Critical behavior of the two-dimensional $2A \to 3A$, $4A \to \varnothing$ binary system

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(Received 1 April 2004; published 31 August 2004)

The phase transitions of the recently introduced $2A \to 3A$, $4A \to \varnothing$ reaction-diffusion model [G.Ódor, Phys. Rev. E **69**, 036112 (2004)] are explored in two dimensions. This model exhibits site-occupation restriction and explicit diffusion of isolated particles. A reentrant phase diagram in the diffusion-creation rate space is confirmed, in agreement with cluster mean-field and one-dimensional results. For strong diffusion, a mean-field transition can be observed at zero branching rate characterized by an $\alpha = 1/3$ density decay exponent. In contrast, for weak diffusion the effective $2A \to 3A \to 4A \to \varnothing$ reaction becomes relevant and the mean-field transition of the $2A \to 3A$, $2A \to \varnothing$ model characterized by $\alpha = 1/2$ also appears for nonzero branching rates.

DOI: 10.1103/PhysRevE.70.026119 PACS number(s): 05.70.Ln, 05.70.Fh, 05.70.Jk, 82.20.Wt

I. INTRODUCTION

The classification of universality classes of nonequilibrium systems is one of the most important tasks of statistical physics [1,2]. Many of the known systems can be mapped onto some reaction-diffusion-type models, the behavior of which has been studied intensively in the past decades [3,4]. In these systems, particle (A) creation, annihilation, and diffusion processes compete, and by tuning the control parameters, phase transition may occur from an active steady state to an inactive, absorbing state of zero density. For a long time, only the critical "directed percolation" (DP) type of universality class has been known [5]. Later, other classes were discovered related to certain conservation laws or symmetries [6–9], to long-range interactions [10–12], to boundary conditions [13–16], or to disorder [17–21]. These findings are all in agreement with the concepts of universality in equilibrium systems.

An extraordinary family of models has triggered a long debate among specialists recently [22–42]. The common behavior of these models is that for particle production and annihilation, at least two particles are needed (henceforth they are called binary systems) and these reactions compete with the diffusion of isolated particles. Since for reactions at least one pair is needed while isolated particles can diffuse, only these models can also be regarded as coupled systems [27]. The representative of this class is the so-called diffusive pair contact process (PCPD) with reactions $2A \to 3A$, $2A \to \varnothing$ [24]. The binary nature was also found to be relevant in the case of reactions of multispecies [33].

The critical behavior of such models has been found to be different from all previously known classes (however, there is still an ongoing debate on the precise values of critical exponents). The lack of symmetries, conservation laws, etc., have been motivating skepticism about the existence of a non-DP class transition, and recently some studies suggested DP class behavior with extremely strong correction to scalings [44–46]. Field-theoretical analysis [23], on the other hand, indicates that the absence of the mass term corresponding to the direct channel to the absorbing state $(A \to \varnothing)$ should be responsible for this "anomalous" behavior with respect to expectations based on equilibrium statistical physics. There is another important difference between binary systems and DP: there is no rapidity symmetry,

$$\phi(x,t) \to -\psi(x,-t), \quad \psi(x,t) \to -\phi(x,-t) \tag{1}$$

between the field (ϕ) and the response field (ψ) variables in the corresponding field-theoretical description, contrary the case of the DP process. Furthermore, the lack of this relation is not a consequence of a symmetry breaking field of some boundary [like the $t=0$ boundary with a long-ranged correlated order parameter field in the case of the pair contact process (PCP) [16]] or some disorder, but it is not there in the definition of these homogeneous, binary systems.[1]

Another odd feature is that bosonic (site-unrestricted) and site-restricted versions of these models show completely different behavior. While site-restricted models investigated numerically exhibit the above continuous phase transition, the bosonic versions do not have steady state, but above an abrupt transition, the density of particles diverges quickly [23,43]. The field-theoretical renormalization-group (RG) analysis [23] predicts an upper critical dimension $d_c = 2$, with logarithmic corrections at $d=2$ for this class (PCPD). Simulations [32] have confirmed the mean-field scaling in two dimension in the case of the $2A \to 4A$, $2A \to \varnothing$ binary production model.

