Non-Universal Extinction Transition for Boundary Active Site

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We present a generalized model of a diffusion-reaction system where the reaction occurs only on the boundary. This model reduces to that of Barato and Hinrichsen when the occupancy of the boundary site is restricted to zero or one. In the limit when there is no restriction on the occupancy of the boundary site, the model reduces to an age dependent Galton-Watson branching process and admits an analytic solution. The model displays a boundary-induced phase transition into an absorbing state with rational critical exponents and exhibits aging at criticality below a certain fractal dimension of the diffusion process. Surprisingly the behavior in the critical regime for intermediate occupancy restriction $N$ varies with $N$. In fact, by varying the lifetime of the active boundary particle or the diffusion coefficient in the bulk, the critical exponents can be continuously modified.

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Nonequilibrium phase transitions can differ significantly from their equilibrium cousins, and are a subject of continuing interest. Recently, Barato and Hinrichsen [1,2] (BH) studied a reaction-diffusion model apparently exhibiting a new universality class of nonequilibrium phase transitions, boundary induced phase transitions. The model they studied was a variant of a model introduced earlier by Deloubrière and van Wijland [3], who however did not discover the novel scaling behavior. In this letter we generalize the model and solve it analytically in a certain limit. Our model exhibits a phase transition and at criticality we find the presence of aging [4,5], a nonequilibrium property observed in such diverse systems as spin-glasses [4], gels [6] and turbulence [7]. Furthermore a critical fractional dimension for the diffusion process is naturally obtained in the context of our model. Interestingly we find that the critical exponents of the model vary continuously with the parameters of the model. We also note that our toy model is interesting in the context of catalytic reactions and biological situations when the reaction occurs on a specific membrane, such as a boundary of a cell.

Our model is defined as follows: As in the BH model, a particle starting on the boundary follows a birth-death process. It produces an offspring (next to the boundary site) with probability $p$ ($A \rightarrow A + O$) and dies with probability $1 - p$ ($A \rightarrow \emptyset$). The particle $A$ continues to reproduce until it dies. The offspring $O$ diffuse freely in the bulk since their birth and up to the time they reach the boundary, and then they start to reproduce again according to the same death-birth process. By varying the rate of offspring production, one expects to reach extinction for $p \rightarrow 0$ (absorbing state) and a growing or stable population for $p \rightarrow 1$, intuitively one expects a transition between those two states as $p$ grows from 0 to 1. In the BH model, there is a constraint that only one particle can exist on the boundary site at any given time. Any other particle trying to enter the boundary site dies immediately. We generalize this to allow up to $N$ particles to coexist simultaneously on the boundary. As shown by BH, the role of the bulk diffusion is just to generate a probability distribution $\psi(t)$ for the arrival of the newly born particle to the boundary site, where it can, if the boundary site is not fully occupied, reproduce some number of times, setting off new processes and then die. Introducing constraints on the occupancy of the bulk sites has no effect on the global dynamics, due to the indistinguishability of different particles [8]. By totally relaxing the constraint on the boundary occupancy, i.e., $N \rightarrow \infty$, we are capable of completely solving the model since technically the unrestricted model is a random branching, or Galton-Watson, process.

In the unrestricted case we can make another simplification, since the time to die is governed by a short-range exponential distribution, we can, without doing any harm to the model, consider all births as happening simultaneously. In this view, the particle generates $k$ children, governed by a geometrical distribution, $p_k = (1 - p)p^k$, and then immediately dies. The basic technique employed in the analysis is the use of the generating functional [9] and parallels the solution of the standard age-dependent branching process [10]. Let us denote by $Z(t, t+s)$ the number of particles that been observed on the boundary during the time interval $(t, t+s)$. We define a generating function for the random variable $Z(t, t+s)$ as the average of $s^{Z(t,t+s)}$ over the distribution of $Z(t, t+s)$

\[
G_{(t,t+s)}(s) = \sum_{Z(t,t+s)=0} P(Z(t, t+s))s^{Z(t,t+s)},
\]

where $P(Z(t, t+s))$ denotes the probability to observe $Z(t, t+s)$ particles on the boundary in the specified time interval. The generating function for the number of offsprings is $G_D(s) = (s^k) = (1 - p)/(1 - ps)$. We set the initial conditions such that at $t = 0$ a single particle was injected into the bulk and it has the probability distribution $\psi(t)$ to return to the boundary at time $t = t_R$. By conditioning on the outcome of the returning time
for the first particle [10], we obtain [11] the equation for \( G(t, t+s) \)

\[
G(t, t+s) = \int_0^t G_0(G(t-u, t-u+s))\psi(u)du + \int_{t+s}^\infty \psi(u)du.
\]

