Phase transitions in nonequilibrium *d*-dimensional models with *q* absorbing states

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A nonequilibrium Potts-like model with q absorbing states is studied using Monte Carlo simulations. In two dimensions and $q=3$ the model exhibits a discontinuous transition. For the three-dimensional case and $q=2$ the model exhibits a continuous transition with $\beta=1$ (mean field). Simulations are inconclusive, however, in the two-dimensional case for $q=2$. We suggest that in this case the model is close to or at the crossing point of lines separating three different types of phase transitions. The proposed phase diagram in the (q,d) plane is very similar to that of the equilibrium Potts model. In addition, our simulations confirm the field-theory prediction that in two dimensions a branching-annihilating random walk model without parity conservation belongs to the directed percolation universality class.

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I. INTRODUCTION

One of the main achievements of statistical physics during the past decades is the understanding of the universal properties of systems near an equilibrium second-order phase transition. Universality classes, characterized by a small number of parameters, allow us to understand why different systems have the same critical properties [1].

One important model in equilibrium statistical physics is the so-called q-states Potts model [2], which can be used to describe a large class of physical systems. Its rich critical behavior is to a large extent understood. It is known that the important parameters that determine its critical behavior are its dimensionality d and the degeneracy of its ground state q.

The relatively complete understanding of equilibrium phase transitions has yet no nonequilibrium counterpart. However, it is becoming evident that some analogies between equilibrium and nonequilibrium systems could be made.

For example, a classification into universality classes is particularly evident for one-dimensional nonequilibrium models with absorbing states [3], which exhibit a phase transition between active and absorbing phase in their stationary state. A prime example of a universality class is the directed percolation (DP) one, which is typical of models with a single absorbing state [4]. The so-called parity-conserving (PC) universality class is typical for models with certain conservation laws or symmetries [5–8].

However, it is necessary to investigate nonequilibrium models in higher dimensions to have a complete characterization of the possible universal properties.

Analytical approach to high-dimensional problems is based mainly on field-theory methods. Recently, interesting results were obtained along this line by Cardy and Täuber [9] who clarified the role of parity conservation and also discovered some new universality classes. However, this technique is applicable only to certain particle systems [10] and a large class of two- and higher-dimensional models with absorbing states cannot be treated within such a method. Accordingly, our understanding of higher-dimensional nonequilibrium models is rather limited. As for continuous phase transitions some models with single absorbing states were shown to fall into the DP universality class [11]. Results were also reported for a two-dimensional model with two absorbing states [8]. These models are often motivated by problems of surface catalysis [12]. In some models with absorbing states discontinuous phase transitions are also known to occur [13,3,14].

A subclass of models with absorbing states are the so-called branching-annihilating random walk (BARW) ones. In BARW models each particle can react (annihilate, branch, diffuse, etc.) according to prescribed rules. It turns out that BARW models for $d>1$ are much different from the above mentioned (surface-catalysis) models. Some of the results obtained from the field-theory method [9] have been confirmed using numerical methods. For example, Szabó and Santos confirmed the existence of logarithmic corrections in two-dimensional parity-conserving BARW models [15]. However, for parity-nonconserving particle systems Monte Carlo simulations [6] seem to be in disagreement with field-theory results [9].

A characterization of the rich critical behavior encountered in models with absorbing states is clearly an important issue. However, lacking a sound theoretical basis, it is by no means obvious as to which parameters are relevant for such a classification. On general grounds one expects that the dimensionality d of the system is a relevant parameter. Moreover, based on the information coming from the one-dimensional case and from equilibrium one expects that the number of absorbing states q is another relevant parameter. Note however that, in some cases, details of the dynamics might also change the critical properties, even without affecting the symmetry of absorbing states [16]. Nevertheless, we can expect that these cases are accidental rather than generic (as it is the case in equilibrium phase transitions when a marginal scaling field is present [17]). Keeping in mind the above objections, and in the absence of a better choice, we consider q as a classification parameter [18].

In the present paper we study a recently introduced nonequilibrium Potts model with q absorbing states. Our numerical results for $d\geqslant 2$ can be summarized as follows.

(i) For $d=2$ and $q=3$ the model has a discontinuous transition.

(ii) For $d=3$ and $q=2$ the model exhibits a continuous transition with an order parameter critical exponent $\beta=1$ (mean field).

(iii) Simulations are inconclusive, however, in the $d=2$ and $q=2$ case, and we suggest that in this case the model is close to or at the crossing point of lines separating three different types of phase transitions.

