Role of diffusion in branching and annihilation random walk models

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Different branching and annihilating random walk models are investigated by the cluster mean-field method and simulations in one and two dimensions. In the case of the $A \to 2A$, $2A \to \emptyset$ model the cluster mean-field approximations show diffusion dependence in the phase diagram as was found recently by the nonperturbative renormalization group method [L. Canet *et al.*, Phys. Rev. Lett. **92**, 255703 (2004)]. The same type of survey for the $A \to 2A$, $4A \to \emptyset$ model results in a reentrant phase diagram, similar to that of the $2A \to 3A$, $4A \to \emptyset$ model [G. Ódor, Phys. Rev. E **69**, 036112 (2004)]. Simulations of the $A \to 2A$, $4A \to \emptyset$ model in one and two dimensions confirm the presence of both the directed percolation transitions at finite branching rates and the mean-field transition at zero branching rate. In two dimensions the directed percolation transition disappears for strong diffusion rates. These results disagree with the predictions of the perturbative renormalization group method.

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Phase transitions in nonequilibrium, dynamical systems, which do not satisfy the detailed balance condition, may appear in models of population, epidemics, catalysis, cooperative transport [1], enzyme biology [2], and markets, for example [3]. Many of the known systems can be mapped onto some reaction-diffusion models, the behavior of which has been studied intensively in recent decades [1,4]. In these systems creation, annihilation, and diffusion processes for particle A compete, and by tuning the control parameters a phase transition may occur from an active steady state to an inactive, absorbing state of zero density. The simplest example of such models exhibiting a phase transition are the branching and annihilating random walk (BARW) models, in which offspring are created by a single ancestor, $A \to (n+1)A$, and particles annihilate, $2A \to \emptyset$.

The classification of universality classes of nonequilibrium systems is one of the most important tasks of statistical physics [5,6]. Universal scaling behavior may occur at continuous phase transitions as in equilibrium systems and the corresponding n-point correlations are homogeneous (but anisotropic) functions of space and time. In the past decades analytical and numerical studies have explored a large variety of such classes [6]. One may pose the important question: Which are the relevant factors determining these classes? By inspecting the widespread literature it appears that in addition to the well known factors of homogeneous equilibrium models with short ranged interactions, i.e., spatial dimensions, symmetries, and conservation laws, there are more things that must be taken into account. For example, due to the possibility of transitions in low dimensions topological effects may play an important role [7]. Furthermore, the initial condition—as a boundary in the time direction—can also be relevant [8,9].

The mean-field classes of general,

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

site occupation number restricted models (with $n > 1$, $m > 1$, $k > 0$, $l > 0$, $m - l \geqslant 0$, and the time scale fixed by setting $\lambda + \sigma = 1$) resulted in a series of different universality classes depending on n and m [10]. This means that above the upper critical dimension (d_c) of the transition *n and m are relevant parameters*. In particular, for the $n=m$ symmetrical case the density of particles in the active phase near the critical point ($\sigma_c > 0$) scales as

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

with $\beta = 1$, while at the critical point it decays as

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

with $\alpha = \beta / \nu_{\|} = 1/n$ [10,11]. On the other hand, for the $n < m$ asymmetric case continuous phase transitions at zero branching rate $\sigma_c = 0$ occur characterized by

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

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

By going beyond the site mean-field approximation it turned out that phase diagrams of the type Eq. (1) models may contain other transition points with nontrivial scaling behavior. In previous papers [12,13] I investigated the $2A \to 3A$, $4A \to \emptyset$ model by generalized (cluster) mean-field (GMF) approximations and simulations in one and two dimensions and showed that the *diffusion* plays an important role: it introduces a different critical point in addition to the one obtained by the site mean-field solution at $\sigma_c = 0$ [Eq. (4)]. The nontrivial critical point at $\sigma_c > 0$ appearing at low diffusion rates exhibits the universal behavior of the transition of the $2A \to 3A$, $2A \to \emptyset$ diffusive pair contact process (PCPD) model owing to the generation of the effective $2A \to \emptyset$ reaction via the quick processes $2A \to 3A \to 4A \to \emptyset$ [15].