The site mean-field solution of general

$$nA \xrightarrow{\sigma} (n+k)A, \quad mA \xrightarrow{\lambda} (m-l)A \tag{2}$$

models (with $n>1$, $m>1$, $k>0$, $l>0$, and $m-l \geqslant 0$) resulted in a series of different universality classes *depending on n and m* [47]. This shows that above d_c, *n and m are relevant parameters* determining the type of continuous phase transitions. In particular, for the $n=m$ symmetrical case the density of particles above the critical point $(\sigma_c > 0)$ scales as

$$\rho \propto |\sigma - \sigma_c|^{\beta}, \tag{3}$$

with $\beta^{MF} = 1$, while at the critical point it decays as

[1]Noh *et al.* claim in their generalized PCPD model, a long-range memory is generated by the diffusing isolated particles [41].

$$\rho \propto t^{-\alpha}, \tag{4}$$

with $\alpha^{MF}=\beta^{MF}/\nu_{\|}^{MF}=1/n$ [38,39] (here MF denotes mean-field value). On the other hand, for the $n<m$ asymmetric case, continuous phase transitions at zero branching rate $\sigma_c=0$ occur with

$$\beta^{MF}=1/(m-n), \quad \alpha^{MF}=1/(m-1). \tag{5}$$

For $n>m$, the mean-field solution provides a first-order transition.

By going beyond site mean-field approximations, it turns out that the above classification is not completely satisfying. In a previous paper [40], I investigated the $2A\to3A$, $4A\to\varnothing$ model by cluster mean-field approximations and simulations in 1D and showed that the *diffusion* plays an important role: it introduces a different critical point besides the one at the $\sigma=0$ branching rate with Eq. (5) exponents. The nontrivial critical point, obtained for low diffusion rate, exhibits the universal behavior of the $2A\to3A$, $2A\to\varnothing$ (PCPD) model owing to the generation of the effective $2A\to\varnothing$ reaction via $2A\to3A\to4A\to\varnothing$ [48].

In this work, I continue the study of this model in two dimension (2D) and show that a similar phase-transition structure and critical behavior can be obtained. This is somewhat surprising, since one may expect that the diffusion is less relevant in higher dimensions due to its short interaction range. A very recent study using exact methods [49] showed that the particle density fluctuation and density correlation function are diffusion-dependent in the bosonic PCPD model for $d>2$. In this work, I give numerical evidence for diffusion dependence in a site-restricted, binary model in $d=2$.

II. THE $2A\to3A$, $4A\to\varnothing$ MODEL

This binary production reaction-diffusion model is defined by the following rules:

$$2A\to3A \quad \text{with rate } \sigma,$$

$$4A\to\varnothing \quad \text{with rate } \lambda=1-\sigma,$$

$$A\varnothing\leftrightarrow\varnothing A \quad \text{with rate } D. \tag{6}$$

Here D denotes the diffusion probability and σ is the production probability of the particles. The site occupancy is restricted to 0 or 1 particle. In [40], the cluster mean-field approximations were determined on 1D lattices for $N=1,2,\ldots,5$ cluster sizes. The corresponding reentrant phase diagram is shown in Fig. 1. Although cluster mean-field approximations based on $d>1$ lattices may result in transition points at other locations, the universal features are expected to be the same. Therefore, I compare the simulation results with this approximation.

A. Simulation results

I performed simulations in two dimensions in $L=(1-7)\times10^3$ linear-sized systems with periodic boundary conditions. The simulations were started from fully occupied lattices. One elementary Monte Carlo step consists of the following processes. A particle and a number $x_1\in(0,1)$ are selected randomly; if $x_1<D$, a site exchange is attempted with one of the randomly selected empty nearest neighbors (NN). The time is updated by $1/n$, where n is the total number of particles. A particle and a number $x_2\in(0,1)$ are selected randomly. If $x_2<\sigma$ and if the number of NN particles is- 1 or 2 or 3, one new particle is created at an empty site selected randomly. If $x_2\geq\sigma$ and the number of NN particles is greater than 2, four randomly selected neighboring particles are removed. The time (t) is updated by $1/n$ again. The density of particles was followed up to $t_{max}\leq10^7$ Monte Carlo steps [throughout the whole paper, the time is measured by Monte Carlo steps (MCS)].

