Absorbing Phase Transitions of Branching-Annihilating Random Walks

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The phase transitions to absorbing states of the branching-annihilating reaction-diffusion processes

\[ mA \to (m + k)A, \ nA \to (n - l)A \]

are studied systematically in one space dimension within a new family of models. Four universality classes of non-trivial critical behavior are found. This provides, in particular, the first evidence of universal scaling laws for pair and triplet processes.

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Even though it is widely believed that far from equilibrium phase transitions can be classified, recent numerical results reveal that we are still far from a satisfactory understanding of even the relevant ingredients deciding to which class a given transition belongs. This is in particular true for transitions from a fluctuating phase to one or several absorbing states (APT, for absorbing phase transitions) where, in spite of a wealth of analytical and numerical studies, rather little is known beyond the existence of the prominent universality class of directed percolation (DP) \([1, 2]\). In terms of reaction-diffusion processes, the DP class is often represented by the simplest branching-annihilating reactions: \(A \to 2A, A \to \emptyset\).

Following an early suggestion by Grassberger \([3]\), a lot of attention has been devoted recently to the case of binary or pair reaction-diffusion processes such as \(2A \to (2 + k)A, 2A \to \emptyset\) or \(A\), which involve two particles both for branching and annihilating \([4, 5, 6, 7, 8, 9, 10, 11, 12, 13]\). Usually designated under the name of “pair contact process with diffusion” (PCPD), it is still unclear as of now if systems of this type can exhibit universal scaling laws or even if (simple) scaling occurs at all at the APT. The origin of the strong deviations to scaling observed is debated \([14, 15]\), and various conclusions have been drawn ranging from diffusion-rate dependent sub-classes \([6]\) to continuously-varying exponents \([12]\) to no scaling to slow crossover to the DP class \([13]\). At the analytical level, a bosonic field theory of PCPD processes exists but is not renormalizable whereas no fermionic version is available \([3, 4, 14]\). Completing this unsatisfactory picture, similar results were reported recently for the “triplet contact process with diffusion” (TCPD) \(3A \to 4A, 3A \to 2A\), where three particles are involved for both reactions \([16]\). Finally, the role of the conservation of parity of the number of particles in APT is not well understood either: it is known to be relevant for some one-dimensional DP-like processes, giving rise to the so-called “parity-conserving” (PC) class \([14, 15]\), whereas it was argued not to influence the critical properties of PCPD systems \([19]\).

In this Letter, we report on a systematic numerical investigation of the reaction-diffusion processes \(mA \to (m + k)A, nA \to (n - l)A\) in one space dimension, from which we draw a considerably clarified picture of the above situation. This is achieved thanks to a new class of very simple models which, contrary to all the works cited above, abandon the “fermionic constraint” usually considered for both theoretical and practical reasons (to avoid the divergence of the density of particles in the active phase, and —hopefully— increase numerical efficiency). Our results include the first evidence of universal (ordinary) scaling for PCPD and TCPD processes, the classification of “hybrid” rules (i.e. those for which \(m \neq n\), and further insights into the conditions under which the conservation of the number of particles modulo 2 or 3 is able to change the “reference” scaling laws.

Following Hinrichsen \([10]\), we may write, for the \(mA \to (m + k)A, nA \to (n - l)A\) processes, the following “mean-field Langevin equation” expected to govern the coarse-grained local density \(\rho\):

\[
\partial_t \rho = a \rho^m - b \rho^n - c \rho^{m+1} + D \nabla^2 \rho + \zeta(x, t),
\]

where \(a, b, c\) are positive constants related to the reaction rates and \(D\) is the diffusion constant. Note that of the two negative terms in Eq. (1) only the lowest-order one is relevant. As usual, the stochastic nature of the process is embodied in \(\zeta\), a delta-correlated noise whose amplitude is a power of \(\rho\) (thus ensuring the absence of fluctuations in the \(\rho = 0\) absorbing phase):

\[
\langle \zeta(x, t)\zeta(x', t') \rangle = \Gamma \rho^\mu(x, t) \delta^d(x - x') \delta(t - t')
\]