Very recent studies by Canet *et al.* [16,17] found similar diffusion dependence in the $A \to 2A$, $2A \to \emptyset$ BARW model. Using the nonperturbative renormalization group (NPRG) method they obtained a different phase diagram than what was expected by perturbative renormalization group (RG) arguments [18]; namely, directed percolation (DP) transitions were found in these models for $d>2$ dimensions with $d_c=4$. Furthermore, those transitions at $\sigma_c>0$ branching rate persist up to infinite dimensions provided λ/D is greater than a threshold value. This threshold value was found to be zero for $d<3$ and finite for $d\geqslant 3$.

In this work I apply dynamical, cluster mean-field approximations for the BARW model and by extrapolations to $N\to\infty$ cluster sizes I determine the phase diagram in one dimension (1D). Furthermore I explore the phase transitions of the $A\to 2A$, $4A\to\emptyset$ model with this method and by simulations in one and two dimensions.

The cluster mean-field method applied for nonequilibrium models first in [19,20] is based on the calculation of N-block probabilities of the model. This method has successfully predicted the phase diagram of many systems (see references in [6]). I apply it for one-dimensional, site restricted lattice versions of the models mentioned before. It is well known that such approximations predict the phase structure qualitatively well in 1D provided N is high enough to take into account the relevant interaction terms. For example, $N>1$ is needed to take into account particle diffusion terms, while $N>2$ was found to be necessary in case of binary production processes exhibiting pair production [12]. The GMF method is an efficient phase diagram exploration method and although it was set up for the $d=1$ lattice in previous cases it provided qualitatively good phase diagrams for higher dimensional, mean-field versions, too (see for example [13,14]).

One can set up a master equations for the P_N block probabilities as

$$\frac{\partial P_N(\{s_i\})}{\partial t} = f(P_N(\{s_i\})), \quad (5)$$

where the site variables take the values $s_i=\emptyset, A$. During the solution of these equations one estimates larger than N sized block probabilities by the maximum overlap approximation:

$$P_{N+1}(s_1,\ldots,s_{N+1}) \simeq \frac{P_N(s_1,\ldots,s_N)P_N(s_2,\ldots,s_{N+1})}{P_N(s_2,\ldots,s_N,\emptyset)+P_N(s_2,\ldots,s_N,A)}. \quad (6)$$

Taking into account spatial symmetries, for the maximal $N=8$ approximations of this work one has to find the solution of equations of 136 independent variables. Using this method first I investigated the model defined by the transition probabilities

$$A\xrightarrow{\sigma}2A, \quad 2A\xrightarrow{\lambda}\emptyset, \quad \emptyset A\overset{D}{\leftrightarrow}A\emptyset. \quad (7)$$

The steady state solutions were determined for $N=1,2,3,\ldots,8$ approximations and the corresponding steady state densities $\rho_s(\sigma,D)$ are calculated numerically. The phase transition points are obtained for several values and are plotted in the σ_c/D vs λ_c/D parametrization [Fig. 1(a)] in order to be comparable with the results of [17]. The phase transition lines for $N>1$ corroborate the phase diagram of [17], with $(\lambda_c/D)_{th}>0$ threshold values and with linear shapes in the $\sigma/D\to\infty$ limit. By inspecting the numerical values of the $(\lambda_c/D)_{th}(N)$ threshold values for $N=2,3,\ldots,8$ (see Table I) one can set up a hypothesis that in general

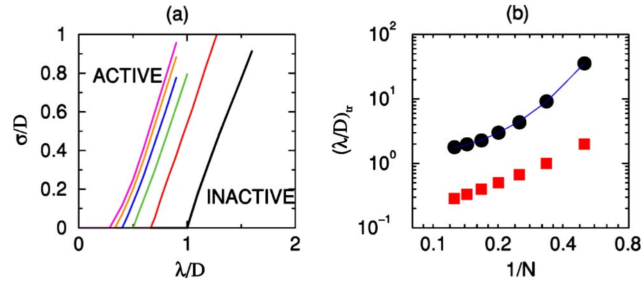

FIG. 1. (Color online) (a) Phase diagram of the $A\to 2A$, $2A\to\emptyset$ model determined by $N=3,4,\ldots,8$ (right to left curves) cluster approximations. (b) The $(\lambda_c/D)_{tr}$ critical end point values of the $\sigma_c>0$ transitions as a function of $1/N$. Boxes correspond to the $A\to 2A$, $2A\to\emptyset$ and circles to the $A\to 2A$, $4A\to\emptyset$ model. The line shows a fitting of the form (10).

