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Nonuniversality in the pair contact process with diffusion

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We study the static and dynamic behavior of the one dimensional pair contact process with diffusion. Several critical exponents are found to vary with the diffusion rate, while the order-parameter moment ratio $m=\overline{\rho^2}/\overline{\rho}^2$ grows logarithmically with system size. The anomalous behavior of m is traced to a violation of scaling in the order parameter probability density, which in turn reflects the presence of *two distinct sectors*, one purely diffusive, the other reactive, within the active phase. Studies restricted to the reactive sector yield precise estimates for exponents β and $\nu_\perp$, and confirm finite size scaling. We also determine the value $m_c=1.334$ for the parity-conserving universality class in one dimension.

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The pair contact process (PCP) [1,2] is a nonequilibrium stochastic model which, like the basic contact process (CP) [3–5], exhibits a phase transition to an absorbing state. While the absorbing state in the contact process corresponds to a unique configuration (an empty lattice), the PCP possesses infinitely many. Numerical and theoretical studies, nevertheless, indicate that the PCP belongs to the same universality class as the CP [namely, that of directed percolation (DP)], but with anomalies in the critical spreading dynamics [1,2,6–12]. An infinite number of absorbing configurations arise in the PCP because all processes (creation and annihilation), require a nearest-neighbor (NN) pair of particles (to be referred to simply as a ''pair'' in what follows). If individual particles are allowed to hop on the lattice, however, there are but two absorbing states: the empty lattice, and the state of a single particle hopping.

Study of the diffusive pair contact process (PCPD) was stimulated by the observation of Howard and Täuber [13] that its Langevin description would involve complex noise. On the basis of numerical results in their pioneering density-matrix renormalization group study, Carlon *et al.* [14], noted that certain critical exponents in the PCPD had values similar to those known for the parity conserving (PC) universality class. Hinrichsen [15] reported simulation results inconsistent with the PCPD being in the PC class, and proposed that the model defines a *distinct* class. In particular, while models in the PC class possess two symmetric absorbing states, the two absorbing states of the PCPD are not related by any symmetry. Interestingly, Park *et al.* found that even when such a symmetry is imposed on the PCPD, its critical exponents remain different from those of the PC class [16]. The distinctive behavior of the PCPD was further confirmed in simulations by Ódor [17], who presented evidence for the existence of two universality classes (for diffusion probabilities greater than, or less than, about 0.3). Henkel and Schollwöck, suggested, on the basis of a study of universal finite-size scaling amplitudes, that for finite diffusion rates, the critical behavior of the PCPD belongs to a single universality class [18]. In a further variant of the PCPD, critical exponents are found to vary with the survival probability for newly created pairs [19]. Our goal in this Rapid Communication is to shed some light on this rather confusing situation by studying moment ratios and probability distributions in the critical PCPD.

The PCP is defined on a lattice, with each site either occupied (by a ''particle'') or vacant. Only pairs of occupied sites exhibit activity; each has a rate of p of mutual annihilation, and a rate of $1-p$ to create a new particle at a NN site, if this site (chosen at random) is vacant. For $p>p_c$ [$\simeq 0.077\,090(5)$ in one dimensional [6]), the system falls into the absorbing state (all activity ceases). The order parameter is the density of pairs.

In the PCPD, in addition to the creation and annihilation processes described above, each particle attempts to hop, at rate D, to a randomly chosen NN site; the move is accepted if the target site is vacant. The model again exhibits a continuous transition to the absorbing state, at a critical annihilation rate $p_c(D)$ that increases with the diffusion rate. Once particles are allowed to diffuse, the nature of the system changes radically. The absorbing state is modified as noted above, and the order parameter is now the particle density not the pair density. In contrast to simpler models like the CP, in which diffusion does not alter the critical behavior [20,21], diffusion represents a *singular perturbation* in the PCP.