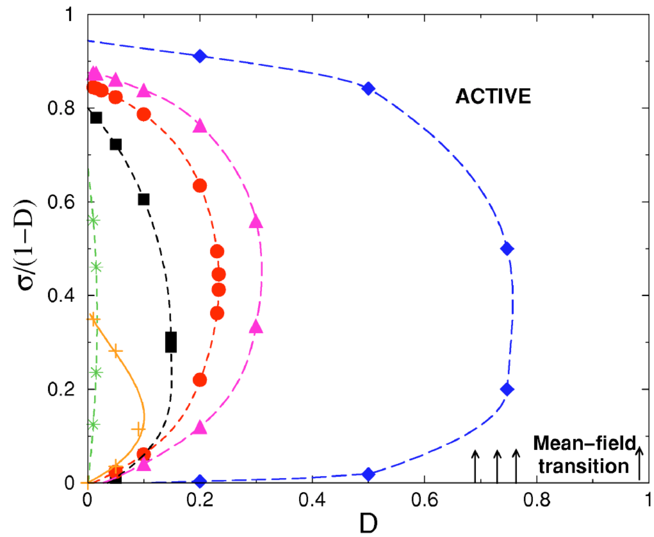

FIG. 1. Phase diagram of the $2A\to3A\to4A\to\varnothing$ model. Stars correspond to $N=2$, boxes to $N=3$, bullets to $N=4$, and triangles to $N=5$ cluster mean-field approximations. Diamonds denote 1D; + signs denote 2D simulation data, where PCPD class transitions are found. The lines serve to guide the eye. At the $\sigma=0$ line, asymmetric, Eq. (5) type mean-field transition occurs.

As one can see in Fig. 2, simulation data and the five-point approximations fit qualitatively well. In both cases, for weak diffusion rates (for $D\lesssim0.1$ in 2D simulations) reentrant phase transitions occur with $\sigma_c>0$, while for strong diffusions a single phase transition at $\sigma_c=0$ branching rate can be found. The transition lines of the cluster mean-field approximations do not converge towards the simulation line as in 1D (see Fig. 1), but the 2D MC curve occurs at lower diffusions. But this is not surprising, since the cluster mean-field calculations are performed on 1D lattices.

I explored the scaling behavior in more detail at $D=0.05$ diffusion near the rightmost transition of Fig. 2 (at $\sigma\sim0.27$). By approaching σ_c from the active phase, the $\rho(t)t^{1/2}$ curves bend down rapidly for long times (beyond $\sim10^6$ MCS). However, this proved to be a finite-size effect: the breakdown of the density curves can be eliminated by increasing L. The largest system I could simulate had a linear size $L=7000$. In this case, no rapid and premature curvatures were observed for $t<2\times10^6$ MCS. As one can see in Fig. 3, for $\sigma>0.2673$ all curves veer up, while for $\sigma<0.2673$ they veer down. A clear straight line—indicating scaling with the

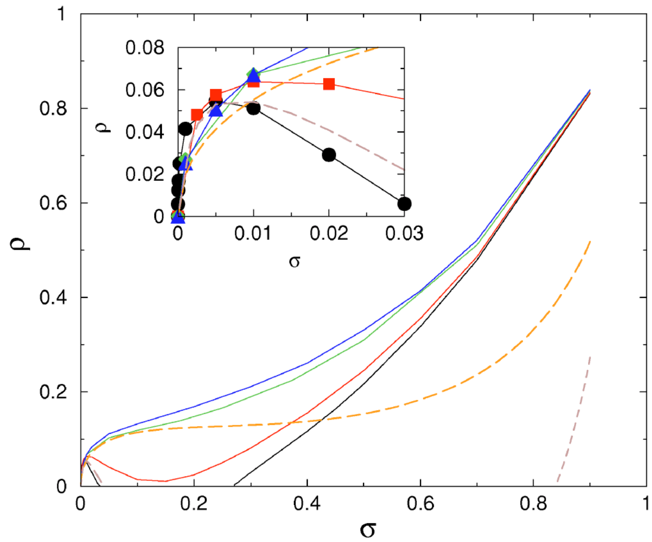

FIG. 2. Simulation results for the steady-state density at diffusions $D=0.5$, 0.35, 0.1, 0.05 (solid lines from top to bottom) and $N=5$ level cluster mean-field approximation data for $D=0.5$, 0.05 (dashed lines from top to bottom). The inset shows the region near $\sigma=0$ magnified.

expected logarithmic correction—cannot be seen clearly. Even the $\sigma=0.2673$ curve shows some up and down curvatures in the last decade of the simulations. However, as can be seen on the local slopes figure (see the inset of Fig. 3) defined as

$$\alpha_{\text{eff}}(t) = \frac{-\ln[\rho(t)/\rho(t/m)]}{\ln(m)}, \tag{7}$$

(where I used $m=2$), the transition is around the expected mean-field value of the PCPD class: $\alpha=0.5$ [23,47]. Other

