Surface Critical Behavior in Systems with Absorbing States

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We present a general scaling theory for the surface critical behavior of nonequilibrium systems with phase transitions into absorbing states. The theory allows for two independent surface exponents which satisfy generalized hyperscaling relations. As an application we study a generalized version of directed percolation with two absorbing states. We find two distinct surface universality classes associated with inactive and reflective walls. Our results indicate that the exponents associated with these two surface universality classes are closely connected. [S0031-9007(98)07023-9]

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The critical behavior of systems with boundaries has been the focus of much research in recent years [1]. So far most work on surface critical behavior and on the analysis of surface universality classes has been within the framework of equilibrium statistical mechanics. However, the same ideas and principles also apply to nonequilibrium systems. A prominent example of such a nonequilibrium process is directed percolation (DP), which is the generic model for systems with a nonequilibrium phase transition from a state with activity (e.g., with a nonzero density of particles) into a so-called absorbing state (with zero activity). An understanding of DP is important for a wide variety of different systems encompassing epidemics, chemical reactions, interface pinning/depinning, spatiotemporal intermittency, the contact process, and certain cellular automata [2]. Recently, however, studies have been made of a number of systems with absorbing states which do not belong to the DP class. One prominent example is a particular reaction-diffusion model called branching and annihilating random walks with an even number of offspring (or BAW for short, where in this paper BAW refers exclusively to the even offspring case) [3]. Other systems in the BAW class (at least in $1 + 1$ dimensions) include certain probabilistic cellular automata [4], monomer-dimer models [5], nonequilibrium kinetic Ising models [6], and generalized DP with two absorbing states (DP2) [7].

In this paper we address the impact of walls on systems with phase transitions into absorbing states. We have developed a general scaling theory which allows for two independent surface exponents, which satisfy generalized hyperscaling relations. As an application, we have investigated the surface critical behavior of DP2. Our numerics indicate that DP2 exhibits a far richer surface structure than DP: we find two different surface universality classes for DP2 with inactive and reflective walls, and our numerical results indicate that the exponents associated with these two classes are closely connected. These results can be successfully contained within our scaling theory. However, we emphasize that the theory is much more general than this and should also apply to other types of systems with walls and absorbing states, e.g., to surface effects in catalytic reactions and systems exhibiting self-organized criticality [8].

Before turning to the surface critical behavior of DP2 (in $1 + 1$ dimensions) and BAW, we begin by discussing the main features of the corresponding bulk systems and then identify some differences and similarities with DP. Many models in the BAW class [3–6] conserve particle number modulo 2, but this appears not to be the fundamental requirement for the emergence of the new universality class. Instead, the key underlying feature seems to be the presence of a symmetry relating the various absorbing states [9]. This has been further demonstrated by Hinrichsen who introduced a generalized version of the Domany-Kinzel model with n absorbing states [7]. This model, which we will refer to as DPn, is defined on a d-dimensional lattice (in space). At time t, the state s_i^t of the ith site can be either active (A) or in one of n inactive states ($I_1, \ldots, I_n$). In $1 + 1$ dimensions, the update probabilities $P(s_i^{t+1} \mid s_{i-1}^t, s_{i+1}^t)$ are given by $P(I_k \mid I_k, I_k) = 1$, $P(A \mid A, A) = 1 - nP(I_k \mid A, A) = q$, $P(A \mid I_k, A) = P(A \mid A, I_k) = p$, $P(I_k \mid I_k, A) = P(I_k \mid A, I_k) = 1 - p$, $P(A \mid I_k, I_l) = 1$, where $(k, l = 1, \ldots, n; k \neq l)$ (see also [7] for a more complete explanation of the model). For $n = 1$ these rules are equivalent to the Domany-Kinzel model which belongs to the DP universality class (apart from one special point which belongs to the compact DP universality class) [10,11]. For $n \geq 2$, the distinction between regions of different inactive states is preserved by demanding that they are separated by active ones. Monte Carlo simulations show that bulk DP2 belongs to the bulk BAW class in $1 + 1$ dimensions [7], whereas this probably does not hold in higher dimensions.

