Critical dynamics of the Baxter-Wu model

M. Santos and W. Figueiredo*
Departamento de Física–Universidade Federal de Santa Catarina 88040-900, Florianópolis, SC, Brazil
(Received 27 October 2000; revised manuscript received 21 December 2000; published 19 March 2001)

The short-time behavior of the Baxter-Wu model is investigated through the relaxation of the order parameter at the critical temperature. We considered Monte Carlo simulations for this model on a triangular lattice, and we studied relaxation starting from the fourfold-degenerate ground state. Using the short-time scaling formalism we found the static critical exponents β and ν of the model and the corresponding dynamical critical exponent z. The values of the static exponents we find agree with the exact ones. To the best of our knowledge, this is the first determination of the dynamical critical exponent of the Baxter-Wu model.

DOI: 10.1103/PhysRevE.63.042101 PACS number(s): 64.10.+h, 64.60.Ht

I. INTRODUCTION

The well known work of Janssen, Schaub, and Schmittmann [1] established that a system relaxing by a dynamical process, that does not conserve the order parameter, exhibits universal behavior at the early stages of its evolution toward equilibrium states. The crucial point in their theory is that the system must be out of equilibrium, exactly at its critical point, in order that we can observe an universal behavior. These ideas have been verified in some models, for which we know the exact value of the critical temperature. For instance, in recent years, many studies were performed for the kinetic Ising and Potts models [2–5]. In this work we investigate the short-time critical dynamics of the Baxter-Wu model, for which the critical temperature is exactly known.

This model was introduced by Wood and Griffiths [6] as a model showing a continuous phase transition but that does not exhibit a invariance by a global inversion of all spins. The model, whose Hamiltonian takes into account only interactions between three nearest-neighbor Ising spins variables on a triangular lattice, was solved exactly by Baxter and Wu [7]. In the thermodynamic limit, the partition function of the model was related to the generating function of a site-coloring problem on a hexagonal lattice. This model is self-dual, with the same critical temperature as the Ising model on a square lattice. In addition, its leading exponents are the same as those exhibited by the four-state Potts model [8]. Recent conformal invariance studies [9,10] showed that the four-state Potts model and the Baxter-Wu model have the same operator content, and this fact put them in the same universality class of critical behavior. Although the Baxter-Wu model does not present invariance by a global inversion of all spins, it displays a special symmetry by a suitable inversion of two spins belonging to two of the three sublattices into which the original triangular lattice can be decomposed [9]. Then the ground-state is fourfold degenerate: three of these states have a magnetization per site equal to $-\frac{1}{3}$, while the remaining state has a magnetization equal to 1. Our interest in studying this model by the short-time formalism is twofold: first, as we know exactly the location of the critical point of the model, the formalism can be applied considering different initial states belonging to the degenerate ground state; second, we want to calculate the dynamical critical exponent of this model because, as far as we know, it was not yet determined. From our Monte Carlo simulations we obtain the static critical exponents of the model that are in agreement with the well-known results found in the literature. The values we found for the critical exponents are independent of the ground-state configuration, we choose to allow the system relax at the critical temperature. On the other hand, despite the fact that the underlying symmetry of the Baxter-Wu model is different from that of the usual Ising model, the dynamical critical exponents of these two models appear to be the same. In Sec. II, we present the model and the scaling relations used in our short-time analysis. In Sec. III, we present our Monte Carlo simulations and the values obtained for the critical exponents, and in Sec. IV we present our conclusions.

II. MODEL AND SCALING RELATIONS

In this section we present the short-time dynamics for the Baxter-Wu model. The transition rate between states follow the well-known Glauber kinetics, where only a single spin can be flipped per unit of time. The Hamiltonian of the Baxter-Wu model is

$$\mathcal{H} = -J \sum_{\langle i,j,k \rangle} \sigma_i \sigma_j \sigma_k , \tag{1}$$

where $\sigma_i = \pm 1$ are the spin variables, and the sum extends over the elementary triangles of the triangular lattice. J is the magnitude of the coupling among three nearest-neighbor spins. The triangular lattice can be decomposed into three sublattices, and each spin of a given sublattice interacts with six nearest-neighbor spins belonging to the two other sublattices. This model is self-dual, and exhibits the same critical temperature as the Ising model on a square lattice. The critical temperature is given by $k_B T_c = 2/\ln(1+\sqrt{2})$ in units of J. The equilibrium critical exponents [8] associated with the correlation length and the order parameter are $\nu = 2/3$ and $\beta = 1/12$, respectively. For this model the order parameter is simply taken as the mean value of the magnetization of the three sublattices. In general, the studies concerning the short-time dynamics assume that the initial state is completely dis-

