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The *n*-site approximation for the triplet-creation model

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Abstract

The nonequilibrium phase transition of the one-dimensional triplet-creation model is investigated using the n-site approximation scheme. We find that the phase diagram in the space of parameters (γ, D), where γ is the particle decay probability and D is the diffusion probability, exhibits a tricritical point for $n \geqslant 4$. However, the fitting of the tricritical coordinates (γ_t, D_t) using data for $4 \leqslant n \leqslant 13$ predicts that γ_t becomes negative for $n \geqslant 26$, indicating thus that the phase transition is always continuous in the limit $n \to \infty$. However, the large discrepancies between the critical parameters obtained in this limit and those obtained by Monte Carlo simulations, as well as a puzzling non-monotonic dependence of these parameters on the order of the approximation n, argue for the inadequacy of the n-site approximation to study the triplet-creation model for computationally feasible values of n.

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1. Introduction

The characterization of discontinuous nonequilibrium phase transitions from an active state to an absorbing state (vacuum) remains an elusive problem in nonequilibrium statistical mechanics of lattice models, despite the availability of powerful Monte Carlo techniques such as the spreading analysis [1] and the conservative ensemble [2]. The difficulty, as usual, seems to be the large transient times necessary for the system to reach the steady-state regime, and the instability of the active state near the transition point which makes the absorption into the vacuum almost certain for long runs in finite lattices. The latter hindrance can be avoided by using an ensemble in which the number of particles is kept fixed, this being the main motivation for the proposal of the conservative ensemble. The spreading analysis, in contrast, is based on the time evolution of a small initial set of particles which are free to multiply and spread over an infinite lattice. In both techniques, however, the measurement of the relevant physical quantities must be carried out only after the dynamics enters the steady-state regime

and, in the case of models that seem to exhibit a discontinuous transition, the transient times may be exceedingly long [3].

The analysis of the spreading dynamics and, in particular, of the survival probability of the particles as a function of time is widely acknowledged as the most powerful technique currently available to estimate the values of the critical parameters at which the transition between the active and the absorbing regimes takes place. Nonetheless, it is not at all clear whether in the case of discontinuous transitions the time dependence of the survival probability in the critical regime is a power law with mean-field critical exponents [4, 5] or an exponential [6]. If the latter alternative turns out to be correct, the spreading analysis would be inappropriate to locate the transition point in the space of control parameters of the model and, as a result, the (discontinuous) nonequilibrium transition could not be characterized by the dynamic critical exponents. Even in that case, however, it would be possible to characterize the transition by the static critical exponent associated with the vanishing of the ultimate survival probability at the critical point (see, e.g., [7]).

In this contribution we try to circumvent these difficulties, which are inherent to approaches based on Monte Carlo simulations, using a deterministic technique—the n-site approximation or mean field cluster analysis [8–12]—to study the one-dimensional triplet-creation model of Dickman and Tomé [13]. In this model, a necessary condition for the creation of a particle in an empty site is the presence of at least three particles occupying contiguous positions in the neighborhood of the empty site. The other ingredients of the triplet model are particle decay and diffusion to neighboring sites. The model exhibits a unique absorbing state, the vacuum, characterized by the absence of particles. The rich critical behavior of the triplet-creation model owns to the competition between diffusion and the particle creation process. On the one hand, in the absence of diffusion, Monte Carlo simulations indicate the onset of a continuous transition to the absorbing state which belongs to the class of universality of the directed percolation (see [14–16] for reviews on the universality class of nonequilibrium phase transitions), as predicted by a conjecture put forward independently by Janssen and Grassberger [17, 18]. On the other hand, for high enough diffusion there is strong numerical evidence that the continuous transition becomes discontinuous at a tricritical point (see, e.g., [5, 13, 19, 20]). This result, however, is not unanimously accepted by the statistical physics community in view of a general argument due to Hinrichsen [3] that first-order transitions cannot occur in fluctuating one-dimensional systems because the surface tension of a domain does not depend on its size (see also [21, 22]).

Here we show that for $n \leqslant 3$ the n-site approximation predicts a discontinuous-transition-only scenario, irrespective of the diffusion strength. The nontrivial tricritical behavior appears for $n \geqslant 4$ where the n-site approximation predicts the same phase diagram as the Monte Carlo simulations (i.e., a continuous transition that becomes discontinuous as the diffusion probability increases from zero to one). However, the extrapolation of the location of the tricritical point to the limit $n \to \infty$ using data for $4 \leqslant n \leqslant 13$ yields nonphysical results. More pointedly, this extrapolation yields a negative value for the tricritical decay probability. In addition we find that even for low values of the diffusion probability the extrapolation of the n-site approximation grossly underestimates the critical value of the decay probability.

Nevertheless, we feel this mean field cluster analysis is necessary because of the relevance of the triplet-creation model—it was proposed as the simplest, *local* nonequilibrium model that exhibits both a continuous and a discontinuous transition into an absorbing state [13] (though this status is now threatened by the pair-creation model [19]). We note that the Domany–Kinzel (DK) cellular automaton [23] exhibits a discontinuous nonequilibrium phase transition, which belongs to the directed compact percolation universality class [24], but lacks a tricritical

point. The first-order transition of the DK automaton is uncontroversial, but since it happens at the boundary of the DK phase diagram it has the same status as the $T = 0$ equilibrium phase transition of the one-dimensional Ising model [22]. A generalization of this automaton to a model with two absorbing states does seem to exhibit a tricritical point (see [25]) but the greater number of absorbing states makes this model somewhat more complicated than that of the triplet-creation model. In this line, we must note that another generalization of the DK automaton—the tricritical directed percolation model [21, 22] (see also [26])—exhibits a tricritical point only in two or more dimensions. In addition, the reasons for the failure (in the sense of extremely poor convergence) of the n-site approximation are not yet understood, and we think that it may be opportune to re-examine this issue. We refer the reader to the seminal paper by ben-Avraham and Köhler to a discussion of a variety of lattice models to which the n-site approximation has been applied [9].