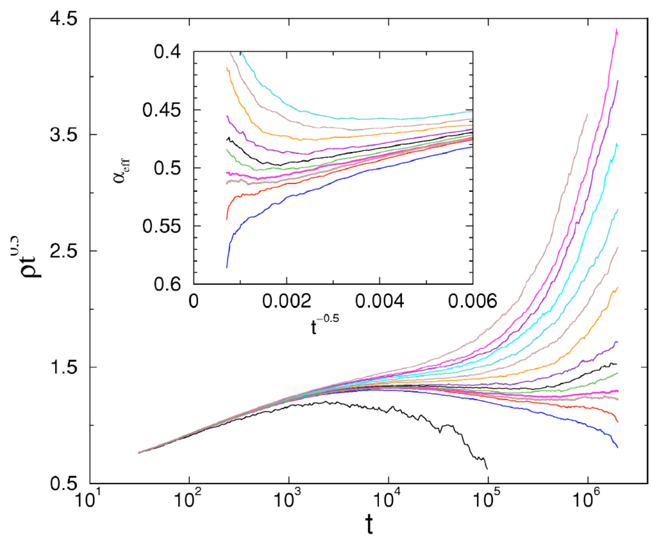

FIG. 3. Density decay times $t^{0.5}$ in the two-dimensional $2A \to 3A$, $4A \to \emptyset$ model at $D=0.05$. Different curves correspond to $\sigma=0.2715$, 0.2708, 0.2704, 0.27, 0.2695, 0.269, 0.2685, 0.268, 0.2677, 0.2675, 0.2673, 0.26715, 0.267, 0.2665, and 0.26 (top to bottom). The inset shows the corresponding local slopes.

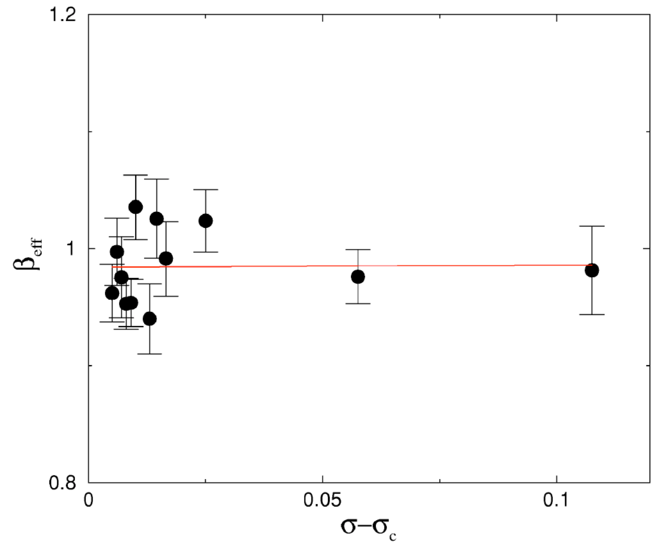

FIG. 4. β_{eff} as the function of $\sigma-\sigma_c$ in the two-dimensional $2A \to 3A$, $4A \to \emptyset$ model near the $\sigma_c=0.2673$ critical point for $D=0.05$. The solid line shows a linear fitting.

curves exhibit strong curvatures for long times, i.e., for $\sigma > 0.2673$ they veer up (active phase), while for $\sigma < 0.2673$ they veer down (absorbing phase).

The steady-state density in the active phase near the critical phase transition point is expected to scale as $\rho(\infty) \propto |\sigma-\sigma_c|^{\beta}$. Using the local slopes method, one can get a precise estimate for β and see the corrections to scaling,

$$\beta_{\text{eff}}(p_i) = \frac{\ln \rho(\infty,\sigma_i) - \ln \rho(\infty,\sigma_{i-1})}{\ln(\sigma_i) - \ln(\sigma_{i-1})}. \tag{8}$$

The steady-state behavior at the $\sigma_c > 0$ transition for $D=0.05$ was investigated using $\sigma_c=0.2673(2)$ from the density decay analysis. Here the local slopes tend to $\beta_{\text{eff}}=0.98(2)$ without showing any relevant correction to scaling (see Fig. 4). This agrees with the mean-field value of the PCPD model again [23,47].

One may expect the same kind of transition all along the $\sigma_c > 0$ transition line. Indeed, simulations showed that the density decays in a similar way at transitions with $D=0.01$, 0.05, and 0.09.

To see the transition near $\sigma_c=0$ (horizontal axis in Fig. 1), I determined the steady-state value of $\rho(\infty,\sigma)$ for several σ's at $D=0.05$ diffusion. The steady-state density was determined by running the simulations in the active phase near $\sigma=0$, by averaging over ~ 100 samples in a time window following the level off that is achieved. The smallest value I tested was $\sigma=10^{-5}$, when I had to go up to $t=10^7$ MCS to reach a steady state (on an $L=2000$-sized system). By looking at the data, it is quite obvious that the transition is at $\sigma_c=0$, as the cluster mean-field approximations predicted.

