Universality in the pair contact process with diffusion

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The pair contact process with diffusion is studied by means of multispin Monte Carlo simulations and density matrix renormalization group calculations. Effective critical exponents are found to behave nonmonotonically as functions of time or of system length and extrapolate asymptotically towards values consistent with the directed percolation universality class. We argue that an intermediate regime exists where the effective critical dynamics resembles that of a parity conserving process.

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I. INTRODUCTION

Out of equilibrium systems may display phase transitions analogous to those found in their equilibrium counterparts. These transitions are classified into distinct universality classes, characterized by a set of critical exponents [1,2]. Particular attention has been paid to one-dimensional systems with transitions from an active state into absorbing states, i.e., frozen configurations from which the system cannot escape. For these systems, so far, only two distinct universality classes have been firmly established: the directed percolation (DP) and the parity conserving (PC) universality class. While the former is ubiquitous and found in several systems with very different dynamical rules, the latter is only known to occur when extra symmetries are present [1,2].

A model which has attracted quite some interest recently, because it may indeed belong to a novel universality class [3] is the so-called pair contact process with diffusion (PCPD). Despite a rather intense activity in the past couple of years [4–12], the understanding of the PCPD and its relation with other known models is still unsatisfactory. In the *fermionic* version of the model—the one studied here—each lattice site is either occupied by a single particle (A) or empty (0). The reactions are

$$\begin{cases} AA0 \to AAA \\ 0AA \to AAA \end{cases} \quad \text{with rate } \frac{(1-p)(1-d)}{2}, \tag{1}$$

$$AA \to 00 \quad \text{with rate } p(1-d),$$

$$A0 \leftrightarrow 0A \quad \text{with rate } d$$

with $0<d<1$, $0<p<1$. The analysis of the critical properties of the PCPD has shown to be much more difficult than all similar models analyzed so far and several scenarios have been proposed. First, a similarity of the exponents $\beta/\nu_\perp$ and $z=\nu_\parallel/\nu_\perp$ (where $\nu_\parallel$ and $\nu_\perp$ are the correlation length exponents along the time and space directions and β the order parameter exponent) with those of the PC class [4] was reported, although in the PCPD there is no conservation of parity. It was later suggested that the PCPD could belong to a new universality class with exponents close to, but different from, the PC values [5]. It has also been argued that there could be two universality classes [6] at small and large diffusion rates (d), or continuously varying exponents [7], or that scaling may even be violated [8]. More recently the option of a slow crossover to DP was also discussed [9], although the general belief is that the PCPD belongs to a novel universality class [7,8,10–12]. Field theoretical methods, which have been successfully applied to other reaction-diffusion models [13] failed so far to clarify the critical properties of the PCPD [3,14].

In this paper we present some insights into the PCPD. We show that accurate numerical results from Monte Carlo (MC) simulations and density matrix renormalization group (DMRG) calculations convincingly demonstrate that for sufficiently long times and system lengths the exponents cross over towards the DP values. Corrections to scaling are, however, rather strong and only an accurate extrapolation of the effective critical exponents allows to identify the final asymptotic critical behavior. We give evidence that in the near-asymptotic region the model shows effective exponents close to the PC class values, which suggests that the critical behavior of the system is described by two competing fixed points.

II. RESULTS ON BULK PARTICLES AND PAIR DENSITIES

Our MC simulations exploit a technique known as multispin coding [15]. The basic idea is that in a simulation of 64 systems, each with L sites, the occupation of site i in the kth simulation is stored in the kth bit of 64-bit word $A[i]$. To perform the reaction $AA0 \to AAA$ in all 64 systems at a randomly chosen site i and its neighbors, one logical operation $A[i+1]=A[i+1] \vee (A[i] \wedge A[i-1])$ suffices, where $\vee$ and $\wedge$ are the logical operations OR and AND, respectively. Other reactions require only slightly more elaborate logical operations. A direct implementation along these lines might result in 64 simulations, each of which statistically correct, but strongly correlated to each other because the site selection is shared. To alleviate this correlation without sacrificing efficiency, we employ random bit patterns that decide which reaction will be attempted in which system. The strong point of multispin coding is its efficiency. As illustrated above, only a few logical operations (each usually carried out in a single clock cycle without delay) suffice to update a site in 64 systems simultaneously. For each combination of d and p

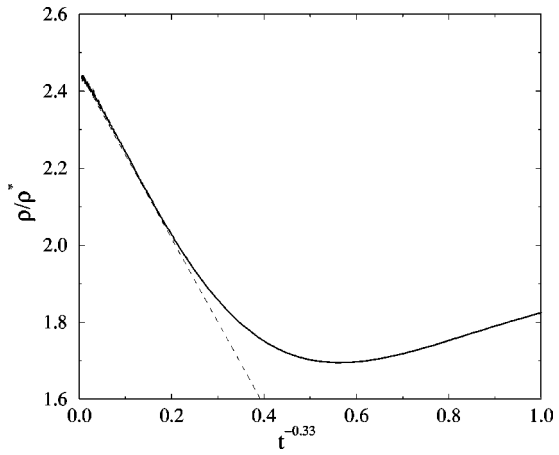

FIG. 1. Ratio of the particle density ρ and pair density ρ^*, as a function of $t^{-\gamma'}$, with $\gamma'=0.33$, for the PCPD with $d=0.5$ and at the estimated critical point $p=0.152\,45$. This ratio approaches a constant.