The rest of the paper is organized as follows. In section 2 we briefly describe the triplet-creation model and in section 3 we present the n-site approximation. The single-site ($n = 1$) and the pair approximation ($n = 2$) are discussed analytically whereas the general case ($n \geqslant 3$) is treated numerically, with emphasis on the location of the tricritical point through the study of the discontinuity of the particle density at the phase transition line. The discrepancy between the predictions of the limit $n \to \infty$ of the n-site approximation and the Monte Carlo simulations is discussed in section 4, where we also present our concluding remarks.

2. The triplet-creation model

The configuration of the n-sites chain can be described in terms of binary occupation variables $\sigma_i = 1, 0$ for $i = 1, \ldots, n$ with the convention that σ_i takes on the value 1 if site i is occupied by a particle and the value 0 if site i is empty. The evolution rules of the triplet-creation model are as follows [13].

A site, say site i, is chosen randomly among the n sites of the chain. Suppose $\sigma_i = 1$. Then there are two possible actions: either the particle decays with probability γ so site i becomes vacant, or it moves to a neighboring site with probability D. In the latter case, either the variables σ_i and σ_{i-1} or σ_i and σ_{i+1} are interchanged. The left and right neighbors are selected with equal probability so, for example, the probability that the particle at site i moves to the right site is $D/2$. Of course, site i remains unchanged with probability $1 - \gamma - D$.

Next, suppose site i is empty, $\sigma_i = 0$. The first step is to choose with equal probability which neighbors of site i—those on the left or those on the right side of i—will affect its current state. Suppose the right side is chosen. As before, there are two possibilities: occupation of site i with probability s, provided that $\sigma_{i+1} = \sigma_{i+2} = \sigma_{i+3} = 1$ (hence the name triplet-creation model) or diffusion with probability D, when the variables σ_i and σ_{i+1} are interchanged. A similar procedure is applied in the case the neighborhood at the left side of i is chosen.

In principle, the one-dimensional triplet-creation model is defined for a chain of infinite length so there is no need to specify the boundary conditions at this model-definition stage. In practice, however, the choice of the boundary conditions depends on the method used to study the critical properties of the model. If the focus is on steady-state properties then the cyclic boundary conditions are used, as in the original paper by Dickman and Tomé [13] or in the conservative ensemble analysis [19], whereas if the focus is on the dynamic properties then the boundary conditions may remain unspecified since the simulation time is chosen such that the particles never reach the boundaries of the chain [5].

This description of the triplet-creation model differs from the original formulation of Dickman and Tomé [13] only by the fact that we have explicitly symmetrized the diffusion

process, which is more convenient for the purpose of solving numerically the equations resulting from the n-site approximation, as the symmetrization speeds up convergence. Since $D+\gamma+s=1$ there are only two independent parameters in the model which we choose to be D and γ.

3. The n-site approximation

The discrete-time stochastic process that defines the triplet-creation model is completely described by the joint probability distribution $P_n(\sigma^n;\tau)$ where $\sigma^n=(\sigma_1,\ldots,\sigma_n)$, given the initial configuration (hence P_n is actually a conditional probability distribution [27]). Since the process is Markovian and the site update rules are independent of τ we can write

$$P_n(\sigma^n;\tau+\Delta\tau)=\sum_{\hat{\sigma}^n} P_{\Delta\tau}(\sigma^n\mid\hat{\sigma}^n)P_n(\hat{\sigma}^n;\tau), \tag{1}$$

where the summation is over all configurations $\hat{\sigma}^n$ that differ from σ^n by 0, 1 or 2 sites, and $\Delta\tau$ is an arbitrary unit of time. Here $P_{\Delta\tau}(\sigma^n\mid\hat{\sigma}^n)$ is the conditional probability for the transition from configuration $\hat{\sigma}^n$ to configuration σ^n in the time interval $\Delta\tau$. We choose this discrete-time formulation rather than the usual continuous-time approach in order to preserve the interpretation of the parameters γ, D and s as probabilities, and so keep their values restricted to the range [0, 1]. Using $P_{\Delta\tau}(\sigma^n\mid\sigma^n)=1-\sum_{\hat{\sigma}^n\neq\sigma^n}P_{\Delta\tau}(\hat{\sigma}^n\mid\sigma^n)$ we can rewrite (1) in a form more convenient for comparison with the continuous-time case,

$$\delta P_n(\sigma^n;\tau)=\sum_{\hat{\sigma}^n}[P_{\Delta\tau}(\sigma^n\mid\hat{\sigma}^n)P_n(\hat{\sigma}^n;\tau)-P_{\Delta\tau}(\hat{\sigma}^n\mid\sigma^n)P_n(\sigma^n;\tau)], \tag{2}$$

where $\delta P_n(\sigma^n;\tau)=P_n(\sigma^n;\tau+\Delta\tau)-P_n(\sigma^n;\tau)$. As usual, the continuous-time formulation is obtained by dividing both sides of equation (2) by $\Delta\tau$, taking the limit $\Delta\tau\to 0$, and defining the ratio $P_{\Delta\tau}(\sigma^n\mid\hat{\sigma}^n)/\Delta\tau$ as the transition rate between configurations $\hat{\sigma}^n$ and σ^n. Thus it is evident that both the discrete and the continuous-time formulations are equivalent in the steady-state regime $\delta P_n(\sigma^n;\tau)=0$. The number of equations in (2) can be reduced considerably by using the parity symmetry $P_n(\sigma_1,\sigma_2,\ldots,\sigma_n)=P_n(\sigma_n,\sigma_{n-1},\ldots,\sigma_1)$ as well as the usual normalization constraint $\sum_{\sigma^n}P_n(\sigma^n;\tau)=1$.

For finite chain sizes, application of the site update rules $P_{\Delta\tau}(\sigma^n\mid\hat{\sigma}^n)$ with a suitable local boundary condition, say the periodic one in which the two extremes of the chain are joined to form a ring (i.e., setting $\sigma_{n+1}=\sigma_1$ and $\sigma_0=\sigma_n$), allows the dynamics to visit any configuration beginning from an arbitrary initial configuration distinct from the absorbing state $\sigma^n=0$ (i.e., the configuration for which $\sigma_i=0$ for $i=1,\ldots,n$). So the unique steady-state solution of equation (1) is $P_n\ (\sigma^n=0;t\to\infty)=1$. In the limit of infinitely large chains $n\to\infty$, a second stable stationary solution of equation (1) appears, the so-called active state, for which the average density of particles ρ is nonzero. In Monte Carlo simulations of relatively large chains (say, $n>100$) the active state is metastable, but unless the parameters γ and D are set very close to their critical values, the probability that the dynamics leaves this state during a simulation run (which lasts typically 10^7 updates per site) is vanishingly small. However, these metastable states have no role in our analysis since we solve for the steady-state solutions of equation (2) directly.

