Phase transitions of the binary production $2A\rightarrow 3A$, $4A\rightarrow\emptyset$ model

Géza Ódor
Research Institute for Technical Physics and Materials Science, P.O. Box 49, H-1525 Budapest, Hungary
(Received 23 July 2003; published 23 March 2004)

Phase transitions of the $2A\rightarrow 3A$, $4A\rightarrow\emptyset$ reaction-diffusion model is explored by dynamical, N-cluster approximations and by simulations. The model exhibits site occupation restriction and explicit diffusion of isolated particles. While the site mean-field approximation shows a single transition at zero branching rate introduced by Ódor [G. Ódor, Phys. Rev. E **67**, 056114 (2003)], $N>2$ cluster approximations predict the appearance of another transition line for weak diffusion (D) as well. The latter phase transition is continuous, occurs at finite branching rate, and exhibits different scaling behavior. I show that the universal behavior of these transitions is in agreement with that of the difffusive pair contact process model both on the mean-field level and in one dimension. Therefore this model exhibiting annihilation by quadruplets does not fit in the recently suggested classification of universality classes of absorbing state transitions in one dimension [J. Kockelkoren and H. Chaté, Phys. Rev. Lett. **90**, 125701 (2003)]. For high diffusion rates the effective $2A\rightarrow 3A\rightarrow 4A\rightarrow\emptyset$ reaction becomes irrelevant and the model exhibits a mean-field transition only. The two regions are separated by a nontrivial critical end point at D^*.

DOI: 10.1103/PhysRevE.69.036112 PACS number(s): 05.70.Ln, 05.70.Fh, 05.70.Jk, 82.20.Wt

Phase transitions in nonequilibrium systems, which do not possess Hermitian Hamiltonian may appear in models of population, epidemics, catalysis, cooperative transport [1], enzyme biology [2], and markets [3], for example. Reaction-diffusion systems are of primary interest since other nonequilibrium models often can be mapped onto them [4]. The classification of universality classes in reaction-diffusion systems [5,6] has recently got some impetus. In these systems particle 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. The fluctuations in the absorbing state are so small, so that systems cannot escape from it, hence such phase transitions may emerge in one dimension already. Several systems with binary, triplet, or quadruplet particle reactions have been investigated numerically and unclassified type of critical phase transitions were found [7–27]. Solid field theoretical treatment exists for bosonic, binary production systems only [26], but this is not applicable for the active and critical states of site restricted models, since it cannot describe a steady state with finite density.

The mean-field solution of general models,

$$nA\xrightarrow{\sigma}(n+k)A,\quad mA\xrightarrow{\lambda}(m-l)A \tag{1}$$

(with $n>1$, $m>1$, $k>0$, $l>0$, and $m-l\geqslant 0$) resulted in a series of universality classes depending on n and m [24]. In particular for the $n=m$ symmetrical case the density of particles above the critical point ($\sigma_c>0$) scales as

$$\rho\propto|\sigma-\sigma_c|^{\beta}, \tag{2}$$

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

$$\rho\propto t^{-\alpha}, \tag{3}$$

with $\alpha^{MF}=\beta^{MF}/\nu_{||}^{MF}=1/n$ [23,24] (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

$$\beta^{MF}=1/(m-n),\quad \alpha^{MF}=1/(m-1). \tag{4}$$

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

The upper critical dimension for such systems is debated [6,21,23,24] but should be quite low ($d_c=1-2$) allowing a few anomalous critical transitions only. For example, $d_c<1$ was confirmed by simulations in case of the asymmetric, binary production $2A\rightarrow 4A$, $4A\rightarrow 2A$ model [25]. It was also pointed out there that $N>1$ cluster mean-field approximation, which takes into account the diffusion of particles, would provide a more adequate description of such models. Earlier studies have shown [28–30] that there exist models with first-order transitions in the site mean-field approximation that changes to continuous one in higher level of cluster approximations. Dependence on the diffusion was found to be important in binary production models [8,10] and it turned out that at least $N>2$ level of approximation is needed for an adequate description [17,20].