Our results together with the already accumulated knowledge, prompted us to partition the (q,d) plane into three regions of different phase transitions: mean-field, non-mean-field, and discontinuous transitions. Somewhat surprisingly, the topology of such a partition is the same as for the equilibrium Potts model. Although nonequilibrium systems, and in particular models with absorbing states, are usually regarded as very much different from equilibrium systems our work shows, however, that despite some differences there are also some qualitative similarities.

In addition, we performed simulations of a $d=2$ BARW model without parity conservation. Our results confirm the field-theory predictions according to which the critical behavior belongs to the directed percolation universality class.

II. NONEQUILIBRIUM POTTS MODEL

Before presenting our model let us recall basic properties of the equilibrium Potts model. First we assign with a lattice site i a q-state variable $\sigma_i=0,1,\ldots,q-1$. Next, we define the energy of this model through the Hamiltonian

$$H=-\sum_{(i,j)}\delta_{\sigma_i\sigma_j}, \tag{1}$$

where summation is over pairs (i,j) which are usually nearest neighbors, and δ is the Kronecker delta function. This equilibrium statistical mechanics model was studied using many different analytical and numerical methods and is a rich source of information about phase transitions and critical phenomena [2].

To study the equilibrium Potts model using Monte Carlo simulations one constructs a stochastic Markov process with suitably chosen transition rates. One of the possible choices corresponds to the so-called Metropolis algorithm. In this algorithm one looks at the energy difference ΔE between the final and initial configuration and accepts the move with probability $\min\{1,e^{-\Delta E/T}\}$, where T is temperature.

A nonequilibrium Potts model having q adsorbing states can be obtained by making the following transformation in the Metropolis dynamics [16]: when all neighbors of a given site are in the same state as this site, then this site cannot change its state (at least until one of its neighbors is changed). Let us notice that any of q ground states of the equilibrium Potts model (1) is an absorbing state of our nonequilibrium Potts model. The one-dimensional version of this nonequilibrium Potts model has already been examined [16]. In addition to recovering the expected critical behavior for $q=2$ and 3, it was found that certain additional modifications of its dynamics might affect the critical behavior. We shall not be concerned with such a variant in the present paper.

Since the dynamics of our models is obtained from a modification of the Metropolis algorithm of an equilibrium system transition probabilities are parametrized by a temperaturelike quantity T. Strictly speaking, for our model the ordinary temperature cannot be defined. Nevertheless, we will refer to this quantity as temperature.

Of course in the realm of nonequilibrium systems there are also other models than those with absorbing states. One of the important questions is whether under certain conditions nonequilibrium systems might be mapped, at least at the coarse-grained level, into equilibrium ones. Some aspects of this problem were studied by Grinstein *et al.* [19]. In a class of models studied by them it is important that all transition probabilities are strictly greater than zero. In models with absorbing states this requirement is clearly violated.

III. MONTE CARLO SIMULATIONS AND RESULTS

In order to study the properties of our model we made extensive Monte Carlo simulations. A natural characteristic of models with absorbing states is the steady-state density of active sites ρ. A given site i is active when at least one of its neighbors is in a state different than i. Otherwise the site i is called nonactive. Upon approaching a critical point ρ develops a power-law singularity characterized by the exponent β. At the first-order transition ρ has a jump. In addition, we also looked at its time dependence $\rho(t)$. In the active phase $\rho(t)$ converges to the positive value, while at criticality $\rho(t)$ usually has a power-law decay $\rho\sim t^{-\delta}$. In the absorbing phase ρ very often decays faster than the power law, however, in some cases (also those studied in the present paper) a power-law behavior is seen, but with a different exponent than for the critical decay.

Moreover, we used the so-called dynamic Monte Carlo method where one sets the system in the absorbing state with activity only locally initiated and monitor some stochastic properties of runs [20]. One of the most frequently used characteristics is the survival probability $P(t)$ that activity survives at least until time t and the average number of active sites $N(t)$ [to calculate $N(t)$ we average over all runs]. At criticality $P(t)$ and $N(t)$ are expected to have power-law decay: $P(t)\sim t^{-\delta'}$ and $N(t)\sim t^{\eta}$. (For some models $\delta=\delta'$, but exceptions from this relation are also known [3]). Our simulations were made for various system sizes and we ensured that the system was large enough so that below presented results are size independent.