We perform extensive simulations of the one-dimensional PCPD, using systems of $L=20,\ 40,\ \ldots,1280$ sites, with durations of 10^4–4×10^6 time steps, and sample sizes of 10^4–10^6 realizations. Initially all sites are occupied. We determine the mean particle density $\overline{\rho}$, and pair density $\overline{\rho_p}$, the moment ratio $m=\overline{\rho^2}/\overline{\rho}^2$, and the survival probability $P_s(t)$. (The overline denotes a stationary average.) The exponential decay of the latter permits us to determine the lifetime τ.

Experience with absorbing-state phase transitons leads us to expect the following scaling properties at the critical point: $\overline{\rho}\sim L^{-\beta/\nu_\perp}$; $\tau\sim L^{\nu_\parallel/\nu_\perp}$; and $m\to m_c$, a universal critical value [6]. We use power-law dependence of $\overline{\rho}$ on system

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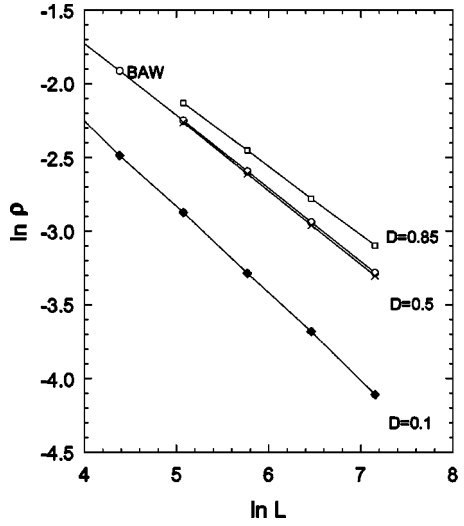

FIG. 1. Particle density ρ vs system size at the critical point in the PCPD and the BAW model.

size to determine the critical annihilation rate $p_c(D)$. For comparison, we applied the same algorithm to the parity-conserving branching-annihilating random walk (BAW) model studied by Zhong and ben-Avraham [22].

Figure 1 shows the scaling of the order parameter with system size, at the critical point, for the PCPD and the BAW; in the PCPD, $\beta/\nu_\perp$ decreases with increasing diffusion rate. (The similarity between the PCPD with $D=0.5$ and the BAW appears to be a coincidence; the scaling of τ is quite different in the two cases.) Figure 2 shows that while the moment ratio m attains a limiting value in the BAW model, it *grows* with L in the PCPD (roughly, $\sim \ln L$), a most unusual behavior. Using the extrapolation procedure of Ref. [6], we find $m_c=1.3340(4)$ for BAW [$m_c=1.1735(5)$ DP in 1+1 dimensions [6]].

At the critical point, the probability distribution $P(\rho;L)$ is expected to exhibit scaling, $P(\rho;L)=\overline{\rho}\mathcal{P}(\rho/\overline{\rho})$ ($\mathcal{P}$ is a normalized scaling function), as was verified for the PCP without diffusion [2]. In the PCPD, the steady growth of m_c with system size precludes scaling. The particle and pair probability distributions, shown (for $D=0.1$) in Fig. 3, evidently do not scale. Instead, the most probable particle number is always 2, and the overwhelmingly most probably number of pairs is *zero*, independent of system size. The distributions exhibit a tail that grows broader with increasing system size; these ''tail events'' are responsible for the observed critical behavior. The tails, which have a Gaussian form, again violate the scaling relation. (The pair distribution exhibits a second maximum, away from $\rho_p=0$, at a value that increases roughly as $L^{0.6}$.)

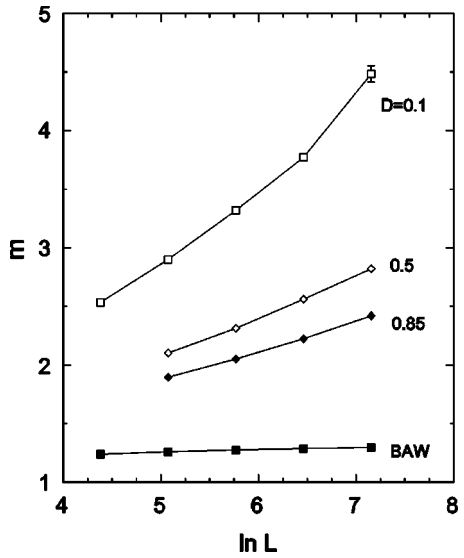

FIG. 2. Moment ratio m vs system size at the critical point in the PCPD and the BAW model.