We see the n-site approximation as a prescription to deal with the sites at or close to the boundaries of the chain, namely, sites $i=1,2,3,n-2,n-1,n$ and to guarantee the stabilization of the stationary solution associated with the active phase. The idea is very intuitive and seems to have been discovered independently many times [8–10]. The basic point is to describe the stochastic dynamics of a n-site spin configuration only in terms of

the joint probability distribution $P_n(\sigma^n;\tau)$ using translationally invariant equations. The imposition of cyclic boundary conditions can accomplish that, but as mentioned above it does not guarantee the stability of the active phase solution. The condition of translational invariance requires that the update rules for the sites close to the boundaries of the chain are the same as for the inner sites. To achieve that we need to introduce *virtual* sites, say $i = -2, -1, 0$ if the left neighborhood of site $i = 1$ is considered, but then we have to introduce the extraneous $n+3$-joint distribution $Y_{n+3} \equiv P_{n+3}(\sigma_{-2}, \sigma_{-1}, \sigma_0, \sigma^n;\tau)$. The n-site approximation is a prescription to write the m-joint probability distributions ($m > n$) in terms of $P_n(\sigma^n;\tau)$ only. The basic assumption involved in this approximation scheme is that the states of any two sites are considered as statistically independent variables if their distance is larger than n (see subsection 3.2 for a detailed application of this assumption). For the example considered we have

$$Y_{n+3} = \frac{P_n(\sigma_{-2}, \sigma_{-1}, \sigma_0, \sigma^{n-3})}{P_{n-1}(\sigma_{-1}, \sigma_0, \sigma^{n-3})} \times \frac{P_n(\sigma_{-1}, \sigma_0, \sigma^{n-2})}{P_{n-1}(\sigma_0, \sigma^{n-2})} \times \frac{P_n(\sigma_0, \sigma^{n-1})}{P_{n-1}(\sigma^{n-1})} \times P_n(\sigma^n), \tag{3}$$

where the $n-1$-site distributions can be easily written in terms of the n-site distributions (we have omitted the dependence on τ to lighten the notation). For example,

$$P_{n-1}(\sigma_{-1}, \sigma_0, \sigma^{n-3}) = \sum_{\sigma_{-2}=0}^{1} P_n(\sigma_{-2}, \sigma_{-1}, \sigma_0, \sigma^{n-3}), \tag{4}$$

and similarly for the other distributions that appear in the denominators of equation (3). Recalling the update rules of the triplet-creation model, if site $i = 1$ is empty (i.e., $\sigma_1 = 0$) and its left neighborhood is chosen for the occupation procedure, then it is necessary that its three virtual neighbors $i = -2, -1, 0$ are occupied (i.e., $\sigma_{-2} = \sigma_{-1} = \sigma_0 = 1$) in order it can be occupied by a particle too. These are the site values that must be feed into equation (3). In addition, we note that expression (3) is valid for $n > 3$ only.

Now consider the task of updating the vacant site $i = 2$ (i.e., $\sigma_2 = 0$) in a configuration σ^n where site $i = 1$ is occupied (i.e., $\sigma_1 = 1$). We need to consider two virtual sites $i = -1, 0$ and the relevant joint distribution $Y_{n+2} \equiv P_{n+2}(\sigma_{-1}, \sigma_0, \sigma^n;\tau)$ is given by

$$Y_{n+2} = \frac{P_n(\sigma_{-1}, \sigma_0, \sigma^{n-2})}{P_{n-1}(\sigma_0, \sigma^{n-2})} \times \frac{P_n(\sigma_0, \sigma^{n-1})}{P_{n-1}(\sigma^{n-1})} \times P_n(\sigma^n) \tag{5}$$

for $n > 2$. As before, the contribution from the virtual sites to the probability of occupation of site $i = 2$ is obtained by setting $\sigma_{-1} = \sigma_0 = 1$ in equation (5).

Finally, let us consider the update of vacant site $i = 3$ (i.e., $\sigma_3 = 0$) in a configuration σ^n where sites $i = 1, 2$ are occupied (i.e., $\sigma_1 = \sigma_2 = 1$). In this case, we need only one virtual site $i = 0$ to complete the triplet so we must compute $Y_{n+1} \equiv P_{n+1}(\sigma_0, \sigma^n;\tau)$, which yields

$$Y_{n+1} = \frac{P_n(\sigma_0, \sigma^{n-1})}{P_{n-1}(\sigma^{n-1})} \times P_n(\sigma^n) \tag{6}$$

which is valid for $n > 1$ only. Setting $\sigma_0 = 1$ yields the contribution of the virtual left neighborhood of site $i = 3$ to its probability of occupation. We note that the distribution Y_{n+1} is also needed when implementing the exchange (diffusion) between site $i = 1$ and the virtual site to its left, $i = 0$. In some sense, the diffusion process at the boundaries can be seen as a particle source ($\sigma_1 = 0$ and $\sigma_0 = 1$) or a particle sink ($\sigma_1 = 1$ and $\sigma_0 = 0$). The three rightmost sites $i = n-2, n-1, n$ are updated using a procedure analogous to that described above. The update of the other $n-6$ internal sites follows the rules of the triplet-creation model.

The formulation described here and the emphasis given to the boundary sites is motivated by the insightful interpretation of the n-site approximation offered by Ferreira and Mendiratta [10]. Finally, we note that the update rules for the sites at or close to the chain boundaries are the only sources of nonlinearities in equation (2), which ultimately guarantees the appearance and stabilization of the fixed point associated with the active regime for finite n.