In this paper I investigate the $2A\rightarrow 3A$, $4A\rightarrow\emptyset$ model and show that the diffusion plays an important role: it introduces a different critical point besides the one at $\sigma=0$ branching rate. I show by simulations that this transition is not mean-field type in one dimension but belongs to the class of the $2A\rightarrow 3A$, $2A\rightarrow\emptyset$ so-called diffusive pair contact process (PCPD) model. The model described here is defined and parametrized following the notation of Ref. [8] by the rules

$$AA\emptyset,\emptyset AA\rightarrow AAA \quad \text{with rate} \quad \sigma=(1-p)(1-D)/2,$$

$$AAAA\rightarrow\emptyset\emptyset\emptyset\emptyset \quad \text{with rate} \quad \lambda=p(1-D),$$

$$A\emptyset\leftrightarrow\emptyset A \quad \text{with rate} \quad D. \tag{5}$$

Here D denotes the diffusion probability and p is the other control parameter of the system.

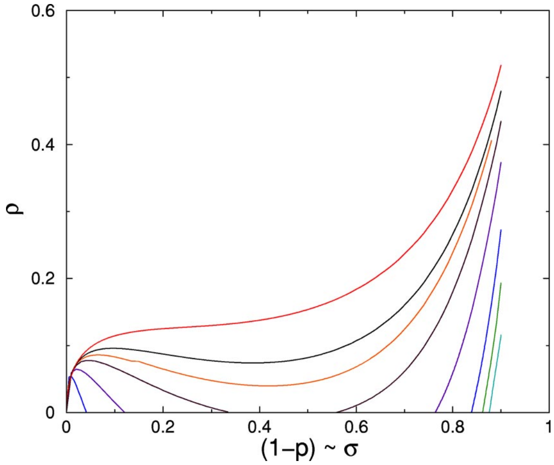

FIG. 1. Steady state density in $N=5$ level approximation for diffusion rates $D=0.5$, 0.4, 0.35, 0.3, 0.2, 0.1, 0.05, 0.01, 0.01 (top to bottom curves). A similar scenario appears for $N=2,3,4$.

Dynamical cluster mean-field approximations have been introduced for nonequilibrium models by Refs. [31,32]. The master equations for $N=1,2,3,4,5$ block probabilities were set up:

$$\frac{\partial P_N(\{s_i\})}{\partial t}=f(P_N(\{s_i\})), \tag{6}$$

where site variables may take values $s_i=\emptyset,A$. Taking into account spatial reflection symmetries of $P_N(\{s_i\})$ this involves 20 independent variables in case of $N=5$. The master equation (6) was solved numerically using the Runge-Kutta algorithm for $N=2,3,4,5$ by several D and p values. The particle $(\rho(p,D))$ and pair $(\rho_2(p,D))$ densities were determined by $P_N(\{s_i\})$. For strong diffusion rates only a mean-field phase transition occurs at $\sigma=0$ with $\beta=1/2$ and $\alpha=1/3$ exponents belonging to the set of classes (4) discovered in Ref. [24].

However for $N>1$ and weak diffusion rates other phase transitions points emerge as well, with $\sigma_c>0$. This means that for intermediate σ and small D values the absorbing state becomes stable, as one can see in Fig. 1. Simulations in one dimension confirm this (see later).

In the active phases in the neighborhood of the $\sigma_c>0$ transition points, power-law fitting of the form (2) to the mean-field data point resulted in $\beta=1$ for all $N>1$ levels of approximations. On the other hand for the pair density in pair approximations one obtains $\beta=1$ again, such as in the case of the PCPD model for low diffusions [8]. This anomaly disappears for $N=3,4,5$ and the fitting results in $\beta=2$ for pairs.