(2)

In the limit of \( s \to 0 \) the generating function goes to \( P(Z(t_t + t_s) = 0) = P_E(t, s) \), i.e. the probability that not a single particle appears on the boundary at the mentioned time interval, taking this limit in Eq. [3] we obtain

\[
P_E(t, s) = \int_0^t \frac{1 - p}{1 - p P_E(t, s)} \psi(u)du + \int_{t+s}^\infty \psi(u)du,
\]

(3)

where we have now used the explicit from of \( G_0(s) \). Eq [3], a non-linear Volterra equation of the second kind, is our main equation for the unrestricted case of the model and it describes the time evolution of a two-time quantity. We haven’t assumed anything as to the form of \( \psi(t) \) and so Eq. [3] is quite general. The long-time behavior of \( P_E \) is, as we shall see, governed entirely by the long time behavior of \( \psi(t) \). For normal diffusion in the bulk, this long-time behavior is \( \psi(t) \sim \psi_\infty t^{-(1+\beta)} \), with \( \beta = 1/2 \), \( \psi_\infty = 1/\sqrt{4\pi D} \), where \( D \) is the diffusion constant (defined as usual). We also consider the more general case of \( 0 < \beta < 1 \), and in such case the constant \( \psi_\infty \) is used for the normalization of \( \psi_\infty \). The case of \( 0 < \beta < 1 \) can be achieved if the diffusion in the bulk is anomalous [12]: e.g., subdiffusion for \( 0 < \beta < 1/2 \) described by models such as the continuous time random walk (CTRW) [12] [13]. Herein we study \( P_E \) exclusively; other quantities such as the mean number of particles can also be obtained from Eq. [2] [11].

We will now explore the behavior of \( P_E(t, s) \) in the asymptotic limit of large \( t \) for different values of the parameters \( p \) and \( \beta \). Inspired by numerical solutions of Eq. [3], we adopt the ansatz

\[
P_E(t, s) = P_\infty - A(s)t^{-\alpha} \quad t \to \infty
\]

(4)

In order to obtain a solution of Eq. [3] we substitute the asymptotic form in Eq. [4] into both sides of Eq. [3], perform an expansion in inverse powers of \( t \) and compare the coefficients in front of the appropriate leading terms. We leave the exact technical details for a longer publication [11] and now provide only the final results.

So doing, in the limit \( t \to \infty \), \( s \) fixed, we obtain

\[
P_\infty = \begin{cases} 1-p/1 & p \geq 1/2 \\ 1-p^\beta & p \leq 1/2 \end{cases}
\]

(5)

which clearly points out the existence of a critical \( p = p_c = 1/2 \). The location of the critical point at \( p = 1/2 \) is due to the fact that at this value, each particle on the boundary produces exactly one offspring. Below this point, the number of particles decreases exponentially with the number of past boundary particles, and above it grows exponentially. The behavior of \( A(s) \) and \( \alpha \) for the off-critical case, \( p \neq p_c \), is given by

\[
A(s) = \begin{cases} \frac{1-p}{1-2p} & p < 1/2 \\ -1 & p > 1/2 \end{cases}, \quad \alpha = \begin{cases} 1 + \beta & p < 1/2 \\ \beta & p > 1/2 \end{cases}
\]

(6)

(7)

The presence of the phase transition as we approach \( p = 1/2 \) from below is clearly manifest in the divergence of the coefficient \( A \). The approach from above is not obvious from the large \( t \) behavior. What happens is that for \( p \geq 1/2 \), \( P_E \) first rises toward unity, as happens below the transition. However, at very large \( t \), the behavior crosses over toward the power-law decay toward \( P_\infty \). The details of this crossover will be presented in our longer presentation [11].

