau=0}$.

A. The second-order transition line

In order to determine the values of the static and dynamic critical exponents at the λ line, where the system passes continuously from the ordered ferromagnetic phase to a paramagnetic phase, we have prepared the system in a completely ordered state, with all the spins assuming their maximum value, $\sigma_i=+\frac{3}{2}$. Then, the system is left to evolve in time at a chosen point of the λ line, with coordinates T_c and Δ_c. In order to get reliable results, the averages were estimated by using 4×10^4 samples for the lattices with the lattice size in the range $8\leqslant L\leqslant 32$, and 10^4 samples for $48\leqslant L\leqslant 128$. For the value $\Delta_c=0$, the critical temperature $T_c=3.287\,94(7)$ was determined very accurately [10] by employing a hybrid algorithm to the spin-$\frac{3}{2}$ two-dimensional Ising model. We show in the next three figures the results we have obtained for this critical point. Figure 1 displays the log-log plot of the $m(t)$ as a function of t for $L=128$. The figure also exhibits the best fit to the data points. From the slope of this straight line, we found the following ratio for the critical exponents: $\beta/\nu z=0.059\,72(5)$. Similarly, in Fig. 2, we show the log-log plot of the second-order Binder cumulant $U_2(t)$ as a function of t, giving the value $d/z=0.919(2)$ for the slope of this curve. We found the value $(\nu z)^{-1}=0.4954(7)$ for the slope of the curve presented in Fig. 3, which is the log-log plot of the logarithmic derivative of m versus t. From these ratios, we can easily determine the values of the critical exponents: $z=2.176(4)$, $\nu=0.928(3)$, and $\beta=0.1206(7)$. We have also considered other points on the λ line for which Δ_c is different from zero. We have employed the same procedure described above to find the critical exponents. In Fig. 4, we summarize the results for the three considered critical exponents β, ν, and z. In this figure, the dotted lines give the exact values for the static exponents β and ν for the two-dimensional Ising model, and the one well accepted estimate [11] for the dynamical exponent z. Despite

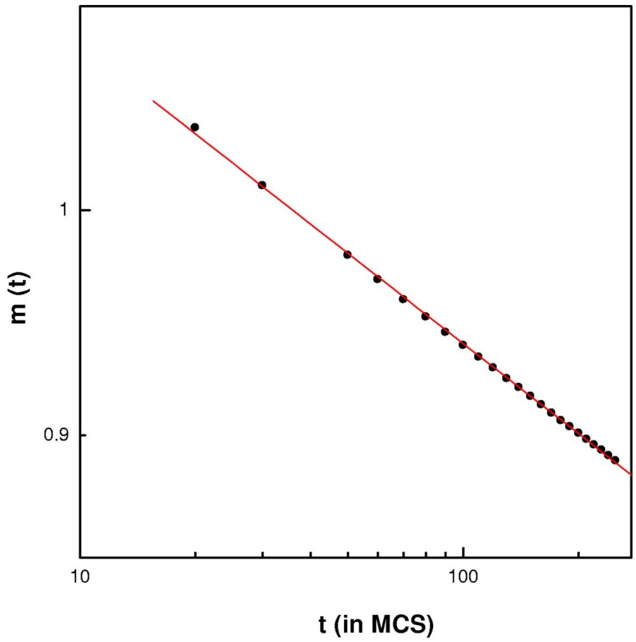

FIG. 1. Log-log plot of the order parameter $m(t)$ vs time t, at the λ line, for $T_c = 3.287\,94(7)$, $\Delta_c = 0$, and $L = 128$. The error bars found in the simulations are less than the size of the points. The straight line is the best fit to the data, which gives $\beta/\nu z = 0.059\,72(5)$ (the error is that obtained from the fitting).

the larger deviation from the dotted lines for $\Delta > 0$, which can be ascribed to the fact that T_c in these cases have not been so accurately determined as for $\Delta = 0$, the critical behavior along the λ line of this model seems to be the same as that of the Ising model in two dimensions.

