Critical behavior of the one-dimensional diffusive pair contact process

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The phase transition of the one-dimensional diffusive pair contact process is investigated by N cluster mean-field approximations and high precision simulations. The $N=3,4$ cluster approximations exhibit smooth transition line to absorbing state by varying the diffusion rate D with $\beta_2=2$ mean-field order parameter exponent of the pair density. This contradicts with former $N=2$ results, where two different mean-field behavior was found along the transition line. Extensive dynamical simulations on $L=10^5$ lattices give estimates for the order parameter exponents of the particles for $0.05\leqslant D\leqslant 0.7$. These data may support former two distinct class findings. However, the gap between low- and high-D exponents is narrower than previously estimated and the possibility for interpreting numerical data as a single class behavior with exponents $\alpha=0.21(1)$, $\beta=0.40(1)$ assuming logarithmic corrections is shown. Finite-size scaling results are also presented.

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I. INTRODUCTION

The exploration of nonequilibrium universality classes is of current interest of research. In this area, most systems investigated exhibit phase transitions to absorbing states with such weak fluctuations from which no return is possible [1,2]. For a long time, only the robust directed percolation (DP) universality class has been known [3,4]. Later, systems with extra conservation laws and symmetries were shown belong to other universality classes [5–8]. In the past few years it turned out that there are novel classes in low-dimensional reaction-diffusion systems, where neither bosonic field theory nor symmetry arguments can give better understanding of the critical behavior [9]. This is probably due to the fact that in low-dimension topological constraints become effective, blocking the motion of reacting particles [10]. While bosonic field theories cannot capture this feature, fermionic field theories have not been successful for such systems yet. In fact the critical classes of such models can be different, depending on fermionic or bosonic particles, which are involved in Refs. [11–14].

Recently, novel universal behavior is reported in some low-dimensional reaction-diffusion models featured by production at pairs and explicit single particle diffusion [13–21]. In these systems, particle production competes with pair annihilation and diffusion. If the production wins steady states with finite particle, density appear in (fermionic) models with hard-core repulsion, while in unrestricted (bosonic) models the density diverges. By lowering the production or annihilation rate a doublet of absorbing states without symmetries emerges. One of such states is completely empty, the other possesses a single wandering particle. In case of fermionic systems, the transition to absorbing states is continuous with novel, yet not completely settled critical behavior.

The existing field theory of binary production reaction-diffusion systems [13], describing bosonic particles could not be solved by standard renormalization procedures, but hinted at a transition with non-DP behavior. At the transition point of the one-dimensional model it predicts a density decay of the form

$$\rho(t,p_c)\propto\left[\frac{\ln(t)}{t}\right]^{1/2}, \tag{1}$$

while in the inactive phase, $\rho(t,p_c)\propto t^{-1/2}$. These were confirmed by simulations [10]. In case of fermionic particles of this model diffusive pair contact process (PCPD) density matrix renormalization group analysis [14], coherent anomaly extrapolation [16], and simulations [15,16] found a different kind of critical phase transition. However, the critical exponents seem to depend on the diffusion strength D and different interpretations of data have been born. These embrace the possibilities of continuously changing exponents, two-universality classes [16], and single class with huge corrections [14,22].

Very recently, well defined set of critical exponents have been reported in different versions of binary production PCPD-like processes [23]. However, these simulations were done at a fixed, high-diffusion per annihilation rate and, as will be shown in Sec. IV, the exponent estimates agree well with those of this paper in the high-diffusion region. Even more recently, two studies [24,25] reported nonuniversality in the dynamical behavior of the PCPD. While the former one by Dickman and Menezes explored different sectors (a reactive and a diffusive one) in the time evolution and gave nontrivial exponent estimates, the latter one by Hinrichsen provided a hypothesis that the ultimate long time behavior should be characterized by DP behavior.

Just before the submission of this paper, a preprint by Kockelkoren and Chaté [26] showed simulation results for a modified version of PCPD which is in between fermionic and bosonic cases. That means they discard the single particle occupation constraint on the lattice but suppress multiple occupancy by an exponentially decreasing creation probability ($p^{N/2}$) of the particle number. They claim that their stochastic cellular automaton (SCA) model shows smaller corrections to scaling than the PCPD and exhibits single universality class transition.