$$(\lambda_c/D)_{th}(N) = 2/(N-1) \quad (8)$$

exactly. Therefore one can extrapolate that in the $N\to\infty$ limit $(\lambda_c/D)_{th}(N)\to 0$ [Fig. 1(b)] in agreement with the results of [17] for 1D. So $N>1$ cluster mean-field approximations, which can take into account diffusion, exhibit similar phase diagrams to the one obtained by the NPRG method for $d\geqslant d_c=4$ and in the asymptotic limit they even reproduce the zero threshold corresponding to 1D.

The other system of interest in this study is the

$$A\xrightarrow{\sigma}2A, \quad 4A\xrightarrow{\lambda}\emptyset, \quad \emptyset A\overset{D}{\leftrightarrow}A\emptyset \quad (9)$$

model, for which perturbative RG predicts $d_c=2/3$ [18]; therefore in all physical dimensions only type (4) mean-field transitions are expected at $\sigma_c=0$. By solving the cluster mean-field equations up to $N=8$, with the $\lambda=1-\sigma$ parametrization, one obtains a reentrant phase structure for low diffusion rates as in the case of the $2A\to 3A$, $4A\to\emptyset$ model [12] (Fig. 2). I have determined the $(\lambda_c/D)_{th}$ threshold values for each N and plotted them as a function of $1/N$ [Fig. 1(b)]. One can see a tendency toward leveling off contrary to the results for the $A\to 2A$, $2A\to\emptyset$ case. By extrapolating to the $N\to\infty$ limit using a form similar to but more general than Eq. (8),

$$(\lambda_c/D)_{th}(N) = a + b/(N-1)^c, \quad (10)$$

the threshold does not vanish: $a=1.2$, $b=34.5$, $c=2.14$, therefore we may expect phase transitions with $\sigma_c>0$ even in one dimension for any $0<D\leqslant 1$ diffusion probabilities.

To test the cluster mean-field results for the $A\to 2A$, $4A\to\emptyset$ model I performed simulations in one dimension with lattice sizes $L=10^5$ and with periodic boundary conditions. The simulations were started from homogeneously filled lattices with probability 1/2. One elementary Monte Carlo step

TABLE I. Numerical N-cluster results for the threshold values of the $A\to 2A$, $2A\to\emptyset$ model

N	2	3	4	5	6	7	8
$(\lambda_c/D)_{th}$	2	1	0.666	0.5	0.4	0.333	0.286

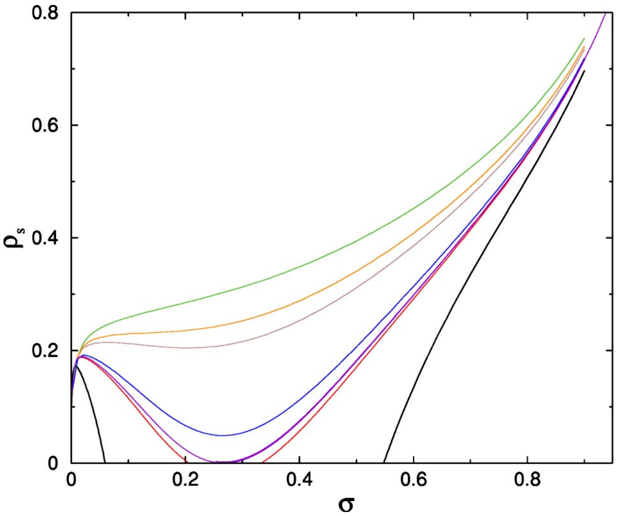

FIG. 2. (Color online) Steady state density results in the $N=7$ approximations of the $A \to 2A$, $4A \to \emptyset$ model. Different curves correspond to $D=1, 0.7, 0.6, 0.4, 0.371, 0.36, 0.2$ (top to bottom). The $\sigma_c > 0$ critical point disappears for $D^* > 0.370\,83$.