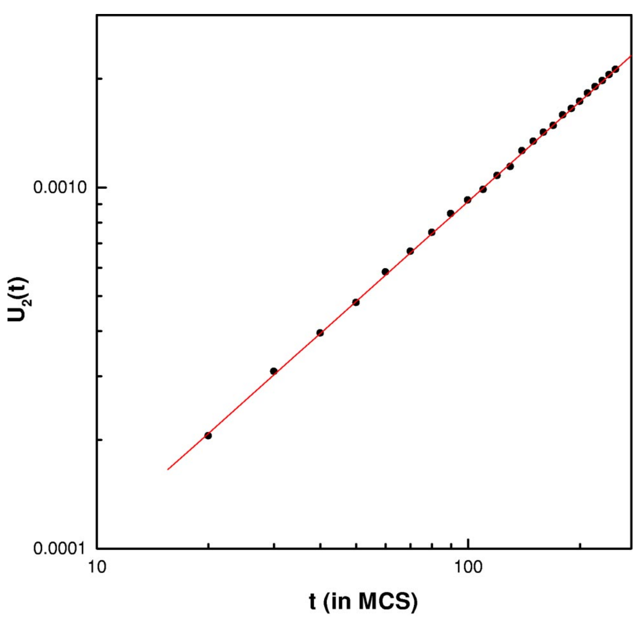

FIG. 2. Log-log plot of the second-order Binder cumulant $U_2(t)$ as a function of time t, at the λ line, for $T_c = 3.287\,94(7)$, $\Delta_c = 0$, and $L = 128$. The straight line is the best fit to the data, which gives $d/z = 0.919(2)$.

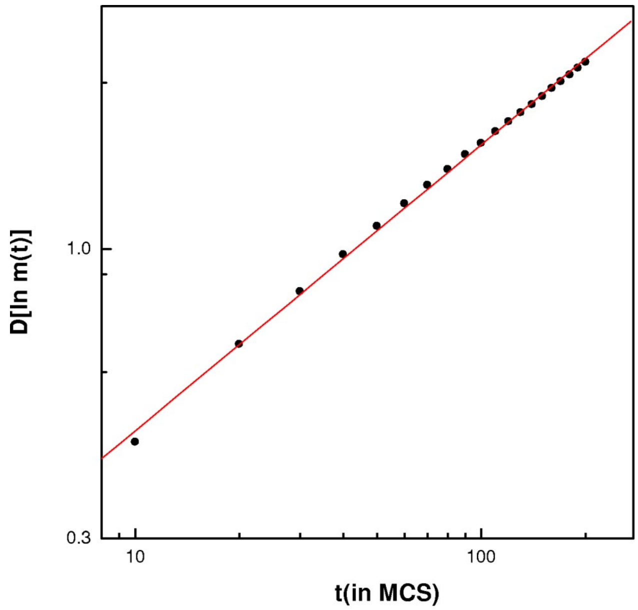

FIG. 3. Log-log plot of $\partial \ln m(t,\tau)/\partial\tau$ as a function of time t, at the λ line, for $T_c = 3.287\,94(7)$, $\Delta_c = 0$, and $L = 128$. The straight line is the best fit to the data, which gives $(\nu z)^{-1} = 0.4954(7)$.

B. Double critical end point

Now we turn our attention to the double critical end point found in the phase diagram of the spin-$\frac{3}{2}$ Blume-Capel model. The coordinates of this point was determined very precisely by Plascak and Landau [1] through Monte Carlo simulations via METROPOLIS sequential single spin-flip up-

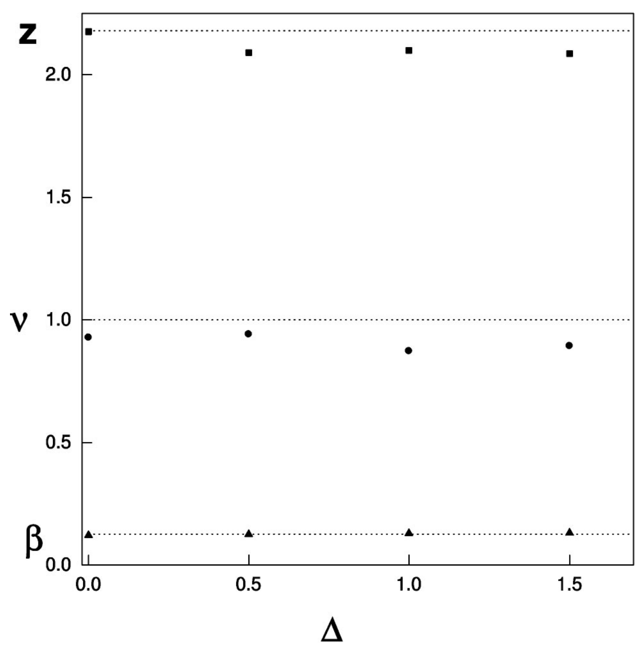

FIG. 4. The exponents z, ν, and β as a function of the crystal field parameter, at the λ line for $L = 128$. The dotted lines mark the exact values of the exponents ν and β of the two-dimensional Ising model, while the dotted line associated with z is the value of Ref. [11].

