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Revisiting the nonequilibrium phase transition of the triplet-creation model

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Abstract. The nonequilibrium phase transition in the triplet-creation model is investigated using critical spreading and the conservative diffusive contact process. The results support the claim that at high enough diffusion the phase transition becomes discontinuous. As the diffusion probability increases the critical exponents change continuously from the ordinary directed percolation (DP) class to the compact directed percolation (CDP). The fractal dimension of the critical cluster, however, switches abruptly between those two universality classes. Strong crossover effects in both methods make it difficult, if not impossible, to establish the exact location of the tricritical point.

PACS. 05.70.Ln Nonequilibrium and irreversible thermodynamics – 87.10.+e General theory and mathematical aspects – 89.75.Fb Structures and organization in complex systems

1 Introduction

The occupation of a resident population by a small colony of mutant replicators or, more simply, the settlement of a colony of spontaneously generated replicators in the vacuum are critical issues in prebiotic evolution [1], which have recently been shown to be nonequilibrium phase transitions [2]. The characterization of the diverse types of replicators according to the conditions necessary to their replications [3] leads to a variety of irreversible dynamical systems that are familiar to the statistical physics community [4–6]. Of particular importance for the setting of a sound prebiotic scenario is the nature of the invasion process, that can be suitably described by the dynamic and static critical exponents associated to the probability of invasion [7].

In this contribution we re-examine the one-dimensional triplet-creation model of Dickman and Tomé [8], in which a necessary condition for replication (i.e., particle creation) is the existence of at least three replicators occupying contiguous positions in the neighborhood of an empty site. (Henceforth we will use the terms replicator and particle interchangeably.) This may be viewed as a generalization of the three-member hypercycle [9,10] in which the presence of all members is required to catalyze the replication of any of the component replicators. Decay and diffusion of the replicator to neighboring sites are considered as well. The rich and controversial critical behavior of the triplet-creation model owns to the competition between diffusion and the triplet replication process.

The motivation for the proposal of that model was to find the simplest, *local* nonequilibrium model that exhibits a discontinuous transition into an absorbing state [8].

In the absence of diffusion, the triplet-creation model exhibits a continuous transition to the unique absorbing vacuum state which belongs to the class of universality of the directed percolation, DP [4-6], as predicted by a conjecture put forward independently by Janssen and Grassberger [11,12]. When diffusion is turned on, however, the situation becomes much less clear. The original analysis of Dickman and Tomé [8] indicates that the continuous transition associated to the low diffusion regime changes into a discontinuous transition for high enough diffusion. (Of course, for infinite diffusion rate, and infinite number of particles as well, the mean-field limit is reached and so the transition is definitely discontinuous.) Their conclusion was disputed by Hinrichsen [13] who presented general arguments against the existence of discontinuous transitions in certain classes of one-dimensional irreversible models and provided numerical evidence, using spreading analysis, that the transition of the triplet-creation model is always continuous, regardless of the value of the diffusion rates. Moreover, the transition was found to be in the DP universality class. More recently, Fiore and de Oliveira [14] used the conservative diffusive contact process, in which the number of particles is kept fixed (see also [15]), to vindicate the original findings of Dickman and Tomé. Here we investigate the nonequilibrium transition of the tripletcreation model using both the spreading and the conservative diffusive techniques and find, in agreement with [14], strong evidence of a discontinuous transitions in the high

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diffusion regime. However, strong crossover effects lead to a continuous variation of the dynamic and static critical exponents, which obey the generalized hyperscaling relation [16], so that a precise location of the tricritical point (i.e., the point at which the transition becomes discontinuous) is very difficult. These crossover effects are probably the cause of the controversies surrounding the triplet-creation model.