In what follows we present the explicit form of the equations that determine the joint distribution $P_n(\sigma^n;\tau)$ for $n = 1$ and 2, termed single-site and pair approximation, respectively. In these cases we are able to derive analytical expressions for the (discontinuous) transition lines and for the jump in the particle density at the transition. Although we can easily write down the explicit equations in the case $n = 3$ as well, they do not yield to an analytical approach. For $n \geqslant 3$ we resort to the numerical solution of equation (2) for the steady-state condition $\delta P_n(\sigma^n) = 0$, so we are left with a system of 2^n coupled equations. We solve those equations using the Newton–Raphson method with the requisite of an error smaller than 10^{-16} per equation. We note that the sole requisite either to iterate or to solve equation (2) for the steady-state is a user supplied routine that returns the right-hand side of that equation for any tentative solution $P_n(\sigma^n;\tau)$ [28].

3.1. The single-site approximation

Since none of the formulae (3), (5), (6) are valid in the single-site ($n = 1$) limit, here we show how the general n-site formulation summarized by equation (2) reduces to the usual (single-site) mean-field equation in this limit. The relevant quantity is simply $P_1(1) = \rho$ as $P_1(0) = 1-\rho$ is given by the normalization condition. Recalling that the only real site is $i = 1$ we introduce the convention to write the state of the virtual sites (i.e., $i = -2, -1, 0, 2, 3, 4$) with an overlying bar. Hence can rewrite equation (2) as

$$\delta P_1(1) = -\gamma P_1(1) + \frac{s}{2} P_4(\bar{1}, \bar{1}, \bar{1}, 0) + \frac{s}{2} P_4(0, \bar{1}, \bar{1}, \bar{1}). \tag{7}$$

The diffusion parameter (D) does not appear explicitly in this equation because its contribution comes from terms such as $DP_2(\bar{1}, 0)$ and $-DP_2(\bar{0}, 1)$ which cancel out because of the parity symmetry. Since in this case the sites are independent we can write $P_4(\bar{1}, \bar{1}, \bar{1}, 0) = P_1^3(1)P_1(0)$ and similarly for the contribution of the right neighborhood of site $i = 1$, so that equation (7) becomes

$$\delta\rho = -\gamma\rho + s\rho^3(1-\rho). \tag{8}$$

The nontrivial solutions at equilibrium are given by the roots of the cubic equation $\rho^2(1-\rho) = \gamma/s$. In the physical regime $\gamma/s > 0$, there is always one negative root. The two positive roots disappear when they coincide, and then the two-fold degenerate root yields the size of the discontinuity of particle density $\Delta\rho$ at the transition between the active and absorbing phases (this happens at the so-called spinoidal point, see figure 1). We find $\Delta\rho = 2/3$ regardless of the values of the control parameters γ and D. The discontinuous transition in the space (γ, D) is also determined by the collapse and consequent disappearance of those two roots. Inserting the value $\rho = 2/3$ in equation (8) with $\delta\rho = 0$ yields $\gamma_c = 4(1-D)/31$. In figure 1 we show all positive steady-state solutions of equation (8). We note that the dependence on the diffusion parameter D is trivial in this case since it appears through the particle creation probability $s = 1-\gamma-D$ only.

3.2. The pair approximation

In the case $n = 2$, equation (2) can be reduced to only two independent equations using the parity symmetry $P_2(0, 1;\tau) = P_2(1, 0;\tau)$ and the normalization condition. As usual (see,

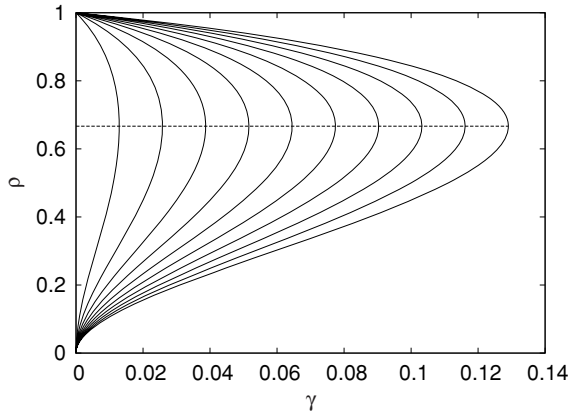

Figure 1. The equilibrium solutions of the one-site approximation equation for (right to left) $D = 0, 0.1, \ldots, 0.9$. The dashed line shows the size of the discontinuity of the particle density $\Delta\rho = 2/3$: for fixed D the stable solutions are those for which $\rho > \Delta\rho$.

e.g., [14]) the pair approximation is posed in terms of the quantities $\phi \equiv P_2(1, 1; \tau)$ and $\rho \equiv P_2(1, 1; \tau) + P_2(1, 0; \tau)$. To illustrate the reasoning that leads to the formulae (3), (5), (6) we will derive the equation for $P_2(1, 1)$ explicitly. Recalling that only $i = 1, 2$ are real sites and omitting τ dependence equation (2) yields

$$\begin{aligned}\delta P_2(1,1) = &-\gamma P_2(1,1) - \frac{D}{4}P_3(1,1,\bar{0}) - \frac{D}{4}P_3(\bar{0},1,1)\\ &+ \frac{D}{4}P_3(\bar{1},0,1) + \frac{D}{4}P_3(1,0,\bar{1}) + \frac{s}{4}P_5(\bar{1},\bar{1},\bar{1},0,1)\\ &+ \frac{s}{4}P_5(1,0,\bar{1},\bar{1},\bar{1}) + \frac{s}{4}P_4(0,1,\bar{1},\bar{1}) + \frac{s}{4}P_4(\bar{1},\bar{1},1,0),\end{aligned} \tag{9}$$

where, as before, we use the convention of writing the virtual site states with an overlying bar. The factor $1/4$ appears here because the probability of choosing a given site for update is $1/2$ (there are only two real sites) and the probability that the left (or the right) neighborhood of that site is selected to verify the possibility of diffusion (site interchange) or creation is also $1/2$.