*Email address: wagner@fisica.ufsc.br

ordered at the critical point, with a vanishing or a very small value of the order parameter. Here we consider a dynamical relaxation process starting from one of the possible configurations of the ground state. That is, we considered relaxation processes which initiate with magnetization 1 or $-\frac{1}{3}$. Usually, for systems with a nondegenerate ground state, the initial state is always that with magnetization equal to 1. This approach was successfully applied to the three-dimensional Ising model [11], extended to the quantum domain (a one-dimensional transverse Ising model at zero temperature) [12], and applied to a competing Ising model in the presence of a magnetic field [13].

Let us consider the equations that describe the relaxation of the Baxter-Wu model from its ground state toward equilibrium. Then the initial magnetization at time $t=0$ can be 1 or $-\frac{1}{3}$ depending on which state we choose to start the relaxation. Very near the critical point we can write the following scaling form for the kth moment of the order parameter,

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

where $\tau=(T-T_c)/T_c$ is the reduced critical temperature, b is the spatial rescaling factor, and L is the linear lattice size. The exponents β and ν are the well-known equilibrium exponents defined above, and z is the dynamical critical exponent. This scaling relation for the order parameter is similar to the one used in the long-time regime studies. Here it is used to investigate the macroscopic short-time regime, as in the work of Jaster *et al.* [11]. For $k=1$, we have the proper magnetization, and choosing the scaling factor to be $b=t^{1/z}$, we obtain

$$M(t,\tau)=t^{-\beta/\nu z}M(1,t^{1/\nu z}\tau), \qquad (3)$$

where it is assumed that the linear dimension L is very large. At the critical point $(\tau=0)$, the magnetization exhibits the power-law behavior

$$M(t)\sim t^{-c_1}, \qquad (4)$$

where $c_1=\beta/\nu z$. Taking the derivative of Eq. (2) with respect to τ and choosing the same scaling factor as before, we can write the following relation at the critical point:

$$DM(t)\sim t^{c_2}, \qquad (5)$$

where $c_2=1/\nu z$, and $DM(t)$ is the logarithmic derivative of $M(t,\tau)$ with respect to τ at the critical point. As the magnetization is different from zero at the initial stages of the evolution, we can also define a time-dependent second-order cumulant. It is given by

$$U(t)=\frac{M^{(2)}}{(M)^2}-1. \qquad (6)$$

From Eq. (2), at the critical point $(\tau=0)$, taking $b=t^{1/z}$, and for large values of L, we can write that

$$M^2\sim t^{-2\beta/\nu z}, \qquad (7)$$

$$M^{(2)}=t^{-2\beta/\nu z}M^{(2)}(1,t^{-1/z}L), \qquad (8)$$

where $M^{(2)}(1,x)\sim x^{-d}$, because at the beginning of the time evolution the spatial correlation length is very small. Therefore, Eq. (6) becomes, for a fixed and large value of L,

$$U(t)\sim t^{-c_3}, \qquad (9)$$

where $c_3=d/z$, and d is the spatial dimensionality of the spin system. Therefore, by measuring the three independent exponents, c_1, c_2, and c_3, we can obtain the static (β,ν) and the dynamical (z) critical exponents. This procedure is easier to implement than the usual one, where we need to prepare the system to have, at the initial time, very small values of the magnetization and correlation length.

III. MONTE CARLO SIMULATIONS

We have measured the magnetizations $M(t)$ and $M^{(2)}(t)$ for lattice sizes with linear dimensions up to $L=258$. We choose this value to be a multiple of 3, because we divided the triangular lattice into three independent sublattices. For the lattice size $L=258$, we have considered 500 Monte Carlo steps, and we have seen that 2000 samples are sufficient to obtain good statistics. We have taken, for the transition probability rate among states, the following one-spin flip Glauber prescription [14]:

$$w_i(\sigma)=\frac{1}{2}\left\{1-\sigma_i^a\tanh\left[\frac{1}{k_BT}\left(\sum_1^6 \sigma^b\sigma^c\right)\right]\right\}, \qquad (10)$$

where the spin to be flipped is the ith spin of the sublattice a. In the above sum we considered all six nearest-neighbor pairs of spins belonging to sublattices b and c, and which are neighbors of the spin σ_i^a. k_B is Boltzmann's constant, and T is the absolute temperature of heat bath.