In the critical state, \( p = p_c \), Eq. [5] remains valid and so \( P_\infty = 1 \) while the behavior of \( A(s) \) and \( \alpha \) shows a transition as a function of \( \beta \). For \( \alpha \), we obtain

\[
\alpha = \begin{cases} 1 - \beta \beta \leq 1/2 \\ \beta \beta > 1/2 \end{cases}
\]

(8)

We can exhibit an analytic expression for \( A(s) \) at \( p_c \), only for \( \beta > 1/2 \):

\[
A(s) = -\frac{\pi csc(\beta \pi)\Gamma(1-b)}{\Gamma(1-2\beta)\Gamma(1+\beta)} \quad (\beta > 1/2)
\]

(9)

For \( \beta < 1/2 \), \( A(s) \) has to be calculated numerically in general. However, in the limit of large \( s \), we have

\[
A(s) \propto s^{1-\beta} \quad (\beta < 1/2).
\]

(10)

The existence of a special \( \beta \) for the behavior at criticality is very non-trivial and it is especially interesting that the critical \( \beta_c \) is equal to 1/2, i.e the normal diffusion case. We can treat this critical \( \beta_c \) as a critical fractal dimension since \( 2\beta \) is just the fractal dimension of the diffusion. For the special case of \( \beta = 1/2 \) our ansatz, i.e. Eq. [4], does not work and one needs to treat this case specially [11]; the result is

\[
1 - P_E(t, s) \propto \frac{1}{\log(s/t)}(s/t)^{1/2} \quad (\beta = 1/2).
\]

(11)

The logarithmic corrections in the behavior support our claims as to the critical nature of \( \beta = 1/2 \). For a two time quantity like the survival probability \( P_S(t, s) = 1 - P_E(t, s) \), one usually expects for a stationary process a dependence only on the time difference \( s \); when the process is non-stationary this is generally not true. When the time dependence is that of a ratio of the two
times this is usually defined as aging, as in our case
$P_S(t, s) \propto (s/t)^{1-\beta}$. The aging behavior for $\beta \leq 1/2$ at
criticality is a signature of the nonequilibrium phase trans-
ition properties, which have been studied extensively in
the context of DP and Contact Process \[13\ \[15\], and the
nonstationarity of the process usually obtained in
glassy dynamics \[4\]. We must note that the obtained re-
result where the probability to observe at least one particle
in time interval $s$ is proportional to $s^{1-\beta}$ ($\beta < 1/2$) is
unexpected in light of the fact that for the off-critical state
($p < p_c$), this probability is proportional to $s$.

Now we treat the limit $s \gg t \gg 1$, where we take first
$s \to \infty$. In this limit we can neglect the second term
on the right hand side of Eq. \[3\] and define $P_E(t, \infty) =
P_E(t)$ simply as the extinction probability of the process.
We are now dealing with a single-time quantity and so
no aging behavior could be obtained. For the solution
we use the same ansatz as in Eq. \[4\], writing
$E$ expected in light of the fact that for the off-critical state
$p$ the origin, we have a phase transition at $p = 1/2$
expected also in numerical simulations \[2\]. This is in
the context of DP and Contact Process \[5, 14, 15\], and
transition properties, which have been studied extensively in

Thus for the survival probability of the process, $P_S(t) =
1 - P_E(t)$, we obtain the power-law behavior $P_S(t) \sim
t^{-\delta}$ with $\delta = \beta/2$. The special properties of $\beta = 1/2$
are not observed in the limit of $s \gg t$, and as already
been mentioned no aging behavior could be observed for
a one-time quantity. The noncommutativity of the limits
t \to \infty - s \to \infty is similar in some sense to the non
commutativity of the same limits present for correlation
function behavior in glassy systems \[4\] and leads to such
non-equilibrium property as ergodicity breaking \[19\ \[17\].