In the absence of branching (i.e. in the inactive phase leading to an absorbing state), the noise dimension \(\mu = n\) and the upper critical dimension of the annihilation process is \(d_c = 2/(n - 1)\). In the critical region, fluctuations are expected to increase the noise strength and thus to reduce \(\mu\) and increase \(d_c\). In the following, we restrict ourselves to \(m, n \leq 4\) (in one dimension, non-trivial APT are mostly expected to occur if \(n < 4\)). Each of the branching-annihilating processes \(mA \to (m + k)A, nA \to (n - l)A\) is defined by the 4 integers \((m, n, k, l)\). Obviously, one must have \(0 < n - l < m\) to insure the existence of at least one absorbing state. For legibility, \(m\) and \(n\) will be coded below by the letters \(s, p, t, q\) (for singleton, pair, triplet, quadruplet). The
PCPD rule $2A \rightarrow 3A$, $2A \rightarrow \emptyset$ is thus noted $pp12$, and $ttxx$ denote TCPD processes. The fermionic constraint adopted in most PCPD and TCPD models studied so far can be seen as counter-productive: the actual implementation of their Monte-Carlo simulations often lead to complicated rules, inefficient for both code elaboration and simulation. More importantly, the fermionic constraint may well be at the origin of the strong deviations to scaling observed. Our branching-annihilating random walk (BARW) models are designed to bypass both of these problems. Particles of a single species $A$ evolve in parallel in two synchronized sub-steps: random walk on the lattice (diffusion) followed by on-site reaction. For simplicity, in the following, the diffusion constant is kept constant: all particles always jump to a randomly chosen nearest-neighbor. Let us consider, to describe our on-site reaction scheme, the PCPD rule $pp12$. (The generalization to all other rules studied here is straightforward.) Suppose that $n_A$ particles are present at a given site. If $n_A = 1$, nothing happens (this is the main PCPD constraint). For $n_A \geq 2$, each of the $\lfloor n_A/2 \rfloor$ pairs into which the local population can be divided branches with probability $p^{\lfloor n_A/2 \rfloor}$ (thus creating each time one new particle for this particular example) otherwise it annihilates. The only parameter is $p$: for large $p$, branching is likely, and one expects to be in the active phase. For small $p$, annihilation dominates (indeed this is the only process at play for $p = 0$), leading to an absorbing state. One key feature is the nonlinearity introduced by raising $p$ to the power $\lfloor n_A/2 \rfloor$: branching/annihilation is inhibited/enhanced for large local populations, preventing the divergence of population of usual bosonic models. All the results presented below were obtained for reaction schemes of this type, but we have checked that the functional form of the nonlinearity as well as other details do not change the critical properties observed.

As recommended when studying APT numerically, we first investigate, for a given rule, the decay of the order parameter from some highly active, correlation-less, initial condition in a large system. Above threshold, activity eventually reaches a constant level in time. Well below threshold, one observes a decay typical of the annihilation process (exponential for $n = 1$, algebraic for $n > 1$). At $p = p_c$, in the usual framework, one expects a non-trivial algebraic decay characterized by the scaling exponent $\delta = \beta/\nu_H$. Once the threshold determined, other scaling exponents can be estimated. In this work, we also give —without showing the data— our estimates of $z$, obtained by the finite-size scaling of the mean lifetime of the system at threshold ($\langle \tau \rangle \sim L^z$), and of $\beta$, given by the decay of the stationary density with the distance to threshold ($\lim_{t \to \infty} \rho(t) \sim (p - p_c)^x$). More precise estimates will appear elsewhere [21]. In the following, the role of conservation (modulo 2 or 3) of the number of particles is discussed at the end. Before proceeding to higher-order rules, we report that $ssxx$ rules are easily verified to exhibit DP-class scaling laws (not shown).

In Fig. 1 we show the critical behavior of the PCPD rule $pp12$. Quite easily, a clean algebraic decay in time of all order parameters is observed over many decades with the exponent $\delta_{PCPD} = 0.200(5)$. At the determined threshold, the mean lifetime scales nicely with system size, yielding the estimate $z_{PCPD} = 1.70(4)$. Finally, the decay of the stationary order parameter with distance to
threshold allows to estimate $\beta_{\text{PCPD}} = 0.375(10)$. These exponent values appear to be universal: this has been checked to the above numerical accuracy for rule pp11 and with less care for several other rules.

Similar results were obtained for TCPD rules. Although scaling usually sets in later than for the PCPD rules, it is well established over a large range of scales. Again, scaling laws are found to be universal within numerical accuracy. Fig. 3 shows typical results obtained for the decay of the particle density at threshold for five different rules, from which we estimate $\delta_{\text{TCPD}} = 0.27(1)$. Other exponents are reported in Table I.

Next, we consider hybrid rules for which $m > n$. At the mean-field level, they are expected to present first-order transitions (see Eq. (1)). Nevertheless, in one space dimension, all the cases we considered show DP scaling, at least for the decay exponent $\delta$. This is true for $n = 1$ (simple radioactive decay), a case where we have studied rules ps11, ts21, and qs11. But this is also true for higher-order annihilation processes, as shown by pair-annihilation rules tp12 (2 variants) and qp12, as well as by triplet-annihilation rule qt12. As seen in Fig. 4, high-order branching process scaling sets in rather late, probably because the initial conditions chosen are not “optimal”. That a given process for which a first-order APT is predicted at mean-field level exhibits a continuous transition in low dimensions is by no means surprising, especially in one dimension, where this has been noticed early [22]. Nevertheless, to our knowledge, satisfactory analytical arguments for our finding are not available.