The growth of both BAW and DP clusters in the bulk close to criticality can be summarized by a set of independent exponents. A natural choice is to consider $\nu_\perp$ and $\nu_\parallel$ which describe the divergence of the correlation lengths in space, $\xi_\perp \sim |\Delta|^{-\nu_\perp}$, and time, $\xi_\parallel \sim |\Delta|^{-\nu_\parallel}$, where $\Delta \equiv p - p_c$ describes the deviation from criticality. We also need the order parameter exponent β, which can be defined in two *a priori* different ways: it is either governed by the percolation probability (the probability that a cluster grown from a finite seed never dies),

$$P(\Delta) \sim \Delta^{\beta_{\rm seed}}, \qquad \Delta > 0\,, \tag{1}$$

or by the density of active sites in the steady state,

$$n(\Delta) \sim \Delta^{\beta_{\rm dens}}, \qquad \Delta > 0\,. \tag{2}$$

For the case of DP, it is known that β is unique: $\beta_{\rm seed} = \beta_{\rm dens}$ in any dimension. This follows from theoretical considerations [12,13] and has been verified by extensive numerical calculations. The relation also holds for BAW in $1 + 1$ dimensions, a result first suggested by numerics and now backed up by an exact duality mapping [14]. However, this exponent equality is certainly not always true—for example, it breaks down for certain systems with infinitely many absorbing states [15,16].

Furthermore, $\beta_{\rm seed} \neq \beta_{\rm dens}$ for BAW in high enough dimension: if we consider the mean-field regime valid for spatial dimensions $d > d_c = 2$, then the system is in an inactive state for only a zero branching rate, whereas any nonzero branching rate results in an active state. The steady-state density (2) approaches zero continuously (as the branching rate is reduced towards zero) with the mean-field exponent $\beta_{\rm dens} = 1$. Nevertheless, for $d > 2$ the survival probability (1) of a particle cluster will be finite for *any* value of the branching rate, implying that $\beta_{\rm seed} = 0$ in mean-field theory. This result follows from the nonrecurrence of random walks in $d > 2$.

From the perspective of formulating field theories for BAW, the $1 + 1$ dimensional case poses considerable difficulties [17]. These stem from the presence of two critical dimensions: $d_c = 2$ (above which mean-field theory applies) and $d_c' \approx 4/3$ (where for $d > d_c'$ the branching reaction is a relevant process at the pure annihilation fixed point, whereas for $d < d_c'$ it is irrelevant there [17]). This means that the (physically interesting) spatial dimension $d = 1$ cannot be accessed using controlled expansions down from the upper critical dimension $d_c = 2$. However, if we assume that a (bulk) scaling theory can be properly justified (as it can be for DP, and BAW for $d > d_c'$), then it is straightforward to relate the above set of exponents to those of other quantities. Keeping the distinction between $\beta_{\rm seed}$ and $\beta_{\rm dens}$, the average lifetime of finite clusters, $\langle t \rangle \sim |\Delta|^{-\tau}$, satisfies $\tau = \nu_\parallel - \beta_{\rm seed}$, and the average mass of finite clusters,

$$\langle s \rangle \sim |\Delta|^{-\gamma}, \tag{3}$$

leads to the following hyperscaling relation:

$$\nu_\parallel + d\nu_\perp = \beta_{\rm seed} + \beta_{\rm dens} + \gamma\,. \tag{4}$$

Note that (4) is consistent with the distinct upper critical dimensions for BAW and DP. Using the above mean-field values for BAW and $\nu_\perp = 1/2$, $\nu_\parallel = 1$, and $\gamma = 1$, we verify $d_c = 2$. In contrast, for DP one has the mean-field exponent $\beta_{\rm seed} = 1$ and $d_c = 4$.

We now turn to the surface critical behavior of DP2 and show how the above relations and exponents are modified in a semi-infinite geometry where we place a wall at $x_\perp = 0$ [$\mathbf{x} = (\mathbf{x}_\parallel, x_\perp)$, with the $\perp$ and $\parallel$ directions being relative to the wall]. In the simulations we start from an absorbing state, where all sites are in the state I_1. We then initiate a cluster by placing a seed (site in state A) next to the wall. However, the analogy with DP is no longer immediate, as our numerical measurements in $1 + 1$ dimensions indicate that DP2 supports an additional surface exponent as well as an additional surface universality class. The type of surface universality class is governed by the choice of boundary condition (BC). We have studied two types of BC: the inactive BC (IBC) where the wall sites are always in the inactive state I_1, and the reflective BC (RBC), where the wall acts like a "mirror" by letting imaginary sites next to the outer side of the wall be the mirror images of those on the inside.