The rest of the paper is organized as follows. In Section 2 we present the set of rules that govern the evolution of the particles in the triplet-creation model with a slight variation from the original proposal. The two techniques used to characterize the stationary and dynamic behavior at the transition point are reviewed in Section 3. In particular, we give emphasis to the description of the conservative diffusive contact process since it is, relatively to the spreading analysis, a new method to study nonequilibrium phase transitions. The results obtained by the application of both methods to the triplet-creation model are then presented and discussed in Section 4. Finally, in Section 5 we present some concluding remarks.

2 The triplet-creation model

To gain in computation speed, instead of describing the configuration of the L-sites chain in terms of binary occupation variables [8], we choose to describe the chain by a list of the particle positions $p_n = 1, \ldots, L$ with $n = 1, \ldots, N$. (In practice, a second list $q_i = 0, 1, \ldots, N$ with $i = 1, \ldots, L$ is needed in order to identify which particle occupies site i. If $q_i = 0$ then site i is vacant.) This procedure was also used in [13] for without it long time spreading simulations would not have been possible. In terms of these lists the evolution rules are as follows (see [17] for a similar approach).

Diffusion: this is the diffusion or hopping process that occurs with probability D. A particle, say n, is chosen at random and one of its nearest neighbors sites, say k, is chosen also at random. If $q_k = 0$ then particle n moves to site k and the lists are updated accordingly, otherwise nothing happens.

Decay: this process occurs with probability

$$\gamma = \frac{1 - D}{1 + \lambda}.\tag{1}$$

A randomly chosen particle, say n, is chosen and then annihilated. This is implemented by simply moving particle N to the position of particle n, with the corresponding changes in the lists, and then by resetting the number of particles to N-1.

Creation: this process takes place with probability $s = \lambda \gamma$. As before, a particle, say n with $p_n = i$, is chosen at random. Then its two nearest-neighbor sites, i-1 and i+1, are checked to verify whether they are both occupied or not. If $q_{i-1}q_{i+1} = 0$ nothing happens, since then particle n will not be part of a triplet, otherwise one of the sites i-2 or i+2 is chosen at random and a new particle, identified by the label N+1, is placed at the chosen site, provided it

is vacant. The number of particles is then reset to N+1, so the newly created particle is placed at the end of the q_i list.

Since $D+\gamma+s=1$ there are only two independent parameters in the model which we choose as D and γ . As we will see in Section 3, the fact that the probability of decay and creation are not independent introduces some complications to the formulation of the conservative diffusive contact process for the triplet-creation model.

The modifications we have introduced in the processes of decay and creation were so as to reduce the number of wasted checks of the original formulation of the model, such as choosing an empty site in any of these two processes. Hence they have no effect whatsoever on the steady-state properties of model. As for the dynamics, we acknowledge that by increasing the number of trials that effectively modify the chain configuration, we may affect in a nontrivial and uncontrollable way the time dependence of some properties of the model. But we do not expect that these effects will alter the asymptotic form of the relevant dynamic quantities, say from exponential to power-law and vice-versa, or the values of the exponents that characterize an eventual power-law decay; otherwise the current effort to classify nonequilibrium phase transitions [4–6] would be utterly vain.

The changes in the hopping process, however, are a different matter. In the original model, a site chosen at random, say i, is interchanged with its right neighbor, site i+1 [8]. (If both sites are occupied or vacant, then their interchange will be a waste of time, which is avoided in our formulation.) Hence in the original model a particle at site i has two opportunities to diffuse — when either site i or site i+1 is chosen — but it has only one chance of hopping in the present framework. There is, fortunately, a simple relationship between the probability of hopping \tilde{D} of the original model and our parameter D, namely, $\tilde{D} = D/\left(2-D\right)$ [17], so our results can be readily compared with those in the literature.

For the sake of concreteness we define a trial as the choice of one of the three processes — diffusion, decay and creation — described above. In the original algorithm, a time step of the dynamics is defined as the realization of L such a trials [8], which is clearly impracticable in the case of the very large (ideally infinite) chains used in the spreading analysis. Instead, we follow reference [17] and define the time increment per trial as 1/N, where N is the number of particles just before the trial. Hence each trial represents on average L/N trials in the original algorithm.

