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Hard-core particle exclusion effects in low-dimensional non-equilibrium phase transitions

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Abstract

We review the currently known universality classes of continuous phase transitions to absorbing states in non-equilibrium systems and present results of simulations and arguments to show how the blockades introduced by different particle species in one dimension cause new robust classes. Results of investigations on the dynamic scaling behavior of some bosonic spreading models are reported.
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1. Introduction

Critical universality is an attractive feature in statistical physics because wide range of models can be classified purely in terms of their collective behavior into classes. While in equilibrium systems the factors determining these classes are quite well understood, in non-equilibrium systems the situation is less clear. The $(1+1)$-dimensional reaction–diffusion systems are important for the understanding of the universality classes of non-equilibrium system because order–disorder phase transitions may occur in such a low dimension unlike in equilibrium systems [1]. However, for the ordered state to be stable it must exhibit only small fluctuations. All of this kind of transitions are such that the ordered state is "absorbing", i.e. when the system falls into it, it cannot escape. In fact for a long time only such phase transitions have been

known where the absorbing state is completely frozen. A few universality classes of this kind are known [2,3], the most prominent and the first one that was discovered is that of the directed percolation (DP) [4]. An early hypothesis [5] was confirmed by all examples up to now. This claims that in one-component systems exhibiting continuous phase transitions to single absorbing states (without extra symmetry, inhomogeneity or disorder) short-ranged interactions can generate DP class transition only. The Lagrangian of the field theory of the DP process $L(\phi(x,t), \psi(x,t))$ exhibits a time reversal symmetry $\phi(x,t) \leftrightarrow \psi(x,-t)$. This results in relations among scaling exponents (see [3]).

The same static scaling behavior was observed in frozen multi-absorbing state systems as well, like in the pair contact process (PCP) [8]. Here the time reversal symmetry is broken owing to an extra term in the Lagrangian describing the effect of frozen particles generating long-time memory in the system [9]. Besides DP, a few more universality classes have been established in the last decade. In models exhibiting

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Table 1
Summary of known $(1 + 1)$-dimensional universality classes[a]

Class ID	Features	Degree of knowledge	References
DP	Time reversal symmetry	RG to ϵ^2, series exp.	[1–6]
PCP	Broken time reversal symmetry	RG, simulations	[8]
NDCF	Global conservation	RG, simulations	[10–12]
CDP	Compact DP, Glauber–Ising	Exactly solved	[13–15]
PC	Parity cons. $+ Z_2$ symmetry	RG, simulations	[16–24]
N-BARW2	N-comp. parity conservation	RG, simulations, DMRG	[18,25,26]
PCPD	Binary production	Simulations	[27–33]
DCF	Global conservation	RG, simulations	[34–37]
N-BARW2s	N-comp. symmetry BARW + exc.	Simulations, MF	[25,38–40]
N-BARW2a	N-comp. asymmetry BARW + exc.	Simulations, MF	[25,38]

[a] DCF and NDCF denote models with coupled (non)diffusive conserved fields.

particle annihilation fluctuating absorbing states with a single wandering particle can occur [7]. In Table 1, we have tried to summarize the most well-known absorbing state phase transition classes of disorder-free, homogeneous models with short-range interactions. The lower seven classes exhibit fluctuating absorbing states. For more details of field theoretical symmetries and their relation to hyperscaling laws, see [9].

A major problem of these models is that they are usually far from the critical dimension and critical fluctuations prohibit mean-field (MF)-like behavior. Further complication is that bosonic field theoretical methods cannot describe particle exclusion that may obviously happen in one dimension. The success of the application of bosonic field theory for models shown in the first part of the table is the consequence of the asymptotically low density of particles near the critical point. However, in multi-component systems, where the exchange between different types is non-trivial, bosonic field theoretical descriptions may fail. Also in case of the binary production (PCPD) models [27], it predicts a non-vanishing density at the transition point and diverges in the active phase contrary to the lattice model version of hard-core particles [28–33]. Fermionic field theories, on the other hand, have the disadvantage that they are non-local and results exist for very simple reaction–diffusion systems only [41,42]. Other techniques like independent interval approximation [43], empty interval method [44] or density matrix renormalization (DMRG) [45] are currently being developed to be able to solve

multi-component reaction–diffusion models. The main aim of this work is to give an overview and present simulation results for these systems.

