On the continuum time limit of reaction-diffusion systems

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Abstract – The parity-conserving branching-annihilating random walk (pc-BARW) model is a reaction-diffusion system on a lattice where particles can branch into \( m \) offsprings with even \( m \) and hop to neighboring sites. If two or more particles land on the same site, they immediately annihilate pairwise. In this way the number of particles is preserved modulo two. It is well known that the pc-BARW with \( m = 2 \) in 1 spatial dimension has no phase transition (it is always subcritical), if the hopping is described by a continuous time random walk. In contrast, the \( m = 2 \) 1-d pc-BARW has a phase transition when formulated in discrete time, but we show that the continuous time limit is non-trivial: When the time step \( \delta t \to 0 \), the branching and hopping probabilities at the critical point scale with different powers of \( \delta t \). These powers are different for different microscopic realizations. Although this phenomenon is not observed in some other reaction-diffusion systems like, e.g., the contact process, we argue that it should be generic and not restricted to the 1-d pc-BARW model.

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It is well known that the short-distance behavior of relativistic quantum field theories is in general anomalous. For instance, Abelian gauge theories like QED have diverging bare charges while the coupling constants of non-Abelian gauge theories like QCD converge to zero at short distances. In simulations of non-linear quantum field theories like QCD this is usually taken into account by making space-time discrete and letting the lattice constant tend to zero after the calculation.

In non-relativistic reaction-diffusion systems one might \textit{a priori} expect something similar, but there it is of course extremely natural to work on spatial lattices, so the problem is considered as much less fundamental (for possible problems associated with spatial discretization, see [1,2]). Indeed it is often taken for granted that spatial discretization is sufficient to render any reaction-diffusion model well defined mathematically. This is, \textit{e.g.}, true for models in the reggeon field theory \cite{3} universality class. As shown in \cite{4}, the reggeon field theory describes a reaction-diffusion system which can be either realized as a process discrete in space and time, in which case it is known as directed percolation \cite{5}, or on discrete space with continuous time, called “contact process” \cite{6}. Indeed, the contact process can be seen as the limit of a particle process in discrete time with hopping diffusion, branching, annihilation, and spontaneous decay where all probabilities are \( O(h) \) with \( h \ll 1 \), and physical time proceeds also slowly so that \( t \) is \( h \) times the number of iteration steps.

In the present note we point out that things are not always so simple. Take a diffusion process on a spatial lattice, where the hopping rate is \( h \ll 1 \). This by itself would correspond to a random walk with rms. end-to-end distance \( R^2 \propto hn \) for a walk with \( n \) steps. In order to have a finite diffusion constant \( D \) independent of \( h \), we then have to define physical time as \( t \propto hn \). Add now some reaction(s) which conceivably can lead to qualitatively new behavior(s) with one or more critical points. Is it still true that the critical points are obtained when all reaction rates also scale \( \propto h \)? We will give an example where this is not the case.

The model we study here is the one-dimensional branching-annihilating random walk (BARW) with two offsprings at each branching event and with pairwise annihilation \cite{7,8}. Since both branching and annihilation change the number of particles by an even amount, the total number of particles is conserved modulo 2. This is also called the parity-conserving BARW (pc-BARW). It was proven rigorously by Sudbury \cite{9} that this model is
always subcritical, if treated in continuous time. This is
often taken as evidence that the model is always subcriti-
ical also when treated in discrete time [8,10,11], and more
complicated models were used to study the corresponding
universality class [2,10,12–14].

We will see that this is not true. More concretely, we
will study two versions of the discrete time 1-d pc-BARW.
In model A hopping and branching reactions are applied
alternatingly. First, all particles can hop with probabil-
ity \( p \), then they can branch with probability \( q \), then again
hop, etc. In model B particles can hop at any time step
with probability \( p \) or branch with probability \( q \), or stay
idle with probability \( 1 - p - q \). In model B we have of-
course the restriction \( p + q \leq 1 \), while no such restriction
holds in model A. In order to guarantee that annihilation
occurs only between particles in the same generation, we
used two data structures: two lists \( L_1 \) and \( L_2 \) of integer
particle positions and a 1-d array \( S \) of characters contain-
ing the occupancy state of each lattice site. Assume that
at time step \( \tau \) the particles are at sites \( i_1, \ldots, i_N \) stored
in \( L_1 \), and \( S \) is empty. To proceed to the next time step, we
first go through \( L_1 \) and update \( S \) at the positions \( i_1 \)
and \( i_n \pm 1 \), taking into account annihilation. Then we go
again through \( L \), check the values of \( S[i_n] \) and \( S[i_n \pm 1] \). If
they are non-zero, the corresponding positions are written
into \( L_2 \) and \( S \) is cleared at this position. Finally, \( L_1 \) is re-
placed by \( L_2 \) and we proceed to the next time step. More
precisely, this algorithm applies to model B. For model A
each time step is composed of two half-steps.

We study these models by simulations where we started
with two particles at adjacent sites, and followed their
evolution until the population dies or until a prefixed
number \( T \) of time steps is reached. We typically used
\( 10^5 \leq T \leq 5 \times 10^7 \), with larger \( T \) corresponding to smaller
values of \( p \) and \( q \). For each value of \( p \) we searched for that
value of \( q \) where the process is critical. For this we simply
monitored the average number \( N(\tau) \) of particles at time
step \( \tau \). In addition we measured the probability \( P(\tau) \) that
the process has not yet died and the average squared dis-
cance \( R^2(\tau) \) of the particles from the origin. Since it is
known that at criticality \( N(\tau) \sim \tau^\eta \) with \( \eta = 0 \pm 0.001 \)
[10,13], it is easy to find the critical point with a relative
error \( < 10^{-3} \) by using \( 10^5 \) runs for each \( p \).