3 Methods

In what follows we present a brief account of the spreading analysis which is based on the time evolution of the model as defined in the previous section. In particular, the number of particles varies in time following the separated creation and annihilation processes. More emphasis is given to the description of the, comparatively less familiar, conservative diffusive contact process, in which the number of particles is kept fixed during the evolution of the colony.

3.1 Spreading analysis

We begin with the spreading analysis [7] since it is probably the simplest and most powerful technique to estimate the values of the critical parameters at which the transition between the active and the absorbing regimes take place. We set an initial colony of replicators — a single triplet for D = 0 and a string of 40 contiguous replicators for D > 0 — in the center of an otherwise empty cell of "infinite" size. This can be accomplished by taking the chain size large enough so that, during the time we follow the evolution of the colony, the replicators can never reach the chain extremes. Here we focus on the time dependence of three key quantities: (i) the average number of replicators N(t); (ii) the survival probability of the colony P(t); and (iii) the average mean-square distance over which the colony has spread $R^2(t)$. For each time t we carry out 10⁵ independent runs, all starting with the same colony. Hence P(t) is simply the fraction of runs for which there is at least one replicator in the chain at time t. We stress that in the calculation of N(t) we take an average over all runs, including those that have already been extinct at time t, whereas $R^2(t)$ is averaged only over the colonies that survived at time t.

The idea behind the estimate of critical parameters by following the spreading of the colony is that the time dependence differs qualitatively depending whether the system is in the supercritical or in the subcritical regime. The mere visual inspection of the plots N(t) (or P(t)) versus t allows one to determine whether the control parameters D and γ are below or above the critical ones. In the case that the transition is continuous, it is conjectured that the following scaling laws will hold [7]

$$N(t) \sim t^{\eta}$$
 (2)

$$N(t) \sim t^{\eta}$$
 (2)
 $P(t) \sim t^{-\delta}$ (3)
 $R^{2}(t) \sim t^{z}$, (4)

$$R^2(t) \sim t^z,\tag{4}$$

where η , δ and z are critical dynamic exponents. Particularly relevant to our purposes is the relation between these exponents and the fractal dimension d_f of the surviving colonies at a given asymptotically large time, namely, $d_f = 2(\eta + \delta)/z$ [7], since the value of this quantity, calculated at the steady-state with a different method, was used by Fiore and de Oliveira [14] as the main criterion to distinguish between the continuous and the discontinuous transition.

In principle, power laws are not expected at a discontinuous transition because correlations are of finite range and so quantities such as the survival probability P(t) and the average number of particles N(t) should decay exponentially with time [8]. Earlier reports on power laws at discontinuous transitions in the two-dimensional Ziff-Gulari-Barshad (ZGB) model [18] and in Conway's game of life [19] were proven artifacts of inadequately short-time simulations [20,21]. On the other hand, the one-dimensional Glauber-Ising model at zero temperature in a magnetic field [13] as well as the one-dimensional Domany-Kinzel cellular automaton [22] are realizations of the compact directed percolation (CDP) which exhibits a

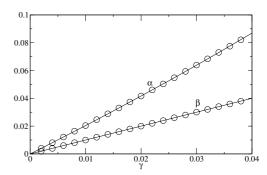


Fig. 1. Stationary weighted (β) and unweighted (α) fractions of active empty sites as function of the decay probability γ for the standard triplet-creation model with cyclic boundary conditions. The solid lines are the fittings $\beta=\gamma$ and $\alpha=\gamma/(1-D-\gamma)$. The parameters are $L=10^4$ and D=0.5.

first-order transition characterized by power laws with the exponents $\eta = 0$, $\delta = 1/2$ and z = 1 for d = 1 [23]. In d=2 and above, models in the CDP class are characterized by the mean-field exponents $\eta = 0$, $\delta = 1$ and z = 1 [24]. Such mean-field-like discontinuous transition was recently reported in a single-component, two-dimensional lattice model of replicators [25]. Thus there seems to be two possibilities only for the critical behavior at a first-order irreversible transition between an active regime and an absorbing state: either there is no power-law behavior at all (as in ZGB and Conway's models) or the critical behavior is mean-field like (as in the abovementioned replicator model [25] and in some monomer-monomer reaction systems [26]). The features of the model that determine which of these two alternatives will hold are still not wellunderstood.