2. Critical dynamical behavior of single-species spreading processes

The bosonic field theory of the DP was established by Grassberger and Sundermayer [46]. Perturbative $\epsilon = 4 - d$ renormalization group analysis [5] up to two-loop-order resulted in estimates for the critical exponents. For the density decay exponent, it gives

$$\alpha_B = 1 - \tfrac{1}{4}\epsilon - 0.01283\epsilon^2, \tag{1}$$

which results in $\alpha_B = 0.13453$ in one dimension. This differs from the most precise simulation and series expansion results of DP $\alpha = 0.1595(1)$ [49] with about 18%. An attempt for fermionic field theoretical solution in one dimension (that does not allow multiple occupancy of sites) was shown in [42] but ran into severe convergence problems and has not resulted in precise quantitative estimates for critical exponents. Although the bosonic field theory is expected to be valid owing to the asymptotically low density at criticality it has never been proven rigorously. On the contrary, a recent study on a special one-dimensional DP model predicts different bosonic and fermionic field theoretical results [47]. As far as we know all simulations of DP (and other spreading models) have been done on lattices allowing single occupancy. Moreover,

there are no more precise estimates for the critical exponents of the one-dimensional bosonic model than those of the ϵ^2 expansion cited above. Therefore, we decided to perform some simulations with bosonic particles to check the scaling behavior at criticality.

First, we investigated the following one-dimensional branching and annihilating process with one offspring (BARW1):

$$A \xrightarrow{\sigma} 2A, \qquad 2A \xrightarrow{\lambda} \emptyset, \qquad A\emptyset \overset{1-\sigma-\lambda}{\underset{}{\leftrightarrow}} \emptyset A \qquad (2)$$

in such a way that the branching and the coagulation processes happen in place. The simulations were run on $L = 10^6$ systems with periodic boundary conditions and with initially randomly distributed $\emptyset$'s and A's of probability 1/2. The density of particles ($\rho(t)$) is measured up to $t_{max} = 2 \times 10^5$ Monte Carlo steps (MCS) and averaged over 10^4 samples. By fixing the branching rate to $\sigma = 0.1$ and varying the annihilating rate, we determined the critical point λ_c with the local slope analysis of data

$$\alpha_{eff}(t) = \frac{-\ln[\rho(t)/\rho(t/m)]}{\ln(m)} \qquad (3)$$

(where we use $m = 8$ usually). In the $t \to \infty$ limit, the critical curve goes to exponent α by a straight line, while in sub (super)-critical cases they were down (up), respectively. As Fig. 1 shows the critical point is at $\lambda_c = 0.12882(1)$ with $\alpha = 0.165(5)$ that agrees well with other simulation and series expansion results 0.1595(1) [49]. By simulating on smaller lattice sizes ($L = 20\,000$) we found strong finite size effects.

Next we performed the same analysis for the one-dimensional two-offspring version BARW (BARW2)

$$A \xrightarrow{\sigma} 3A, \qquad 2A \xrightarrow{\lambda} \emptyset, \qquad A\emptyset \overset{1-\sigma-\lambda}{\underset{}{\leftrightarrow}} \emptyset A \qquad (4)$$

that exhibits mod 2 particle number conservation and its critical behavior is known to belong to the PC class [16,18]. Now we fixed $\lambda = 0.2$ and as Fig. 2 shows the critical point is at $\sigma_c = 0.04685(5)$ with the corresponding decay exponent $\alpha = 0.290(3)$. This value agrees with that of the PC class again 0.285(2) [17].

