

Moment ratios for the pair-contact process with diffusion

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(Received 22 May 2006; published 31 July 2006)

We study the continuous absorbing-state phase transition in the one-dimensional pair contact process with diffusion (PCPD). In previous studies [Dickman and de Menezes, *Phys. Rev. E* **66**, 045101(R) (2002)], the critical point moment ratios of the order parameter showed anomalous behavior, growing with system size rather than taking universal values, as expected. Using the quasistationary simulation method we determine the moments of the order parameter up to fourth order at the critical point, in systems of up to 40 960 sites. Due to strong finite-size effects, the ratios converge only for large system sizes. Moment ratios and associated order-parameter histograms are compared with those of directed percolation. We also report an improved estimate [$p_c=0.077\ 092(1)$] for the location of the critical point in the nondiffusive pair contact process.

DOI: [10.1103/PhysRevE.74.011124](https://doi.org/10.1103/PhysRevE.74.011124)

PACS number(s): 02.50.Ga, 05.10.-a, 05.40.-a, 05.70.Ln

I. INTRODUCTION

The pair contact process (PCP) [1] is a nonequilibrium stochastic model that exhibits a phase transition to an absorbing state [2–4]. Several studies have established that the PCP belongs to the robust directed percolation (DP) universality class [5]. In contrast with the contact process, which has the vacuum as its unique absorbing state, the PCP exhibits an infinite number of absorbing configurations, since both creation and annihilation require a nearest-neighbor pair of particles. Allowing particles in the PCP to hop on the lattice, one obtains the so-called pair contact process with diffusion (PCPD). Here there are only two absorbing states: the vacuum, and the subspace with only a single particle.

While a version of the pair contact process with diffusion was proposed by Grassberger in 1982 [6], current interest in the problem follows its rediscovery by Howard and Täuber [7] who questioned the validity of the Langevin description for this process. The first numerical studies of the PCPD [8] suggested that critical the PCPD would fall in the “parity conserving” (PC) class, but increasing computational effort revealed that this was not the case, and that the critical behavior of the model was masked by huge corrections [9,10]. Since then, diverse scenarios, some of them contradictory, have been proposed in order to clarify this question. At present there are two principal schools of thought: in one, the PCPD belongs to a universality class distinct from DP, with a unique set of critical exponents, or possibly continuously varying exponents due to a marginal perturbation [11–13]. The opposing school holds that the PCPD should be attracted to a DP fixed point after a huge crossover time [14,15]. A recent review on these and other scenarios can be found in Ref. [16]. In this work we study the PCPD via quasistationary (QS) simulations [17], focussing on the order parameter and its moments.

The balance of this paper is organized as follows: In the next section we review the definition of the model and detail

our simulation method. In Sec. III we present our results, and Sec. IV is devoted to discussion and conclusions.

II. MODEL AND SIMULATION METHOD

The PCP is defined on a lattice, with each site either occupied or vacant. All changes of configuration involve a pair of particles occupying nearest-neighbor sites, called a *pair* in what follows. A pair annihilates itself at a rate of p , and with rate $1-p$ creates a new particle at a randomly chosen site neighboring the pair, if this site is vacant. In the PCPD, in addition to the creation and annihilation processes already mentioned, each particle attempts to hop, at rate D , to a randomly chosen nearest-neighbor (NN) site; the move is accepted if the target site is vacant. The PCPD exhibits a continuous phase transition to the absorbing state, at a critical annihilation rate $p_c(D)$. Several variants of the model, differing in how each process (creation, annihilation or diffusion) is selected, have been studied in the literature [16]. Here we use the implementation of Ref. [11]. The model is defined on a ring of L sites. We maintain a list of pairs to improve efficiency. At each step of the evolution we first choose between diffusion (with probability D) and reaction (with probability $1-D$). In a reaction step, we select a pair at random, and choose between creation and annihilation with probabilities p and $1-p$, respectively. If we choose diffusion, a particle is selected at random; it attempts to hop to one of its neighbor sites (if the latter is vacant). The time increment associated with each step is $\Delta t=1/(N_{\text{pair}}+DN_{\text{part}})$, where N_{pair} and N_{part} are the number of pairs and particles in the lattice at time t . Thus each lattice site is effectively visited once (on average) per time unit. The most obvious definition of the order parameter in the PCPD is the *pair density* ρ_2 , the number of pairs per site. Since creation (and destruction) of particles requires pairs, one might expect the particle density ρ_1 to scale in a similar manner. (We in fact confirm numerically that ρ_1 and ρ_2 exhibit similar scaling properties.)