We begin by working out the more cumbersome expression $P_5(\bar{1}, \bar{1}, \bar{1}, 0, 1)$. First, we write the identity

$$\begin{aligned}P_5(\bar{1},\bar{1},\bar{1},0,1) &= P_{1|4}(\bar{1}\,|\,\bar{1},\bar{1},0,1) \times P_4(\bar{1},\bar{1},0,1)\\ &= P_{1|4}(\bar{1}\,|\,\bar{1},\bar{1},0,1) \times P_{1|3}(\bar{1}\,|\,\bar{1},0,1) \times P_3(\bar{1},0,1)\\ &= P_{1|4}(\bar{1}\,|\,\bar{1},\bar{1},0,1) \times P_{1|3}(\bar{1}\,|\,\bar{1},0,1)\\ &\quad \times P_{1|2}(\bar{1}\,|\,0,1) \times P_2(0,1),\end{aligned} \tag{10}$$

and then use the statistical independence of non-neighboring sites, $P_{1|4}(\bar{1}\,|\,\bar{1},\bar{1},0,1) = P_{1|1}(\bar{1}\,|\,\bar{1})$, $P_{1|3}(\bar{1}\,|\,\bar{1},0,1) = P_{1|1}(\bar{1}\,|\,\bar{1})$, $P_{1|2}(\bar{1}\,|\,0,1) = P_{1|1}(\bar{1}\,|\,0)$ to finally obtain an expression only in terms of joint distributions,

$$P_5(\bar{1},\bar{1},\bar{1},0,1) = \frac{P_2(\bar{1},\bar{1})}{P_1(\bar{1})} \times \frac{P_2(\bar{1},\bar{1})}{P_1(\bar{1})} \times \frac{P_2(\bar{1},0)}{P_1(0)} \times P_2(0,1), \tag{11}$$

where we have used the definition of the conditional probability. A similar reasoning allows us to write

$$P_4(\bar{1}, \bar{1}, 1, 0) = \frac{P_2(\bar{1}, \bar{1})}{P_1(\bar{1})} \times \frac{P_2(\bar{1}, 1)}{P_1(1)} \times P_2(1, 0), \tag{12}$$

$$P_3(\bar{0}, 1, 1) = \frac{P_2(\bar{0}, 1)}{P_1(1)} \times P_2(1, 1), \tag{13}$$

and

$$P_3(\bar{1}, 0, 1) = \frac{P_2(\bar{1}, 0)}{P_1(0)} \times P_2(0, 1). \tag{14}$$

At this point, use of the parity symmetry suffices to write $\delta P_2(1, 1)$ given by equation (9) in terms of $P_2(1, 1)$ and $P_2(1, 0)$ only. It is still necessary to derive an equation for $\delta P_2(1, 0)$, but this can be done quite straightforwardly using the procedure described above. The final dynamic equations for the pair approximation, posed in terms of the usual variables ϕ and ρ, are

$$2\delta\rho = -\gamma\rho + s(\rho - \phi)\frac{\phi^2}{\rho^2} \tag{15}$$

$$2\delta\phi = -2\gamma\phi + s\frac{\phi^2}{\rho^2}(\rho - \phi)\left(1 + \frac{\rho - \phi}{1 - \rho}\right) - D(\phi - \rho^2)\frac{\rho - \phi}{\rho(1 - \rho)}. \tag{16}$$

In contrast with the single-site approximation, now the diffusion parameter D introduces a nontrivial contribution to the master equation. Since the diffusion process does not depend on the particle creation mechanism the last term in equation (16) is identical to that obtained for simpler models, as the simple contact process [14, 29]. In the equilibrium regime, it is equation (15) which determines the onset of the phase transition. In fact, the reduced variable $\tilde{\phi} = \phi/\rho$ is given by the same cubic equation discussed in the single-site approximation and so $\tilde{\phi} = 2/3$ at the transition line. This implies that the equation of the transition line $\gamma_c(D)$ is also identical to that obtained in the single-site approximation. However, the size of the discontinuity $\Delta\rho$ at the transition differs in the two approximation schemes. Imposing the steady-state condition in equation (16) yields

$$\Delta\rho = \frac{1 + 2D/3\gamma_c}{2 + D/\gamma_c}, \tag{17}$$

where $\gamma_c = 4(1 - D)/31$. For $D \to 1$ we find $\Delta\rho = 2/3$ as in the single-site approximation. We note that the equations for the transition line $\gamma_c(D)$ coincide in the cases of the single-site and pair approximations only. Figure 2 shows all positive steady-state solutions of equations (15)–(16).

3.3. The general n-site approximation

As pointed out before, for $n \geqslant 3$ we have to resort to a numerical implementation of equation (2). In particular, the configurations σ^n (i.e., the arguments of the joint distribution P_n) are represented by n-bit integers, which allows an easy implementation of the boundary-sites update rules by the Fortran bit manipulation intrinsic functions. For example, suppose the configuration σ^n is represented by the integer I. Then using the ISHFT(I, k) function which shifts I to left or to right by k bits and the IBSET(I, i) function that sets bit i of I to 1, we can write the configuration $\{\sigma_0 = 1, \sigma^{n-1}\}$ represented by the n-bit integer I' using

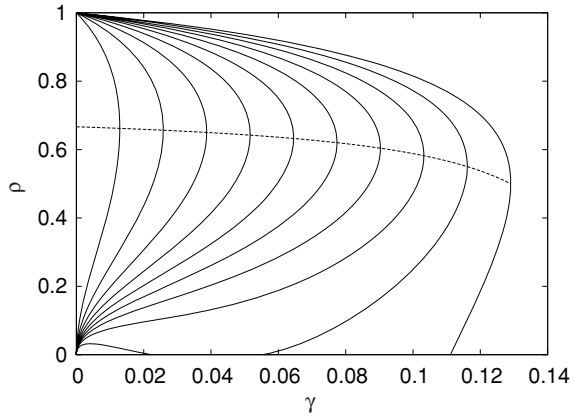

Figure 2. The positive equilibrium solutions of the two-site approximation equations for (right to left) $D = 0, 0.1, \ldots, 0.9$. The dashed curve shows the size of the discontinuity of the particle density $\Delta\rho$ as given by equation (17). The stable solutions for fixed D are those for which $\rho > \Delta\rho$.