Hybrid rules for which the branching process is of lower order than the annihilation reaction ($m < n$) are also easily investigated within our family of models. First, we note that whenever $n = 4$, no non-trivial APT was found in any of the rules sqxx, pqxx, tqxx or qqxx that we have considered. In other words, $p_c = 0$ and the decay is then that of the mean-field prediction ($t^{-1/3}$), in agreement with the fact that the upper critical dimension of the decay process is $\frac{3}{2} < 1$. For $m < n < 4$, we find that the universality class of the critical behavior is determined by the order of the branching process: $m = 1$ rules such as sp12, st13, st23 exhibit DP-scaling, in agreement with the analytical arguments of [18]. Pair-braniching rules ($m = 2$) pt12 and pt13, after a rather long crossover time, show scaling compatible with the PCPD class (Fig. 4). That $m$ sets the universality class in this case is actually not too surprising: it is clear at the mean-field level of Eqs. (1), and can also be deduced from “vertex generation arguments” such as those developed in [18].

We now turn our attention to the rules for which the total number of particles is conserved modulo 2 (parity conservation) or modulo 3. Phase space is then divided into 2 or 3 disjoint sectors, each of which may or may not possess an absorbing state. For example, the even sector of parity-conserving rule sp22, the archetypical rule of the PC class, includes an absorbing state (the empty configuration) whereas its odd sector does not. For parity-conserving PCPD rule pp22, on the other hand, each sector has an absorbing state. We studied at least one rule in each of the relevant sub-families (namely pp, tt, sp, pt, qp, qt for parity conservation, and st, pt, tt, qt for conservation mod 3). We find that when-
ever every sector includes an absorbing state, mod2 or mod3 conservation does not change the “reference” scaling class. Thus rule pp22 is in the PCD class (as suggested in [14]), rules tt22 and tt33 in the TCPD class (Fig. 3). Interestingly, rules tp22, qp22, qt22, and qt33 are found to be in the DP class, like their non-conserving counterparts, and thus constitute the first examples of DP-class rules with mod2 or mod3 conservation (Fig. 3).

Conversely, conserving rules with at least one non-absorbing sector do not offer such a clear conclusion: as expected, rules sp22 and sp42 fall into the PC class (not shown). As argued in [13], rule st33 does not have a non-trivial APT. This is also observed for rule pt33, probably for similar theoretical reasons. The only possible case left is that of parity-conserving hybrid rules pt(2k)2. There the even sector is non-absorbing because the empty state—which is absorbing—cannot be reached from any other configuration. Numerical simulations of rules pt22 and pt42, however, do not show any significant difference from their non-conserving cousins (Fig. 4). This result, which needs confirmation due to the lateness of scaling, seems to refute the suggestion of [19] that influence of parity conservation may be equivalent to having a non-absorbing sector of phase space. Instead we would like to propose that rules sp(2k)2 are the only ones in the PC class because they are the only BARW processes equivalent to generalized two-state Voter models, as defined in [24], i.e. spin models with up/down symmetry, no bulk noise, and an order/disorder transition. This remark, which will be developed in [25], calls for renaming the PC class the Voter class.

We now summarize and discuss our results. We first note that our BARW models, at criticality, exhibit ordinary scaling after some crossover scale, and do not seem to be plagued by the strong deviations observed with even the simplest fermionic PCDP or TCPD rules [13, 15]. Numerical results of basic fermionic models can be shown to converge to the critical behavior found here [24]. To our numerical accuracy, the scaling exponents recorded at criticality lead to conclude to the existence of three basic universality classes: DP, PCDP, and TCPD. Table II summarizes our current estimates of the basic exponents δ, z, and β, pending more precise ones [25]. Extrapolating from our numerical findings, we believe that the critical behavior of all processes considered here is as follows (Table II): rules with four-particle annihilation (n = 4) do not have non-trivial APT, indicating (in partial agreement with [16]) that δc ≤ 1 in this case. Hybrid processes fall into one of these basic classes: m > n rules exhibit DP critical behavior, whereas the class of m < n rules is set by m. Finally, we have shown that mod2 (parity) or mod3 conservation seems to act only on sp(2k)2 rules, suggesting that the PC class should be seen as the (one-dimensional, generalized) Voter class.

Obviously, our numerical findings need to be confirmed by analytical approaches. We hope that, at the very least, they will trigger some new lines of attack to the difficult issues at play. At the numerical level, ongoing work aims at obtaining more comprehensive results, including the study of spreading exponents and the case of higher space dimensions.

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| m \ n | 1   | 2   | 3   | 4   |
|-------|-----|-----|-----|-----|
| DP    | DP/PC | DP/∅ | 0   |
| DP    | PCDP | PCDP/∅ | 0   |
| DP    | DP   | TCPD | 0   |
| DP    | DP   | DP   | 0   |

TABLE II: Universality class of BARW processes. “∅” stands for no non-trivial APT (p_c = 0). The second markings indicate the change of class whenever mod2 or mod3 conservation plays a role. See text for details.

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