In the studies reported here we sample the *quasistationary* (QS) distribution of the process (that is, conditioned on survival), which is very useful in the study of processes with an absorbing state. (In fact, conventional simulations of “sta-

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tionary” properties of lattice models with an absorbing state actually study the quasistationary regime, given that the only true stationary state for a finite system is the absorbing one). We employ a recently devised simulation method that yields quasistationary properties directly [17]. This is done by maintaining, and gradually updating, a set of configurations visited during the evolution; when a transition to the absorbing state is imminent the system is instead placed in one of the saved configurations. Otherwise the evolution is exactly that of a conventional simulation. (The updating of the set of saved configurations is done by replacing, at each time step, with a small probability p_{rep} one of the saved configurations with the current one.)

The above scheme was shown [17] to yield precise results, in accord with the exact QS distribution for the contact process on a complete graph, and with conventional simulations of the same model on a ring [17]. The scheme has also been shown to yield results that agree, to within uncertainty, with the corresponding results of conventional simulations for a sandpile model [18]. The advantage of the method is that a realization of the process can be run to arbitrarily long times. Thus, whereas in conventional simulations a large number of realizations must be performed to have a decent sampling of the (quasi)stationary state, here every realization provides useful information, once the initial transient has relaxed. This leads to an order of magnitude improvement in efficiency, in the critical region. For further details on the method see Ref. [17].

The PCPD dynamics is characterized by (1) single-particle diffusion and (2) reactions involving a pair, motivating us to ignore the “purely diffusive” subspace. This means that we modify slightly the dynamics of the model, *restricting it to the subspace with at least one pair*, which we call the *reactive* subspace. The motivations for studying the modified process are as follows: (1) In Ref. [11] excluding the subspace without pairs yielded better behaved moment ratios; (2) eliminating the large fraction of time expended on the nonreactive intervals yields a major improvement in efficiency. We may further justify our choice by noting that any scaling properties necessarily involve reactions, that is, the existence of pairs.

We impose this restriction as follows. The initial configuration (all sites occupied) has a large number of pairs. Applying the QS simulation method, we accumulate a list of configurations during the evolution. Then, whenever a visit to a configuration (absorbing or not) without pairs is imminent, the system is instead placed in a configuration selected randomly from the list. In other words, the QS method, previously used to sample quasistationary properties, is used here to *restrict* the dynamics to the subspace of interest. A subtle difference between the two applications of the method is that, while in the usual QS simulations [17] the method provides a just sampling of properties conditioned on survival, in the present case we eliminate certain nonabsorbing configurations (and the histories involving them) as well. For the reasons given above, we do not expect this to color our results for large system sizes.

III. SIMULATION RESULTS

We performed extensive simulations of the PCPD on rings of $L=1280, 2560, \dots, 40960$ sites, using the QS

TABLE I. Critical exponent values for the PCP, PCPD, and DP. DP values from Ref. [23].

D	p_c	β/ν_{\perp}	z
0 (PCP)	0.077092(1)	0.2519(3)	1.584(7)
0.1	0.106405(15)	0.505(10)	2.08(15)
0.5	0.120354(3)	0.385(11)	2.04(5)
0.85	0.129925(8)	0.386(5)	1.88(12)
DP		0.25208(5)	1.5807(1)

method restricted to the reactive subspace. Each realization of the process is initialized with all sites occupied, and runs for 10^9 time steps. Averages are taken in the QS regime, after discarding an initial transient which depends on the system size. In practice we accumulate histograms of the time during which the system has exactly $1, 2, \dots, n, \dots$ pairs, and similarly for particles. The histograms are used to evaluate moments; we denote by $m_{j,1}$ the j th moment of the particle number probability distribution; $m_{j,2}$ denotes the corresponding moment of the pair number distribution. (Thus the order parameter ρ_2 could also be denoted $m_{1,2}$.) The QS lifetime τ is taken as the mean time between attempts to leave the reactive subspace.