3.2 Conservative diffusive contact process

We now turn to the conservative diffusive contact process [14,15] in which, together with the hopping probability D, the number of replicators N is kept fixed whereas the decay probability γ [or, equivalently, λ , see Eq. (1)] is derived from the analysis of the chain configuration at the stationary state. To see how γ can be obtained in this way we introduce the properly weighted fraction of active empty sites,

$$\beta = \frac{1}{N} \sum_{i} \frac{s}{2} n_{triples}^{(i)} \tag{5}$$

where the sum is over all empty sites and $n_{triples}^{(i)}=0,1,2\,$ is the number of triples adjacent to vacant site i. An active empty site is a vacant site that has a nonzero probability of being occupied. In the stationary regime the number of replicators that decay equals in average the number of replicators that are created in the active empty sites, so one has $\langle \beta \rangle = \gamma$. (The average here is over the distribution of occupied and vacant sites in the steady-state regime.) We have verified the correctness of this relation by carrying out extensive simulations (see Fig. 1) with the standard ensemble of variable particle number in a closed

chain (i.e., using cyclic boundary conditions). Hence we can infer the value of γ by measuring the average fraction of active empty sites in the stationary regime, $\langle \beta \rangle$.

There is, however, a difficulty to apply this scheme for the triplet-creation model. In the conservative diffusive contact process there are two known parameters — the diffusion probability D and the number of replicators N — but in order to calculate β using equation (5) we need the value of the creation probability s, which depends on γ , the quantity we ultimately set out to derive. The situation here is fundamentally different from that of models for which the creation and the decay procedures are independent so that the corresponding conservative contact process can easily be formulated [25]. This hindrance can be circumvented by eliminating the factor s from the definition of the fraction of active empty sites and considering, instead, the quantity [14]

$$\alpha = \frac{1}{N} \sum_{i} \frac{1}{2} n_{triples}^{(i)} \tag{6}$$

where, as before, the sum is over all empty sites. In Figure 1 we present the dependence of the two average fractions β and α on the decay probability γ (for simplicity, henceforth we will omit the average symbols when referring to these quantities), obtained through simulations of the standard (i.e., the number of particle is free to vary according to the creation and decay procedures) triplet-creation model with cyclic boundary conditions. The purpose of this figure is merely to illustrate the correctness of the relation $\gamma = \beta$. Since from equations (5) and (6) we have $\beta = s\alpha$ we can easily derive the relation between γ and α , namely,

$$\gamma = \alpha \frac{1 - D}{1 + \alpha} \tag{7}$$

or, equivalently, $\lambda=1/\alpha$. Hence the choice of β or α is immaterial since γ can easily be inferred from any of them. We note in passing that the relation between the leading parameter of the conservative diffusive contact process α and the parameter of the original formulation λ was not made explicit in [14].

The basic idea of the conservative contact process is the occupation of the active empty sites by the transference of randomly chosen replicators to those sites, rather than by the creation of new replicators. In this way the number of replicators does not change and the processes of creation and annihilation are replaced by a single jumping process [15]. In the conservative diffusive contact process there are two procedures only: diffusion that occurs with probability D and jumping, which combines both creation and decay, that occurs with probability 1 - D. Since the diffusion procedure does not change the number of replicators, it can be implemented exactly as described in the definition of the model [14]. The jumping process is implemented as follows. We choose a replicator at random and check whether it is at the center of a triple. If so, then we pick at random one of the sites adjacent to the triple. If this site is vacant we choose another replicator at random and transfer it to the vacant site. This

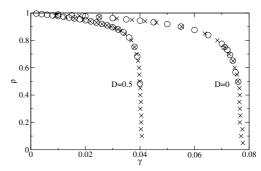


Fig. 2. Average density of particles as function of the decay probability of the standard (\bigcirc) and the conservative (\times) versions of the triplet-creation model for diffusion probabilities as indicated and chain size $L=10^4$.

scheme is completely equivalent to that used by Fiore and de Oliveira [14].