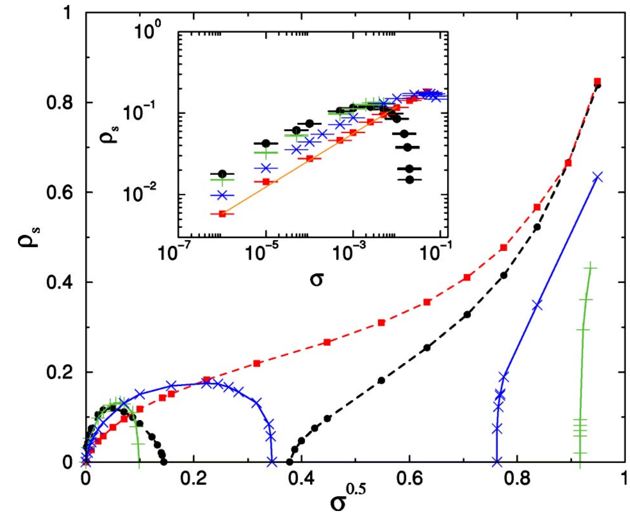

FIG. 3. (Color online) Simulation results for the steady state density of the $A \to 2A$, $4A \to \emptyset$ model. Crosses correspond to $D=1.0$ and + signs to $D=0.2$ diffusion in 1D. Circles denote $D=0.01$ and squares $D=1$ data in 2D. Error bars are smaller than the symbol sizes. The lines serve to guide the eye. The inset shows the data magnified in the neighborhood of the $\sigma=0$ transition point. The solid line shows a power-law fitting with the exponent $\beta=0.33(1)$.

consists of the following substeps. A particle and a direction are selected randomly. A particle hopping is attempted in the given direction with probability D provided the nearest neighbor (NN) site is empty. The time (t) measured by Monte Carlo steps (MCS) is updated by $\Delta t=1/n$, where n is the total number of particles. Again a particle and a direction are selected randomly and either four NN particles in the given direction are removed with probability λ or an offspring is created in an empty NN site in the direction selected before with probability $1-\lambda$. The time is updated by $\Delta t=1/n$. The density of particles $\rho(t)$ is followed for up to 10^7 MCS (throughout the whole paper the time is measured in Monte Carlo steps). The phase transition points have been located for several diffusion rates and are shown on Fig. 3. A qualitative agreement with the low- D results of the finite N-cluster mean-field approximations can be observed. However, the $\sigma_c > 0$ transition persists even for $D=1$ diffusion probability in agreement with the $N \to \infty$ extrapolations.

The density decay near a $\sigma_c > 0$ critical point at $D=0.2$ has been investigated in more detail. The density at σ_c is expected to decay as Eq. (3). Figure 4(a) shows the local slopes of α defined as

$$\alpha_{eff}(t) = \frac{-\ln[\rho(t)/\rho(t/m)]}{\ln(m)} \qquad (11)$$

(where I used $m=2$). As one can see curves with $\sigma > 0.8398$ veer up (active phase), while those with $\sigma < 0.8398$ veer down (absorbing phase). A clean scaling with exponent $\alpha=0.159(1)$ can be observed at $\sigma=0.839\,80(2)$, corroborating the $(1+1)$-dimensional DP class exponent value [$\alpha=0.159\,464(6)$ [21]]. In the inactive phase $\rho(t)$ vanishes exponentially in agreement with the DP behavior again. One may expect the same kind of transition all along the $\sigma_c(D) > 0$ transition line. Indeed simulations showed that the density decays in a similar way at transition points with $D=0.01, 0.05, 0.09$.

The simulations for this model were repeated in two dimensions in $L=4\times 10^3$ linear sized systems with periodic boundary conditions. These 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 NN's. The time is updated by $1/n$. A particle and a number $x_2 \in (0,1)$ are selected randomly. If $x_2 < \sigma$ and if the number of NN empty sites is greater than 0, one new particle is created at an empty site selected randomly. If $x_2 \geqslant \sigma$ and the number of NN particles is greater than two, four randomly selected neighboring particles are removed. The time (t) is updated by $1/n$ again. The density of particles was followed up to $t_{max} \leqslant 10^7$ MCS. As one can see the simulation data (Fig. 3) and the seven-point approximations (Fig. 2) fit qualitatively well (this is