The number of saved configurations ranges from 10 000, for $L=1280$, to 500 for $L=40960$. Values of p_{rep} range from 10^{-4} to 2×10^{-6} . (During the relaxation phase we use a p_{rep} 10 times larger, to eliminate the influence of the initial configuration.) The results of QS simulations were found to agree with results of conventional simulations [11], for system sizes $L=80, 160, \dots, 1280$. We study three diffusion rates, $D=0.1, 0.5$, and 0.85 , as in Ref. [11]. For comparison, we also study the (nondiffusive) PCP, whose scaling properties are known to be those of directed percolation. The QS results for the $D=0$ case confirm DP behavior in the nondiffusive PCP, as can be verified from the values of the exponents and moment ratios listed in Tables I and II. Further, we improved the estimate for the critical point of the PCP, obtaining $p_c=0.077092(1)$. (This is consistent with the previous best estimate, $p_c=0.077090(5)$, of Ref. [19].)

The first step in analyzing our results is to determine, for each D value studied, the critical annihilation probability $p(D)$. We use the following criteria for criticality: power-law dependence of (1) ρ_1 and ρ_2 and (2) τ on system size L (i.e., the usual finite-size scaling relations $\rho \sim L^{-\beta/\nu_{\perp}}$ and $\tau \sim L^z$); (3) constancy of the moment ratio $r_{211;2} \equiv m_{2;2}/m_{1;2}^2$ with system size. The three criteria were found to be mutually consistent within the error margins. Figure 1 shows the data for ρ_2 for $D=0.5$; the QS order parameter for various p values near p_c is plotted versus L on log scales. The data for the four largest sizes are well fit by a straight line of slope $-\beta/\nu_{\perp} = -0.385$. Plotting $L^{\beta/\nu_{\perp}}\rho_2$ (see inset), allows us to eliminate as off-critical p values for which the plot shows a significant curvature, leading to the estimate $p_c = 0.120353(2)$. A similar analysis of the particle density ρ_1 yields $p_c = 0.120357(5)$ while that for the lifetime τ gives $0.120352(3)$, leading to the overall best estimate $p_c = 0.120354(3)$ for $D=0.5$. For all three diffusion rates stud-

TABLE II. Critical moment ratio values for the PCP, PCPD, and the DP, parity-conserving (PC), and conserved-DP (CDP) universality classes.

D	$r_{211;2}$	$r_{312;2}$	$r_{422;2}$	K_4/K_2^2	Reference
0 (PCP)	1.1738(2)	1.303(3)	1.558(2)	-0.493(3)	[19]
0.1	1.140(15)	1.27(2)	1.55(3)	0.1(2)	This work
0.5	1.166(8)	1.310(15)	1.61(2)	0.0(1)	This work
0.85	1.170(6)	1.31(1)	1.61(4)	-0.1(1)	This work
DP	1.1736(2)	1.301(3)	1.554(2)	-0.505(3)	[19]
PC	1.3340(4)				[11]
CDP	1.142(8)				[18]

ied, the values of β/ν_\perp from analysis of ρ_1 and ρ_2 agree to within uncertainty. [For $D=0.5$, for example, we find $\beta/\nu_\perp = 0.378(11)$ and $0.385(11)$, respectively, using the particle and pair densities.]

Analysis of the moment ratio is also useful in setting limits on p_c : As can be seen in Fig. 2, this quantity appears to grow with system size for $p < p_c$, and vice versa. For $D=0.85$, for example, we find $p_c=0.129\,92(1)$ from analysis of ρ_2 , $p_c=0.129\,93(1)$ from analysis of τ , and $p_c=0.129\,925(8)$ from analysis of the moment ratio $r_{211;2}$. (For $D=0.5$, on the other hand, the moment ratio data do not yield an estimate of precision comparable to that furnished by ρ_1 , ρ_2 , and τ .)