A. $d=2$, $q=3$

Simulations for $d=2$ models were performed on the square lattice. The temperature dependence of the density of active sites ρ is shown in Fig. 1. For $T<1.237$ it is virtually impossible to reach an active steady-state value of ρ, which suggests that the model undergoes a discontinuous phase transition. Such a scenario is confirmed by the data in Figs. 2–4. In Fig. 2 one can see that upon approaching the transi-

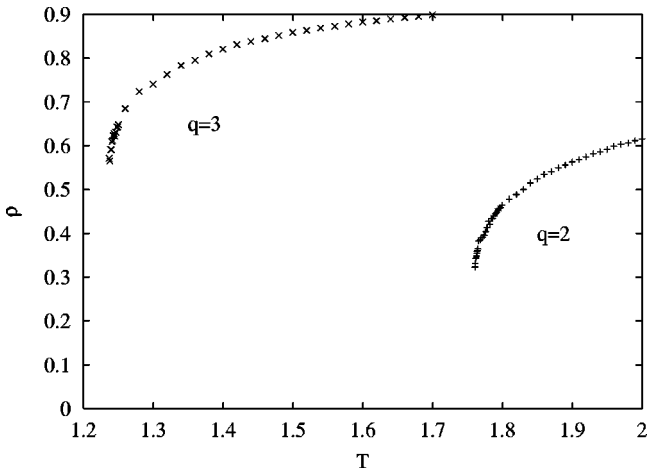

FIG. 1. The density of particles ρ as a function of temperature T for the $d=2$ nonequilibrium Potts model. Close to the transitions we used the lattice of the linear size $L=600$.

tion point $\rho(t)$ develops a longer and longer plateau. At the transition point, which we locate around $T=1.237$, the density $\rho(t)$ has basically an infinitely long plateau. Such a behavior is a clear indication of the discontinuous nature of the transition.

Let us notice that below the transition temperature $\rho(t)$ decays as $t^{-1/2}$. A simple scaling argument can be used to show that such a behavior is related to the average domain size growth $l\sim t^{1/2}$. Indeed, let us consider the $d=2$ system of the linear size L. It contains $(L/l)^2$ subdomains of the linear size l and thus the total perimeter of these subdomains scales as L^2/l. Since active sites are located mainly at the domain walls their density scales as $L^2/lL^2=l^{-1}$. Assuming now that l increases as $t^{1/2}$ we obtain that $\rho\sim t^{-1/2}$. The characteristic length that increases as $t^{1/2}$ is typical for coarsening in the broken-symmetry phase of the original Potts model [21,22]. It also appears in the evolution of one-dimensional

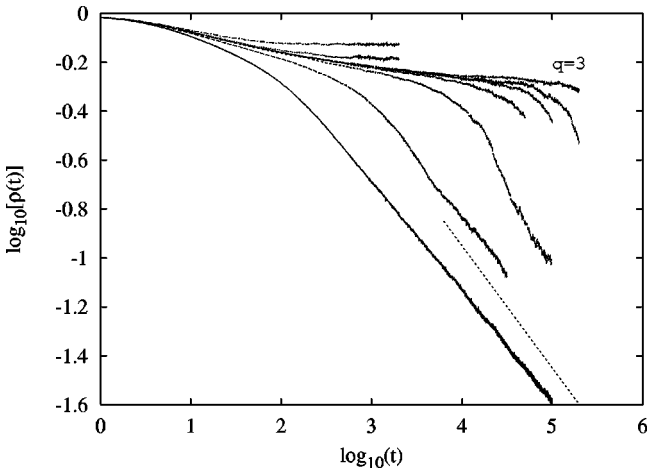

FIG. 2. The time dependence of the density $\rho(t)$ for the $d=2$ model and (from top) $T=1.3$, 1.25, 1.237, 1.2365, 1.236, 1.235, 1.23, 1.2, and 1.1 ($L=500$). Each line is an average of 100 independent runs, which starts from random initial configurations. The dotted straight line has a slope corresponding to $\delta=0.5$.

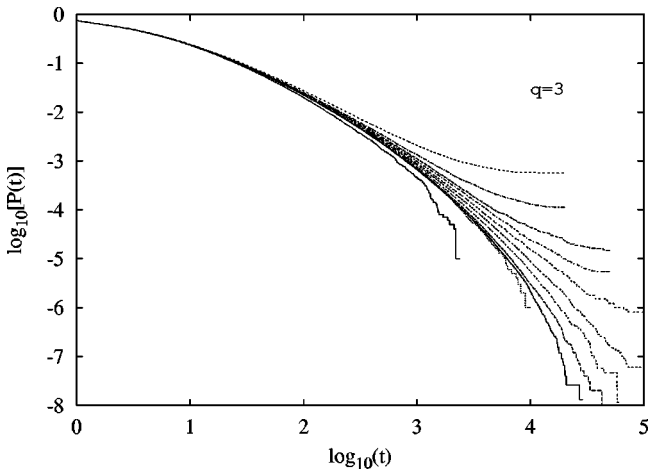

FIG. 3. The time dependence of the survival probability $P(t)$ for the $d=2$ model and (from top) $T=1.25$, 1.245, 1.242, 1.241, 1.24, 1.239, 1.238, 1.237, 1.2365, 1.236, and 1.23 ($L=500$). Lines for $T=1.2365$, 1.237, and 1.238 are obtained averaging over 10^8 independent runs.

nonequilibrium systems that belong to the parity-conserving universality class.