The two-universality class scenario was backed by pair-mean-field approximation [14] that showed two different mean-field behavior by varying D and simulations [16] for the order parameter density exponents. Such kind of mean-field behavior is absent if we replace the annihilation process $AA \to \emptyset$ by a coagulation $AA \to A$ [18]. By the investigation of the parity conserving version of the PCPD, the mean-field and pair-mean-field approximations resulted in similar phase diagrams, but higher order cluster mean-field showed a single mean-field class behavior [21]. Hence the authors concluded that for appropriate description of such binary production models at least $N=3$ clusters are needed. Then mean-field behavior was indeed found in $d=d_c=2$ by simulations [21].

In the present work, I show $N=3,4$ cluster mean-field results for the PCPD model that again suggest a single mean-field universality class. This does not necessarily imply that below $d_c=2$ only one class should exist. Higher precision simulations than that of Ref. [16] are also presented in the second part of this paper that provide better exponent estimates but still left this question open. I show that a single universality class scenario can be accepted if we assume logarithmic corrections to data.

II. THE PCPD MODEL

A PCPD-like binary spreading process was introduced in an early work by Grassberger [27]. Its preliminary simulations in one dimension showed a non-DP type transition, but these results have been forgotten for a long time. The PCPD introduced by Carlon *et al.* [14] is controlled by two independent parameters: the probability of pair annihilation p and the probability of particle diffusion D. The dynamical rules are

$$AA\emptyset,\emptyset AA \to AAA \quad \text{with rate} \quad (1-p)(1-D)/2,$$
$$AA \to \emptyset\emptyset \quad \text{with rate} \quad p(1-D),$$
$$A\emptyset \leftrightarrow \emptyset A \quad \text{with rate} \quad D. \tag{2}$$

The *site mean-field* approximation gives a continuous transition at $p_c=1/3$. For $p \leqslant p_c$ the particle and pair densities exhibit singular behavior,

$$\rho(\infty,p) \propto (p_c-p)^{\beta}, \quad \rho_2(\infty,p) \propto (p_c-p)^{\beta_2}, \tag{3}$$

while at $p=p_c$ they decay as

$$\rho(t,p_c) \propto t^{-\alpha}, \quad \rho_2(t,p_c) \propto t^{-\alpha_2}, \tag{4}$$

with the exponents

$$\alpha=1/2, \quad \alpha_2=1, \quad \beta=1, \quad \beta_2=2. \tag{5}$$

According to *pair-mean-field* approximations the phase diagram can be separated into two regions (see Fig. 1). While for $D>1/7$ the pair approximation gives the same $p_c(D)$ and exponents as the site mean-field, for $D \leqslant 1/7$ the transition line breaks and the exponents are different

$$\alpha=1, \quad \alpha_2=1, \quad \beta=1, \quad \beta_2=1. \tag{6}$$

In the entire inactive phase the decay is characterized by the exponents

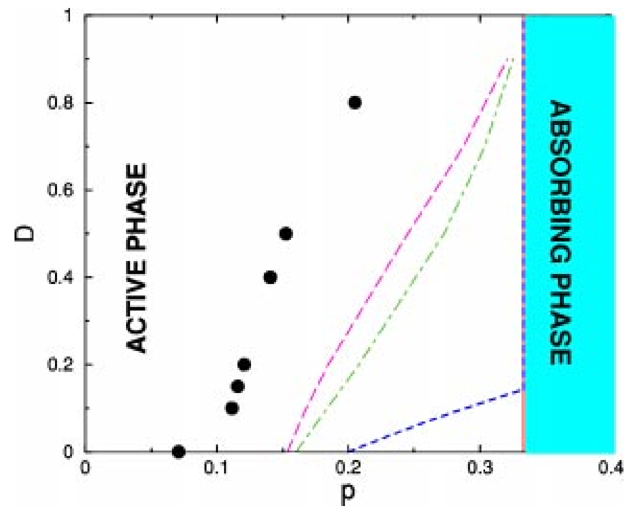

FIG. 1. Schematic phase diagram of the one-dimensional PCPD model. Circles correspond to simulation and DMRG results; solid line, site mean-field ($N=1$); dashed line, pair approximation ($N=2$); dot-dashed line, $N=3$; and long-dashed $N=4$ cluster mean-field results discussed in Sec. III.