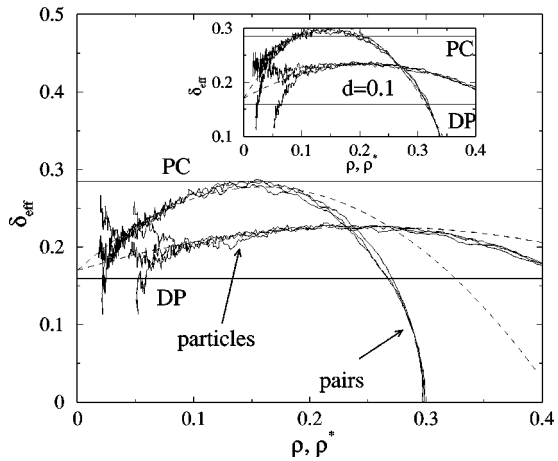

FIG. 2. Plot of $\delta_{\rm eff}$ at $d=0.5$ and $p=0.1524$, $p=0.152\,45$, and $p=0.1525$ (from bottom to top) obtained from the decay of the particles and pairs densities. The dashed lines are parabolic fits to the data. The two horizontal lines show the ratio $\beta/\nu_\parallel$ for the DP and PC class. Inset: $d=0.1$ and $p=0.1110$, $p=0.111\,05$, $p=0.1111$.

we simulated 64 systems with $L=100\,000$ sites over 3×10^6 Monte Carlo time units, in about 15 h on a single-processor workstation. We also simulated 16×64 systems with $L=100\,000$ sites over 10^7 Monte Carlo time units on a parallel computer, for $d=0.5$ and $p=0.152\,45$, our estimate for the critical point.

A standard procedure to obtain critical exponents by means of Monte Carlo simulations is to study the decay of the particle density $\rho(t)$ as a function of time t, starting from a random configuration of particles. At the critical point one has $\rho(t)\sim t^{-\beta/\nu_\parallel}$. To monitor the decay it is convenient to define the effective exponent $\delta_{\rm eff}\equiv-\partial\ln\rho(t)/\partial\ln t$. Typically $\delta_{\rm eff}$ is plotted as a function of $1/t$. At the critical point, in the limit $t\to\infty$, it approaches a finite value ($\delta_{\rm eff}\to\beta/\nu_\parallel$), while it deviates upwards or downwards with respect to this value in the inactive and active phases, respectively. This criterion allows to estimate the critical point location and the ratio $\beta/\nu_\parallel$ [1]. Some care, however, has to be taken when corrections to scaling are particularly strong, for example, when $\rho(t)\sim t^{-\beta/\nu_\parallel}(1+ct^{-\gamma})$ with $\gamma<1$ and c a constant. In this case $\delta_{\rm eff}$ plotted as a function of $1/t$ approaches $\beta/\nu_\parallel$ with an infinite slope. The ideal situation would be to plot $\delta_{\rm eff}$ as a function of $1/t^\gamma$ as in that case the approach to the asymptotic value would be linear. Further on in this paper we will give numerical evidence that the correction-to-scaling exponent γ is close to $\beta/\nu_\parallel$ (which is much smaller than 1). A natural choice is therefore to plot $\delta_{\rm eff}$ as a function of the particle density ρ instead of $1/t$, to avoid infinite slopes.

Besides the decay of the particle density ρ, we also consider the decay of the pair density $\rho^*\equiv\langle AA\rangle$. Before presenting the results for the critical exponents we analyze the behavior of the ratio ρ/ρ^* at the critical point. Such a quantity, which is shown in Fig. 1 for $d=0.5$, approaches a constant value (≈2.45) asymptotically for long times. The most important consequence of this fact is that in PCPD one can extract the critical exponent $\beta/\nu_\parallel$ both from the decay of the particle and pair densities [16]. Numerically the ratio is much better behaved than the individual densities ρ and ρ^*, as fluctuations in the individual densities are highly correlated and largely cancel each other in the ratio.

The data of Fig. 1 also provide an estimate of the leading correction term in the asymptotic limit $t\to\infty$, which appears to be of the type $\rho/\rho^*\sim C(1+Dt^{-\gamma'})$ with $\gamma'\approx0.33$, as shown by the linear approach to the asymptotic behavior of the data when plotted versus $t^{-0.33}$. This exponent is much larger than its equivalent γ in the particle and pair densities, which implies that the leading corrections for ρ and ρ^* cancel in the ratio ρ/ρ^*. We tested that a similar cancellation also occurs in the process $A\to3A$, $2A\to0$, which belongs to the PC universality class [1]: the leading correction in ρ and ρ^* scales as $t^{-0.6}$, whereas the leading correction in the ratio ρ/ρ^* scales as $1/t$.