Results of the dynamic Monte Carlo also support the discontinuous nature of the transition. Indeed, both for $P(t)$ (Fig. 3) and $N(t)$ (Fig. 4) the data are systematically bending and no clear power-law behavior is observed.

Thus, as a summary, for the $d=2$, $q=3$ case our model undergoes a discontinuous phase transition.

B. $d=2$, $q=2$

In the $q=2$ case the density of active sites is a similar function of temperature as in the $q=3$ case (Fig. 1). Let us notice however, that now the jump in ρ is almost twice smaller than previously. We should also be aware of the fact that an observed jump might be a finite-size effect. (Large

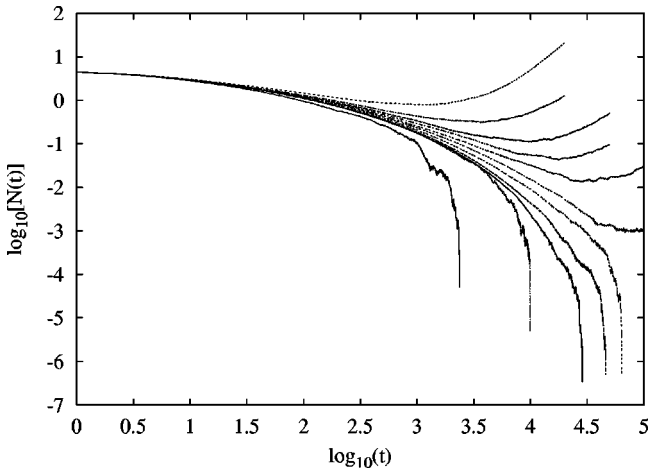

FIG. 4. The time dependence of the number of active sites $N(t)$ for the $d=2$, $q=3$ model and (from top) $T=1.25$, 1.245, 1.242, 1.241, 1.24, 1.239, 1.238, 1.237, 1.2365, 1.236, and 1.23 ($L=500$). Lines for $T=1.2365$, 1.237, and 1.238 are obtained averaging over 10^8 independent runs.

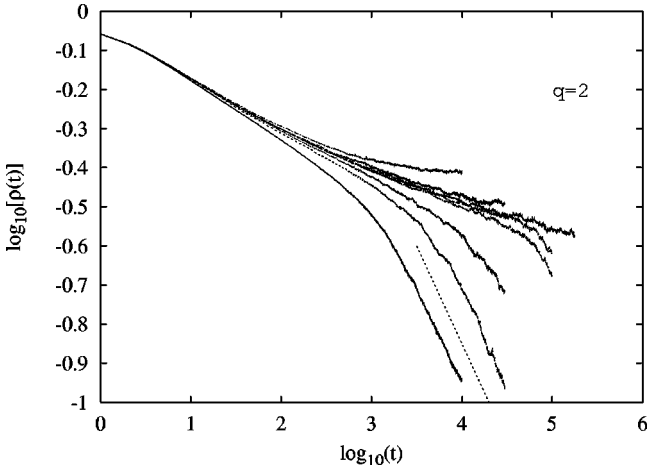

FIG. 5. The time dependence of the density $\rho(t)$ for the $d=2$ model and (from top) $T=1.77$, 1.76, 1.7585, 1.758, 1.757, 1.75, 1.74, and 1.71 ($L=500$). Each line is an average of 100 independent runs, which starts from random initial configurations. The dotted straight line has a slope corresponding to $\delta=0.5$.

fluctuations might drive the system into an absorbing state even though temperature is above the critical temperature.) As further results show, it is rather difficult to clarify the nature of the transition in this case. First, let us notice that time dependence of $\rho(t)$ does not develop a clear plateau as in the $q=3$ case. [We estimate the critical point in this case as $T_c=1.7585(3)$.] Neither is there a pronounced power-law behavior seen in Fig. 5. If $\rho(t)$ does decay as $t^{-\delta'}$ at criticality then δ' is very small [$\delta'=0.07(2)$], which suggests that the true exponent δ' might be equal to zero. Sometimes to improve the estimation of δ one can use the so-called local slopes method [3]. In this method δ is calculated from the equation

$$\delta(t)=\frac{\log_{10}\left[\dfrac{\rho(t)}{\rho(t/m)}\right]}{\log_{10}(m)}, \tag{2}$$

where m is a certain constant. Application of this method to our data and $m=5$ is shown in Fig. 6. At criticality the data converge (with some scattering) to the value 0.06 but such a small value means that the possibility $\delta=0$ still cannot be excluded.