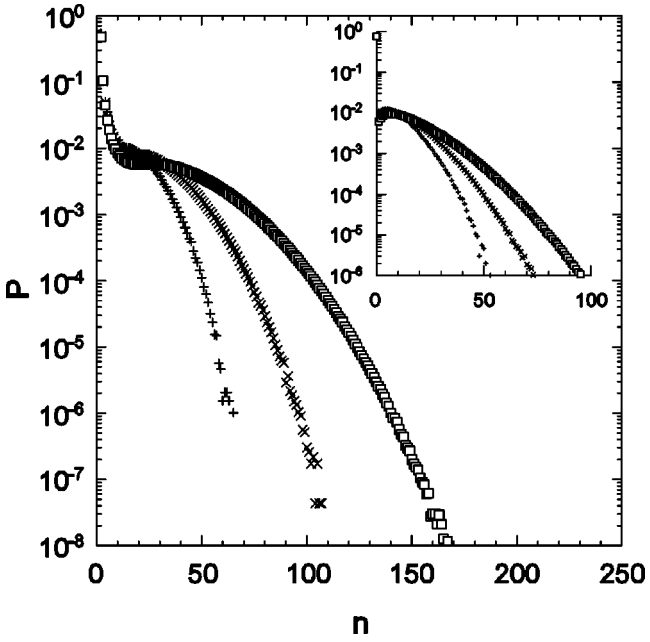

FIG. 3. Probability distribution of the number of particles n at the critical point, for $D=0.1$; +, $L=80$; ×, $L=160$; □, $L=320$. The inset shows the corresponding probability distributions for the number of pairs, n_p. Note that the most probable value of n_p is zero.

The particle and pair probability distributions confirm lack of scaling, and, perhaps more importantly, provide a clue to the enigmatic behavior of the process. In the PCPD, being in the active (i.e., nonabsorbing) state implies that there are at least two particles, but not neccessarily any pairs; at p_c, the process apparently favors configurations with no pairs. (For $D=0.1$, for example, the probability of having no pairs is about 0.8, and shows no sign of decreasing as L grows; for $D=0.5$ this probability is about 0.58, and for $D=0.85$, about 0.5.) In this ''purely diffusive'' sector, the activity is that of a set of random walkers, but the particle number does not change, and critical fluctuations are not generated. From time to time the system ventures into the ''reactive'' sector (at least one pair), and may exhibit a burst of creation and annihilation reactions. We expect the latter activity to possess scale invariance at p_c. Since $P(\rho;L)$ is a superposition of distributions associated with the two sectors, lack of scaling is quite understandable. In the purely diffusive sector, the particle-number distribution is highly

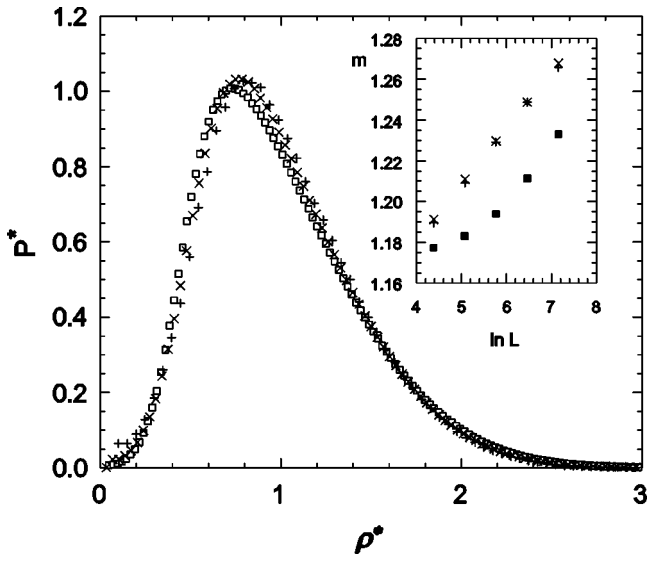

FIG. 4. Scaling plot of the probability distribution in the reactive sector, at the critical point, for the same parameter values as in Fig. 3. Inset: moment ratio m vs system size in the reactive sector; filled squares, $D=0.1$; $+$, $D=0.5$; $\times$, $D=0.85$.