At the $\sigma_c>0$ critical points the dynamical behavior is power-law type (3) with $\alpha=1/2$ for $N=3,4,5$. Again the pair approximation gives the strange result: $\alpha=1$ (such as in Ref. [8]). The failure of the pair approximation also appears in the inactive region, where it results in exponential density decay. In contrast with this the $N=3,4,5$ approximations show power laws here with $\alpha=1$ for particles and $\alpha=2$ for pairs. The above α and β exponents occurring by low diffusions at the critical points and inactive phases in the phase diagram away from the $\sigma=0$ transition are different from those of the site mean-field values (4). This can be explained by accepting that the dominant decay process for $\sigma>0$, $D<D^*$, is $2A\to\emptyset$ (via $2A\to3A\to4A\to\emptyset$) instead of the $4A\to\emptyset$—which is the only mode of decay at $\sigma=0$. Altogether one can find very similar cluster mean-field behavior as in case of the PCPD model [8,20].

One can also observe that by increasing D from zero the PCPD-like transitions disappear at some D^* value when the $\rho(\infty)$ steady state curve touches the $\rho=0$ axis. For $D\geqslant D^*$ there is no absorbing state in the system and a critical end point appears with $\beta=2$ (parabolic) singularity at σ_c^*. For $N=5$ the end point is located at $D^*=0.301(1)$, $p_c^*=0.53(1)$.

To test these analytical findings I have performed simulations in one dimension. These were carried out on $L=(1-5)\times10^5$ sized systems with periodic boundary conditions. The initial states were half-filled lattices with randomly distributed A's and the density of particles is followed up to 5×10^8 Monte Carlo steps (MCS's). One MCS consists of the following processes. A particle, a direction, and a number $x\in(0,1)$ are selected randomly; if $x<D$, a site exchange is attempted with one of the randomly selected empty nearest neighbors; else if $D\leqslant x<(D+\lambda)$, four neighboring particles are removed; else one particle is created at an empty site in the randomly selected direction following a pair of A's. In each MCS the time is updated by $1/n$, where n is the number of particles.

First I followed the density of particles for a small σ (at $p=0.95$) at diffusion rates $D=0.5$ and $D=0.2$. In both cases a power-law decay with $\alpha=0.5$ exponent could be observed, hence an inactive phase with decay of the $AA\to\emptyset$ process—valid in one dimension [34]—was identified.

The critical points were determined by calculating the local slopes defined as

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

(where I used $m=2$) for $D=0.2,0.5,0.747$. As Fig. 2 shows the local slopes curve for $D=0.5$, $p=0.15850(2)$ extrapolates to $\alpha=0.21(1)$. This value agrees with that of the PCPD model [20,21]. Other curves exhibit curvature for long times, i.e., for $p<0.1585$ they veer up (active phase), while for $p>0.1585$ they veer down (absorbing phase). The local slopes figure shows similar strong correction to scaling as in case of the PCPD model, i.e., some curves that seem to be supercritical veer down after $t>\sim10^6$ MCS's. Similar results are obtained by other $\sigma_c>0$ transitions. For $D=0.2$, when the critical point is at $p=0.0892(1)$, the local slopes for the density decay predicts $\alpha=0.21(2)$. Repeating the simulations at $D=0.9$ no absorbing phase has been found (up to $p\leqslant0.9999$), the steady state density disappears monotonously as $\sigma\to0$. At $\sigma=0$ the density decays with $\alpha=1/3$ valid for the $4A\to\emptyset$ process in one dimension [35].

The steady state density in the active phase near the critical phase transition point is expected to scale as $\rho(\infty)\propto|p$

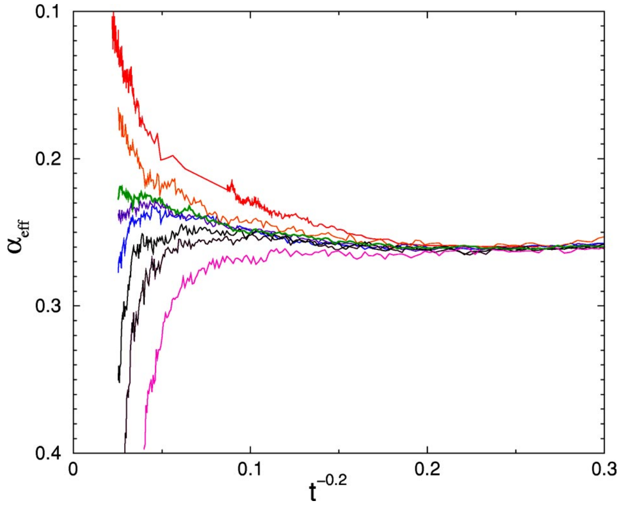

FIG. 2. α_{eff} in the one-dimensional $3A\to4A$, $4A\to\emptyset$ model at $D=0.5$. Different curves correspond to $p=0.1583$, 0.1584, 0.1585, 0.15852, 0.15853, 0.1586, 0.1587, 0.159 (top to bottom).