Figure 1 shows the log-log plot of the magnetization versus time. In this figure we represent the data obtained from two different initial conditions for the fourfold-degenerate ground state: one with magnetization $M(0)=1$ (curve a) and the other with $M(0)=-\frac{1}{3}$ (curve b). For the latter value of the magnetization, there are three distinct configurations of the ground state, and the data correspond to the absolute value of the mean obtained from these configurations. In the same figure we also show the best linear fit to the data points. From the slope of the curve a we found the value $c_1^a=0.0578(2)$, while for curve b we found $c_1^b=0.0668(3)$. Figure 2 exhibits the log-log plots of the logarithmic derivative of the magnetization with respect to the reduced temperature at the critical point, versus time. The slope of these curves gives the values of c_2. For the initial condition $M(0)=1$ we obtain $c_2^a=0.768(3)$, and for the initial condition $M(0)=-\frac{1}{3}$, $c_2^b=0.817(4)$. Finally, Fig. 3 shows the log-log plots of the second-order cumulant versus time, and the corresponding best fits to the data points. The slopes are given by $c_3^a=0.967(3)$ and $c_3^b=1.02(1)$.

Therefore, the critical exponents β, ν, and z can be determined for the Baxter-Wu model. Considering the initial

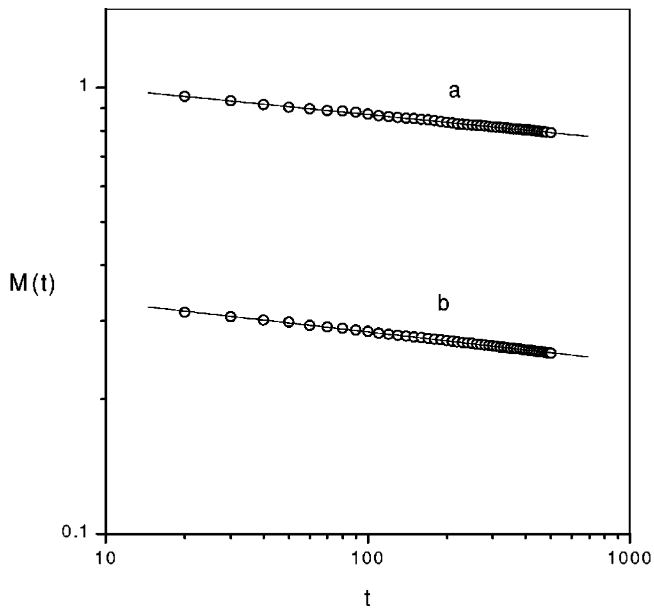

FIG. 1. Log-log plot of the absolute magnetization $M(t)$ vs time, in units of Monte Carlo steps (MC's), at the critical temperature of the Baxter-Wu model. Curve a shows data points for $M(0)=1$, and curve b initial magnetization $M(0)=-\frac{1}{3}$. The straight lines give the best fit to the data points.

condition $M(0)=1$, which corresponds to the coefficients c_i^a, we obtain the following values:

$$\beta=0.0753\pm0.0014,$$

$$\nu=0.629\pm0.005,$$

and

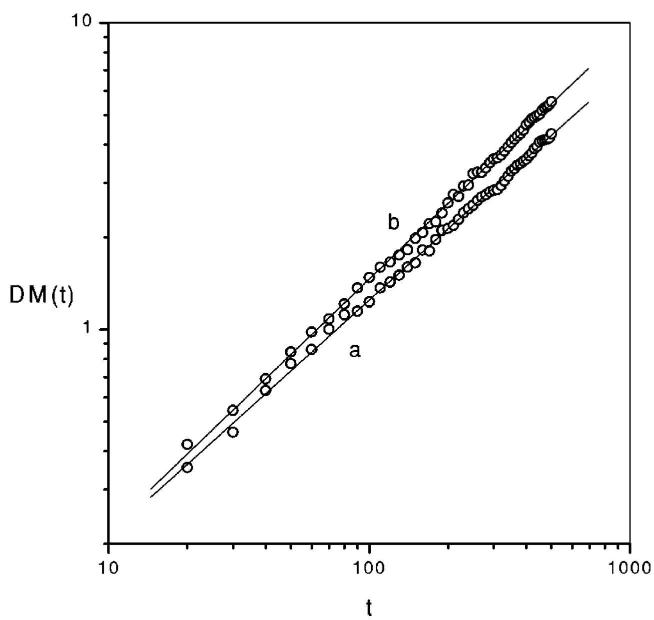

FIG. 2. Log-log plot of the logarithmic derivative of the magnetization with respect to the reduced temperature $DM(t)$ vs time, at the critical temperature. The straight lines give the best fit to the data points. Curve a: $M(0)=1$. Curve b: $M(0)=-\frac{1}{3}$.