peaked at $n=2$, with a mean value of 3.2–3.5, independent of system size.

These observations motivate us to *exclude* the purely diffusive sector by studying properties *conditioned on having at least one pair* in the system, as was done in Ref. [19] for different reasons. Note that this does not modify the dynamics of the system in any way; we simply restrict the averages to configurations having one or more pairs. Figure 4 shows the order parameter distribution in the reactive sector, plotted in the reduced variables $\rho^*=\rho/\overline{\rho}$ and $P^*=\overline{\rho}P$. The distribution is now similar to that found in the nondiffusive PCP [2], with a maximum at a nonzero value of the order parameter, and shows evidence of scaling. Thus the behavior in the reactive sector is much closer to that familiar from the contact process and the PCP.

Closer examination reveals, however, that the scaling collapse is imperfect. Studies of larger systems confirm that the maximum of the scaled order parameter distribution gradually shifts to smaller values of ρ^*, and that the distribution becomes broader, with increasing L. While we do not claim to have a complete understanding of this ''defect,'' a possible explanation is that for large L, configurations with a single pair represent a system with only a small reactive region, the remainder residing in the purely diffusive sector. We defer a full investigation of this rather subtle question to future work.

TABLE I. Critical exponents for the PCPD and the BAW model; figures in parentheses denote uncertainties. BAW results are taken from Ref. [22].

D	p_c	$\beta/\nu_\perp$	β	$\nu_\parallel/\nu_\perp$	δ
0	0.077090(5)	0.2523(3)	0.2765	1.577(4)	0.1595
0.1	0.10648(3)	0.503(6)	0.546(6)	2.04(4)	0.249(5)
0.5	0.12045(3)	0.430(2)	0.468(2)	1.86(2)	0.236(3)
0.85	0.13003(1)	0.412(2)	0.454(2)	1.77(2)	0.234(5)
BAW		0.497(5)	0.922(5)	1.74(1)	0.286(2)

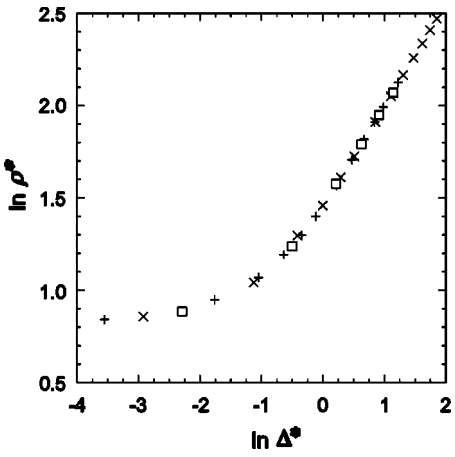

FIG. 5. Scaling plot of the order parameter in the reactive sector for $D=0.1$; $+$, $L=640$; $\times$, $L=1280$; $\square$, $L=2560$.

Once we restrict the sample to the reactive regime, we eliminate a large source of uncertainty (i.e., the erratic switching between the two sectors), and are able to obtain more precise results. Using, as before, the criterion of power-law dependence of $\overline{\rho}$ on system size, we determine the critical parameter p_c and the ratio $\beta/\nu_\perp$ to good precision; these values are given in Table I. Restricting the averages to the reactive sector changes the value of p_c by 0.1% or less. There are more pronounced changes in $\beta/\nu_\perp$: without the restriction, we obtain 0.585, 0.50, and 0.465 for $D=0.1$, 0.5, and 0.85, respectively. (We regard these as poorer estimates, colored by the superposition of the two sectors.) Figure 4 (inset) shows the critical moment ratio m_c versus system size, in the reactive sector. Its value is now comparable (for the system sizes studied here) to that for the DP and PC classes, but a slow growth (roughly linear in $\ln L$) is again evident. (Restricting the sample to configurations with two pairs leads to a reduction in m, but not in its rate of growth with system size.)