Figure 2 shows a plot of $\delta_{\rm eff}$ at $d=0.5$ as a function of ρ and ρ^*, calculated in the PCPD from the decay of particles and pairs, respectively. Three different values for p have been plotted around the critical point which we estimate as $p_c=0.152\,45(5)$. For $p>p_c$ (inactive phase) and $p<p_c$ (active phase) $\delta_{\rm eff}$ rapidly veers up and down, as expected. At the critical point, $\delta_{\rm eff}$ approaches the y axis with a finite slope, indicating that the leading correction to scaling is most likely described by an exponent roughly equal to δ itself. A parabolic fit through the data yields as a common estimate for the critical exponent $\beta/\nu_\parallel=0.17$. Similar calculations were repeated for other values of the diffusion coefficient $d=0.05$, 0.1, 0.2, and 0.9 (the inset of Fig. 2 shows the case $d=0.1$), with the same results which we can summarize with the estimate $\beta/\nu_\parallel=0.17(1)$. This value is consistent with the DP class exponent $\beta/\nu_\parallel=0.159$.

An alternative way to calculate critical exponents would be to use a linear fit of the densities versus time on a double-logarithmic scale. However, such fits are hazardous when dealing with very slow convergence, as is the case here, and may lead to wrong estimates for the critical exponents. We illustrate this in Fig. 3 which shows the plot of the average particle density as a function of the time in a double-

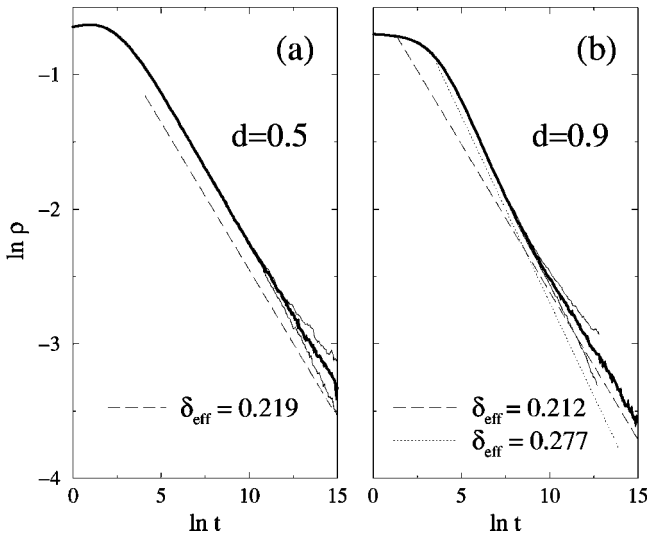

FIG. 3. Log-log plots of ρ (particle density) vs t. (a) $d=0.5$, $p=0.1524$, $p=0.152\,45$, and $p=0.1525$ (from top to bottom). (b) $d=0.9$ and $p=0.2330$, $p=0.2335$, and $p=0.234$ (from top to bottom). The critical point densities are plotted as thick solid lines. The dashed lines are linear fits to the data, shifted for clarity.

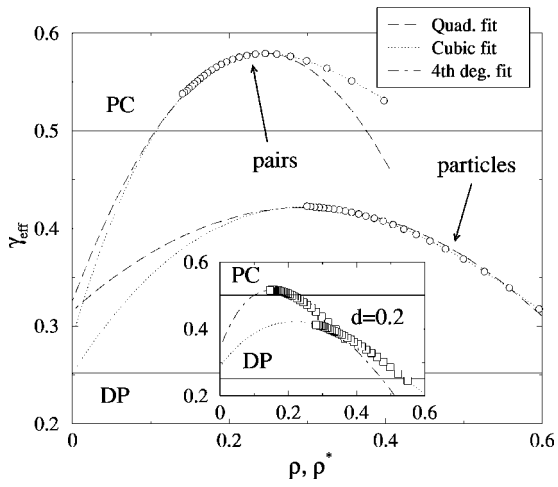

FIG. 4. Plots of $\gamma_{\rm eff}$ for $d=0.5$ at the system critical point ($p=0.152\,45$) for lattices up to $L=60$ calculated from the decay of particle (circles) and pair (squares) densities as function of the lattice lengths. The dotted and dashed lines are fits in powers of the densities. Inset: $\gamma_{\rm eff}$ for $d=0.2$.

logarithmic scale for $d=0.5$ and $d=0.9$. In the former case a straight line (dashed) fits extremely well the critical density decay leading to the estimate $\delta_{\rm eff}=0.219$. The analysis of the effective exponent (see Fig. 2), however, provides a closer inspection of the local slopes of the double-logarithmic data. This analysis reveals some remaining curvature, and the final estimate of the exponent is significantly lower, compared to that obtained from the fit in the double-logarithmic scale. In the case of higher diffusion [see Fig. 3(b)] the curvature is more pronounced and clearly visible also in the double-logarithmic plot, which can be fitted by two straight lines with slopes $\delta_{\rm eff}\approx 0.277$ in the range $4\lesssim \ln t\lesssim 8$, and with $\delta_{\rm eff}\approx 0.212$ for $10\lesssim \ln t\lesssim 15$. Notice that the former exponent is consistent with that expected for the PC class ($\delta_{\rm PC}=0.286$ [1]).