In Figure 2 we present the comparison of the average density of particles at the stationary state obtained with a single sample of the traditional (T) and the conservative (C) versions of the triplet-creation model for two values of the diffusion probability. At first sight the excellent agreement between these two models with very different rules for the creation and decay processes is truly remarkable. (We note that, leaving diffusion aside, creation occurs with probability s in the traditional formulation, whereas it occurs with probability one in the conservative formulation.) But the reason for that is actually quite prosaic (see [27] for a formal argument). For a given value of N, model C leads to a stationary state characterized by a particular value of α , as defined in equation (6). The problem is to find the value of γ (or λ) in model T that produces a stationary state characterized by exactly the same value of α , though these stationary states may differ in many other aspects as, for instance, in the fluctuations of the number of particles. In view of equation (5) and of the fact that $\gamma = \beta$ at the stationary state of model T the answer is given simply by equation (7). Hence the agreement between models T and C, at least with regard to properties related to α , follows trivially from this argument.

In addition, Figure 2 provides a good illustration of the difficulty to carry out simulations with the traditional ensemble very near the transition point since the instability of the active state for long runs in finite lattices leads most of the samples to fall into the absorbing state. This hindrance, however, can be avoided by using an ensemble in which the number of replicators is kept fixed, this being the motivation for the proposal of the conservative contact process [15].

4 Results

From the qualitative aspect, Figure 2 already demonstrates the main effect of diffusion in the model. Diffusion disrupts the triplets so that the active phase can be maintained only by increasing the probability of creation s, or

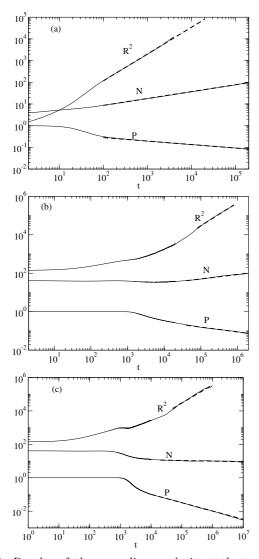


Fig. 3. Results of the spreading analysis at the transition points γ_c for (a) D=0 and $\gamma_c=0.07683(3)$; (b) D=0.95 and $\gamma_c=0.00450(1)$; and (c) D=0.98 and $\gamma_c=0.001886(2)$. The numbers in parentheses represent the uncertainty of the last digit. The dashed lines are the fittings with the scaling laws (2)–(4)

equivalently, by decreasing the probability of decay γ as shown in the figure. In the following we will concentrate on three values of the diffusion probability: D=0, for the purpose of comparison only since there is no dispute that the continuous transition in this case is in the directed percolation universality class; D=0.95, which corresponds to $\tilde{D}=0.905$, roughly the value for which Hinrichsen [13] has run the simulations that led to the conclusion that the transition of the triplet-creation model is continuous in opposition to the findings of Dickman and Tomé [8]; and D=0.98, which corresponds to $\tilde{D}=0.961$ for which the conservative diffusive approach predicts a discontinuous transition [14].