A possible weak point in our analysis is that we assume finite size scaling (i.e., the power-law dependence of $\overline{\rho}$ on system size), in determining p_c, whilst the results for m indicate that there is still a (relatively weak) violation of scaling. We therefore check our method by studying the order parameter (again restricted to the reactive sector) in the supercritical regime, $p<p_c$. We verify that the order parameter follows a power law, $\overline{\rho}\sim(p_c-p)^\beta$, and in so doing obtain the estimates for β given in Table I. This exponent decreases steadily with D, as found in Ref. [17]. (A direct comparison with Ref. [17] is not possible since the latter study uses a parallel-update scheme, in contrast to the sequential updating used here.)

In fact, our results verify finite size scaling relation, $\overline{\rho}=L^{-\beta/\nu_\perp}\mathcal{R}(L^{1/\nu_\perp}\Delta)$, where $\Delta=p_c-p$ and the scaling function $\mathcal{R}(x)\sim x^\beta$ for $x\gg 1$; the data collapse is evident in Fig. 5. From this analysis we obtain $\nu_\perp=1.10$, 1.09, and 1.10 for

$D=0.1$, 0.5, and 0.85, respectively, suggesting that this exponent does not vary with the diffusion rate.

We also studied the decay of the particle density starting from a fully occupied lattice at the critical point, restricting the sample to the reactive sector. (In the early stages of the evolution, the probability for the system to be in the reactive sector is nearly unity, but at later times this probability decays much more rapidly than the survival probability itself.) The order parameter decays as $\rho \sim t^{-\delta}$. From a data-collapse analysis of $\rho(t)$, using the finite-size scaling form, $\rho = L^{-\beta/\nu_\perp}\mathcal{F}(t/L^{\nu_\parallel/\nu_\perp})$, we obtain the estimates for $z = \nu_\parallel/\nu_\perp$ listed in Table I. (Without the restriction to the reactive sector we find 1.87(1) for $D=0.1$, 1.82(1) for $D=0.5$ and 0.85. Further results on dynamic properties will be reported in Ref. [23].) Our results satisfy $(\nu_\parallel/\nu_\perp)(\nu_\perp/\beta)\delta = 1$ (as expected, given the scaling relation $\beta = \nu_\parallel \delta$), to within uncertainty.

In summary, we have performed extensive studies of the PCPD, including the probability distributions for the order parameter and number of pairs. Our results clearly exclude the model from both the parity-conserving and the DP universality classes. The criticial exponents β, η, and $\nu_\parallel$ vary with the diffusion rate, while $\nu_\perp$ appears to be independent of this parameter. An interesting open question is whether the PCPD can be described by a single universality class (with unusually strong corrections to scaling) [18], two distinct universality classes (one for high diffusion rates, the other for low, but finite D), as suggested by Ódor [17], or even exponents that vary continuously with D. Our data are not sufficient to distinguish between these hypotheses. We note, however, that we observe relatively little change in the exponent values for $D=0.5$ and 0.85, compared with the changes between $D=0.1$ and 0.5. A similar observation applies to the size dependence of m shown in Fig. 4.

The growth of the moment ratio m with system size signals a violation of scaling in the associated probability distribution, which we have argued is a consequence of there being two sectors, one reactive, the other purely diffusive, within the active phase. Restricting averages to the reactive sector, we find good evidence of finite size scaling of the order parameter, and a much weaker violation of scaling for the probability distribution. We expect that decomposition of configuration space into sectors will prove useful in understanding other systems exhibiting bursts of activity separated by long quiescent periods.

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