Phase transition of the one-dimensional coagulation-production process

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Recently an exact solution has been found by M. Henkel and H. Hinrichsen [J. Phys. A **34**, 1561 (2001)] for the one-dimensional coagulation-production process: $2A\to A$, $A\emptyset A\to 3A$ with equal diffusion and coagulation rates. This model evolves into the inactive phase independently of the production rate with $t^{-1/2}$ density decay law. This paper shows that cluster mean-field approximations and Monte Carlo simulations predict a continuous phase transition for higher diffusion/coagulation rates as considered by the exact solution. Numerical evidence is given that the phase transition universality agrees with that of the annihilation-fission model with low diffusions.

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One-dimensional, nonequilibrium phase transitions have been found to belong to a few universality classes, the most robust of them is the directed percolation (DP) class [1,2]. According to the hypothesis of Refs. [3,4] all continuous phase transitions to a single absorbing state in homogeneous systems with short ranged interactions belong to this class provided there is no additional symmetry and quenched randomness present.

Recent studies on the annihilation fission (AF) process $2A\to\emptyset$, $2A\to 3A$ [5–8] found evidence that there is a phase transition in this model that does not belong to any known universality classes. This model without the diffusion—the so called pair contact process where pairs of particles can annihilate or create new pairs—was introduced originally by Jensen [9] and while the static exponents were found to belong to DP class the spreading ones show nonuniversal behavior. By adding single particle diffusion [6] Carlon *et al.* introduced the pair contact process with diffusion (PCPD) particle model. The renormalization group analysis of the corresponding bosonic field theory was given by Ref. [5]. This study predicted a non-DP class transition, but it could not tell to which universality class this transition really belongs. An explanation based on symmetry arguments is still missing but numerical simulations suggest [10,8] that the behavior of this system can be well described (at least for strong diffusion) by coupled subsystems: single particles performing annihilating random walk coupled to pairs (B) following DP process: $B\to 2B$, $B\to\emptyset$. The system has two nonsymmetric absorbing states: one is completely empty, in the other a single particle walks randomly. Owing to this fluctuating absorbing state this model does not oppose the conditions of the DP hypothesis.

The most well known exception from the robust DP class is the parity conserving (PC) class, where a mod 2 conservation of particles can be found [11] and in multiabsorbing state systems an exact Z_2 symmetry is satisfied too [12]. Some exponents of the PCPD model are close to those of the PC class but the order parameter exponent β has been found to be very far away from both of the DP and PC class values [8]. In fact this system does not exhibit either a Z_2 symmetry or a parity conservation that appear in models with PC class transition. It is conjectured [13] that this kind of phase transition appears in models where (i) solitary particles diffuse, (ii) particle creation requires two particles, and (iii) particle removal requires at least two particles to meet. In this paper the following one-dimensional coagulation-production processes will be investigated.

(a) Spatially symmetric coagulation-production processes:

$$A\emptyset A \xrightarrow{f} 3A, \tag{1}$$

$$2A \xrightarrow{c/2} A\emptyset, \quad 2A \xrightarrow{c/2} \emptyset A, \tag{2}$$

$$A\emptyset \overset{d}{\leftrightarrow} \emptyset A. \tag{3}$$

(b) Spatially asymmetric coagulation-production processes:

$$AA\emptyset \xrightarrow{f/2} 3A, \quad \emptyset AA \xrightarrow{f/2} 3A, \tag{4}$$

$$2A \xrightarrow{c/2} A\emptyset, \quad 2A \xrightarrow{c/2} \emptyset A, \tag{5}$$

$$A\emptyset \overset{d}{\leftrightarrow} \emptyset A. \tag{6}$$

Both versions fulfill conditions (i)–(iii.) but Henkel and Hinrichsen [13] show that for $d=c$ the symmetric version always evolve into the inactive state with $\rho\propto t^{-0.5}$ scaling law. They argue that the asymmetric version displays a nonequilibrium phase transition. The difference is said to be similar to the hard-core effects observed in one-dimensional models [14–18].