As a check on our procedure for determining p_c , we also performed, for $D=0.85$ initial decay studies [20,21]. In these studies the order parameter ρ_2 is followed as a function of time, starting, as in the other studies, with all sites occupied. (In this case the system does not leave the reactive subspace on the time scale of the simulation so the QS procedure is not needed.) Here the expected behavior is $\rho_2 \sim t^{-\theta}$. Using deviations from the power law to identify off-critical values, a study of systems of 10^6 sites, to a maximum time of 10^8 ,

yields $p_c=0.129\,915(15)$, fully consistent with the QS results. Analysis of the data for $t \geq 5 \times 10^5$ furnishes $\theta = 0.19(1)$, consistent with previously reported results [13,20].

Our present estimates for p_c are slightly lower than those reported in Ref. [11], a difference of less than 0.1%. These differences highlight the strong finite-size corrections affecting the PCPD (in Ref. [11] system sizes range from 80 to 1280), and appear in other absorbing state problems, such as the restricted sandpile model [18].

Using our results for the three largest system sizes ($L=10\,240$, $20\,480$, and $40\,960$) we obtain estimates for the critical exponent ratios β/ν_\perp and $z=\nu_\parallel/\nu_\perp$. These are reported in Table I. The chief contribution to the uncertainties in the exponent ratios comes from the uncertainty in p_c . We note that although the exponent z appears to depend systematically on diffusion rate D , our results are in fact consistent with $z=2$ in all cases. By contrast, the value of β/ν_\perp for $D=0.1$ is significantly different than that found for $D=0.5$ and 0.85 . The latter value [$\beta/\nu_\perp=0.385(11)$] does not yield a good fit to the data for $D=0.1$ even if a logarithmic correction term is introduced in the fitting function.

In nonequilibrium statistical physics, obtaining values for moment ratios has proved an efficient method for identifying the universality class [19]. Here we analyze, in addition to $r_{211;2}$ mentioned above, the ratios

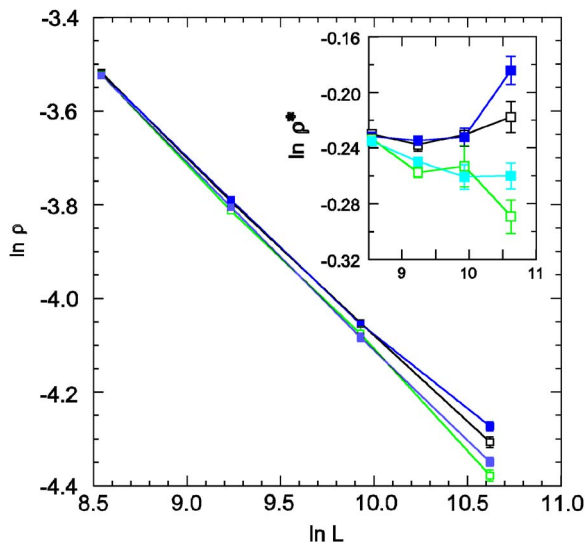


FIG. 1. (Color online) Quasistationary order parameter versus system size for $p=0.120\,345$, $p=0.120\,350$, $p=0.120\,355$ and $p=0.120\,360$, from top to bottom. $D=0.5$. Inset, $\ln L^{\beta/\nu_\perp} \rho$ versus $\ln L$ for the same values of p .

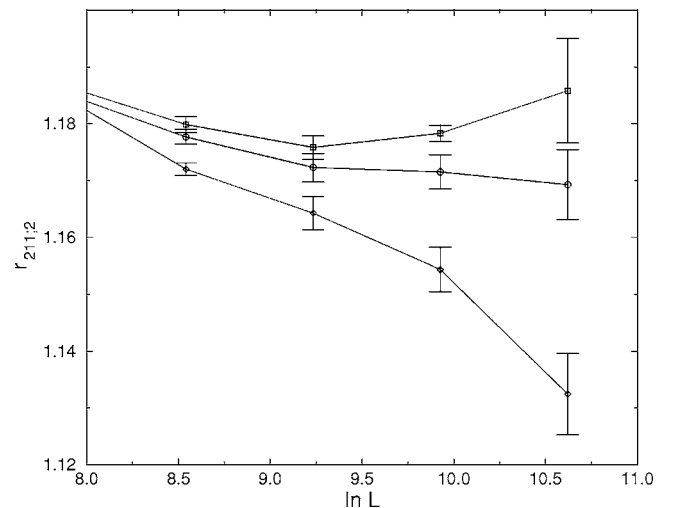


FIG. 2. Quasistationary moment ratio $r_{211;2}$ versus system size for $p=0.129\,90$, $p=0.129\,93$, and $p=0.129\,95$, from top to bottom $D=0.85$.