Again an extrapolation of the effective exponent (as done in Fig. 2) shows convergence to a value consistent with DP. Note that the value $\beta/\nu_{\parallel}\approx 0.21$ is consistent with the most recent Monte Carlo estimates for the PCPD [9,11,17]. In particular, Kockelkoren and Chaté [11] performed a series of Monte Carlo simulations for a bosonic version of the PCPD where the constraint of one particle per site is released. Their estimation of critical exponents is based on a straight-line fit to a double-logarithmic plot of ρ versus t, from which they find $\beta/\nu_{\parallel}=0.200(5)$. This bosonic version of the model is claimed to suffer less from corrections to scaling than the fermionic case. Notice, however, that also in the fermionic PCPD studied here the density decay at $d=0.5$ [see Fig. 3(a)] is rather straight in a double-logarithmic plot for simulation times similar to those in Ref. [11]. The advantage of the effective exponent analysis performed here is that it allows to extrapolate the numerical results to time scales *beyond* those actually simulated.

Next we present some DMRG results. DMRG [18] allows to calculate accurate stationary state probabilities for chains of moderate lengths [19]. As usual in DMRG, we used open boundary conditions. In the PCPD on a lattice of finite length there are only two stationary states: a state with no particles and a state occupied by a single diffusing particle. To induce a finite density of particles we added a reaction $0\to A$ at the two boundary sites. The particle density decays from the two boundaries and forms a U-shaped profile. For chains of various lengths we calculated the density of particles $\rho(L)$ and of pairs $\rho^*(L)$ at the central site of a system of length L. At the critical point these quantities decay in the limit $L\to\infty$ as $\rho(L)\sim\rho^*(L)\sim L^{-\beta/\nu_\perp}$.

Figure 4 shows the effective exponent $\gamma_{\rm eff}=-\partial\ln\rho(L)/\partial\ln L$ versus ρ for $d=0.5$ at the critical point. As in Fig. 2, we include also the data for the pairs. Dotted and dashed lines are fits with polynomials in the densities. Again, a test of good convergence is that both exponents extrapolate to the same asymptotic value. This requirement seems indeed to be fulfilled and we find as extrapolation $\beta/\nu_\perp=0.27(4)$. This exponent is again consistent with the DP value $\beta/\nu_\perp=0.252$ [1]. Similar results have also been found for other values of the diffusion coefficient d. Extrapolations for $d=0.2$ are shown in the inset of Fig. 4. At small d the maxima in $\gamma_{\rm eff}$ shift to longer L, thus extrapolations are somewhat less stable. In this case we take the estimate obtained from the particles $\beta/\nu_\perp=0.28(5)$.

Previous DMRG results [4] were restricted to the density of particles and to smaller systems than that studied here. The data for the effective exponent showed a monotonic behavior (except at very strong diffusion) and were analyzed using an extrapolation with polynomes in $1/L$. These extrapolations lead to a value consistent with the PC class exponent $\beta/\nu_\perp=0.50$ [4]. The present calculation, extended to the density of pairs and to longer systems, reveals that nonmonotonicity in the effective exponent is a common feature at all d. This nonmonotonicity leads to a rather strong decrease of the extrapolated exponent compared to the estimates of Ref. [4].

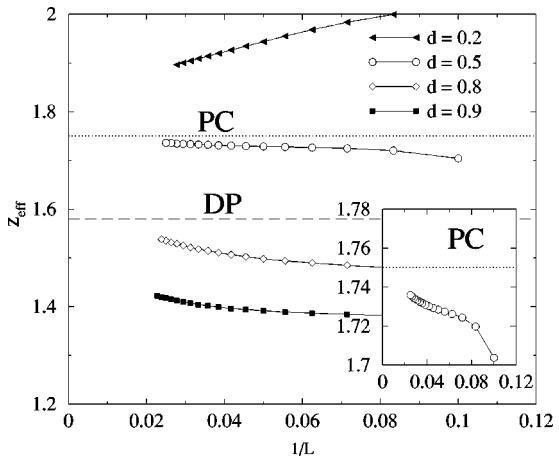

FIG. 5. Plot of the effective exponent z_{eff} as a function of $1/L$ for $d=0.2$, 0.5, 0.8, and 0.9. Inset: blowup of the data for $d=0.5$.