In our opinion, from the steady-state and time-dependent measurements of ρ the most likely possibility is that the transition is of first order and the plateau will develop (in Fig. 5) but only at a larger time scale.

However, the dynamic Monte Carlo results raise some doubts on such an interpretation. Indeed, in Fig. 7 we can see that $P(t)$ has a clear power-law decay for at least three decades in time with the exponent $\delta'=0.90(2)$. In addition, $N(t)$ seems to remain constant at the transition point, which suggest that $\eta=0$ (see Fig. 8). To support our dynamic Monte Carlo results let us notice that Hinrichsen reported basically the same values for dynamical exponents for another two-dimensional model with $q=2$ [8].

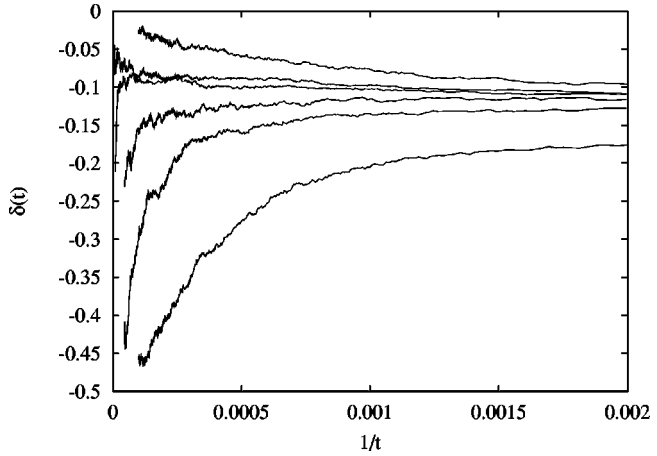

FIG. 6. The exponent $\delta(t)$ as a function of $1/t$ for the $d=q=2$ model and (from top) $T=1.77$, 1.7585, 1.757, 1.75, 1.74, and 1.71 ($L=500$). Each line is an average of about 100 independent runs.

The fact δ' is close to unity and $\eta=0$ prompted Hinrichsen to suggest that the model exhibits a mean field behavior. In such a case, however, one should have $\delta=1$, which is clearly in contradiction with the behavior of $\rho(t)$, which we observe. A power-law behavior of $P(t)$ and $N(t)$ is typical for continuous transitions, which seems to be in conflict with the behavior of ρ. However, the possibility that we have a discontinuous transition accompanied by some dynamical power-law characteristics, although exotic at first sight, cannot be ruled out. We will return to this problem in the following section.

Let us also notice (Fig. 5) that, similarly to the $q=3$ case, for $T<T_c$ the density $\rho(t)$ seems to decay in time as $t^{-1/2}$.

C. $d=3$, $q=2$

As a last case in this section, we consider our model on the simple cubic lattice and for $q=2$. Of course, simulations

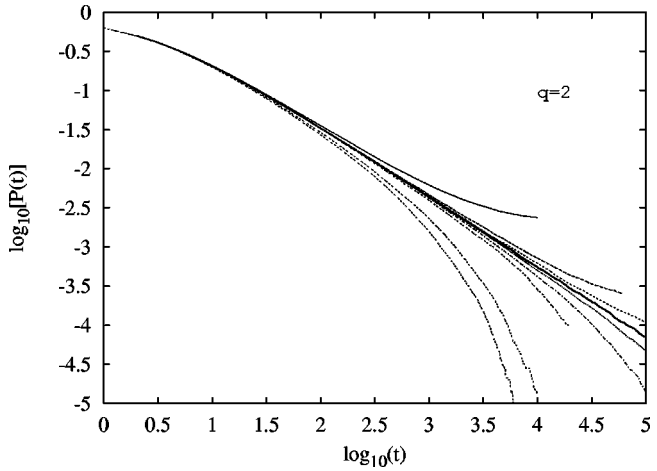

FIG. 7. The time dependence of the survival probability $P(t)$ for the $d=2$ model and (from top) $T=1.77$, 1.76, 1.759, 1.7585, 1.758, 1.757, 1.755, 1.74, and 1.73 ($L=500$). Each line is an average of about 10^6 independent runs.