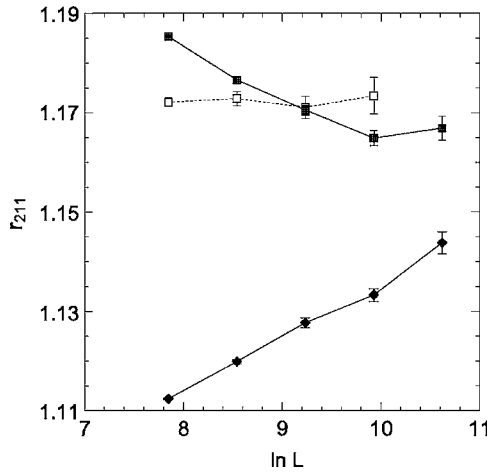


FIG. 3. Moment ratios $r_{211;2}$ (pairs), (upper set), and $r_{211;1}$ (particles), (lower set) versus $\ln L$ for $p=0.120354$ and $D=0.5$. Dashed line, moment ratio $r_{211;2}$ for the critical PCP.

$$r_{312;2} \equiv \frac{m_{3;2}}{m_{2;2}m_{1;2}} \quad (1)$$

and

$$r_{422;2} \equiv \frac{m_{4;2}}{m_{2;2}^2} \quad (2)$$

and the corresponding ratios for particles. Scaling arguments imply that such ratios assume universal values at the critical point, as has been amply verified in equilibrium, and for models with an absorbing state such as the contact process and the PCP [19]. Analysis of such ratios is of particular interest in the present context, given the perplexing result of Ref. [11], namely, apparently *unlimited growth* in $r_{211;2}$ with increasing system size, suggesting that the PCPD does not follow the usual scaling behavior observed at absorbing-state phase transitions. The present large-scale simulations show that the PCPD moment ratios do in fact exhibit the expected behavior.

Figure 3 shows the moment ratios for pairs and particles in the critical PCPD, with $D=0.5$ and the PCP. On the basis of these data we estimate $\lim_{L \rightarrow \infty} r_{211;2} = 1.166(8)$ for the PCPD with $D=0.5$. While the results for $r_{211;2}$ appear to converge for the system sizes studied, the data for the *particle* moment ratio $r_{211;1}$ continue to grow with system size and cannot be extrapolated to the infinite-size limit. (We note in passing that the values for particles and pairs suggest that the two ratios become equal at a system size on the order of 5×10^5 , for $D=0.5$. Since universality implies similar scaling of particle and pair densities at the critical point, we may take this as an order of magnitude estimate for the system size at which corrections to scaling are finally superseded. The moment ratio data for $D=0.85$ are consistent with this estimate, while those for $D=0.1$ suggest convergence only at even larger sizes, on the order of $L \sim 10^7$.) Table II lists estimates of the limiting ($L \rightarrow \infty$) moment ratios for the PCPD and some other known universality classes. The ratios for $D \geq 0.5$ are rather similar to those for directed percolation.