Hard-core particle exclusion effects can really change both the dynamic [14–16] and static [17,18] behavior of one-dimensional systems by introducing blockades in the particle dynamics but in this work I argue that this kind of hard-core effects are not responsible for the lack of phase transition. One can quickly check by simulations that for $d\leqslant c$ the density in the asymmetric version decays in much the same way—with $\rho\propto t^{-0.5}$ scaling law—as in case of the symmetric version. Furthermore I shall show that if the coagulation rate is smaller than the diffusion rate particles can escape before removal, an active phase will emerge with a continuous phase transition belonging to the same class that was found in the AF model for weak diffusion. Therefore both versions exhibit qualitatively the same phase diagram.

To prove this first I shall apply cluster mean-field approximations (GMF) [19,20], which can predict phase diagrams qualitatively well. The mean-field equation for the steady state of both versions is

$$0=f(1-p_A)p_A^2-cp_A^2, \tag{7}$$

where p_A is the probability of A-s at a given site. Note that the diffusion rate d does not play a role in this approximation. By introducing the parametrization $c=p(1-d)$, $f=(1-p)(1-d)$—that is similar to that of the PCPD model—this has the solution,

$$\rho=p_A=\frac{2p-1}{p-1}, \tag{8}$$

for $p<1/2$ and $\rho=0$ if $p\geqslant 1/2$. Therefore an active state appears in the mean-field approximation already.

For higher order cluster mean-field approximations similar scenario can be found, but one has to treat the two versions separately. The density in pair approximation for the symmetric version is

$$\frac{(p-1)p^2-2dp(p^2+2p-2)+d^2(p^3+5p^2+4p-4)}{(p-1)p^2-2dp(p^2+2p-2)+d^2(p^3+5p^2-4)}. \tag{9}$$

One can easily prove that if the coagulation rate is equal to the diffusion rate $d=p(1-d)/2$ this gives a single $\rho=0$ absorbing state solution in agreement with [13].

The steady state solution with positive density is possible if

$$d>\frac{p^2-p}{p^2+3p-2}. \tag{10}$$

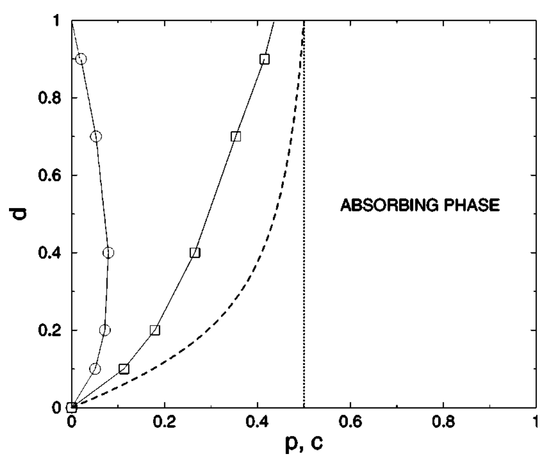

FIG. 1. Phase diagram of the symmetric coagulation-production model. Dotted line: mean-field approximation, dashed line: pair approximation, squares: simulation results. The circles show d_c as the function of c. Lines connecting symbols are used to guide eyes only.

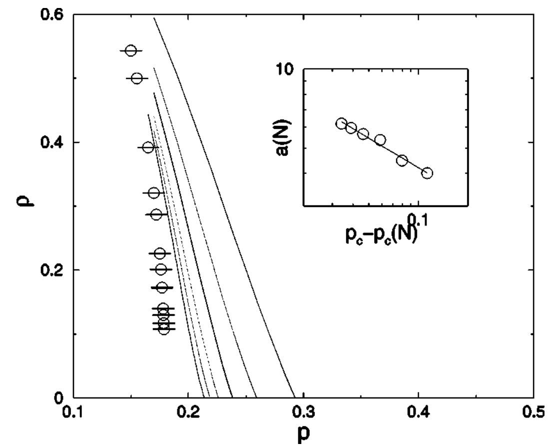

FIG. 2. Cluster mean-field approximations in the symmetric coagulation-production model for $d=0.2$. The curves correspond to steady state density solutions as the function of p, for $N=2,3,4,5,6,7$ (right to left). The circles with error bars represent simulation results. Inset: Corresponding coherent anomaly amplitudes with a power-law fitting.