Finally, we performed bosonic simulations for the sub-critical behavior of the following one-dimensional binary spreading process:
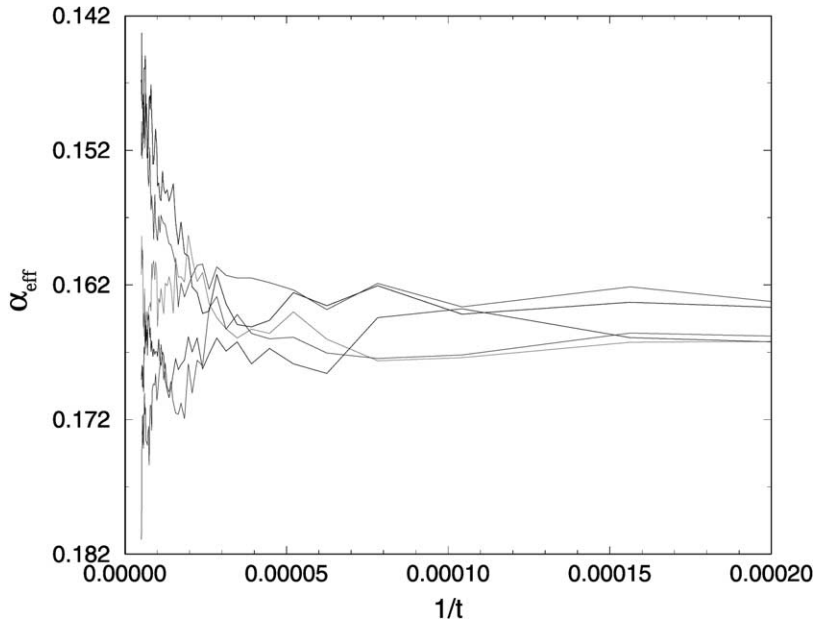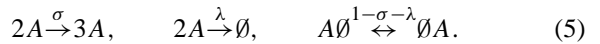
$$2A \xrightarrow{\sigma} 3A, \qquad 2A \xrightarrow{\lambda} \emptyset, \qquad A\emptyset \overset{1-\sigma-\lambda}{\underset{}{\leftrightarrow}} \emptyset A. \qquad (5)$$

Fig. 1. Local slopes of the density decay in a bosonic DP model. Different curves correspond to $\lambda = 0.12883, 0.12882, 0.12881, 0.1288, 0.12879$ (from bottom to top).
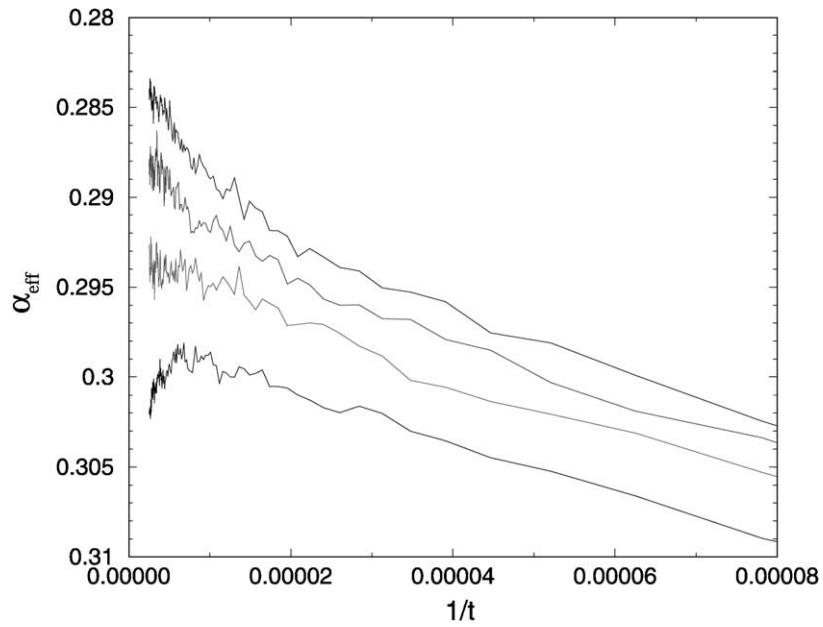
Fig. 2. Local slopes of the density decay in a bosonic BARW2 model. Different curves correspond to $\sigma = 0.466, 0.468, 0.469, 0.47$ (from bottom to top).
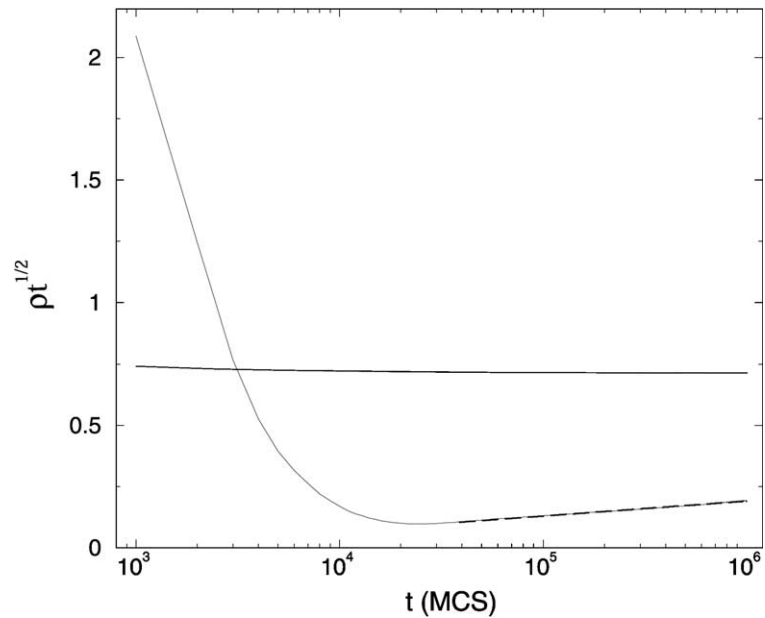