Thus, in the case of normal diffusion, i.e. $\beta = 1/2$,
for our modified model with unrestricted occupation of
the origin, we have a phase transition at $p = 1/2$ with a
critical exponent for the survival probability of $\delta = 1/4$, 
observed also in numerical simulations \[2\]. This is in
contrast with the original model, with a larger critical $p$,
but more importantly, a survival exponent of $\delta \approx 0.17$.
The change in the phase transition point is clear, since in
the original $N = 1$ model, some children die upon their
attempted return to the origin and so the critical $p$ has
to be larger than $1/2$ to compensate. The change in ex-
ponent is not unexpected. For directed percolation, the
critical exponents in a model of unrestricted occupancy
are the mean-field exponents, which differ from the ex-
ponents in the restricted occupancy version \[18\].

In the case of directed percolation, for any finite $N$
the critical exponents are those of the $N = 1$ model. For
large $N$, there is a crossover in the scaling between the
mean-field scaling of the $N = \infty$ model and the directed
percolation exponents \[18\]. Based on this analogy, one
would expect a similar behavior in the present case, with
the critical behavior for any finite $N$ being identical to
the $N = 1$ model.

To test this hypothesis, we have measured the survival
exponent $\delta$ at criticality for various $N$. The results are
shown in Fig. \[4\] We see that, contrary to our naive
expectation, there is a different exponent for each $N$. The
measured best fit exponents are, for example, $\delta = 0.160$
for $N = 1$, $\delta = 0.171$ for $N = 2$, $\delta = 0.180$ for $N = 3$ and
$\delta = 0.192$ for $N = 4$. There is no sign of any crossover
behavior. One test for this is shown in Fig. \[2\] where we show
$P_S(t) t^\delta$, in a linear($y$)-log($x$) scale. We see that
the graphs all exhibit the same characteristic oscillation
in $\ln(x)$ \[19\] that makes accurate determination of an
exponent so difficult, but they show no secular trend.

Varying $N$ is not the only way to interpolate between
the two models and thereby vary $\delta$. We can instead intro-
duce a parameter $\Delta$ which controls the lifetime of a par-
ticle on the active site after reproduction (in the original
model, $\Delta = 1$). As $\Delta$ decreases, the interference between
different particles is reduced, and the theory approaches
the noninterference, Galton-Watson, limit. We can also

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{The survival probability vs. time for $N = 1, 2, 3,$
and 4, together with power-law fits for the cases $N = 1$ and
$N = 4$.}
\end{figure}
increase $\Delta$ beyond one, and make the interference effect stronger, thereby reducing the exponent below the original BH value. Actually the precise dimensionless parameter which controls the exponent $\delta t = \delta t^* \ll D \Delta$, which presents a surprising dependence of the critical exponent $\delta$ on the diffusion coefficient ($D$) in the bulk. This is demonstrated in Fig. 1 where the survival exponent is plotted as a function of $\Delta$. We see that as opposed to the discrete parameter $N$, now the exponent varies continuously, decreasing with $D \Delta$.

Finally we note that the relevance of the limit for which we managed to solve the model analytically is much broader when one considers higher dimension systems. We have studied herein a one dimensional system where the boundary is zero dimensional, while if one considers a $d$ dimensional system where the boundary is of dimension $d-1$, a line or a membrane, in such a case even if $D \Delta$ does not approach zero, the probability that two particles would try to occupy the same site (since there an infinite number of sites on boundary) during the time $D \Delta$ is small and this would lead to a larger applicability of our analytical solution. Another type of system where our results could be applied is systems with anomalous diffusion behavior described by the Continuous Time Random-Walk model [12], for such systems the results stays valid even if the size of the system is finite as for a finite system with regular diffusion our results are modified for times long enough [11].

In summary, we have extended to finite active site occupancy $N$ and solved analytically the $N \rightarrow \infty$ limit of the Barato-Hinrichsen model, yielding the scaling exponents of the extinction transition in this limit. We have also show that below a critical fractal dimension for the diffusion process in the bulk, there is aging behavior at the transition. In addition, we have seen that the exponents are in fact not universal, varying with $N$ or the scaled lifetime of the particles on the active site. This is of course very different from the situation that obtains in the superficially similar contact process, which exhibits universal Directed Percolation scaling.

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