On the Continuum Time Limit of Reaction-Diffusion Systems

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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 δt. 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.

I. INTRODUCTION

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 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. Indeed it is often taken for granted that spatial discretization is sufficient to render any reaction-diffusion model well defined mathematically. This is e.g. true for models in the Reggeon field theory [1] universality class. As shown in [2], 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 [3], or on discrete space with continuous time, called 'contact process' [4]. 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 $R_n^2 \propto hn$. 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 [5, 6]. 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 preserving BARW (pc-BARW). It was proven rigorously by Sudbury [7] that this model is always subcritical, if treated in continuous time. This is often taken as evidence that the model is always subcritical also when treated in discrete time [6, 8, 9], and more complicated models were used to study the corresponding universality class [8, 10, 11]. 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 probability 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 happens 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 containing the occupancy state of each lattice site. Assume that at time step τ 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 replaced 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

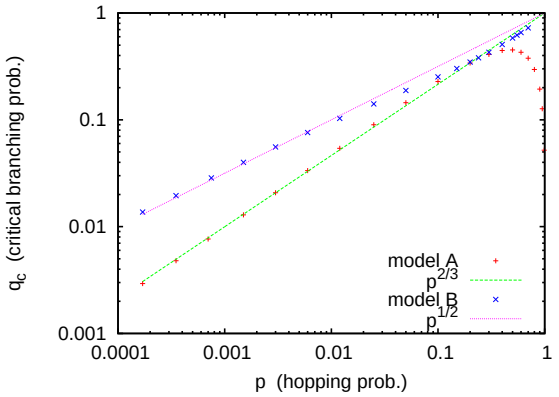

FIG. 1. (Color online) Log-log plots of critical branching probabilities against hopping probabilities for models A and B. Symbols represent Monte Carlo results whose errors are much smaller than the symbol sizes. Straight lines represent scaling for $p \to 0$.

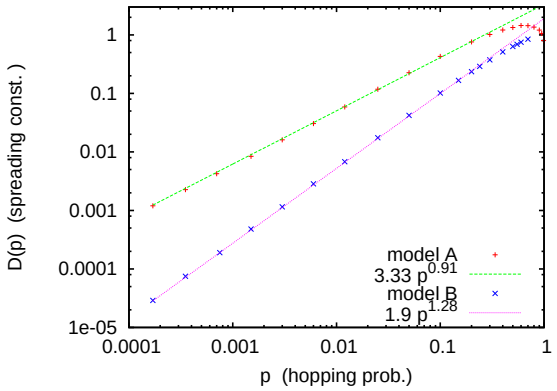

FIG. 2. (Color online) Log-log plots of spreading constants defined as prefactors in the scaling law $R^2(\tau) \sim \tau^z$ at criticality. Again, errors are much smaller than the symbol sizes, and straight lines represent the scaling for $p \to 0$.

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 $10^5 \leq T \leq 5\times10^7$, 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 τ. In addition we measured the probability $P(\tau)$ that the process has not yet died and the average squared distance $R^2(\tau)$ of the particles from the origin. Since it is known that at criticality $N(\tau) \sim \tau^\eta$ with $\eta = 0 \pm 0.001$ [8, 11], it is easy to find the critical point with a relative error $< 10^{-3}$ by using $\sim 10^5 - 10^7$ 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 $p \to 0$ for $q \to 1$). This is not surprising. It is also not surprising that $q \to 0$ when $p \to 0$. But we definitely do not see that the ratio q/p stays finite when $p \to 0$, as expected in a "normal" continuous time limit. Rather we find power laws

$$q \sim p^\alpha \tag{1}$$

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

This immediately explains why Sudbury [7] found only a subcritical phase in the continuum time limit: To see critical behavior in the limit $p \to 0$ 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 [8, 11] result $R^2(\tau) \sim \tau^z$ with $z \approx 1.15$. Therefore we can estimate the p-dependent 'spreading constant' $D(p)$ as

$$D(p) = \lim_{\tau\to\infty} R^2(\tau)/\tau^z. \tag{2}$$

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,

$$P(t) \sim p^\rho t^{-\delta} \tag{3}$$

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

Eq. (2) would suggest that we define the continuous time spreading constant $D = \lim_{p\to 0} p^{-\sigma} D(p)$. This in turn would suggest that we have to define *physical* time t as $t = p^\sigma \tau$, 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 [8, 10, 11]. 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 paper 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 [8, 10, 11]. Since the simplicity of the numerically obtained critical exponents is still enigmatic [8] –

in particular, there is no explanation why η is compatible with being exactly equal to zero –, one might want to redo simulation with very high precision. Either one of the models proposed in this paper would be a good candidate. In preliminary runs of model A with $p = 1/2$ we indeed found $z = 1.149(1)$ and $\delta = 0.2873(8)$ which exclude the conjectures $z = 8/7$ and $\delta = 2/7$ of [8], but for η our results are still compatible with the conjecture $\eta = 0$.

Finally, we should stress that the pc-BARW as defined in [7] 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 [12–14]. In view of this, it is suggestive that the problems encountered in the present note result simply from the fact that one rate was assumed to be infinite. Whether this is true or not is not clear.

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