Fig. 3. Density decay in the bosonic annihilation–fission model. The upper curve corresponds to the inactive phase $\lambda = 0.5$, the lower one to the transition point $\lambda = 0.1$. The dashed line shows logarithmic fitting of the form equation (6).

In the fermionic version of this model, continuous phase transition was found [28–30] with new critical behavior. On the other hand, the field theory of the bosonic model [27] predicted discontinuous phase transition at $2\lambda = \sigma$ with diverging particle density in the active phase. Our present simulations confirm this. While in the inactive phase, the $2A \rightarrow \emptyset$ process (see Section 3.1) governs the evolution it is guessed [48] that at the transition point the $3A \rightarrow \emptyset$ dominates with the following scaling law in one dimension:

$$\rho(t) \propto \left(\frac{\ln t}{t}\right)^{1/2} + \mathrm{O}\left(\frac{1}{t}\right). \tag{6}$$

The simulations at $\sigma = 0.2$ in systems with size $L = 10^6$ confirmed these expectations as shown in Fig. 3. At the transition point for $t > 4 \times 10^4$ MCS, we applied the form equation (6) and found a good fitting with $\rho(t) = ((0.0266(1) - 0.1765(1) \ln(t))/t)^{1/2}$. Though the identification of a universality class requires the determination of three independent critical exponents, we believe that the above numerical data give enough support for the expected critical behaviors.

3. Critical dynamical behavior of multi-species annihilating random walks

First, we recall some well-known results (see refs. in [50]) for simple reaction–diffusion systems that lack particle creation. From the viewpoint of phase transitions, this describes the behavior in the inactive phase or as we shall show in the N-BARW models right at the critical point.

3.1. Models $A + A \rightarrow \emptyset$ and $A + B \rightarrow \emptyset$

The simplest reaction–diffusion model $A + A \rightarrow \emptyset$ (ARW), in which identical particles follow random walk and annihilate on contact is exactly solvable in one dimension [51,52], the particle density decays as

$$\rho(t) \propto t^{-1/2}. \tag{7}$$

ARW was also shown to be equivalent to the $A + A \rightarrow A$ model by [53] and renormalization group approach provided universal decay amplitudes to all orders in

epsilon expansion. It was also shown [14] that the motion of kinks in the compact version of directed percolation (CDP) [13] and in the Glauber–Ising model [15] at zero temperature are also described exactly by (7).

Two types of particles undergo diffusive random walk and react upon contact to form an inert particle in the simplest two-component reaction–diffusion model $A + B \rightarrow \emptyset$. For $d < 4$ and for equal initial density of A and B particles (ρ_0), which are randomly situated in space the density decays asymptotically as [54] $\rho_A(t) = \rho_B(t) \propto C_d \sqrt{\rho_0} t^{-1/4}$ where C_d is a dimension-dependent constant. This slow decay is due to the formation of clusters of like particles that do not react and their asymptotical segregation for $d < 4$. The asymptotically dominant process is the diffusive decay of the fluctuations in the initial conditions. Since this is a short-ranged process, the system will have a long-time memory—appearing in the amplitude dependence—for the initial density.