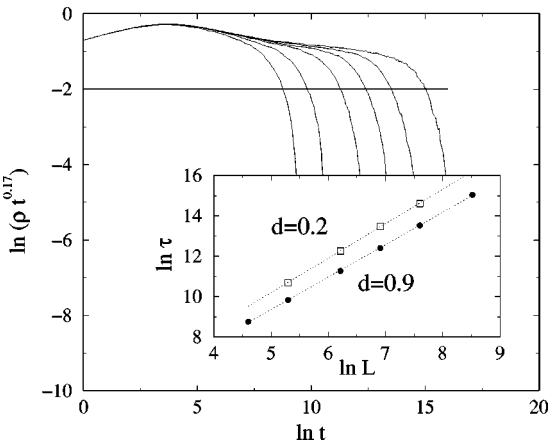

FIG. 6. Scaled particle density for $d=0.9$ at the estimated critical point $p=0.2335$ for $L=100$, 200, 500, 1000, 2000, and 5000. Inset: plot of $\ln\tau$ vs $\ln L$ for two values of the diffusion constant. We estimate $z=1.61(3)$ for $d=0.9$ and $z=1.70(3)$ for $d=0.2$.

III. RESULTS ON THE DYNAMICAL EXPONENT

From the ratio of the exponents $\beta/\nu_\perp$ and $\beta/\nu_\parallel$ one can estimate the dynamical exponent $z=\nu_\parallel/\nu_\perp$. Since both $\beta/\nu_\perp$ and $\beta/\nu_\parallel$ are consistent with DP, also the dynamical exponent z agrees with the DP value $z_{\text{DP}}=1.58$. It is, however, instructive to show the results of an independent calculation of z. This quantity can be obtained from a finite-size scaling analysis of Δ, the gap of the master operator, which is the inverse of the relaxation time of the system (see Ref. [19] for details). As a function of the system length L the gap decays as $\Delta\sim L^{-z}$.

Figure 5 shows a plot of the effective exponent $z_{\text{eff}}=-\partial\ln\Delta/\partial\ln L$ versus $1/L$. The calculations are similar to those reported in Ref. [4], but now for longer systems (up to $L=46$ compared to $L=30$ of Ref. [4]). The critical point locations were obtained from Monte Carlo simulations, which for this purpose are faster and more efficient than DMRG. Therefore we concentrated our computational efforts on a single value of $p=p_c$ and could obtain results for longer systems. As is clear from Fig. 5, the exponent z_{eff} is rather sensitive to the value of the diffusion rate d. As the estimates of $\beta/\nu_\perp$ and $\beta/\nu_\parallel$ are instead rather stable as a function of d we contribute this sensitivity to rather strong finite-size effects. Notice that the finite L corrections change sign from the weak to the strong diffusion regime. The border value is around $d=0.5$ where z_{eff} has a very weak dependence on L. The data (see inset) run extremely close to the PC value $z_{\text{PC}}=1.75$. At higher diffusion rates $d\approx 0.8$–0.9 the effective exponent z_{eff} for the range of sizes investigated is much lower than z_{PC}. At the strongest diffusion investigated, extrapolations with different forms for the correction to scaling terms as $1/L$ or $1/\sqrt{L}$ yield values in the range $1.5\lesssim z\lesssim 1.65$, which should be compared with the DP value $z_{\text{DP}}=1.58$. Current Monte Carlo estimates from various authors [5,6,11] place the exponent z in the range 1.7–1.8 and the calculations were mostly performed in the weak diffusion regime.

We also performed a series of Monte Carlo simulations to calculate the exponent z using finite-size scaling analysis. At the critical point and on a finite system the particle density decays as $\rho=t^{-\beta/\nu_\parallel}f(tL^{-z})$, with f a scaling function. For finite L, ρ follows a power-law decay up to a characteristic time τ after which it drops exponentially. One expects that τ scales as $\tau\sim L^z$. To estimate τ we calculated ρ for lattices up to $L=5000$ and $t=10^7$ Monte Carlo time units. Figure 6 shows a plot of $\ln(t^{\beta/\nu_\parallel}\rho)$ versus $\ln t$ for various L and $d=0.9$. The intersection of the data with a horizontal line at $t^{\beta/\nu_\parallel}\rho=k$ (with k a constant) provides an estimate of τ. As we work in a region where the particle density is rather low and fluctuations are large, and as the calculation of z requires very smooth data, we performed averages over a large number of samples ($>10^3$). For the calculation we used $\beta/\nu_\parallel=0.17$, which is the value determined above, and $k=-2$ (see Fig. 6). The inset shows a double-logarithmic plot of τ versus L for $d=0.2$ and $d=0.9$ at their critical points. In the former case we restricted ourselves to $L=2000$ as the relevant times are typically longer at weak than at stronger diffusion, as expected. Notice that in both cases the data are well fitted by straight lines yielding the estimates $z=1.70(3)$ for $d=0.2$ and $z=1.61(3)$ for $d=0.9$, where the latter value is consistent with the dynamical exponent of directed percolation $z_{\text{DP}}=1.58$. The results generally confirm the DMRG findings according to which the dynamical exponent is generically smaller, for finite L, at higher diffusivity. We also notice that by varying the value of $\beta/\nu_\parallel$ entering in the y axis of Fig. 6 one changes the estimate for z. For instance, if we take $\beta/\nu_\parallel=0.20$, as calculated in Ref. [11], this leads to an increase of 0.03 in the estimated value for z. The estimate of z is rather stable for changes in the constant k.