$$\alpha=1, \quad \alpha_2=2. \tag{7}$$

III. CLUSTER MEAN-FIELD RESULTS FOR PCPD

Generalized, *cluster mean-field* approximation introduced by Refs. [28,29] was applied for the dynamical rules (2) of the 1D fermionic lattice model. The master equations for $N=1,2,3,4$ block probabilities were setup;

$$\frac{\partial P_N(\{s_i\})}{\partial t} = f(P_N(\{s_i\})), \tag{8}$$

where site variables may take values, $s_i=\emptyset,A$. The equations could be solved numerically for the $[\partial P_N(\{s_i\})]/\partial t = 0$ steady state condition. Taking into account, spatial reflection symmetries of $P_N(\{s_i\})$ this involves ten independent variables in case of $N=4$. The particle $(\rho(p,D))$ and pair $(\rho_2(p,D))$ densities were expressed by $P_N(\{s_i\})$ and the phase transition point $p_c(D)$ was located for several values of D. At $p_c(D)$ quadratic fitting of the form

$$a(p-p_c(D)) + b(p-p_c(D))^2 \tag{9}$$

was applied for $\rho(p,D)$ and $\rho_2(p,D)$. The $N=1$ and 2 solutions reproduced the results of [14] for particle and pair densities. For $N=2$ the two regions, corresponding to different leading order singularity of $\rho_2(p,D)$ with $\beta_2=1,2$ were located by least square fit with the form (9). For $N=3,4$ approximations smooth $p_c(d)$ phase transition lines were determined that are shown in Fig. 1 and tabulated in Table I. The quadratic fitting (9) resulted in leading order singularities $\beta=1$ for particles and $\beta_2=2$ for pairs everywhere. These are in contradiction with the $N=2$ approximation results similarly to the parity conserving binary process model case [21]. For that model simulations in two dimension, strengthened the single mean-field class behavior along

TABLE I. Summary of $N=2,3,4$ cluster mean-field approximation results.

	$N=2$			$N=3$			$N=4$		
D	p_c	β	β_2	p_c	β	β_2	p_c	β	β_2
0.9	0.3333	1	2	0.3252	1	2	0.3208	1	2
0.7	0.3333	1	2	0.3036	1	2	0.2875	1	2
0.5	0.3333	1	2	0.2727	1	2	0.2452	1	2
0.2	0.3333	1	2	0.2079	1	2	0.1845	1	2
0.1	0.2888	1	1	0.1840	1	2	0.1680	1	2
0.05	0.2421	1	1	0.1721	1	2	0.1606	1	2
0.0002	0.2002	1	1	0.1604	1	2	0.1537	1	2

$p_c(D)$ and it was conjectured that the pair approximation is an odd one. Here, again I conclude that at least $N>2$ level of approximation is necessary to obtain a correct mean-field behavior.

The single mean-field class property does not necessarily mean that below d_c, a single class behavior should occur all along the $p_c(D)$ transition line. For example, in a similar model that exhibits an additional global particle number conservation [8] such situation was found. Therefore, I investigated this question by extensive simulations.

IV. SIMULATION RESULTS

The simulations were performed on $L=10^5$ sized rings with random sequential update version of PCPD evolving by the following rules. A particle and a direction are selected randomly. One of the following reaction is performed: (a) a nearest neighbor exchange in the selected direction with probability D; (b) an annihilation with the nearest neighbor particle in the selected direction with probability $p(1-D)$; (c) a creation of a new particle in the selected direction at the second nearest neighbor empty site with probability $(1-p)(1-D)$ if the nearest neighbor is filled with a particle.

The number of particles N_p is followed and the time is updated by $1/N_p$ following a reaction [throughout the whole paper the time is measured by Monte Carlo steps (MCS)]. The initial conditions were random distribution of particles with an occupation probability 0.5.

It was suggested in Ref. [24] that one may get smaller corrections to scaling if one excludes the purely diffusive sector by averaging over states having at least one pair in the system. In the present simulations I did not find much effect (within statistical error margin) of such restrictions for the long time behavior. The reason for this is that in the large-size limit one should get the same exponents whether or not one excludes the purely diffusive sector, because all the scaling behavior is associated with the reactive sector. Excluding the purely diffusive sector one eliminates some noise, and one source of finite-size corrections.