$-p_c|^{\beta}$. Using the local slopes method one can get a precise estimate for β and see the corrections to scaling:

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

The steady state density was determined by running the simulations in the active phase: $\epsilon=p_c-p_i>0$, by averaging over ~100 samples in a time window following the level-off is achieved. As one can see in Fig. 3 the effective exponent tends to $\beta=0.40(2)$ as $\epsilon\to\emptyset$ both for $D=0.5$ and $D=0.2$ diffusions. These values are in agreement with that of the one-dimensional PCPD model [20,21]. Again assuming logarithmic corrections as in Ref. [20] of the form

$$\rho(\infty,\epsilon)=\{\epsilon/[a+b\ln(\epsilon)]\}^{\beta} \tag{9}$$

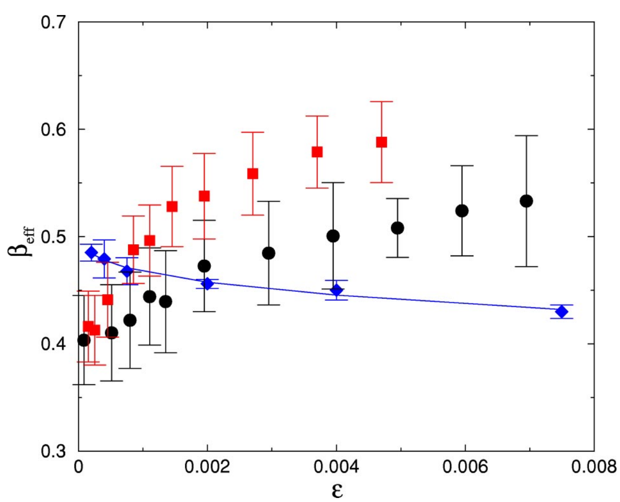

FIG. 3. β_{eff} as the function of ϵ in the one-dimensional $2A\to3A$, $4A\to\emptyset$ model. The bullets correspond to $D=0.5$, and the boxes to $D=0.2$, and the diamonds to $D=0.9$ diffusion rate. The solid line shows a quadratic fitting of the form (10).

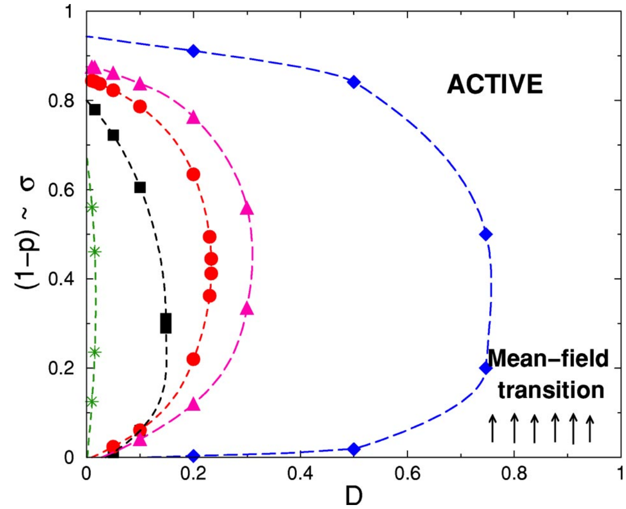

FIG. 4. Phase diagram. Stars correspond to $N=2$, boxes to $N=3$, bullets to $N=4$, and triangles to $N=5$ cluster mean-field approximations. Diamonds denote one-dimensional simulation data. The lines serve to guide the eye. At the $\sigma=0$ line a mean-field transition occurs.

one can obtain $p=0.1585(1)$ and $\beta=0.38(1)$ for $D=0.5$ and $p=0.0892(1)$ and $\beta=0.41(3)$ for $D=0.2$, which agrees with the previous values within numerical accuracy [11,24]. Altogether one cannot see relevant logarithmic corrections for the diffusion rates investigated here.