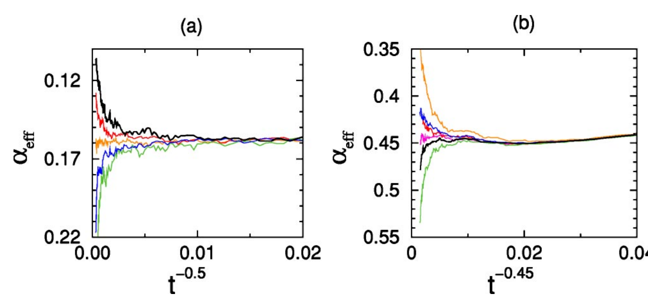

FIG. 4. (Color online) (a) Local slopes of the density decay exponent α as a function of $t^{-0.5}$ of the one-dimensional $A \to 2A$, $4A \to \emptyset$ model at $D=0.2$. Different curves correspond to $\sigma=0.8399$, $0.839\,85$, 0.8398, $0.839\,75$, 0.8397 (top to bottom). The critical point is located at $\sigma_c=0.839\,80(2)$. (b) The same as in (a) in two dimensions, for $\sigma=0.1426$, $0.142\,62$, $0.142\,63$, $0.142\,64$, $0.142\,65$, 0.1427 (top to bottom).

true for other $N>1$ levels as well). In both cases for weak diffusion rates reentrant phase transitions occur with $\sigma_c>0$, while for strong diffusion only a single phase transition at $\sigma_c=0$ branching rate can be found. The density decay at $D=0.01$ is analyzed near the phase transition point. The local slope figure shows a separatrix for the critical value $\sigma_c=0.142\,63(1)$ as can be seen on Fig. 4(b). One can read off the corresponding decay exponent $\alpha=0.445(5)$, which agrees with the $(2+1)$-dimensional DP value [$\alpha=0.4505(10)$ [22]].

I also investigated the steady state behavior at the $\sigma_c=0$ transition. The steady state density in the active phase near the critical phase transition point is expected to scale as Eq. (2). As the inset of Fig. 3 shows, by applying power-law fitting in the $10^{-6}\leqslant\sigma\leqslant10^{-3}$ region one obtains $\beta\simeq0.33(1)$ in both one and two dimensions at different diffusion rates. This agrees with the mean-field value (4) for this model. The density at $\sigma_c=0$ decays as $\rho\propto t^{-1/3}$ trivially, dictated by the $4A\to\emptyset$ process.

In conclusion, numerical evidence is provided that the $A\to2A$, $4A\to\emptyset$ branching and annihilating random walk process exhibits diffusion dependent phase transitions that are not accessible by perturbative renormalization. In particular, N-cluster mean-field approximations (with extrapolations to the $N\to\infty$ limit) resulted in a reentrant (D-σ) phase diagram, with phase transitions at $\sigma_c>0$ for $0<D\leqslant1$ diffusion probabilities. Simulations have shown that along this transition line DP critical behavior occurs in one and two dimensions. This type of critical behavior is the consequence of an effective $A\to\emptyset$ reaction generated by $A\to2A\to3A\to4A\to\emptyset$ of slowly moving particles. In one dimension this line of phase transitions persists for all $0<D\leqslant1$ diffusions, while in 2D it disappears for high diffusion rates. For any D and d values a mean-field transition characterized by $\beta=1/3$ occurs at $\sigma_c=0$.

A similar reentrant phase diagram has been observed in case of the one-dimensional $A\to2A$, $3A\to\emptyset$ model [23], in a variant of the NEKIM model [24], and in the $2A\to3A$, $4A\to\emptyset$ model [12,13]. 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. Another study using exact methods [25] showed that the particle density fluctuations undergo a diffusion dependent phase transition in the bosonic PCPD model for $d>2$. A very recent, nonperturbative RG study [17] has found a similar diffusion dependent phase diagram in the $A\to2A$, $2A\to\emptyset$ model. That work points out that nonperturbative effects arise and there is a threshold $(\lambda/D)_{th}(d)$ above which DP and below which a type (4) mean-field transition at $\sigma_c=0$ appears. The present N-cluster approximations confirm those results and produce a similar phase diagram as in [17] for any finite N, with a threshold value $(\lambda_c/D)_{th}(N)=2/(N-1)$. In the $N\to\infty$ limit this corroborates the vanishing threshold in 1D [17].

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