This gives the phase boundary in pair approximation that is a continuous unlike in case of the PCPD model [6] (see Fig. 1). There is an other solution with positive density for $d<p/(p+2)$ but that is unstable. In the two extreme cases: $d=0$ and $d=1$ there is no phase transition. For $d=0$ the system evolves to frozen states with isolated particles, while for $d=1$ there is only random walk of particles with exclusion. The pair density in the pair approximation

$$c=\frac{((p-1)p-d(p^2+3p-2))^2(p-1)^{-1}}{(p-1)p^2-2dp(p^2+2p-2)+d^2(p^3+5p^2-4)} \tag{11}$$

has a leading order singularity all along the phase transition line

$$c\propto(p_c-p)^2, \tag{12}$$

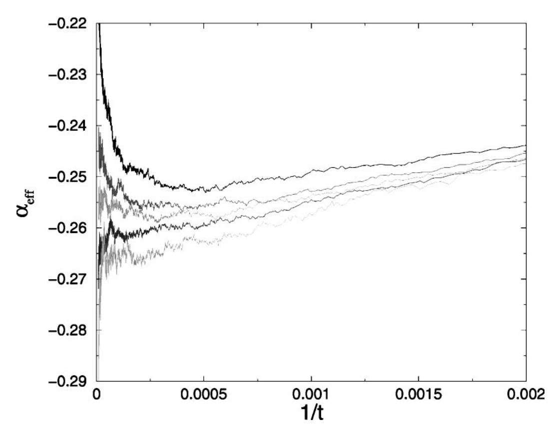

FIG. 3. Local slopes of the density decay in the symmetric coagulation production process. Different curves correspond to $p=0.1795$, 0.1797, 0.1798, 0.1799, 0.18 (from bottom to top). Throughout the whole paper t is measured in units of Monte Carlo sweeps (MCS).

TABLE I. Summary of results.

d	0.1	0.2	0.4	0.7
p_c	0.1129(1)	0.17975(8)	0.2647(1)	0.3528(2)
α		0.263(9)	0.268(8)	0.275(8)
β		0.57(1)	0.58(1)	0.57(1)
β_{CAM}		0.57(3)		

suggesting one universality class unlike in the case of PCPD model [6].

The GMF solutions for $N=3,4,5,6,7$ block sizes have been determined numerically at $d=0.2$. The approximation level is constrained by the numerical stability of the fixed point solution in the multidimensional space of N-block probability variables. As Fig. 2 shows the ρ_N density curves of different approximations converge to the simulation results.

Using these data an estimate can be given for the order parameter density exponent $\rho \propto |p-p_c|^\beta$ using the Coherent anomaly method (CAM) [21], which has been proven to give precise estimates for the DP [22] and PC [23] classes. According to CAM the amplitudes $a(N)$ of the cluster mean-field singularities scale in such a way that

$$a(N) \propto |p_c(N)-p_c|^{\beta-\beta_{MF}} \tag{13}$$

the exponent of true singular behavior can be estimated. From the mean-field solution (8) one read off that $\beta_{MF}=1$. The critical point p_c can be estimated either by extrapolating on the GMF results or by simulations. Linear extrapolation at $d=0.2$ for $p_c(1/N \to 0)$ gives: $p_c=0.182(2)$. Monte Carlo simulations on large systems—discussed below—give a more precise estimate: $p_c=0.179\,75(8)$. The amplitudes $a(N)$ near $p_c(N)$ are determined by linear fitting from the $\rho_N(p)$ data and shown in the inset of Fig. 2 as the function of $p_c(N)-p_c$. A power law with exponent $\beta-\beta_{MF}=-0.43(3)$ can be fairly well applied for points corresponding to $N>2$ approximations giving an estimate: $\beta=0.57(3)$, which agrees well with former results for the AF model with small diffusion rates [8].