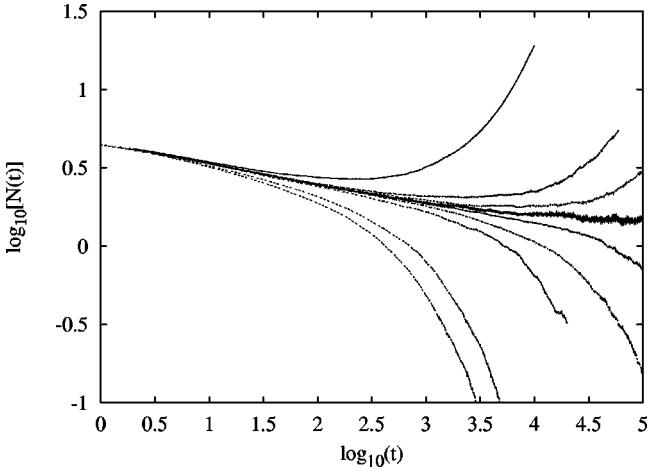

FIG. 8. The time dependence of the number of active sites $N(t)$ for the $d=2$, $q=2$ model and (from top) $T=1.77$, 1.76, 1.759, 1.7585, 1.758, 1.757, 1.755, 1.74, and 1.73 ($L=500$). Each line is an average of about 10^6 independent runs.

for three-dimensional systems are very demanding. Therefore we were not able to perform detailed time-dependent simulations nor the dynamic Monte Carlo. However, the steady-state density ρ as measured for $L=40$ and 60 is basically size independent (Fig. 9). Nearly linear behavior of ρ in the vicinity of the transition suggests that in this case $\beta=1$, which indicate a mean-field nature of the transition.

D. (q,d) phase diagram

In this section we sketch the overall behavior of our model in the (q,d) plane. Our proposal (Fig. 10) is based on the already accumulated knowledge, above presented results, and a minimalistic assumption that the resulting phase diagram should not be too complicated. Essentially, we suggest that the (q,d) plane can be divided into three regions of different types of phase transitions: (i) non-mean-field, (ii) mean-field, and (iii) first-order transitions.

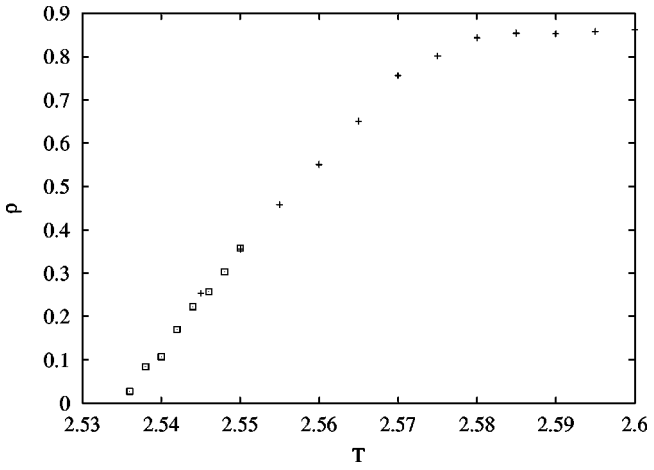

FIG. 9. The density of particles ρ as a function of temperature T for the three-dimensional $q=2$ nonequilibrium Potts model with $L=60$ (□) and 40 (+).

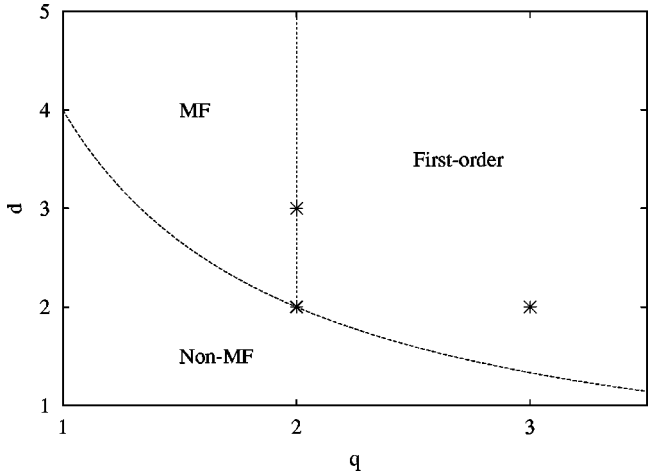

FIG. 10. The location of various types of phase transitions for d-dimensional models with q absorbing states. Models for which numerical results are reported in this paper are denoted as stars.