A. Density decay simulations

The critical point p_c for diffusion rates $D=0.05$, 0.1, 0.2, 0.5, 0.7 was located by following the time evolution of the density decay. These simulations were done in two parts. First runs up to $t_{max}\sim 10^5$ MCS and with high statistical averages ($\sim 10^4$) were performed that allowed local slopes estimates of the density ($\rho(t)$) decay exponent α and p_c. These simulations were extended by long time runs up to 10^7–10^8-MCS with 100–200 sample numbers. The two sets of data are fitted together and are shown on Figs. 2–6.,

On all plots one can see up and down veering $\rho(t)$ curves in the long time limit—corresponding to active and absorbing phases—separated by a roughly straight line—corresponding to p_c. As one can see for high-diffusion rates ($D\geqslant 0.2$) scaling with exponent $\alpha\sim 0.21$ seems to a set for

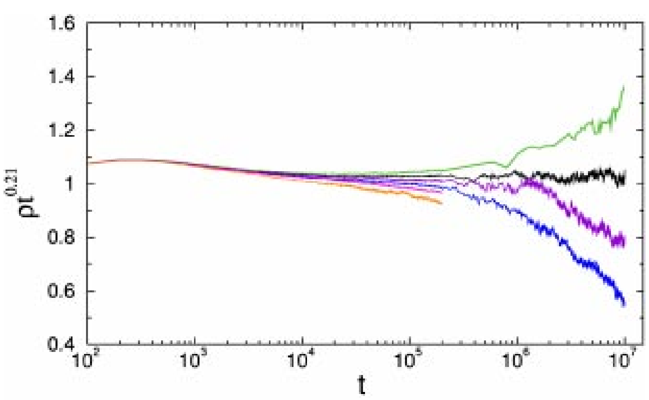

FIG. 2. Density decay times $t^{0.21}$ in one-dimensional PCPD at $D=0.7$ and $p=0.1574$, 0.157 45, 0.1575, 0.157 55, 0.1576, 0.1577 (top to bottom curves).

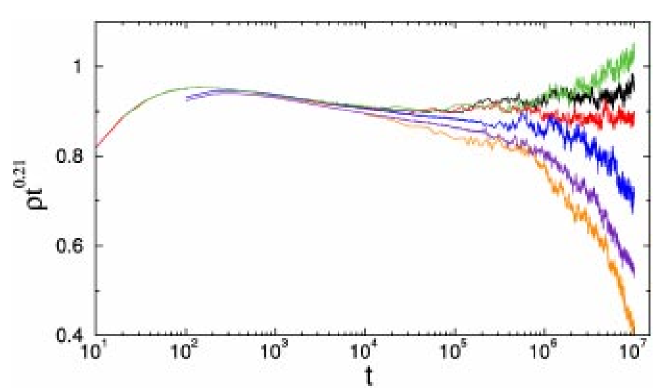

FIG. 3. Density decay times $t^{0.21}$ in one-dimensional PCPD at $D=0.5$ and $p=0.133$ 51, 0.133 52, 0.133 53, 0.133 56, 0.1336, 0.133 63 (top to bottom).

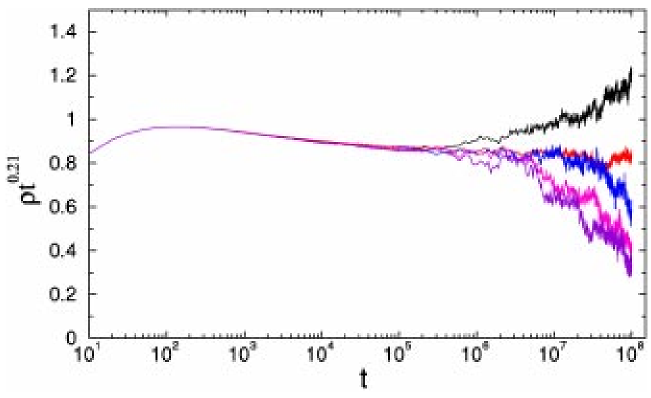

FIG. 4. Density decay times $t^{0.21}$ in one-dimensional PCPD at $D=0.2$ and $p=0.111\,215$, 0.112 17, 0.112 18, 0.112 19, 0.1122 (top to bottom).