The results of the spreading analysis are presented in Figure 3. As already said, for D=0 one recovers the dy-

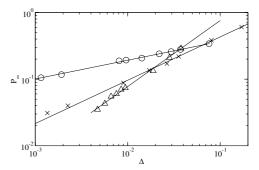


Fig. 4. Logarithm plot of the ultimate survival probability P_{∞} as function of the distance to the transition point $\Delta=1-\gamma/\gamma_c$ for D=0 (\bigcirc), D=0.95 (\times), and D=0.98 (\triangle). The straight lines are the fittings from which the exponent β' is calculated.

namic exponents of the directed percolation $\eta = 0.322(5)$, $\delta = 0.164(5)$, and z = 1.24(2), which yield $d_f = 0.78(1)$. (Henceforth the numbers in parentheses will represent the statistical uncertainty in the last digits.) To avoid possible corrections to scale, the dynamic exponents were calculated using the method of the local slopes [17]. The main point of Figure 3a is to show the easy with which the asymptotic power-law behavior is reached in this case: mere 10^3 time steps are sufficient to evaluate the dynamic critical exponents within a reasonable precision. The situation, however, is very different for high values of the diffusion probability. For instance, Figure 3b shows the results for D = 0.95, the diffusion rate considered in the numerical analysis of reference [13]. The critical spreading is characterized by the exponents $\eta = 0.258(4), \delta = 0.266(6), \text{ and}$ z = 1.35(2) which, surprisingly, lead to the same value of the fractal dimension obtained in the fixed-position limit, $d_f = 0.78(1)$. The initial period of leveling off in the evolution of P(t) is an effect of the large initial colony which guarantees survival in the first 10^3 time steps. After this initial stage, P(t) enters a regime of exponential decay which eventually crosses over to a power-law decay. The critical exponents we find differs substantially from the DP exponents reported in reference [13]. Finally, Figure 3c shows the critical spreading curves for D=0.98 which are characterized by $\eta=-0.026(6),\ \delta=0.49(2),$ and z=1.02(1), resulting in $d_f=0.91(5).$ This result provides strong evidence for a discontinuous transition since these exponents are very close to those of the CDP ($\eta = 0$, $\delta = 1/2$, and z = 1).

In addition to the three dynamic exponents, the spreading analysis applied to the supercritical regime ($\gamma < \gamma_c$) permits the calculation of the exponent β' which controls the approach to the critical point of the ultimate survival probability $P_{\infty} = \lim_{t \to \infty} P(t)$, namely, $P_{\infty} \sim \Delta^{\beta'}$ where $\Delta = 1 - \gamma/\gamma_c$. Figure 4 summarizes the results. We find $\beta' = 0.282(6)$ for D = 0, $\beta' = 0.65(1)$ for D = 0.95, and $\beta' = 0.99(3)$ for D = 0.98. As before, the exponents for D = 0 and D = 0.98 are in excellent agreement with those of the DP and CDP, respectively, but for D = 0.95 the exponent β' settles to a value intermediate to those extremes.

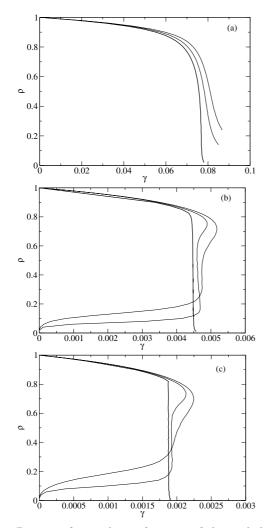


Fig. 5. Density of particles as function of the probability of decay in the conservative diffusive contact process for different chain sizes (left to right at $\rho=0.6$): $L=10^4$ (thick line), L=200, and L=100. The panels are (a) D=0, (b) D=0.95, and (c) D=0.98.

A qualitative picture of the outcome of the conservative diffusive contact process is attained by inspection of Figure 5 that shows the particle density ρ as function of the decay parameter for different chain sizes. Note that if the non-monotonic dependence of ρ on γ for small chains or the apparent steepness of the transition region are used as indicators of a first-order transition, then the transition for D=0.95, which clearly exhibits these features, should be considered as discontinuous. A more careful analysis focusing on the close vicinity of the transition point γ_c is presented in Figure 6. Assuming that the density of particles vanishes as $\rho \sim \Delta^{\beta}$ we find $\beta=0.282(5)$ for D=0, as expected, and $\beta=0.25(5)$ for D=0.95. As illustrated in the figure, the data for D=0.98 are not amenable to this kind of fitting and then we assume $\beta=0$.