3.2. The effect of exclusion

A simple reaction–diffusion model of two types $A + A \rightarrow \emptyset$, $B + B \rightarrow \emptyset$ with exclusion $AB \nleftrightarrow BA$ is offered by the generalized Domany–Kinzel (GDK) stochastic cellular automaton model of Hinrichsen [24] introduced originally to realize phase transitions from active (Ac) to multiple inactive absorbing states: I1, I2. We investigated numerically [55] this model in a special point of its phase diagram where compact domains of I1 and I2 grow separated by AcI1 $= A$ and AcI2 $= B$ kinks that cannot penetrate each other (CDP2). There are special pairwise initial conditions in the model (because the domains are bounded by kinks of the same type): $\cdots A \cdots A \cdots B \cdots B \cdots B \cdots B \cdots A \cdots A \cdots$.

The dynamical behavior of critical systems is usually investigated from two extreme initial conditions: (a) homogeneous system with randomly distributed species and (b) empty system with a single initial seed of particles. In the former case (a) and pairwise initial conditions our numerical simulations show a density decay of kinks (or particles of the corresponding reaction–diffusion system) $\rho \propto t^{-\alpha}$

characterized by a power-law with an exponent larger than $\alpha = 0.5$ that would have been expected in case of two copies of ARW systems that do not exclude each other. Furthermore, the deviation of α from 0.5 showed an initial density dependence. We provided a possible explanation based on symmetry between types that a marginal perturbation emerges here that causes this non-universal scaling. We showed an analogy with the DP confined by parabolic boundary conditions [56] by assuming that the kinks exert a parabolic space–time confinement on the decaying domains. Non-universal scaling can also be observed at surface critical phenomena similarly to here where kinks produce "multi-surfaces" in the bulk. However, simulations and independent interval approximations on a similar model predict a $t^{-1/2}/\ln(t)$ behavior [57]. Perhaps a fermionic field theoretical study could help to understand better the situation. In case of random distribution of A's and B's, the density decays slower owing to the accumulation of AB pairs. An exact mapping onto the $A + B \rightarrow \emptyset$ model predicts $\rho_A = \rho_B \propto t^{-1/4}$ that was confirmed by simulations [25].

In case (b) above, one usually measures the survival probability of clusters originated from a seed. In critical systems, this scales like $P(t) \propto t^{-\delta}$. When we inserted a seed of I2's in the sead of I1 and Ac's of the GDK model at the CDP2 point we found very strong dependence of δ on $\rho_0(I1)$ [55]. Also the above picture with parabolic boundary conditions has gained further support here.

4. Phase transition generated by offspring production

If we add particle creation by branching to the systems mentioned before we may expect a phase transition, where a steady state with constant particle density occurs. For N component parity conserving systems (N-BARW2, $N = 2$ types, two offsprings) it was shown by field theory [18] that the $A \rightarrow 3A$ like processes are not relevant and the models with $A \rightarrow A2B$ and $B \rightarrow B2A$ (ordering of offsprings is not relevant) branching terms do exhibit continuous

phase transitions at $\sigma = 0$ branching rate. The universality class is expected to be independent from N and to coincide with that of the $N \rightarrow \infty$ (N-BARW2) model. The critical dimension is $d_c = 2$ and for $d = 1$ the exponents are

$$\beta = 1, \qquad Z = 2, \qquad \alpha = 1/2,$$
$$\nu_\parallel = 2, \qquad \nu_\perp = 1 \qquad\qquad (8)$$

exactly.

4.1. The parity conserving 2-BARW2 model with exclusion

The effect of exclusion in the 2-BARW2 model was investigated in [25] and for $d = 2$ the field theoretical predictions were confirmed. In one dimension, however, two phase transitions of different types were observed depending on the arrangement of offsprings relative to the parent. Namely if the parent separates the offsprings: $A \xrightarrow{\sigma} BAB$ (2-BARW2s) the steady-state density will be higher than in the case when they are created on the same site: $A \xrightarrow{\sigma} ABB$ (2-BARW2a) for a given branching rate because in the former case they are unable to annihilate with each other. This results in different order parameter exponents for the symmetric and the asymmetric cases ($\beta_s = 1/2$ and $\beta_a = 2$). This is in contrast to the widespread beliefs that bosonic field theory (where $AB \leftrightarrow BA$ is possible) can well describe these systems because in that case [18] the scaling behavior is different (8). This finding led [38] to the conjecture that in one-dimensional reaction–diffusion systems, a series of new universality classes should appear if particle exclusion is present. Note, however, that only the off-critical exponents are different, since in both cases the transition is at $\sigma = 0$ and the on-critical ones are those described in Section 3.2. In [25] a set of critical exponents satisfying scaling relations have been determined for these two new classes shown in Table 2.