$t \gtrsim 3\times 10^4$ MCS. This is in agreement with the first results provided for PCPD for high-diffusion rates [16] and with the results of Refs. [17,24,26] for strong diffusions.

In cases $D=0.05$ and 0.1 straight lines on the log-log plot appear from $t \gtrsim 3\times 10^2$ MCS with an exponent $\alpha=0.245(5)$. This is in agreement with the results of Ref. [23] who considered the case with coagulation and annihilation rates three times the diffusion rate. This exponent is about 10% smaller than that was found in Ref. [16] but the two distinct class behavior seems to be supported.

Although the upper critical dimension of PCPD is expected to be at $d_c=2$ [21] one may not exclude the possibility of a second critical dimension ($d_c'=1$) or topological effects in one dimension that may cause logarithmic corrections to scaling. For this reason, I tried to apply logarithmic fitting to the data of the form

$$\rho(t,p_c)=[(a+b\ln(t))/t]^{\alpha}. \tag{10}$$

One can find the corresponding exponents in Table II which are all in agreement with the value $\alpha=0.21(1)$ in both the low- and high-diffusion regions. Here, I applied least squares fitting for the most critical-like curves such that the relative error in the sum of squares was at most 0.0001. To confirm

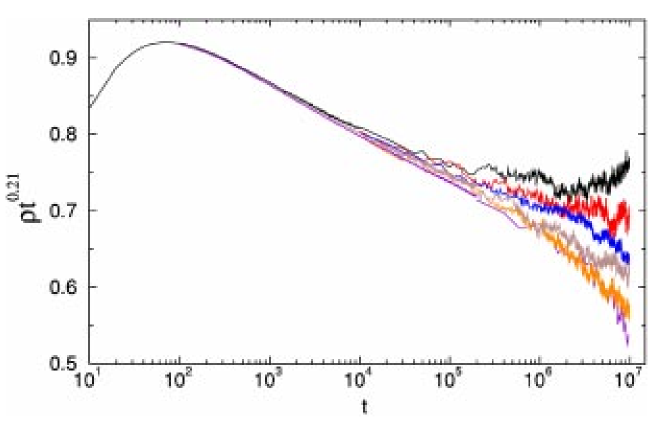

FIG. 5. Density decay times $t^{0.21}$ in one-dimensional PCPD at $D=0.1$ and $p=0.106\,86$, 0.106 88, 0.106 89, 0.1069, 0.106 91, 0.106 92 (top to bottom).

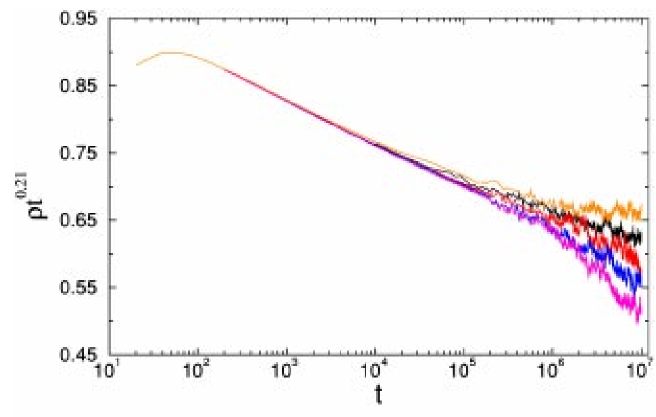

FIG. 6. Density decay times $t^{0.21}$ in one-dimension PCPD for $D=0.05$ and $p=0.104\,36$, 0.104 38, 0.1044, 0.104 41, 0.104 42 (top to bottom).

these results other critical exponents were also investigated using the precise p_c values shown in this section.