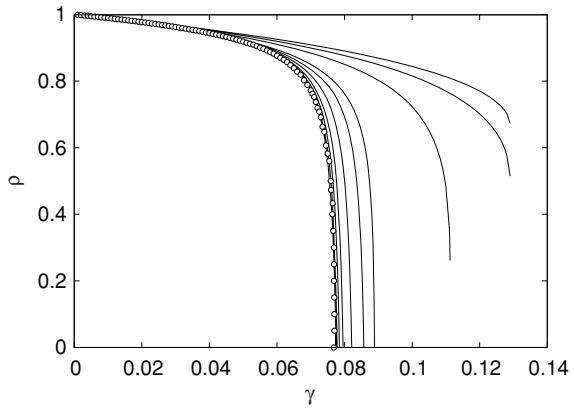

Figure 3. The density of particles at equilibrium ρ as a function of the decay probability γ for $D = 0$ and (right to left) $n = 1, 2, \ldots, 10$. The symbols $\circ$ are the results of the conservative ensemble Monte Carlo simulations of a chain of size 2×10^4 with periodic boundary conditions, except for the point at $\rho = 0$, namely, $\gamma_c = 0.07685 \pm 10^{-5}$ which was estimated using the spreading analysis.

the operation $I' = \mathrm{ISHFT}(I, -1)$ followed by $I' = \mathrm{IBSET}(I', n-1)$. (We recall that in the binary representation of a n-bit integer, the positions of the leftmost and rightmost bits are $n-1$ and 0, respectively.) This is essentially the 'window' method used in [9].

We choose an initial configuration (initial guess) such that $P(\sigma^n = 1; 0) \approx 1$ in order to bias the Newton–Raphson method to find the stable steady-state solution of equation (2). Unless stated otherwise, the Monte Carlo data used to evaluate the predictions of the n-site approximation were obtained by us.

In the absence of diffusion, $D = 0$, both the one- and two-site approximation fail to predict the continuous phase transition between the absorbing and active phases. The natural question is then whether increasing n will improve this situation. The answer is given in figure 3 where we show the equilibrium density of particles ρ for $n = 1$ to $n = 10$: in the position-fixed limit the transition becomes continuous only for $n \geqslant 4$ (see also [13]). The

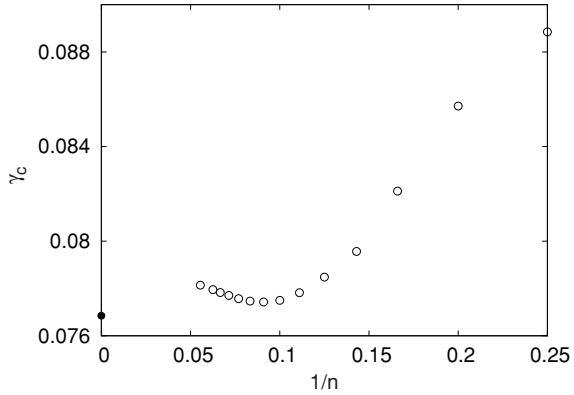

Figure 4. Dependence of the critical value of the decay probability at which the density of particles vanishes continuously on the order n of the n-site approximation ($4 \leqslant n \leqslant 18$). The diffusion probability is $D = 0$ and the filled circle indicates the spreading analysis estimate of γ_c.

approximation scheme seems to converge nicely to the results of the Monte Carlo simulations solely because of the scale used to draw figure 3. In reality, close to the critical point (i.e., for small ρ), the mean-field particle density vanishes as $\rho_n \sim [\gamma - \gamma_c(n)]$ regardless of the value of $n \geqslant 4$, whereas in the Monte Carlo simulations we have $\rho \sim [\gamma - \gamma_c]^{0.28}$ [14–16]. More disturbing, however, is the fact (not shown in figure 3) that for $n > 11$ the estimate of $\gamma_c(n)$ starts to increase with n and shows no tendency to converge to the critical point estimated via the spreading analysis, as illustrated in figure 4. (Of course, this estimate of γ_c agrees very well with the estimate obtained using the data of the conservative ensemble simulations shown in figure 3.) This non-monotonic behavior leads to the crossing between the curves $\rho \times \gamma$ for $n > 12$ and the curves for $n = 8, 9, 10$ and 11 (see figure 4), but this phenomenon could not be observed in the scale of figure 3. It is interesting that the regime where $\gamma_c(n)$ increases with n begins at $n = 12$, which is exactly the cluster size at which the number of internal sites equals the number of sites that follow the update rules (3), (5), (6) rather than the rules of the triplet-creation model. At present we have no explanation for the puzzling non-monotonic behavior of $\gamma_c(n)$ illustrated in figure 4 (see section 4).

The possible existence of a minimum cluster size (i.e., order of approximation n) below which the n-site approximation can yield even qualitatively wrong results was suggested by ben-Avraham and Köhler, using an argument based on the competition between the two mechanisms that govern the dynamics of the domains growth, drift and diffusion [9]. However, since the drift velocity and the (effective) diffusion coefficient (which is nonzero even if $D = 0$) of the domains are not readily accessible, this information is of limited practical value from a quantitative perspective. Qualitatively, however, it suggests that, all other things being equal, the larger the diffusion coefficient, the larger the cluster size n necessary for the n-site approximation to guarantee the correct characterization of the critical properties of the system. Hence we should expect a poor convergence of this approximation scheme (in the sense that a large value of n is required to obtain reliable predictions) in the case that an explicit diffusion procedure is incorporated in the dynamical rules of the model.

In the case $D = 0$, we can obtain results up to $n = 18$ by directly iterating equation (2) until the steady-state is reached. This is a safe procedure that is guaranteed to converge but which becomes useless for $D > 0$ because in that case the convergence to the steady-state is exceedingly slow. Nevertheless, we use this method to provide a good initial guess to the Newton–Raphson method.

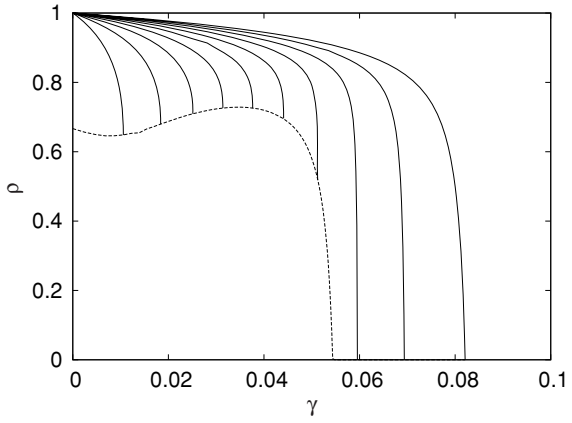

Figure 5. The density of particles at equilibrium ρ as a function of the decay probability γ for $n = 6$ and (solid lines from right to left) $D = 0, 0.1, \ldots, 0.9$. The dashed line shows the the size of the discontinuity of the particle density $\Delta\rho$ at the phase transition. This discontinuity disappears at the tricritical point $D_t = 0.2602 \pm 10^{-5}$, $\gamma_t = 0.0544 \pm 10^{-5}$.