By growing a DP cluster near an IBC wall, it has been observed numerically in $d = 1, 2$ that certain exponents are altered [18,19]. This behavior has been explained by a scaling theory [20] that explicitly takes surface critical phenomena into account and connects IBC with the *ordinary* transition [21]. Apart from the above (three) independent bulk exponents, an additional universal surface exponent must be included, which satisfies a generalized hyperscaling relation [20]. The survival probability (1) for a cluster started close to the wall has the form

$$P_1(t, \Delta) = \Delta^{\beta_{1,\rm seed}}\, \psi_1(t/\xi_\parallel), \qquad \Delta > 0\,, \tag{5}$$

where the subscript "1" refers to the wall. However, in analogy with the bulk case, an order parameter can also be defined by the density of active sites on the wall in the steady state,

$$n_1(\Delta) \sim \Delta^{\beta_{1,\rm dens}}, \qquad \Delta > 0\,. \tag{6}$$

More generally the steady-state density (2) is now given by $n(\Delta, x_\perp) = \Delta^{\beta_{\rm dens}}\, \varphi(x_\perp/\xi_\perp)$, where the scaling function φ behaves in such a way that $n(\Delta, x_\perp)$ for $x_\perp/\xi_\perp \ll 1$ crosses over to the surface behavior (6).

For the case of DP, the surface exponents fulfill $\beta_{1,\rm seed} = \beta_{1,\rm dens}$, as can be shown by a field-theoretic derivation of an appropriate correlation function [20]. However, for DP2 this exponent equality is no longer true. Our numerical results in $1 + 1$ dimensions yield two distinct surface exponents, $\beta_{1,\rm seed} \neq \beta_{1,\rm dens}$, although the corresponding bulk exponents coincide, as expected. The values of these surface exponents depend on the boundary conditions, and, by changing from IBC to RBC or vice versa, we observe that the assignment of the exponents is interchanged (see below). Further investigations are needed in order to determine whether the wall may have broken a (duality) symmetry present in the bulk (which forces the bulk exponents to coincide) and whether the operation of this symmetry relates IBC to RBC and vice versa. In contrast for surface DP, we note that IBC and RBC belong to the same surface universality class.

By keeping $\beta_{1,\rm seed}$ and $\beta_{1,\rm dens}$ distinct, we can now set up a general scaling theory for the surface critical behavior in systems with absorbing states. An ansatz for the coarse-grained density of active sites ρ_1 at the point $(\mathbf{x}, t)$ of a cluster grown from a single seed located next to the wall, has the form

$$\rho_1(x, t, \Delta) = \Delta^{\beta_{1,\mathrm{seed}} + \beta_{\mathrm{dens}}} f_1(x/\xi_\perp, t/\xi_\parallel). \quad (7)$$

The Δ prefactor comes from (5) for the probability that an infinite cluster can be grown from the seed, and from (2) for the (conditional) probability that the point $(\mathbf{x}, t)$ belongs to this cluster. The shape of the cluster is governed by the scaling function f_1, and we assume that the density is measured at a finite angle away from the wall. If the density is measured along the wall, we have instead

$$\rho_{11}(x, t, \Delta) = \Delta^{\beta_{1,\mathrm{seed}} + \beta_{1,\mathrm{dens}}} f_{11}(x/\xi_\perp, t/\xi_\parallel), \quad (8)$$

as we pick up a factor $\Delta^{\beta_{1,\mathrm{dens}}}$ rather than $\Delta^{\beta_{\mathrm{dens}}}$ for the probability that $(\mathbf{x}, t)$ at the wall belongs to the infinite cluster. In $1 + 1$ dimensions, (8) reduces to $\rho_{11}(t, \Delta) = \Delta^{\beta_{1,\mathrm{seed}} + \beta_{1,\mathrm{dens}}} f_{11}(t/\xi_\parallel)$.

Starting from a seed on the wall, the average lifetime of finite clusters, $\langle t \rangle \sim |\Delta|^{-\tau_1}$, satisfies $\tau_1 = \nu_\parallel - \beta_{1,\mathrm{seed}}$. The average size of finite clusters follows from integrating the cluster density (7) over space and time:

$$\langle s \rangle \sim |\Delta|^{-\gamma_1}, \quad (9)$$

where the surface (susceptibility) exponent γ_1 is related to the previously defined exponents via

$$\nu_\parallel + d\nu_\perp = \beta_{1,\mathrm{seed}} + \beta_{\mathrm{dens}} + \gamma_1. \quad (10)$$

The only difference from (4) is that we have now included a wall. Analogously, by integrating the cluster wall density (8) over the $(d - 1)$-dimensional wall and time, we obtain the average (finite) cluster size on the wall,

$$\langle s_{\mathrm{wall}} \rangle \sim |\Delta|^{-\gamma_{1,1}}, \quad (11)$$

where

$$\nu_\parallel + (d - 1)\nu_\perp = \beta_{1,\mathrm{seed}} + \beta_{1,\mathrm{dens}} + \gamma_{1,1}. \quad (12)$$