IV. RESULTS ON SURFACE DENSITIES

Boundary quantities are easily accessible in DMRG techniques [20], as one is basically forced to work with open boundary conditions. Surface criticality in absorbing phase transitions has been the subject of several studies in the past years both for models in the DP [21] and in the PC [22] universality classes. In the latter case, it is known that there

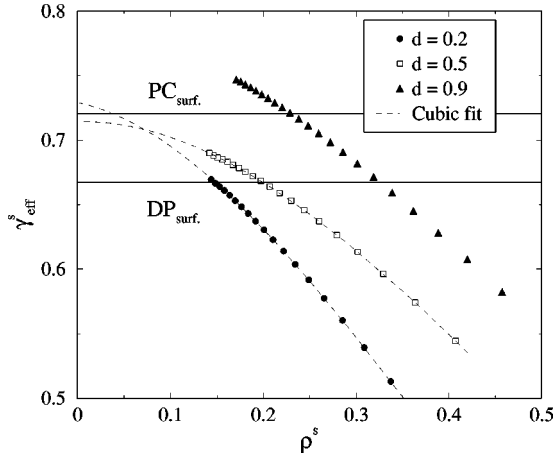

FIG. 7. Plots of $\gamma^s_{\rm eff}$ for three different values of the diffusion constant. Horizontal lines are the reference exponents for the DP and PC universality classes.

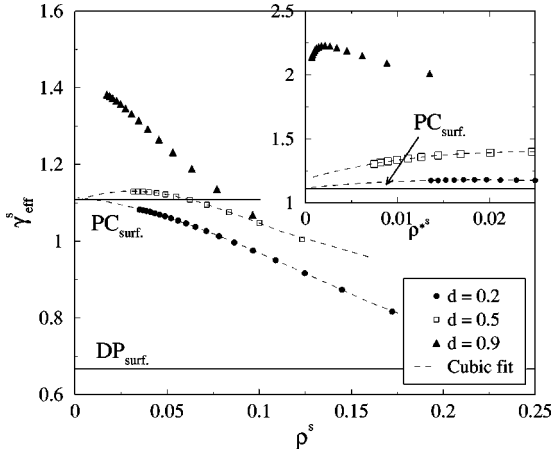

FIG. 8. Plots of $\gamma^s_{\rm eff}$ vs ρ^s for different values of the diffusion constant and absorbing boundary conditions. Inset: $\gamma^s_{\rm eff}$ vs ρ^{*s} calculated from the surface pair density.

are two distinct surface exponents depending on the type of boundary conditions applied [22]. The results of a DMRG calculation of the surface critical exponents for a reaction-diffusion model in the PC class are presented in the Appendix. Here, we report on the surface critical exponent calculations for the PCPD, using the same types of boundary conditions as in the Appendix.

As in the calculation of the bulk particle density of the preceding section we inject particles through the reaction $0 \to A$ at the boundary site labeled by the position $i=1$ in order to induce a finite density of particles in the system, and we measure the particle density $\rho^s(L)$ at the opposite boundary site $i=L$. Asymptotically for $L\to\infty$, we expect $\rho^s(L) \sim L^{-\beta^s/\nu_\perp}$, where β^s is the order parameter surface exponent. The two different boundary conditions (BCs) applied at the site $i=L$ are: (a) No particles are allowed to leave the system from the boundary site and (b) particles may diffuse out of the system, i.e., the reaction $A\to 0$ (with rate d) is added at that site. We refer to these as *reflecting* and *absorbing* boundary conditions, respectively.

In Fig. 7 we plot the effective exponent $\gamma^s_{\rm eff} = -\partial \ln \rho^s(L)/\partial \ln L$ versus ρ^s in the case of reflecting BCs. Horizontal lines show the ratio $\beta^s/\nu_\perp$ for DP ($=0.667$ [19,21]) and PC ($=0.72$ [22]). In the DP case the different BCs produce the same critical exponent. Effective exponents in this case grow monotonically, contrary to what is found for bulk exponents. Notice that a cubic fit yields a quite stable estimate $\beta^s/\nu_\perp = 0.72(1)$ in the range $d \lesssim 0.5$, a value actually consistent with the surface exponent for the PC class (see Appendix). Only at higher d we observe some deviation from PC. The fact that the extrapolated surface exponents vary with d, while our current estimates for the bulk exponents are independent on d, is an indication that the former are not yet the correct asymptotic ones.