The expectation is that by turning on the diffusion process the continuous transition found by $n \geqslant 4$ will eventually become discontinuous at a tricritical point. Figure 5 shows that this is indeed the case. The important quantity regarding the location of the tricritical point is the discontinuity of the particle density at the transition $\Delta\rho$ since it goes continuously to zero as one approaches the tricritical point on the discontinuous transition line. It is quite a challenge to determine numerically the value of $\Delta\rho$ because, as illustrated in figure 5 (see also figures 1 and 2), the derivative of ρ with respect to γ diverges at γ_c. Our procedure to tackle this problem was to fix a target value of density $\tilde{\rho}$ and perform a bisection in γ to find the value of this parameter such that the steady state of the master equation yields $\rho = \tilde{\rho}$. We can easily draw the curve $\rho \times \gamma$ using this procedure and, in the case, $\tilde{\rho} < \Delta\rho$ the bisection converges to γ_c and $\rho = \Delta\rho$.

The jump of the particle density $\Delta\rho$ at the transition is shown in figure 6 for $3 \leqslant n \leqslant 12$. In all cases we find that $\Delta\rho$ vanishes as $A(D - D_t)$ where the amplitude A increases exponentially with increasing n. More pointedly, we find $A \approx 0.2\exp(0.8n)$, which explains the steepness of the curves $\Delta\rho \times D$ for $n > 9$. Note that in the limit where the diffusion process is dominant, i.e. for $D \to 1$ we find $\Delta\rho \to 2/3$, in disagreement with the Monte Carlo simulations of the conservative contact process which yield $\Delta\rho \to 5/6$ [19]. For the sake of completeness, in figure 7 we show the transition lines (i.e., the phase diagram of the model) obtained using different orders of approximation n.

Finally, in figures 8 and 9 we plot the estimates of the tricritical point coordinates as a function of the order n of the n-site approximation. In these figures the Monte Carlo estimates (filled circles) were extracted from [19]. Considering our previous experience with the critical point summarized in figure 4, the tricritical data are surprisingly well fitted by the functions $D_t = D_t^\infty + a_d n^{-1/\nu_\perp}$ and $\gamma_t = \gamma_t^\infty + a_\gamma n^{-1/\nu_\perp}$ where $\nu_\perp = 1.101$ is the critical exponent of the correlation length [14]. (The linear fitting yields essentially the same result.) The nonphysical estimate for γ_t^∞ implies that the limit $n \to \infty$ of the n-site approximation exhibits a continuous transition between the absorbing and active phases regardless of the value of the diffusion probability D. According to figure 9 this continuous-transition-only scenario is predicted to occur for $n > 25$.

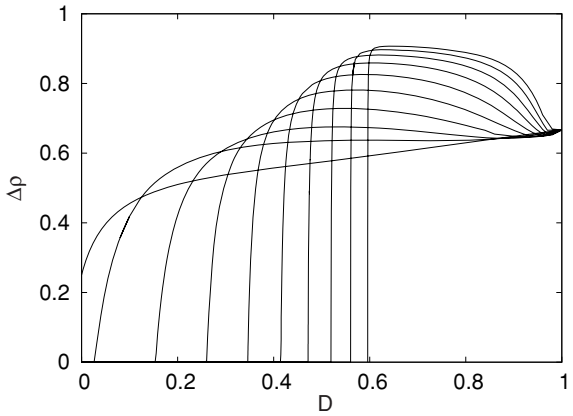

Figure 6. The size of the discontinuity of the density of particles at equilibrium $\Delta\rho$ at the phase transition as a function of the diffusion probability D for (left to right at $\Delta\rho = 0.4$) $n = 3, 4, \ldots, 12$. The values of Δ (and hence γ) at which $\Delta\rho$ vanishes yields the location of the tricritical point. For $D = 1$ we find the single-site approximation value $\Delta\rho = 2/3$, regardless of the approximation order n.

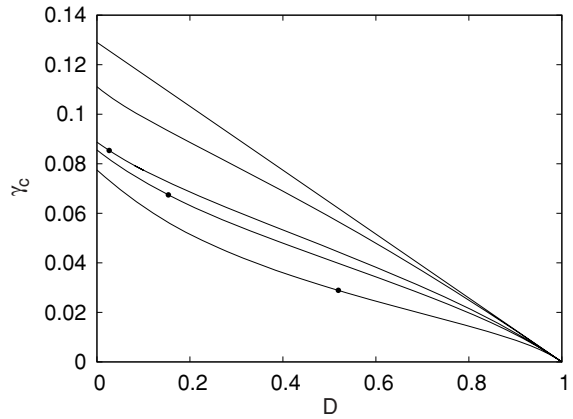

Figure 7. The critical value of the decay probability $\gamma_c(D)$ above which the active phase ($\rho > 0$) disappears for (top to bottom) $n = 2, 3, 4, 5$ and 10. The symbols • indicate the locations, $\gamma_c(D_t)$, of the tricritical points for $n \geqslant 4$. The transition becomes continuous for $D \leqslant D_t$. For $n \leqslant 3$, the transition is always discontinuous.