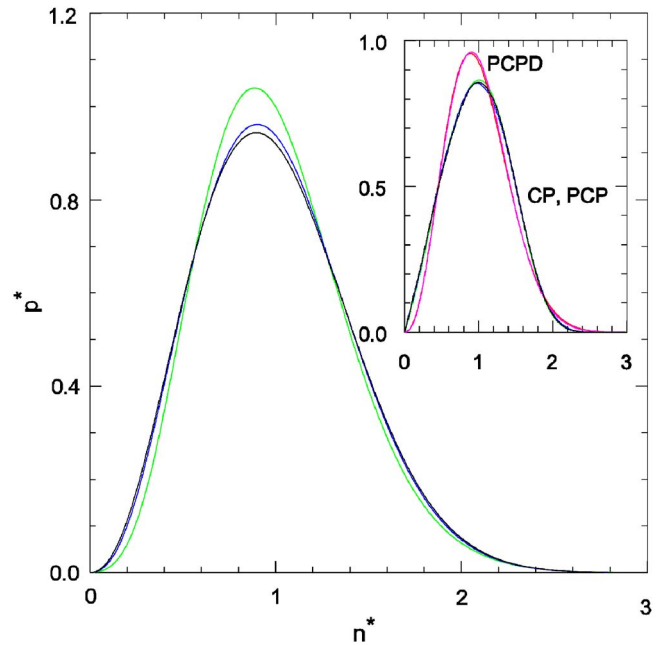


FIG. 4. (Color online) Scaled histograms for the critical PCPD with $D=0.1, 0.5$, and 0.85 (from top to bottom). Inset, scaled histograms for the critical PCPD ($D=0.5$, $L=10240$ and 20480), the critical CP (same sizes) and the critical PCP ($L=10240$).

The cumulant ratio K_4/K_2^2 (here K_j denotes the j th cumulant of the order parameter probability distribution) is not in good accord with the DP value, although the estimates for the PCPD are rather imprecise.

Another quantity that is useful for determining the universality class is the scaled order parameter histogram, defined as $p^*(n^*) = \bar{n}p(n)$, where n denotes the number of pairs and \bar{n} its mean value. (Here $n^* \equiv n/\bar{n}$.) Figure 4 compares the scaled histograms for the PCPD with $D=0.1, 0.5$, and 0.85 . The latter two are quite similar, while the curve for low diffusion rate has a somewhat narrower peak. In the inset of Fig. 4 we compare the scaled histogram for the PCPD with $D=0.5$ to that of the critical contact process and PCP. While the CP and PCP have virtually identical histograms, it is clear that even for the largest sizes studied the PCPD histogram is very different. (A striking difference between the PCPD on the one hand and CP/PCP on the other is the behavior near $n^*=0$: in the latter case the probability increases linearly with n , while former exhibits a distinctly parabolic shape. The parabolic form is not an artefact of the QS simulation method, as it is already observed in Ref. [11], using conventional simulation.)

In the case of $D=0.85$, we accumulated data for several values of the annihilation rate p in the vicinity of p_c . This permits us to estimate the correlation length exponent ν_\perp , using the finite-size scaling relation

$$m(\Delta, L) \propto \mathcal{F}_m(L^{1/\nu_\perp} \Delta), \quad (3)$$

where $\Delta = p - p_c$ and \mathcal{F}_m is a scaling function. This leads to

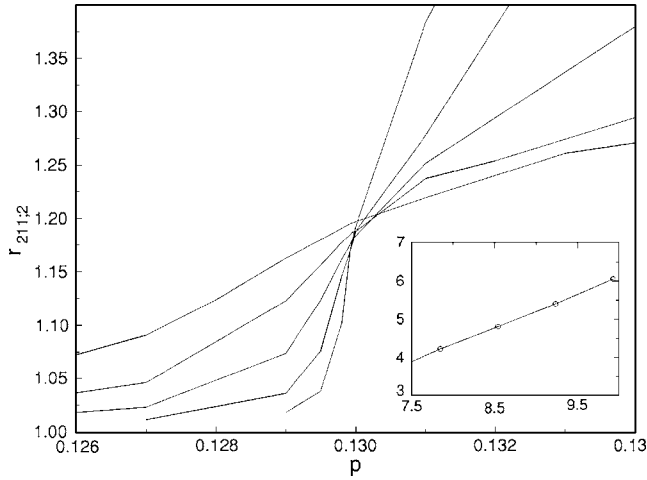


FIG. 5. Quasistationary moment ratio $r_{211;2}$ versus p for system sizes $L=1280, L=2560 \dots L=20480$ and $D=0.85$. Inset, $\ln \partial m / \partial p$ versus $\ln L$ at criticality.

$$\left. \frac{\partial m}{\partial p} \right|_{p_c} \propto L^{1/\nu_{\perp}}. \quad (4)$$

The data of Fig. 5 yield the estimate $\nu_{\perp} = 1.09(1)$, confirming the results of Ref. [11].