Note that if the γ susceptibility exponents obtained from (10) and (12) are negative, then they should be replaced by zero in (9) and (11). The above scaling theory is generic since it allows for $\beta_{1,\mathrm{seed}}$ and $\beta_{1,\mathrm{dens}}$ to be independent surface exponents. When the scaling theory is applied to DP, it can be fully justified (with $\beta_{1,\mathrm{seed}} = \beta_{1,\mathrm{dens}}$) [20]. However, if we apply the theory to BAW [22], it would again be desirable to obtain a secure renormalization-group justification for the scaling behavior. In particular, it would be important to determine from the field theory whether two *independent* surface exponents are present. However, given the fundamental difficulties encountered already in the *bulk* field-theoretic analysis of BAW in $1 + 1$ dimensions [17], this kind of analysis for the surface is unlikely to give a complete justification of the scaling theory.

In order to confirm our scaling theory we have performed numerical simulations for DP2 in $1 + 1$ dimensions with walls constrained by IBC or RBC (see [23] for details). We have also performed simulations for DP2 without a wall and obtained results for the exponents in complete agreement with [7]. There are several estimates for β_{dens} ($= \beta_{\mathrm{seed}}$) available [24]: we have used $\beta_{\mathrm{dens}} = 0.922(5)$ [25].

We extract the critical exponents from several measured quantities. Using (5), we find that the survival probability for the cluster to be alive at time t has the following behavior at criticality ($\Delta = 0$)

$$P_1(t) \sim t^{-\delta_{1,\mathrm{seed}}}, \qquad \delta_{1,\mathrm{seed}} = \beta_{1,\mathrm{seed}}/\nu_\parallel. \quad (13)$$

Integrating the densities (7) and (8) gives expressions for the activity at criticality as a function of time [23], e.g.,

$$N_1(t) \sim t^{\kappa_1}, \qquad \kappa_1 = d\chi - \delta_{\mathrm{dens}} - \delta_{1,\mathrm{seed}}, \quad (14)$$

where we have introduced the envelope (or "roughness") exponent $\chi = \nu_\perp/\nu_\parallel$, and $\delta_{\mathrm{dens}} = \beta_{\mathrm{dens}}/\nu_\parallel$. Note that (14) corresponds to the hyperscaling relation (10) at criticality with $\gamma_1 = \nu_\parallel(1 + \kappa_1)$, since $\langle s \rangle \sim \int dt\, N_1(t)$. For further confirmations of our numerical data we also considered the cluster size distributions at criticality. The cluster size s scales as $s \sim \xi_\perp^d \xi_\parallel n(\Delta) \sim \Delta^{-1/\sigma}$, with $1/\sigma = d\nu_\perp + \nu_\parallel - \beta_{\mathrm{dens}}$. The probability to have a cluster of size s then reads [23]

$$p_1(s) \sim s^{-\mu_1}, \qquad \mu_1 = 1 + \frac{\beta_{1,\mathrm{seed}}}{d\nu_\perp + \nu_\parallel - \beta_{\mathrm{dens}}}. \quad (15)$$

In Table I we list our estimates for the critical exponents for DP2, where $\delta_{1,\mathrm{dens}} = \beta_{1,\mathrm{dens}}/\nu_\parallel$ is obtained from (8) by measuring the activity at the wall [23], and $\mu = 1 + \beta_{\mathrm{seed}}/(d\nu_\perp + \nu_\parallel - \beta_{\mathrm{dens}})$ corresponds to (15) in the absence of a wall. The results are in complete accordance with our theoretical analysis: bulk exponents are unaltered, whereas the wall introduces two separate surface exponents. We have also carried out bulk and surface simulations for $\Delta > 0$ and confirmed that our data could be collapsed according to an appropriate survival probability scaling function [see (5) for the surface case], using our exponent estimates. This numerically confirms the validity of the relation $\delta = \beta/\nu_\parallel$ for the bulk as well as for both sets of corresponding surface exponents [27]. We further observe that the IBC and

TABLE I. Critical exponents obtained from our simulations. For comparison we also list the exponents for DP with an IBC wall in the first column [18,19,26].