Some comments are in order. As it is defined only through dynamical rules, our model is trivial for $q=1$. However, the $q=1$ case corresponds to models with a single absorbing state (directed percolation, contact process). It is known that the critical dimension d_c in this case equals 4 and for d smaller (larger) than d_c we have a continuous non-mean-field (mean-field) transition. Firmly established are also results along the $d=1$ line. It is known that $q=2$ case corresponds typically to the PC universality class. For $q\geqslant 3$ one expects [8,23] that the model typically belongs to the same universality class as a N-BARW model studied by Cardy and Täuber [9], although, under more restrictive dynamics the PC criticality might also appear [16]. In any case, the critical behavior is of non-mean-field type. Taking into account the mean-field behavior obtained in the case $d=3$, $q=2$, we assume that this case falls into the same region as DP above critical dimension. On the other hand, the discontinuous transition in the $d=2$, $q=3$ case implies the existence of the third region. Actually we performed some simulations also for $d=2$, $q=4$ case. Basically the behavior is similar to the $q=3$ case except that the jump is larger and the first-order character of the transition is even more transparent. We expect that such a behavior persists for all $q>3$. Provided that for $d>2$ there are no qualitative changes, the diagram must have a structure as shown in Fig. 10.

It is thus clear that our most difficult case $d=q=2$ is located somewhere close to the point where all three regions meet. We have no strong arguments to locate this point exactly at the crossing point, but such a location would certainly explain unusual behavior as seen in our Monte Carlo simulations. We do not exclude, however, the possibility that $d=q=2$ case is off the crossing point but somewhere close to it, which would still explain the numerical difficulties in this case.

The resulting diagram looks very similar to the diagram of the equilibrium Potts model [2]. In the equilibrium model the non-mean-field part is basically shifted by 2 upwards (critical dimensions for ordinary percolation and the Ising model are 6 and 4, respectively). However, the diagram for

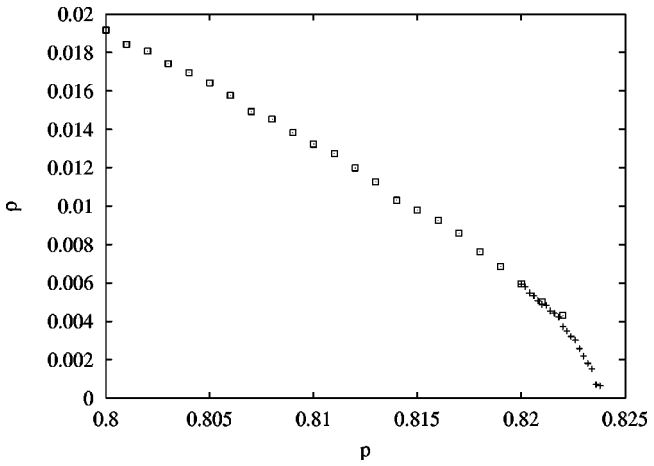

FIG. 11. The density of particles ρ as a function of the diffusion rate p for the two-dimensional BARW model with $L=1000$ ($\square$) and 2000 ($+$).

the equilibrium Potts model is much more meaningful than in our case. Indeed, in the Fortuin-Kasteleyn representation, the Potts model is well defined for any, even noninteger q, which justifies continuous lines on its phase diagram. In our case, we do not have a representation of our model with continuous q. The key property that would be required for such a representation is the existence of an analog of the partition function. Such a quantity exists for nonequilibrium systems only in very special cases [24]. Provided that a certain partition function exists for our model (no matter how complicated), and that using this function one can find a corresponding Fortuin-Kasteleyn representation (no matter how complicated), continuous lines in our diagram would be meaningful.

Of course, the presented diagram does not encompass all models with absorbing states. It is well known that, for example, there are $d=2$, $q=1$ models with first-order transitions [3]. But as we already mentioned, similar situations

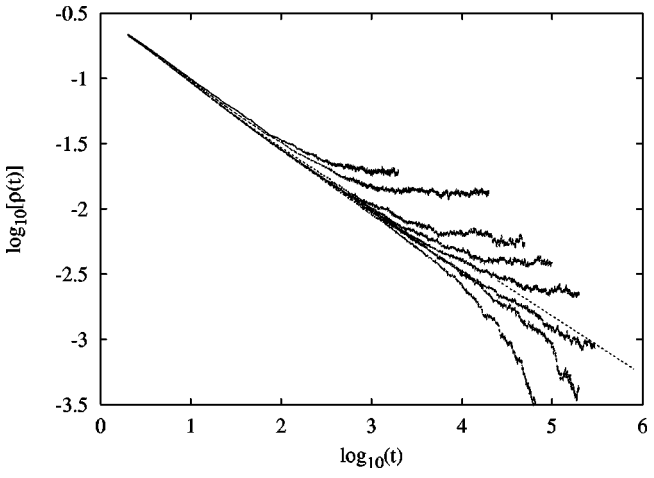

FIG. 12. The time dependence of density of particles $\rho(t)$ for the two-dimensional BARW model. Simulations were made for (from top) $p=0.8$, 0.81, 0.82, 0.822, 0.823, 0.8237, 0.824, and 0.825. The dotted line has a slope corresponding to the DP value $\delta=0.451$.