In case of $D=0.9$, $\sigma_c=0$ one can see $\beta=0.50(1)$ in agreement with the $N=3,4,5$ cluster mean-field approximation results. A quadratic fitting of the form

$$\beta_{eff}=\beta-a\epsilon^{x}-b\epsilon^{2x} \tag{10}$$

results in $a=0.195$, $b=0.158$, $x=0.214$, and $\beta=0.51(1)$. This suggests that the effective $2A\to\emptyset$ process is weaker now than the $2A\to3A$, leaving the transition at $\sigma_c=0$. The phase diagram for different levels of approximations as well as MC data are shown in Fig. 4. As one can see approximations tend towards the simulated points by increasing N.

Similar reentrant phase diagram has been observed in case of the unary production, triplet annihilation model ($A\to2A,3A\to\emptyset$) [36], and in a variant of the NEKIM model [37]. 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, the details have not been worked out.

Finite size scaling investigations at $D=0.5$ and $p_c=0.1585$ were performed for system sizes: $L_i=32,64,128,\ldots,4096$. The quasi-steady-state density (averaged over surviving samples) is expected to scale according to

$$\rho_s(\infty,p_c,L)\propto L^{-\beta/\nu_\perp}, \tag{11}$$

while the characteristic lifetime for half of the samples to reach the absorbing state scales with the dynamical exponent Z as

$$\tau(p_c,L)\propto L^Z. \tag{12}$$

These quantities were analyzed by the local slopes:

$$Z_{eff}(L)=\frac{\ln\tau(L_i)-\ln\tau(L_{i-1})}{\ln L_i-\ln L_{i-1}}, \tag{13}$$

$$\beta/\nu_\perp(L)=\frac{\ln\rho_s(L_i)-\ln\rho_s(L_{i-1})}{\ln L_i-\ln L_{i-1}}. \tag{14}$$

Linear extrapolation to $L\to\infty$ results in $Z=1.80(15)$ and $\beta/\nu_\perp=0.40(3)$. These values corroborate that the transition is of PCPD type.

In conclusion, the N cluster mean-field study of the binary production $2A\to3A$, $4A\to\emptyset$ model has shown the appearance of another critical transition with nonzero production rate for low diffusions. While the pair approximation results in somewhat odd results—such as in the case of other binary production systems [33]—the $N=3,4,5$ levels coherently exhibit PCPD-like mean-field critical behavior for these phase transition points and within the absorbing phase. This transition line disappears at a critical end point for $D\geqslant D^*$ characterized by $\beta=2$ order parameter singularity, and for high diffusion rates the $\sigma_c=0$ critical point remains only in the system, predicted by the site mean-field approximation. The utmost importance of diffusion dependence and the corresponding $N>2$ cluster mean-field approximations is demonstrated in this study.

Extensive simulations in one dimension have confirmed the existence of the nontrivial transition for low diffusions. By these transition points the critical behavior agrees with that of the latest results obtained for the PCPD model. Therefore this model does not fit in the table of universality classes suggested for such models in one dimension [21]. The reason behind this discrepancy might be that in Ref. [21] low diffusions have not been investigated or there is a lack of complete site exclusion in their model. Site exclusion has been shown to be relevant in multispecies reaction-diffusion systems and in binary production systems [38].

An interesting, open problem is the exploration of the phase structure of this system in higher dimensions. The agreement of one-dimensional results with those of the cluster mean field shows that similar rich phase structure may emerge in higher dimensions, too. That would mean that the effective $2A\to\emptyset$ reaction is generated via $2A\to3A\to4A\to\emptyset$ again. These results raise the possibility that such a mechanism also emerges by unary production systems (for example, by $A\to2A$, $4A\to\emptyset$) and one should find a directed percolation [7] transition instead of the mean-field one suggested by perturbative renormalization study [35] of such models. This would affect the classification of fundamental universality classes of RD systems and may point out the weak points of the perturbative renormalization. Another important point to be investigated is the scaling behavior at the critical end point.