	DP (IBC)	DP2	DP2 (IBC)	DP2 (RBC)
δ_{dens}	0.159 47(3)	0.287(5)	0.288(2)	0.291(4)
β_{dens}	0.276 49(4)	0.922(5)	0.93(1)	0.94(2)
$\delta_{1,\mathrm{seed}}$	0.4235(3)		0.641(2)	0.426(3)
$\beta_{1,\mathrm{seed}}$	0.7338(1)		2.06(2)	1.37(2)
$\delta_{1,\mathrm{dens}}$	0.4235(3)		0.415(3)	0.635(2)
$\beta_{1,\mathrm{dens}}$	0.7338(1)		1.34(2)	2.04(2)
μ	1.108 25(2)	1.225(5)		
μ_1	1.2875(2)		1.500(3)	1.336(3)

RBC boundary conditions lead to *different* exponents thus showing the existence of two distinct surface universality classes. Furthermore, $\beta_{1,\mathrm{seed}} \neq \beta_{1,\mathrm{dens}}$, although by changing BCs we observe to good accuracy that $\beta_{1,\mathrm{seed}}^{(\mathrm{IBC})} = \beta_{1,\mathrm{dens}}^{(\mathrm{RBC})}$, $\beta_{1,\mathrm{seed}}^{(\mathrm{RBC})} = \beta_{1,\mathrm{dens}}^{(\mathrm{IBC})}$. As noted above, this suggests that the two BCs for DP2 are related by a symmetry. By universality, we expect the same relations to apply to BAW [23].

By using the explicit definitions of IBC and RBC we can argue that $\beta_{1,\mathrm{seed}}$ and $\beta_{1,\mathrm{dens}}$ should indeed depend on the BCs. There will be more activity next to the wall for IBC than for RBC, since the latter can have regions of I_2 located at the wall. Once created, these I_2 regions will survive until the activity returns to the wall. Thus, from the wall density (6), it follows that $\beta_{1,\mathrm{dens}}^{(\mathrm{IBC})} \leq \beta_{1,\mathrm{dens}}^{(\mathrm{RBC})}$. On the other hand, the existence of these I_2 regions implies that the survival probability (5) for IBC will be smaller than for RBC, leading to $\beta_{1,\mathrm{seed}}^{(\mathrm{IBC})} \geq \beta_{1,\mathrm{seed}}^{(\mathrm{RBC})}$. However, from the observation that $\beta_{1,\mathrm{seed}} + \beta_{1,\mathrm{dens}}$ is independent of the BC, it follows that the average mass on the wall (11) is the same for IBC and RBC. We have also studied several other BCs and found that these give the same scaling behavior as either RBC or IBC depending on whether or not the above-mentioned I_2 regions can disappear only at the wall or also in the bulk [23]. In terms of the BAW model, however, the distinction between the two BCs is slightly different: IBC respects the "parity" symmetry of the bulk, whereas RBC breaks it.

For DP it has been customary to investigate whether the critical exponents can be fitted by (simple) rational numbers [26]. Such a fitting has also been tried for bulk BAW with the following guesses in $1 + 1$ dimensions: $\kappa = \chi - 2\delta = 0$ and $\chi = 4/7$ [3]. These estimates lead immediately to $\delta = 2/7$ (and $\beta/\nu_\perp = 1/2$). It is intriguing to note that our numerical results for DP2 in addition suggest that $\mu_1 = 3/2$ for IBC and $4/3$ for RBC. From Eq. (15), it then follows that $\delta_{1,\mathrm{seed}} = 9/14$ for IBC and $3/7$ for RBC. We would need one more relation in order to obtain the last independent exponent. In fact, we observe numerically that $2\nu_\parallel - \beta_{1,\mathrm{seed}} - \beta_{1,\mathrm{dens}} = 3$ [28] is valid to within 1% [29].

In conclusion, we have presented a generic scaling theory of surface critical behavior in systems with absorbing states. In particular, we have for the first time studied the surface critical behavior of DP2, a model belonging to the BAW universality class in $1 + 1$ dimensions. Numerical simulations of the DP2 model with two different types of boundary conditions have uncovered two surface universality classes. Our most important result is that *two* surface exponents are required to describe the surface critical behavior. The results also indicate that the exponents associated with these two surface universality classes are closely connected. We emphasize that our theory is generic for systems with absorbing states and therefore should also apply to surface effects in, for example, systems exhibiting self-organized criticality. It would also be possible to generalize our theory to allow for edges and corners, which would introduce new exponents and other hyperscaling relations.

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[29] The other DP2 exponents then follow: $\beta_{\mathrm{dens}} = \beta_{\mathrm{seed}} = 12/13$, $\nu_\parallel = 42/13$, $\nu_\perp = 24/13$; also $\beta_{1,\mathrm{seed}} = 27/13$ and $\beta_{1,\mathrm{dens}} = 18/13$ for IBC and vice versa for RBC.