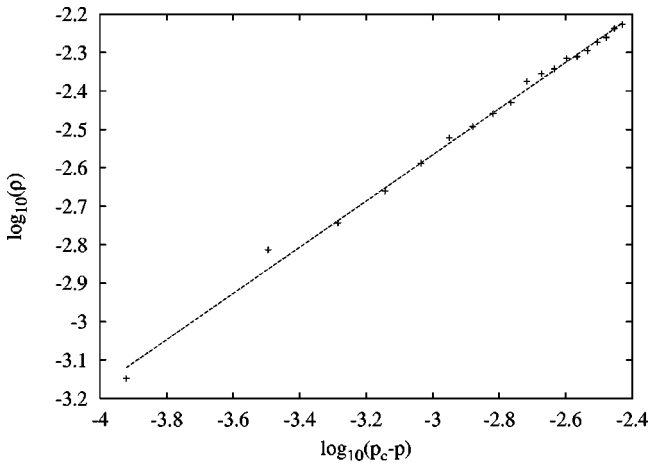

FIG. 13. The density of particles $\rho(t)$ as a function of p_c-p for the two-dimensional BARW model ($p_c=0.8237$). Only results for $L=2000$ runs are shown here. The linear fit (dotted line) obtained using the least-square method has a slope corresponding to $\beta=0.6$.

occurs for equilibrium systems where certain factors (anisotropies, additional interactions, etc.) might change more generic behavior. The presented diagram is valid only for the presented Potts model and its applicability to other systems requires additional examination.

IV. PARITY-NONCONSERVING BARW MODEL IN TWO DIMENSIONS

In the present section we examine the two-dimensional BARW model without parity conservation. In this model particles are located on sites of a square lattice. In addition to diffusion, which takes place at the rate p, particles can branch, at the rate $1-p$, according to the following reaction:

$$X \rightarrow 2X, \tag{3}$$

where the offspring particle is placed on the randomly chosen nearest neighbor of a parent particle. Moreover, two particles that happen to be placed at the same site annihilate instantaneously

$$2X \rightarrow 0. \tag{4}$$

This model was already examined by Takayasu and Tretyakov [6]. They suggested that the model undergoes a continuous transition around $p=0.85$ and the density of particles decays linearly at the transition point ($\beta=1$). This result contradicts more recent field-theory approaches that suggests that in this case the model should belong to the DP universality class [9].

Since such a disagreement requires an explanation, we performed Monte Carlo simulations of this model. Our system size was much larger than in Takayasu and Tretyakov simulations and we approached much closer to the critical point. One can see (Fig. 11) that although around $p=0.8$ (which was the largest value of p simulated by Takayasu and Tretyakov) the density seems to decay linearly, it has a pronounced bending close to the transition point. To obtain more

accurate estimation of the critical point we examined the time dependence of $\rho(t)$ (see Fig. 12). From these analyses we obtain the following estimation of the critical point $p_c = 0.8237(5)$. One can also see that at criticality $\rho(t)$ has a power-law decay with the exponent close to the DP value $\delta = 0.451$.

Having the critical point we can estimate exponent β and the corresponding data are shown in Fig. 13. The least-square fit gives $\beta = 0.60(3)$, which is certainly compatible with the DP value 0.584(4).

To summarize this section, our results confirm the field-theory prediction that BARW models without parity conservation belong to the DP universality class.

V. CONCLUSIONS

In the present paper we examined d-dimensional nonequilibrium models with q absorbing states. As our main result we obtained the diagram shown in Fig. 10. Interestingly, this diagram bears some similarity to the diagram of equilibrium Potts model. In addition, we clarified the nature of the phase transition in the $d=2$ BARW model without parity conservation. Together with the work of Szabó and Santos [15] for the parity-conserving case, it confirms predictions of the field theory for $d=2$ BARW models by Cardy and Täuber [9].

Although it requires considerable numerical efforts, it would be desirable to clarify the behavior of the $d=q=2$ model. Our results are inconclusive in this case, but a possibility that an interesting critical behavior could be found should motivate further study.

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