The effective order-parameter exponent (Fig. 5) tends to $\beta=0.505(5)$ as $\sigma \to 0$, corroborating the cluster mean-field prediction: Eq. (5). Assuming a correction to scaling of the form

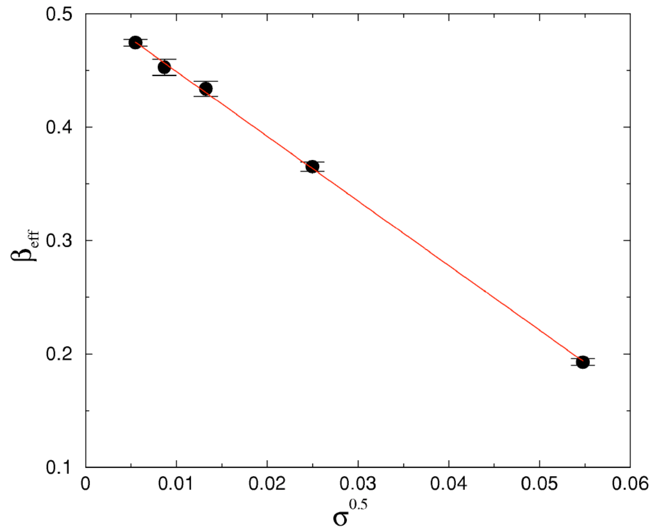

FIG. 5. β_{eff} as the function of $\sigma^{0.5}$ in the two-dimensional $2A \rightarrow 3A$, $4A \rightarrow \varnothing$ model near the $\sigma_c=0$ phase transition at $D=0.05$. The solid line shows a linear fitting.

$$\beta_{\mathrm{eff}} = \beta - a t^{-\beta_1}, \tag{9}$$

fitting results in $\beta_1=0.5$ as can be read off from Fig. 5.

III. CONCLUSIONS

In conclusion, I have investigated the (D-σ) phase diagram of the two-dimensional $2A \rightarrow 3A$, $4A \rightarrow \varnothing$ model with site restriction and explicit particle diffusion. Extensive simulations gave numerical evidence that a reentrant phase diagram emerges as in one dimension and predicted by cluster mean-field approximations [40]. This somewhat surprising result means that diffusion plays a relevant role even in $d=2$ dimension. For high diffusion rates, only a mean-field transition at $\sigma=0$ branching rate can be found, while for low diffusion another transition type at $\sigma_c > 0$ appears. This latter transition shows the mean-field characteristics of the PCPD model because the effective $2A \rightarrow \varnothing$ reaction (via $2A \rightarrow 3A \rightarrow 4A \rightarrow \varnothing$) becomes relevant. The understanding of this diffusion dependence is a challenge for field theory. Existing perturbative field theory does not predict such behavior.

A similar reentrant phase diagram has been observed in the case of a unary production, triplet annihilation model, $A \rightarrow 2A$, $3A \rightarrow \varnothing$ [50]; in a quadruplet model, $A \rightarrow 2A$, $4A \rightarrow \varnothing$ [51]; and in a variant of the NEKIM model [52]. In all cases, the diffusion competes with particle reaction processes, and the bare parameters should somehow form renormalized reaction rates which govern the evolution over long times and distances. An interesting question is whether this scenario extends above $d=2$ dimensions as the cluster mean-field approximation predicts. Two very recent nonperturbative RG studies [53,54] find a similar phase diagram in the case of the $A \rightarrow 2A$, $2A \rightarrow \varnothing$ model for $d \geqslant 3$ dimensions. These works point out that nonperturbative effects arise and there is a threshold $(\lambda / D)_{\mathrm{th}}(d)$ above which DP occurs, while below it a type (5) mean-field transition at $\sigma_c=0$ appears.

The simulations also showed that at the $\sigma_c > 0$ transition, the finite-size effects and corrections to scaling are very strong. I had to go up to (7000×7000)-sized systems and $t_{\max}=2 \times 10^6$ MCS to see the appearance of the expected mean-field scaling with exponents $\alpha=0.5$, $\beta=1$. Showing clear scaling for more than a decade with the predicted logarithmic corrections [23] is beyond the scope of this study, yet these simulation results for a 2D binary system are by far the largest scale published so far. On the contrary, the scaling at the $\sigma_c=0$ critical point is clear with $\beta=0.505(5)$ and correction to the scaling exponent $\beta_1=0.5$.

ACKNOWLEDGMENTS

The author thanks M. Henkel, I. Georgiev, and U. Täuber for useful comments. Support from the Hungarian research fund OTKA (Grant No. T-046129) is acknowledged. Access to the NIIFI Cluster-GRID, LCG-GRID, and to the Supercomputer Center of Hungary is acknowledged with appreciation.

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