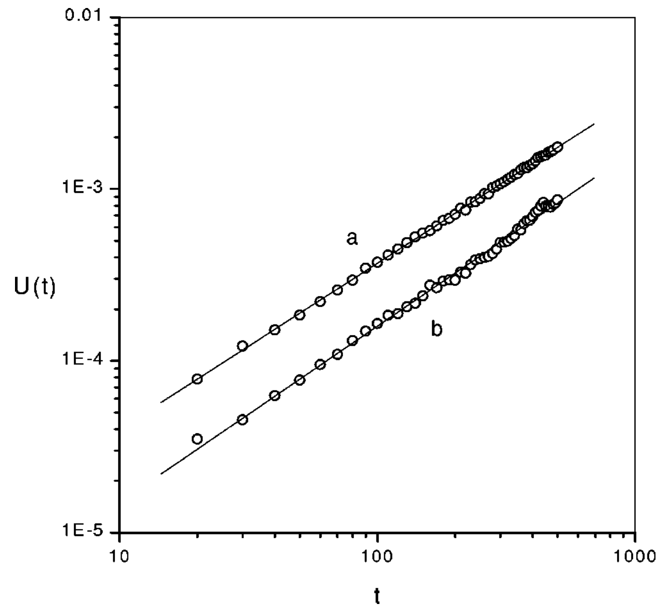

FIG. 3. Log-log plot of the second-order cumulant $U(t)$, vs time, at the critical temperature. The straight lines give the best fit to the data points. Curve a: $M(0)=1$. Curve b: $M(0)=-\frac{1}{3}$.

$$z=2.07\pm0.01.$$

On the other hand, for the initial condition $M(0)=-\frac{1}{3}$, the critical exponents, which are related to the coefficients c_i^b, are given by

$$\beta=0.0817\pm0.0023,$$

$$\nu=0.621\pm0.009,$$

and

$$z=1.96\pm0.02.$$

Within the statistical precision of our measurements, the values we found for the static critical exponents β and ν agree with the exact ones [8]. On the other hand, the values we found for the dynamical critical exponent z are very close to that of the Ising model when the transition rate is of the Glauber type. This appear to indicate that the dynamical universality class is not affected by the underlying symmetry of the Hamiltonian. When the relaxation process is driven by the single spin-flip Glauber prescription, which does not conserve the order parameter, the evolution toward equilibrium states proceeds with the same rate z. Tang and Landau [15] performed Monte Carlo simulations for the two-dimensional q-state Potts models, with $q=2$, 3, and 4. Their results seems to confirm that the dynamical critical exponent z, which governs the long-time relaxation, is the same for the three considered values of q. For instance, their best estimates for the $q=4$ Potts model is $z=2.19$. As the values we found for z are close to these figures, this support the idea that the four-state Potts model and the Baxter-Wu model are also in the same dynamical universality class.

Our results also indicate that the scaling laws for the short-time dynamics are not very sensitive to the initial value

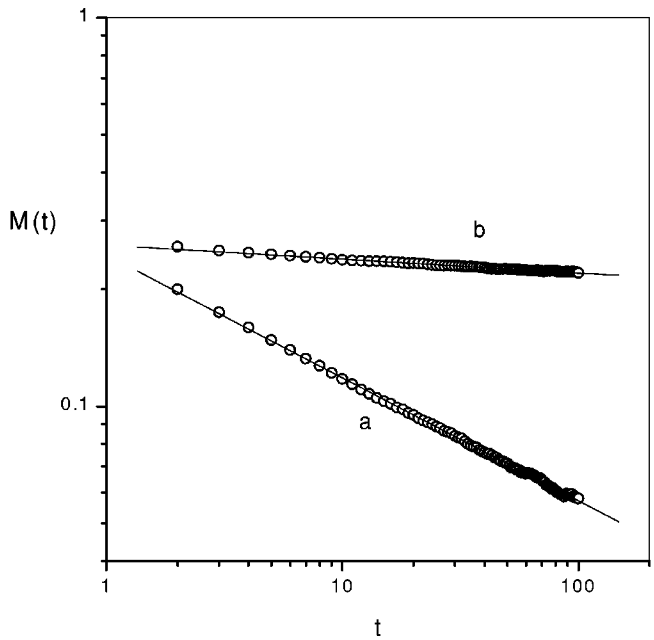

FIG. 4. Log-log plot of the absolute magnetization $M(t)$ vs time, in units of Monte Carlo steps (MC's), at the critical temperature of the Baxter-Wu model. Curve *a* shows data points for $M(0)=-1$, and curve *b* the initial magnetization $M(0)=+\frac{1}{3}$. The straight lines give the best fit to the data points.