Figure 8 shows $\gamma^s_{\rm eff}$ versus ρ^s for the case of absorbing boundary conditions. Again for weak diffusion the exponent seems to extrapolate rather convincingly to values close to the PC class ($\beta^s/\nu_\perp \approx 1.11$, see Appendix), while for strong diffusion it increases to much larger values. Also in this case there is no clear signature of nonmonotonic behavior, except for the case $d=0.5$ where the data for the largest systems pass through a maximum.

We also analyzed the effective exponent data from the pair density ρ^{*s} which are shown in the inset of Fig. 8 in the case of absorbing BCs, and plotted as functions of ρ^{*s}. In the range $d \lesssim 0.5$ the data extrapolate close to the PC surface exponent $\beta^s/\nu_\perp \approx 1.11$ as for the particle density. At very strong diffusion ($d=0.9$) the surface effective exponent shows a nonmonotonic behavior with a maximum around $\gamma^s_{\rm eff} \approx 2.2$. Notice that particle and pair exponents in this case are rather far apart from each other and it is quite hard to find a common extrapolation value. We would expect for $\gamma^s_{\rm eff}$ a similar behavior as for the bulk exponents, i.e., an increase followed by a decrease towards the asymptotic value. We suspect that in the present surface exponent calculation the decreasing side has barely been reached. So we tend to distrust the extrapolation as estimates of the genuine asymptotic behavior. They rather provide some insight on the preasymptotic region and actually point to a similarity with PC surface exponents at weak diffusion.

V. DISCUSSION

To conclude, by combining Monte Carlo and DMRG calculations we analyzed the critical properties of the pair contact process with diffusion. This model has been the subject of increasing attention in recent years. Although the debate around it has not yet been settled, the main belief is that the PCPD belongs to a novel universality class which differs from the known DP and PC classes.

In our opinion, however, the most plausible scenario for the PCPD is that it ultimately falls into the DP universality class. The asymptotic behavior is, however, masked by rather strong finite size and time effects, characterized by small correction-to-scaling exponents, as our Monte Carlo simulations for the decays of the particle density ρ, the pair density ρ^*, and the ratio ρ/ρ^* have demonstrated.

The exponents $\beta/\nu_\parallel$ and $\beta/\nu_\perp$ extrapolated both from ρ

and ρ^* appear to be stable as functions of the diffusion constant d and actually consistent with the DP class values. The data show a nonmonotonic behavior both in time and system size, which in our opinion points to a crossover phenomenon between two competing types of critical behavior. The surface exponents, which we also investigated, turned out to be instead rather sensitive to the value of d; a sign, in our opinion, that the extrapolated values are probably not the true asymptotic ones. Interestingly enough, particularly at weak diffusion, the extrapolated values are rather stable and consistent with those expected for the PC class.

In early numerical studies of the PCPD [4–6], restricted to shorter simulation times and system lengths compared to those considered here, several quantities as $\beta/\nu_\perp$, $\beta/\nu_\parallel$, and $\nu_\parallel/\nu_\perp$ were found to be quite consistent with the PC class values. It is now generally agreed that the PCPD does not belong to the PC universality class, as more extensive simulations performed by several groups have shown convincingly [7–11]. Still one would like to understand if the observed similarity with the PC exponent is purely fortuitous or if there is some deeper reason for it. In our opinion the evidence given above that also the surface exponents extrapolate towards PC values in an intermediate regime strongly suggests that there is a genuine nonasymptotic PC-like regime, with a crossover to DP behavior at longer time scales.

A prototype model in the PC class is the branching annihilating random walk with even offsprings (BARWe), defined by the reactions $A\to 3A$, $2A\to 0$ plus diffusion [1,2], which differs from the PCPD only for the reaction which creates particles. We argue that the early stages of the critical dynamics, when the system has a rather high particle density, are dominated by the annihilation process $2A\to 0$, so that the substitution of the BARWe reaction $A\to 3A$ with that of the PCPD $2A\to 3A$ may result in a very weak perturbation of the system. Therefore a transient PC-like regime may be observed for $t\lesssim\tau_c$, where τ_c is some crossover time. This argument may help to explain features observed in the PCPD, and should be equally valid for other models where the annihilation is of the type $2A\to 0$ and with different creation rules $nA\to(n+k)A$ with $n\geqslant 2$, $k>0$; for such systems we expect a transient PC regime as well.

The study of reaction-diffusion systems where the annihilation and creation reactions involve $n\geqslant 2$ particles has recently drawn some attention [11,17,23]. In particular, we mention here the two cases recently considered by Ódor [17] (i) $3A\to 5A$, $2A\to 0$ and (ii) $4A\to 5A$, $2A\to 0$. In model (i) he estimates $\beta/\nu_\parallel\approx 0.28$ (consistent with PC) for small diffusion rates and $\beta/\nu_\parallel\approx 0.24$ at stronger diffusion. Invoking some logarithmic corrections he claims that all values extrapolate to $\beta/\nu_\parallel\approx 0.22$ [17]. In the case (ii) the estimate is $\beta/\nu_\parallel\approx 0.28$ both at high and low diffusions [17], again consistent with the PC class value. The above observations suggest that these types of systems follow closely a critical behavior as described here for the PCPD, and it is thus plausible that they fall for sufficiently long times into the DP class. However, it may turn out to be quite difficult to show this numerically, as we expect that increasing the number of particles involved in the creation and annihilation reactions will lead to models even harder to simulate and analyze than the PCPD.