B. Steady state simulations

To estimate directly the order parameter exponent describing the scaling

$$\rho(\infty,\epsilon)\propto \epsilon^{\beta} \tag{11}$$

off-critical, steady state densities had to be measured. Here, again I used $L=10^5$ system sizes. The density decay was followed for each D and $\epsilon_i=p_c-p_i$ values on logarithmic time scales until saturation effect was observed. Following that averaging of $\rho(t)$ was done for about 100 samples within a time window that exceeds the saturation by a decade. I measured the effective exponents defined as

$$\beta_{eff}=\frac{\ln[\rho(\infty,\epsilon_i)]-\ln[\rho(\infty,\epsilon_{i-1})]}{\ln(\epsilon_i)-\ln(\epsilon_{i-1})}, \tag{12}$$

which are expected to converge to the true critical values in the $\epsilon\to 0$ limit.

As one can see on Fig. 7 the local slopes for $D=0.7$ and $D=0.5$ converge to $\beta=0.40(1)$ in agreement with the high-diffusion rate results provided in Ref. [16]. This value is also close to Hinrichsen's estimate [0.38(6)] for the cyclically coupled model [17] and to Kockelkoren's value [0.37(2)] for the suppressed bosonic SCA model [26].

TABLE II. Summary of simulation results assuming logarithmic corrections of the forms (10) and (13).

D	p_c	β	α
0.7	0.157 45(1)	0.39(1)	0.214(5)
0.5	0.133 53(1)	0.414(16)	0.206(7)
0.2	0.112 18(1)	0.402(8)	0.217(8)
0.1	0.106 88(1)	0.407(7)	0.206(7)
0.05	0.104 39(1)	0.411(10)	0.216(9)

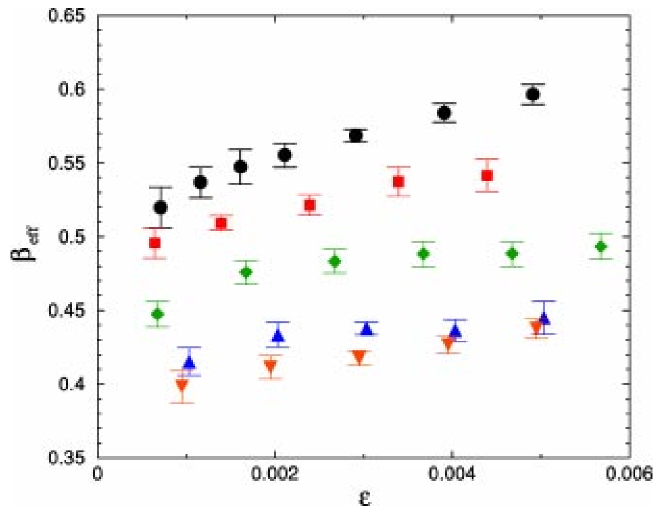

FIG. 7. Effective β exponents for different diffusion rates. The circles correspond to $D=0.05$; the squares to $D=0.1$ the diamonds to $D=0.2$; the up triangles to $D=0.5$; and the down triangles to $D=0.7$.

However, for $D=0.05$ and $D=0.1$ extrapolations suggest $\beta=0.50(2)$. This is in agreement with Park's recent results (~ 0.5) [23] but somewhat off the low-diffusion data of Ref. [16] [0.57(2)] and from Dickman's estimates (0.55–0.45) [24]. The reason for these deviations is likely to be related to strong finite-size effects, the complex way of scaling and the uncertainties of the p_c values used.

In case of the $D=0.2$ curve one may observe an extrapolation to some intermediate value, but the curvature of the last points may also suggest a tendency towards the high-D data. Note that in the earlier, lower scale simulations [16] the data for $D=0.2$ showed low-D critical behavior, strengthening the assumption that some kind of very slow crossover may occur here (although those results were obtained for a SCA version of PCPD).

Similarly to the dynamical simulations, I tried the possibility if logarithmic corrections to scaling of the form

$$\rho(\infty,\epsilon)=[\epsilon/(a+b\ln(\epsilon))]^{\beta} \tag{13}$$

could eliminate these differences. As one can see in Table II the exponents for all D values satisfy scaling with $\beta=0.40(1)$ with logarithmic corrections of the form (13).