4.2. The parity non-conserving model with exclusion (2-BARW1)

Hard-core interactions in the two-component, one-offspring production model (2-BARW1) were

Table 2
Summary of critical exponents in one dimension in N-BARW like models[a]

Process	$\nu_\parallel$	Z	α	β
N-BARW2	2	2	1/2	1
N-BARW2s	2.0(1)|0.915(2)	4.0(2)|1.82(2)[b]	0.25(1)|0.55(1)[b]	0.50(1)|1.00(1)
N-BARW2a	8.0(4)|3.66(2)	4.0(2)|1.82(2)[b]	0.25(1)|0.55(1)[b]	2.0(1)|1.00(1)

[a] The non-blocking data are quoted from [18]. Data divided by "|" correspond to random vs. pairwise initial condition cases [26,55,62].
[b] Exponents exhibit slight initial density dependence.

investigated in [39]. Without interaction between different species one would expect DP class transition. By introducing an $AB \not\leftrightarrow BA$ blocking in the

$$A \xrightarrow{\sigma} AA, \qquad B \xrightarrow{\sigma} BB, \tag{9}$$

$$AA \xrightarrow{1-\sigma} \emptyset, \qquad BB \xrightarrow{1-\sigma} \emptyset \tag{10}$$

model a DP class transition at $\sigma = 0.81107$ was found indeed. On the other hand, if we couple the two sub-systems by the production

$$A \xrightarrow{\sigma/2} AB, \qquad A \xrightarrow{\sigma/2} BA, \tag{11}$$

$$B \xrightarrow{\sigma/2} AB, \qquad B \xrightarrow{\sigma/2} BA, \tag{12}$$

$$AA \xrightarrow{1-\sigma} \emptyset, \qquad BB \xrightarrow{1-\sigma} \emptyset \tag{13}$$

without exclusion bosonic field theory [58] predicts unidirectionally coupled DP class [59] transitions. With hard-core exclusion, a continuous phase transition will emerge at rate $\sigma = 0$—therefore the on-critical exponents will be the same as described in Section 3.2—and the order parameter exponent was found to be $\beta = 1/2$. This assures that this transition belongs to the same class as that of the 2-BARW2s model. The parity conservation law that is relevant in case of one-component systems (PC versus DP class) is irrelevant here. This finding reduces the expectations for a whole new series of universality classes in one-dimensional systems with exclusions. In fact the blockades introduced by exclusions generate robust classes. In [39] a hypothesis was set up that in coupled branching and annihilating random walk systems of N-types of excluding particles for continuous transitions at $\sigma = 0$ two universality classes exist, those of 2-BARW2s and 2-BARW2a, depending on whether the reactants can immediately annihilate (i.e. when

similar particles are not separated by other type(s) of particle(s)) or not. Recent investigations in similar models [40,60] are in agreement with this hypothesis and the extension to binary spreading processes was proposed in [61].

5. Summary

We have shown how blockades generated by particle exclusion in some one-dimensional reaction–diffusion type systems affect critical scaling behavior.

We confirmed by bosonic simulations that the single-component unary BARW1 and BARW2 processes exhibit the same dynamical scaling as the corresponding models with exclusion. In case of the one-component binary spreading process, the bosonic and fermionic versions differ. While the former one has a discontinuous phase transition, the latter exhibits a continuous transition. We determined numerically the dynamic scaling behavior of the bosonic version.

Without particle production initial condition-dependent dynamical scaling was found in multi-component ARW models. This critical behavior was shown to give the set of on-critical exponents if we generate phase transition by particle branching since the transitions occur at the $\sigma = 0$ rate. The off-critical exponents were found to be insensitive to parity conservation law and depend only on the spatial arrangement of parent and offspring. Two generic universality classes: 2-BARW2a and 2-BARW2s were explored by numerical simulations. In these models, the hard-core exclusions generate extra fluctuations in the absorbing state and the passive steady states posses long-range correlations.

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