Very recently Kockelkoren and Chaté analyzed a similar set of models [11]. In their formulation the fermionic constraint of only one particle per site is released. All the reactions of the type $nA\to(n+k)A$ and $2A\to 0$ with $n>2$ were found to belong to the DP class. Surprisingly, in all those models the convergence to DP exponents seems to be quite fast (at least for $\beta/\nu_\parallel$) and not plagued by the strong corrections found in the fermionic models. It would be interesting to study the same models at different values of the diffusion constant, as in the PCPD the onset of crossover behavior is quite strongly influenced by the value of d.

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APPENDIX: SURFACE CRITICAL BEHAVIOR IN THE PARITY CONSERVING PROCESS $2A\to 0$, $A\to 3A$

We present here some results on the surface critical behavior of the parity conserving process defined by the reactions $2A\to 0$, $A\to 3A$ and with single particle diffusion. We show how DMRG produces accurate surface critical exponents for this model, which are in good agreement with former Monte Carlo simulation results. For the single particle diffusion and pair annihilation we used the same rates as in Eq. (1), while we assign a rate $(1-p)(1-d)$ to the reaction $0A0\to AAA$. We restrict ourselves to a single value of the diffusion constant $d=0.5$.

We first estimated the critical point at $p=p_c\approx 0.577(2)$ by means of Monte Carlo simulations using a standard approach. As mentioned above, for surface universality in PC processes there are two possible types of boundary conditions leading to two distinct surface exponents [22]. In the first case, the system is truncated at one edge and no particles

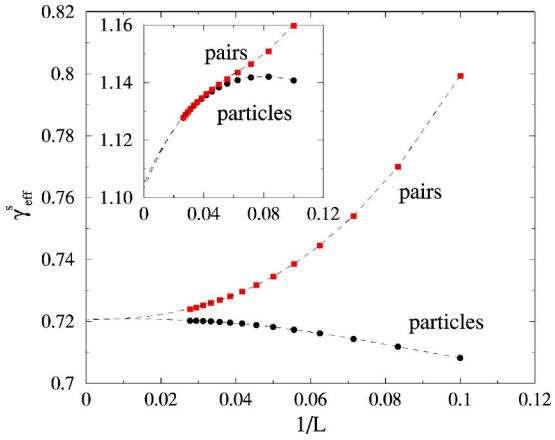

FIG. 9. Plot of the surface effective exponent $\gamma^s_{\rm eff}$ vs $1/L$ for the parity conserving process $A\to 3A$ and $2A\to 0$ in the case of reflecting boundary conditions. Inset: $\gamma^s_{\rm eff}$ vs $1/L$ for absorbing boundary conditions. Dashed lines are extrapolated curves through the DMRG data. Extrapolated values are in good agreement with Monte Carlo simulations results of Ref. [22] (see text).

are allowed to cross the boundary site; we refer to this as *reflecting* boundary conditions. In the second case, particles are allowed to drop from the boundary. We implemented this type of boundary condition adding the boundary reaction $A \rightarrow 0$ (with rate d) which mimics the diffusion of particles out of the system. We refer to this implementation as *absorbing* boundary conditions.

Figure 9 shows the effective surface exponent $\gamma^s_{\rm eff}$ versus $1/L$ in the case of reflecting boundary conditions, calculated both from the particle (circles) and pair (squares) densities. The same quantities are plotted in the inset in the case of absorbing boundary conditions. Notice that indeed the results confirm the existence of two distinct sets of surface exponents and that the data from pairs and particles merge for sufficiently long chains, indicating that both quantities decay with the same exponent. Our estimates $\beta^s/\nu_\perp \approx 0.720(2)$ in the former case and $\beta^s/\nu_\perp \approx 1.10(1)$ in the latter are obtained from a polynomial extrapolation in $1/L$. As the finite-size effects are rather small (see Fig. 9), the extrapolated values are not very sensitive to the type of correction to scaling term used in the extrapolation.

The Monte Carlo simulation results [22] for the critical exponents are $\beta^s = 1.34(2)$ and $\beta^s = 2.04(2)$, for inactive and active boundary conditions, respectively. Combining these results with the PC class correlation length exponent $\nu_\perp = 1.83(3)$ [1], one finds $\beta^s/\nu_\perp = 0.73(1)$ (reflecting BCs) $\beta^s/\nu_\perp = 1.11(1)$ (absorbing BCs), in very good agreement with the DMRG calculations.

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