Monte Carlo simulations of the symmetric process started from fully occupied lattices of size $L=40\,000$ show a phase transition for $d=0.2$ and $p_c=0.179\,75(10)$ (see Fig. 3). The local slopes of the density decay,

$$\alpha_{eff}(t) = \frac{-\ln[\rho(t)/\rho(t/m)]}{\ln(m)}, \tag{14}$$

(where we use $m=8$ usually) at the critical point go to exponent α by a straight line, while in sub(super)-critical cases they veer down(up) respectively.

For the critical point $[p_c=0.179\,75(8)]$ one can estimate that the effective exponent tends to $\alpha=0.263(9)$, see Table I, which agrees with results for the AF model [7,8] again. For other d-s similar results have been found.

In the supercritical region the steady states have been determined for different $\epsilon=p-p_c$ values. Following level-off

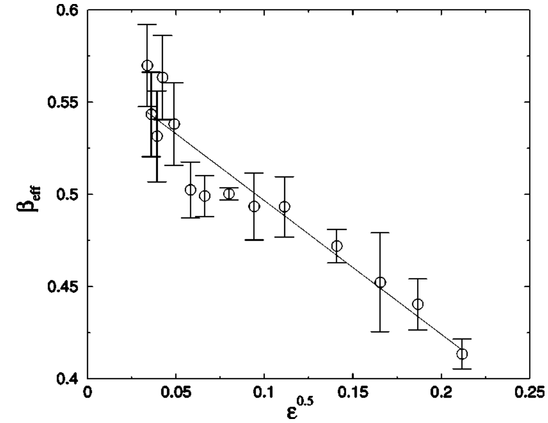

FIG. 4. Effective order parameter exponent results. Linear extrapolation results in $\beta=0.57(1)$.

the densities were averaged over 10^4 MCS and 1000 samples. By looking at the effective exponent defined as

$$\beta_{eff}(\epsilon_i) = \frac{\ln \rho(\epsilon_i) - \ln \rho(\epsilon_{i-1})}{\ln \epsilon_i - \ln \epsilon_{i-1}}, \tag{15}$$

one can read off: $\beta_{eff} \to \beta \simeq 0.57(1)$, see Fig. 4 which is in good agreement with the exponent of the AF model for weak diffusion determined by coherent anomaly method and simulations [8].

The simulations and the cluster mean-field approximations show that if the diffusion rate is lowered this phase transition disappears and the system will decay with the $\rho \propto t^{-0.5}$ law independently of f in *both* versions. As expected the asymmetric version exhibits a phase transition with the same universal properties as the symmetric version. For example, for $d=0.2$ the transition point is at $c=0.359(1)$, $f/2=0.4409(1)$ with the decay exponent $\alpha=0.27(1)$.

In conclusion coagulation-production models exhibit a phase transition if the diffusion is fast enough. The spatial symmetry of the production process has been found to be irrelevant as in case of the AF process [8]. The critical behavior agrees well with that of the AF model in its weak diffusion rate region. An open question is that why can not one see the cyclically coupled behavior in this model similarly as in the PCPD model as $d \to 1$. The corrections to scaling are getting very strong in this limit that make numerical solutions very confusing, but one has to realize that the $B \to \emptyset$ process of pairs (present in AF) is missing in this model. Therefore a *single* universality class in this model and *two distinct classes* in the AF model are likely. This conjecture is strengthened by the pair mean-field results: one obtains analytically the *same* singular behavior here and *two distinct singular behaviors* in case of the PCPD model along the phase transition line.

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