of the magnetization. What seems to be very important in this approach is to choose an initial state which is a ground state of the system. We call attention that in the literature [11,13] the initial state is chosen to be one that is completely ordered. However, this works very well whenever the ground state is nondegenerate. Nevertheless, the condition of being completely ordered is not sufficient to give reliable values for the critical exponents in the short-time regime. Figure 4 exhibits a log-log plot of the magnetization versus time for two different initial configurations, which do not belong to the ground-state set. Curve *a* gives the time evolution for the initial state with $M(0)=-1$, and curve *b* gives the time evolution for the initial state $M(0)=+1/3$. The slope of curves *a* and *b* are 0.316 and 0.035, respectively. On the other hand, from the plot of the second-order cumulants, which gives a direct value for the dynamical critical exponent *z*, we obtain $z=1.38$ $[M(0)=-1]$ and $z=2.33$ $[M(0)=+1/3]$. Relating these values with those found for the slopes of Fig. 4 we found that $\beta/\nu=0.44$ $(M(0)=-1)$ and $\beta/\nu=0.08$ $(M(0)=+1/3)$. Although the state with $M(0)=-1$ be completely ordered, the results obtained are very bad. On the other hand, if the initial state is selected from the ground-state set, it gives good results, even if it is not completely ordered, as is the case of curve *b* in Fig. 1. Usually, the exponent *z* is determined by the long-time regime of the relaxation process by measuring the decay of the magnetization of the system. This procedure presents some difficulties because at the critical point the relaxation times are very long, and we need simulate very large systems to obtain a reliable value of *z*. The present method, that exploits the initial stages of evolution of the system, is free of the critical slowing down difficulties, and can be applied to systems not too large. The price paid using this method is the statistics: we need to consider a very large number of samples in order to obtain critical exponents almost free of noise.

IV. CONCLUSIONS

We have employed the short-time dynamics to investigate the critical properties of the Baxter-Wu model on a triangular lattice. Using Monte Carlo simulations with the Glauber transition rate, we found static critical exponents β and ν that agree with the exact ones known for this model. We also determined the dynamical critical exponent *z* of the model; to the best of our knowledge, an estimate of this exponent for the Baxter-Wu model has not yet been obtained. Although the two-dimensional Ising model and the Baxter-Wu model present different Hamiltonian symmetries, belonging to different equilibrium universality classes, they appear to exhibit the same dynamical critical behavior. We also have shown that the initial value of the magnetization is irrelevant for the scaling relations involved in the relaxation process. However, the initial configuration must be one chosen from the ground state of the model.

ACKNOWLEDGMENT

This work was supported by the Brazilian agencies CNPq and FINEP.

[1] H.K. Janssen, B. Schaub, and B. Schmittmann, Z. Phys. B: Condens. Matter **73**, 539 (1989).
[2] D.A. Huse, Phys. Rev. B **40**, 304 (1989).
[3] Z.B. Li, U. Ritschel, and B. Zheng, J. Phys. A **27**, L837 (1994).
[4] Z.B. Li, L. Schulke, and B. Zheng, Phys. Rev. Lett. **74**, 3396 (1995).
[5] K. Okano, L. Schulke, K. Yamagishi, and B. Zheng, Nucl. Phys. B **485**, 727 (1997).
[6] D.W. Wood and H.P. Griffiths, J. Phys. C **5**, L253 (1972).
[7] R.J. Baxter and F.Y. Wu, Phys. Rev. Lett. **31**, 1294 (1973).
[8] R. J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, New York, 1982).
[9] F.C. Alcaraz and J.C. Xavier, J. Phys. A **30**, L203 (1997).
[10] F.C. Alcaraz and J.C. Xavier, J. Phys. A **32**, 2041 (1999).
[11] A. Jaster, J. Mainville, L. Schulke, and B. Zheng, J. Phys. A **32**, 1395 (1999).
[12] M. Santos, Phys. Rev. E **61**, 7204 (2000).
[13] M. Santos and W. Figueiredo, Phys. Rev. E **62**, 1799 (2000).
[14] R.J. Glauber, J. Math. Phys. **4**, 294 (1963).
[15] S. Tang and D.P. Landau, Phys. Rev. B **36**, 567 (1987).