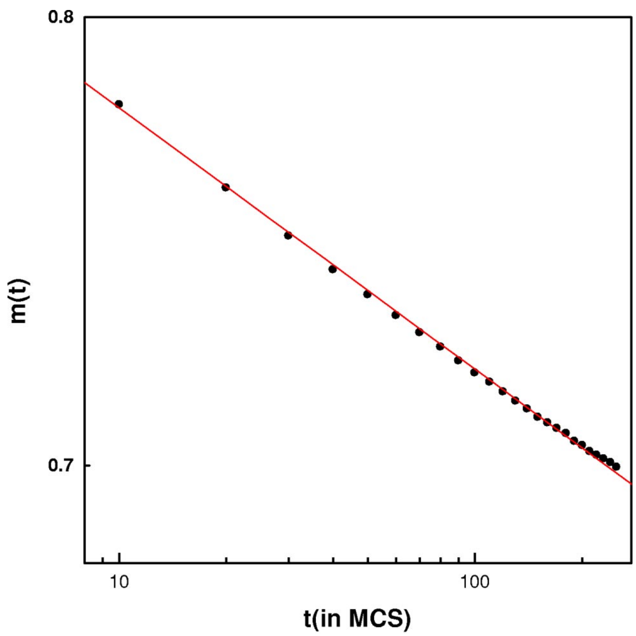

FIG. 5. Log-log plot of the order parameter $m(t)$ vs time t, at the double critical end point, whose coordinates are $T_d=0.593\,74(7)$ and $\Delta_d=1.986\,47(5)$, for $L=64$. The straight line is the best fit to the data, which gives $\beta/\nu z=0.0342(1)$.

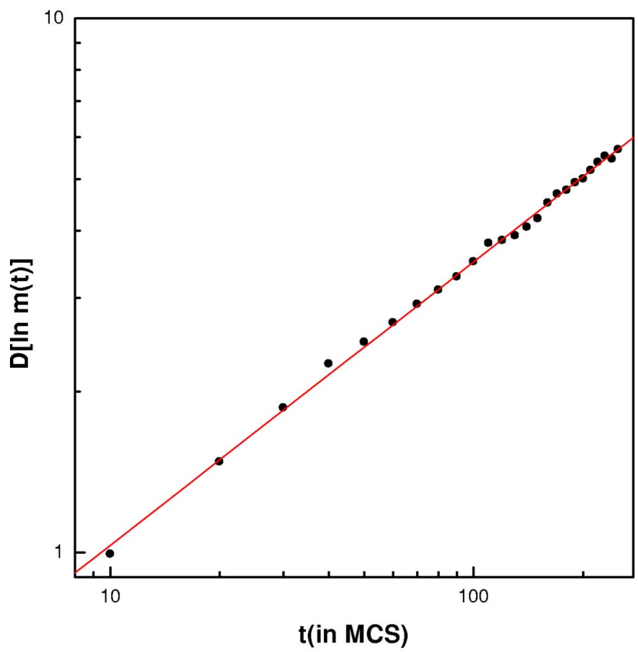

FIG. 7. Log-log plot of the $\partial \ln m(t,\tau)/\partial\tau$ vs time t, at the double critical end point, for $L=64$. The straight line is the best fit to the data, which gives $(\nu z)^{-1}=0.528(3)$.

dates, by employing a histogram reweighting and finite-size scaling techniques. In their analyses, they used square lattices with lattice sizes ranging from $L=12$ to $L=64$. They found the following values for the coordinates of the double critical end point: $T_d=0.593\,74(7)$ and $\Delta_d=1.986\,47(5)$. The values of the magnetization they found for the two largest lattices are for $L=48$, $M_d=0.6285$ and for $L=64$, $M_d=0.6313$. We show in Figs. 5, 6, and 7, the log-log plots of $m(t)$, $U_2(t)$ and the logarithmic derivative of $m(t)$ versus t,