The author thanks F. Iglói, G. Szabó, and U. Täuber for their useful comments. Support from the Hungarian research fund OTKA (Grant No. T-25286) is acknowledged. The author thanks the access to the NIIFI Cluster-GRID and to the Supercomputer Center of Hungary.

[1] For references see J. Marro and R. Dickman, *Nonequilibrium Phase Transitions in Lattice Models* (Cambridge University Press, Cambridge, 1999).
[2] H. Berry, Phys. Rev. E **67**, 031907 (2003).
[3] J.-P. Bouchaud and A. Georges, Phys. Rep. **195**, 127 (1990).
[4] H. Hinrichsen, Adv. Phys. **49**, 815 (2000).
[5] G. Ódor, Rev. Mod. Phys (to be published), e-print cond-mat/0205644.
[6] U. Täuber, Adv. Solid State Phys. **43**, 659 (2003).
[7] P. Grassberger, Z. Phys. B: Condens. Matter **47**, 365 (1982).
[8] E. Carlon, M. Henkel, and U. Schollwöck, Phys. Rev. E **63**, 036101 (2001).
[9] H. Hinrichsen, Phys. Rev. E **63**, 036102 (2001).
[10] G. Ódor, Phys. Rev. E **62**, R3027 (2000).
[11] H. Hinrichsen, Physica A **291**, 275 (2001).
[12] G. Ódor, Phys. Rev. E **63**, 067104 (2001).
[13] J.D. Noh and H. Park, Phys. Rev. E **69**, 016122 (2004).
[14] M. Henkel and U. Schollwöck, J. Phys. A **34**, 3333 (2001).
[15] M. Henkel and H. Hinrichsen, J. Phys. A **34**, 1561 (2001).
[16] K. Park, H. Hinrichsen, and In-mook Kim, Phys. Rev. E **63**, 065103(R) (2001).
[17] G. Ódor, M.A. Santos, and M.C. Marques, Phys. Rev. E **65**, 056113 (2002).
[18] G. Ódor, Phys. Rev. E **65**, 026121 (2002).
[19] K. Park and I. Kim, Phys. Rev. E **66**, 027106 (2002).
[20] G. Ódor, Phys. Rev. E **67**, 016111 (2003).
[21] J. Kockelkoren and H. Chaté, Phys. Rev. Lett. **90**, 125701 (2003).
[22] R. Dickman and M.A.F. de Menenzes, Phys. Rev. E **66**, 045101 (2002).
[23] K. Park, H. Hinrichsen, and I. Kim, Phys. Rev. E **66**, 025101 (2002).
[24] G. Ódor, Phys. Rev. E **67**, 056114 (2003).
[25] G. Ódor, Braz. J. Phys. **33**, 431 (2003).
[26] M.J. Howard and U.C. Täuber, J. Phys. A **30**, 7721 (1997).
[27] G. Ódor, Phys. Rev. E **65**, 026121 (2002).
[28] G. Ódor, N. Boccara, and G. Szabó, Phys. Rev. E **48**, 3168 (1993).
[29] G. Ódor and A. Szolnoki, Phys. Rev. E **53**, 2231 (1996).
[30] N. Menyhárd and G. Ódor, J. Phys. A **28**, 4505 (1995).
[31] H.A. Gutowitz, J.D. Victor, and B.W. Knight, Physica D **28**, 18 (1987).
[32] R. Dickman, Phys. Rev. A **38**, 2588 (1988).
[33] R. Dickman, W.R.M. Rabelo, and G. Ódor, Phys. Rev. E **65**, 016118 (2001).
[34] B.P. Lee, J. Phys. A **27**, 2633 (1994).
[35] J.L. Cardy and U.C. Täuber, J. Stat. Phys. **90**, 1 (1998).
[36] R. Dickman, Phys. Rev. B **40**, 7005 (1989); Phys. Rev. A **42**, 6985 (1990).
[37] N. Menyhárd and G. Ódor, Phys. Rev. E **68**, 056106 (2003).
[38] G. Ódor and N. Menyhárd, Physica D **168**, 305 (2002).