IV. DISCUSSION

We perform large-scale simulations of the pair contact process with diffusion, and find that ratios of various moments of the order parameter approach finite limiting values for large system sizes, allowing us to present the first numerical estimates of such ratios for this model. This resolves the apparent anomaly reported in [11], of a moment ratio growing without limit.

Two basic questions prominent in recent discussions of the PCPD are (1) Does the model exhibit continuously variable critical exponents, or a unique set, independent of diffusion rate D ? (2) In the latter case, are the exponents those of directed percolation? Despite the large computational effort, we are unable to answer these questions definitively. Our results nevertheless provide some clues. With regard to the first question, the results reported in Tables I and II show very good agreement for the two larger diffusion rates studied ($D=0.5$ and 0.85), but those for $D=0.1$ are quite different. Our values for the critical exponents are consistent with earlier studies ([11,12] for low D and [11,22] for high D).

For low diffusion rate ($D=0.1$) we find evidence of stronger corrections to scaling, and/or a slower rate of convergence with increasing L , as noted above in the analysis of the moment ratios. Our results of $z=2.08(15)$ and $\beta/\nu_{\perp}=0.505(10)$ are consistent with previous results for low-diffusion rate [11,12]. While this argues in favor of nonuniversal behavior, we cannot rule out the possibility of a unique set of exponents, as suggested, for example, by Ódor

[22], who asserted that, including a logarithmic correction, the same value for β/ν_{\perp} holds for both high and low diffusion rates. (We note, however, that we were unable to fit all the data using the same value for β/ν_{\perp} , even including a logarithmic correction.) In our opinion, it is still unclear if the observed difference in the exponents and moment ratios for $D=0.1$, as compared with larger diffusion rates, is due to corrections to scaling. Such corrections would have to be exceptionally large to account for the observed differences, and must exhibit a rather irregular behavior, given the close agreement in the results for $D=0.5$ and 0.85 . An equally if not more natural interpretation is that the critical exponents and moment ratios really do depend on D .

If we accept, provisionally, that the PCPD critical properties are independent of D (with huge corrections to scaling for small diffusion rates), it is still not obvious that these properties are characteristic of the DP universality class. The values for β/ν_{\perp} and z are quite far from those of DP, even for larger diffusion rates, where corrections to scaling appear to be less severe. It is true that our estimates for ν_{\perp} (for $D=0.85$), and for the moment ratios (for both $D=0.5$ and 0.85) are close to the DP values, but the qualitatively different form of the order parameter histograms again prevents identification of the PCPD as belonging to the DP universality class, even for higher diffusion rates. Thus our results tend to support the conclusion of Ref. [21], that PCPD scaling is distinct from that of DP.

Large-scale studies of time-dependent behavior [20] suggested a value for the initial decay critical exponent θ different from that of DP. A subsequent study [15] led to the suggestion that apparent values of critical exponents vary as one increases the simulation time and system size, reflecting strong corrections to scaling, and that observed exponent values be interpreted as upper limits on the true values. The results of the quasistationary simulations are not affected by finite-time corrections, although finite size effects are still present.

In summary, we have applied the quasistationary simulation method to the pair contact process with diffusion, restricted to the subspace with at least one pair. Our results indicate that the anomalous behavior of the critical order-parameter moment ratios does not persist for large systems. Restricting the dynamics to the reactive sector, these ratios appear to converge to finite values, as expected. Taken at face value our results imply a variation of scaling properties with diffusion rate, but the opposite interpretation is tenable if one invokes strong corrections to scaling for small D . Regardless of whether or not the critical exponents vary with D , it seems premature to conclude that the PCPD will eventually cross over to the DP class.

ACKNOWLEDGMENTS

The authors are grateful to Géza Ódor and Haye Hinrichsen for helpful comments. This work was supported by CNPq and FAPEMIG, Brazil.

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