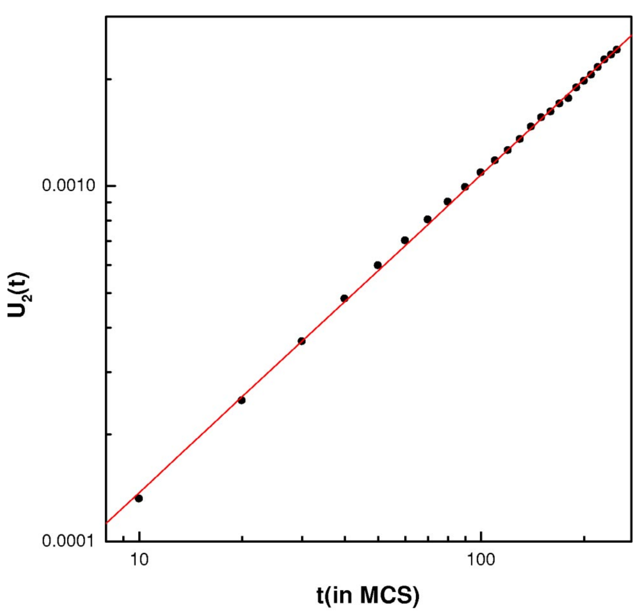

FIG. 6. Log-log plot of the second-order Binder cumulant $U_2(t)$ vs time t, at the double critical end point, for $L=64$. The straight line is the best fit to the data, which gives $d/z=0.922(2)$.

respectively. For this point, the order parameter is $m(t)=M(t)-M_d$, where $M(t)$ is the total magnetization at time t and M_d is the magnetization at the DCE. In this way, this order parameter becomes zero at the DCE. We found the following slopes for these straight lines: for $L=48$, $\beta/\nu z=0.0338(1)$, $d/z=0.908(3)$, and $(\nu z)^{-1}=0.557(5)$. On the other hand, for $L=64$ the slopes are $\beta/\nu z=0.0342(1)$, $d/z=0.922(2)$, and $(\nu z)^{-1}=0.528(3)$. Although we do not have precise values of the magnetization for larger lattices, it is easy to see that the ratio $\beta/\nu z$ is almost insensitive to thelattice sizes considered. For instance, the critical exponents for $L=64$ are $z=2.169(5)$, $\nu=0.873(8)$, and $\beta=0.065(1)$. By considering only these two lattice sizes ($L=48$ and $L=64$), and extrapolating the corresponding critical exponents to an infinite lattice, we see that $\nu=1.05$, which is near the value found by Plascak and Landau [1]. However, the value we estimated for β is 0.077, which is very different from the expected 0.125 for the two-dimensional Ising model. Based on these estimates, we believe that the double critical end point does not belong to the same universality class of the two-dimensional Ising model.

IV. CONCLUSIONS

In this study, we investigated the critical behavior of the generalized two-dimensional Blume-Capel model of spin-$\frac{3}{2}$. The critical exponents were determined by the short-time dynamic scaling and Monte Carlo simulations. We have found that, along the continuous transition line separating the ferromagnetic and paramagnetic phases, the critical exponents are in the same universality class of the two-dimensional Ising model. On the other hand, at the double critical end point, where two critical phases coexist, although the static exponent ν we obtain is almost the same as determined previously [1], we estimated for the exponent β, associated with the order parameter, the value $\beta = 0.077$, which is quite different from the exact 0.125 of the two-dimensional Ising model. Then, we think the behavior of the model at the double critical end point is not in the same universality class of the two-dimensional Ising model. That is, while at the λ line the critical behavior is the same as the corresponding Ising model, it changes drastically at the double critical end point. Nevertheless, the dynamic critical exponent z presents essentially the same value at both the λ line and at the double critical end point.

ACKNOWLEDGMENTS

This work was supported by the Brazilian agencies CNPq and FUNCITEC. We are also very grateful to Dr. João Antonio Plascak for giving us the values of the magnetization at the double critical end point and for the enlightening discussions.

[1] J. A. Plascak and D. P. Landau, Phys. Rev. E **67**, 015103(R) (2003).
[2] H. K. Janssen, B. Schaub, and B. Schmittmann, Z. Phys. B: Condens. Matter **73**, 539 (1989).
[3] Z. B. Li, L. Schülke and B. Zheng, Phys. Rev. Lett. **74**, 3396 (1995).
[4] Z. Li, L. Schülke, and B. Zheng, Phys. Rev. E **53**, 2940 (1996).
[5] K. Okano, L. Schülke, K. Yamagishi, and B. Zheng, Nucl. Phys. B **485**, 727 (1997).
[6] B. Zheng, Phys. Lett. A **277**, 257 (2000).
[7] R. da Silva, N. A. Alves, and J. R. Drugowich de Felício, Phys. Rev. E **66**, 026130 (2002).
[8] A. Jaster, J. Mainville, L. Schülke, and B. Zheng, J. Phys. A **32**, 1395 (1999).
[9] M. Santos and W. Figueiredo, Phys. Rev. E **62**, 1799 (2000).
[10] J. A. Plascak, Alan M. Ferrenberg, and D. P. Landau, Phys. Rev. E **65**, 066702 (2002).
[11] D. Stauffer, Physica A **244**, 344 (1997).