C. Finite-size scaling

Finite-size scaling investigations at p_c were performed for system sizes $L=32,64,128,\ldots,1024$. The quasi-steady state density (averaged over surviving samples) is expected to scale according to

$$\rho_s(\infty,p_c,L)\propto L^{-\beta/\nu_\perp}, \tag{14}$$

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

$$\tau(p_c,L)\propto L^{Z}. \tag{15}$$

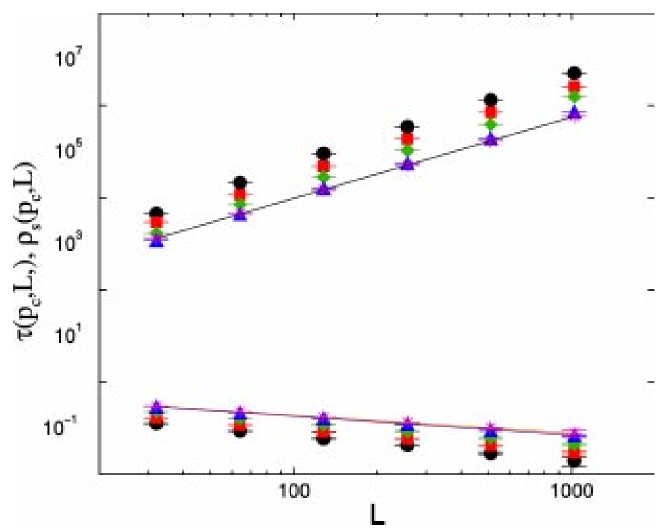

FIG. 8. Finite-size scaling of τ_L (upper points) and $\rho_L(\infty)$. The circles correspond to $D=0.05$; the squares, $D=0.1$; the diamonds, $D=0.2$; the up triangles, $D=0.5$; and the down triangles, $D=0.7$. The lines show power-law fittings applied for $D=0.7$ data points.

Since the system sizes are much smaller than those shown in Secs. IV A and IV B one may expect stronger corrections to scaling. Indeed the power-law fitting for $\beta/\nu_\perp$ results in values in the range 0.385–0.535 and for Z in the range 1.75–2 depending on D. These results are shown of Fig. 8. Again the low-D data are in agreement with those of Refs. [14], [23], and [24], while the high-D data with those of Refs. [14], [26], and [17]. Just considering these ranges one cannot distinguish this transition from the PC class [with $\beta/\nu_\perp=0.500(5)$ and $Z=1.75(1)$ [7]] that caused initial debates in the literature [14–16]. Assuming single universality class corresponding to high-D data we may expect $\beta/\nu_\perp=0.38(1)$ and $Z=1.75(15)$.

V. CONCLUSIONS

In this paper, I addressed the long standing question of diffusion dependence of the phase transition of the PCPD model. The $N=3,4$ level cluster mean-field calculations confirmed a single mean-field universality class scenario similarly to the parity conserving version of this model [21]. Again the best conclusion one can draw from these data is that the $N=2$ pair approximation is an odd one and we need at least $N>2$ level of mean-filed to get the correct scaling behavior for binary production models.

The extensive simulations have confirmed at least one set of the exponents—those for high diffusion—of the early results given in Ref. [16]. Data in the low-diffusion range are in good agreement with other recent simulation results suggesting a different universality class. Although the scaling seems to set in much earlier in the low-diffusion region than in the high-diffusion range, a slow crossover to high-D behavior can be verified numerically assuming logarithmic corrections. Similar conclusions can also be drawn from steady state simulation results. Although the two-universality class picture proposed in Ref. [16] cannot be excluded, data with logarithmic corrections assumption provides a strong support for a single class transition. The field theoretical arguments confirming or excluding logarithmic corrections would be necessary. Note that in one-dimensional coupled systems logarithmic corrections are not rare at all. The interpretation of PCPD as a coupled, two-component system [17] raises the possibility that topological constrains occurring in one dimension are responsible for such behavior.

The finite-size simulations could not give decisive support for any of the possible dependences of the diffusion of this transition, but the range of results are in agreement with those of other numerical results of the literature.

The values of mean-filed exponents, the upper critical dimension, and the lack of time reversal symmetry in this model seem to exclude the possibility of further crossovers to an ultimate DP critical behavior. Finally, the insensitivity to parity conservation in binary production models brings up the question of insensitivity for other conservation laws as well, hence binary production, diffusive models with global particle number conservation may belong to the same class.

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