Results are shown in fig. 1. For \( q = O(1) \) we found
also \( p = O(1) \) (except for model A, where it seems that
\( q \rightarrow 0 \) for \( p \rightarrow 1 \)). This is not surprising. It is also not
surprising that \( q \rightarrow 0 \) when \( p \rightarrow 0 \). But we definitely
do not see that the ratio \( q/p \) stays finite when \( p \rightarrow 0 \), as
expected in a “normal” continuous time limit. Rather we
find power laws

\[
q \sim p^\alpha
\]

when \( p \rightarrow 0 \), with \( \alpha = 0.50(2) \) for model A and \( \alpha =
0.67(2) \) for model B. We conjecture that the exact ex-
ponents are 1/2 and 2/3.

This immediately explains why Sudbury [9] found only
a subcritical phase in the continuum time limit: to see
critical behavior in the limit \( p \rightarrow 0 \) at physical time scales
corresponding to non-zero diffusion rate, one would have
to take the branching rate to infinity.

For a more precise statement, we obtained from \( R^2(t) \)
also the speed of spreading. In all cases we verified the
previous [10,13] result \( R^2(\tau) \sim \tau^2 \) with \( z \approx 1.15 \)
Therefore, we can estimate the \( p \)-dependent “spreading
constant” \( D(p) \) as

\[
D(p) = \lim_{\tau \rightarrow \infty} R^2(\tau)/\tau^2.
\]

As seen from fig. 2, \( D(p) \) scales for small \( p \) as \( D(p) \sim p^\sigma \),
with \( \sigma_A = 0.91(3) \) and \( \sigma_B = 1.28(3) \). In a similar way
we found that the survival probabilities also scaled with
power laws,

\[
P(t) \sim p^\rho t^{-\delta},
\]

where the exponent \( \rho \) was the same for both models, \( \rho_A =
\rho_B = -0.11(1) \).

Equation (2) would suggest that we define the continuous
time spreading constant \( D = \lim_{p \rightarrow 0} p^{-\sigma} D(p) \). This,
in turn, would suggest that we have to define physical
time \( t = p^\rho \tau \), if we want to have \( R^2(t) \approx Dt^z \) with a
finite value of \( D \).

Unfortunately, this redefinition of time would lead to
singular survival probabilities, because \( \sigma \neq \rho \) for both
models. Therefore, in order to obtain finite renormalized
parameters we also have to rescale space.

We presented these details in spite of the fact that there
exists no fundamental reason for using a continuous time
limit for the pc-BARW, and although more complicated
continuous time models in its universality class are known
[10,12,13]. But there might exist models where things are
even more complicated, and where one has a good reason
to prefer a continuous time formulation. The present pa-
per might give an indication of what is needed in order to
deal with such a situation.

Apart from that, both models A and B are simpler
than any previously proposed realization of the pc-BARW,
and much faster to simulate than the continuum models of [2,10,12–14]. Simple rational critical exponents were conjectured in [10]. In particular, the exponent \( \eta \) (which controls the growth of the average critical cluster size with time) is compatible with being exactly equal to zero, the value that would hold for critical branching processes. This enigmatic result —which urgently calls for an explanation— was recently verified in a high statistics simulation [15], where, however, the exponents \( z \) and \( \delta \) (describing the spatial extent and the survival probability) were found to be no simple rationals. In preliminary runs of model A with \( p = 1/2 \) we verified the results of [15] and obtained also a non-trivial estimate \( \beta = 0.965(5) \) (the order parameter exponent). This disagrees both with the estimates \( \beta = 0.922(4) \) of [13] and the mean-field prediction \( \beta = 1 \). Details will be given elsewhere, together with detailed studies of cluster structures and scaling laws related to them.

We should stress that the pc-BARW as defined in [9] has an infinite annihilation rate. Whenever two particles meet on the same site, they annihilate immediately, so that double occupancies of sites are avoided. This would not be a natural assumption in any field theoretic treatment [16–18]. Indeed, in [16–18] a model was discussed with finite annihilation rate, where sites can be occupied also by double occupancies of sites are avoided. This would not meet on the same site, they annihilate immediately, so that.

Fig. 2: (Color online) Log-log plots of spreading constants defined as prefactors in the scaling law \( R^2(\tau) \sim \tau^\beta \) at criticality. Again, errors are much smaller than the symbol sizes, and straight lines represent the scaling for \( p \to 0 \).

problems encountered in the present letter result simply from the fact that one rate was assumed to be infinite. Indeed, in a “non-fermionic” version of model A with finite annihilation rate we found that the critical point appears at finite reaction and hopping rates. Whether the infinity of the annihilation rate is the only reason for the problems discussed in the present paper is not clear.

Finally, we should comment on a similar result for the Sudbury model discovered in [2]. In that model, the continuum \( \text{time} \) limit is assumed. As a consequence, there is no extinction and one is always in the supercritical phase. But that does not mean that the continuous \( \text{space} \) limit is trivial. Indeed, as found in [2], one has to take an infinite ratio between the branching and jumping rates in this limit.

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