Since the four critical exponents must obey the generalized hyperscaling relation [16]

$$h = (1 + \beta/\beta') \delta + \eta - dz/2 = 0$$
 (8)

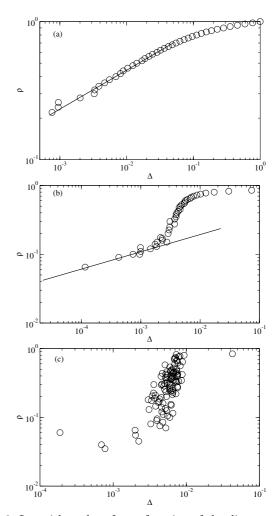


Fig. 6. Logarithm plot of ρ as function of the distance to the transition point $\Delta=1-\gamma/\gamma_c$ for $L=10^4$ and (a) D=0, (b) D=0.95, and (c) D=0.98. The straight lines are the fittings from which the exponent β is calculated.

with d=1, we can easily evaluate the consistency of the set of exponents for each value of the diffusion rate. We find h=0.03 for D=0, h=-0.05 for D=0.95, and h=-0.04 for D=0.98 which indicate that, despite the unusual values of the exponents, the results for intermediate diffusion D=0.95 are as reliable as those for the undisputable limiting situations of very low and very high diffusion probabilities.

5 Conclusion

Our results corroborate the original findings of Dickman and Tomé [8]: the triplet-creation model exhibits a discontinuous transition in the high diffusion regime. In stark contrast with that work, however, we use as indicator of the discontinuous transition not the absence of power-law decay at the critical point, but rather the presence of a power-law behavior characterized by the exponents of the compact directed percolation (CDP) $\eta=0$,

 $\delta = 1/2$, z = 1, and $\beta' = 1$. In fact, while we recovered these exponents for high values of the diffusion probability (D = 0.98), we found strong crossover effects for not so high values of this parameter (D = 0.95), leading to a seemingly continuous variation of the critical exponents. We note that for D = 0.9 (data not shown) we have found the exponents of the directed percolation (DP). Interestingly, we found that the fractal dimension d_f of the colonies is not so affected by the crossover effects. In fact, that quantity was used by Fiore and de Oliveira [14] as the indicator to locate the tricritical point. The calculation of d_f within the conservative diffusive contact process framework is based on the scaling relation between the (fixed) number of particles N and the average distance R between the two particles located at the extremities of the chain, $N \sim R^{d_f}$. In a sense the situation here is reminiscent of models with infinitely many absorbing states, for which only a combination of the dynamic exponents (the sum $\eta + \delta$ in that case) is universal [16, 28]. Nonetheless, the sole coincidence of the values of d_f for D = 0 and D = 0.95, whereas all other exponents differ so markedly (e.g., β'), should be viewed as a weak evidence, rather than a conclusive indication, for a continuous transition

The triplet-creation model provides a simple, but surprisingly difficult, test case to study the crossover from DP to CDP. The fact that the critical exponents seem to change continuously from those of DP for D < 0.9 to those of CDP for D > 0.98 is puzzling, since what is normally observed (and expected) is a transient behavior in which the different universality classes dominate within different time regimes [26,29,30]. However, since the exponents β' , β and the set of dynamic exponents η , δ , z are calculated through independent techniques it is unlikely that, by increasing the chain size or the total evolution time, one would be able to recover the familiar exponents of the DP or CDP universality classes. Clearly, further research is needed to clarify the crossover from these two classes in the triplet-creation model. Despite the interest on this model [8,13,14], the systematic evaluation of the entire set of critical exponents was still lacking. The aim of this contribution was to fill this gap and, in doing so, we have unveiled a rich crossover phenomenon whose elucidation will pose a hard challenge to the current techniques for characterization of nonequilibrium critical behavior.

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