To access the solidity of the $n \to \infty$ predictions summarized in figures 8 and 9 we consider a much simpler situation, namely, the estimate of the critical value of the decay probability γ_c when the diffusion probability is nonzero. The result for $D = 0.2$ and $n \geqslant 6$ (the transition is always continuous in this parameter range, see figure 7) is shown in figure 10. In contrast to the results for $D = 0$ (see figure 4), figure 10 shows that the data is fitted very well by the functional form $\gamma_c = \gamma_c^\infty + an^{-1/\nu_\perp}$ although the extrapolated estimate γ_c^∞ falls short of reproducing the Monte Carlo result. It is clear then that the cluster size used in our analysis ($n \leqslant 14$) is too small to yield a reliable estimate of the critical and tricritical parameters. Regarding figure 10, we note that at some point $\gamma_c(n)$ must increase with increasing n in order to reproduce the Monte Carlo estimate for $n \to \infty$. The fact that this non-monotonic behavior

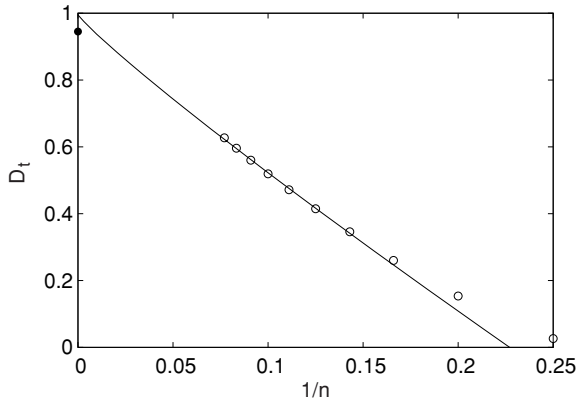

Figure 8. Dependence of the value of the tricritical diffusion probability at which the jump $\Delta\rho$ of the density of particles vanishes continuously on the order n of the n-site approximation ($4 \leqslant n \leqslant 13$). The filled circle indicates the value $D_t = 0.945$ predicted by the conservative contact process [19], whereas the extrapolation to $n \to \infty$ yields $D_t^{\infty} = 0.995 \pm 0.008$.

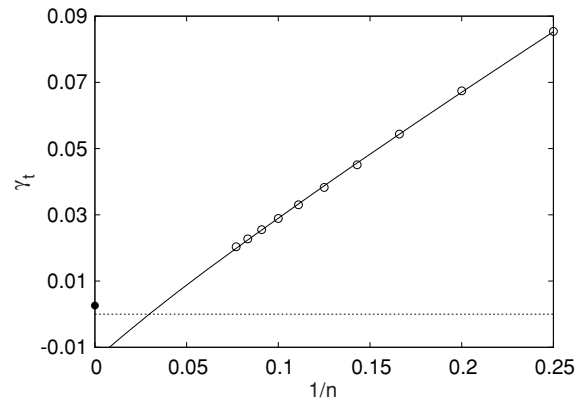

Figure 9. Same as figure 8 but for the tricritical decay probability. The filled circle indicates the value $\gamma_t = 0.0026$ predicted by the conservative contact process [19]. The extrapolation to $n \to \infty$ yields the nonphysical value $\gamma_t^{\infty} = -0.0135 \pm 0.0002$.

is not observed in this figure, whereas it is evident in figure 4 for $n \geqslant 12$, is in agreement with the suggestion that the increase of the diffusion strength hinders the convergence of the n-site approximation. In this line, we find for the single-creation model [29] too that the introduction of the diffusion process ruins the excellent agreement between the critical point estimate obtained by the extrapolation $n \to \infty$ and by the Monte Carlo simulations [10] (see, however, [30] for a more auspicious conclusion in a model that includes pair-creation and pair-annihilation processes).

4. Discussion

It is tempting to think that the effect of the mean-field approximation on the sites close to the boundaries will become less and less important as n increases, so that the approximation

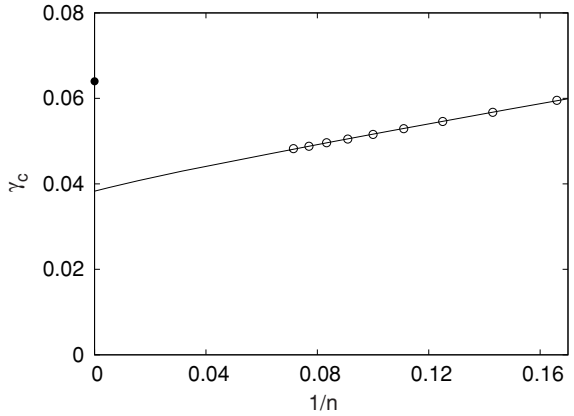

Figure 10. Critical value of the decay probability as function of the order n of the n-site approximation for $D = 0.2$ (open circles). The filled circle indicates the spreading analysis estimate of $\gamma_c = 0.0645 \pm 0.0005$. Here $6 \leqslant n \leqslant 14$.

scheme will converge monotonically to the exact result in the limit $n \to \infty$. Alas, the fact is that this benign-convergence scenario rarely happens. For instance, in the monomer–monomer model for heterogeneous catalysis [31] the single-site and the pair approximations predict the right phase diagram but this agreement is spoiled when higher orders of the approximation ($n \geqslant 3$) are considered. In the words of ben-Avraham and Köhler, 'things look worse when one expects the approximation to improve' [9].

Nevertheless, for sufficiently large n we expect the n-site approximation to yield reliable predictions for the values of the critical parameters. In fact, in the active phase the correlation length $\xi \sim (\gamma_c - \gamma)^{-\nu_\perp}$ is finite and so for $n \gg \xi$ the approximation will describe very precisely the steady-state density of particles ρ and, consequently, it must produce an accurate estimate of the critical parameters. In practice, however, we may never be able to see this regime as the computational demand of the approximation scheme increases exponentially with n, thus limiting the analysis to relatively small cluster sizes.

According to ben-Avraham and Köhler, the n-site approximation works well in one dimension for models that exhibit the same phase diagram in higher dimensions [9]. Although we know virtually nothing about the phase diagram of the triplet-creation model in two dimensions, we know that a very similar model—the tricritical directed percolation model—exhibits a tricritical point in two dimensions [21, 22, 26] and so it is plausible to assume that this conclusion holds for the two-dimensional triplet-creation model as well. Hence, the troubled convergence of the n-site approximation reported here may be an (admittedly weak) indication that the triplet-creation model does not exhibit tricritical behavior in one dimension.

Clearly, much more work is necessary to resolve the controversy over whether the one-dimensional triplet-creation model (or, for that matter, any other one-dimensional nonequilibrium model) exhibits a tricritical behavior. We recall that evidences from Monte Carlo simulations [5, 13, 19] indicate that in the large diffusion limit ($D > D_t \approx 0.945$ according to the conservative ensemble estimate [19]) the nonequilibrium transition between the active and the absorbing phases becomes discontinuous. (The transition is unarguably continuous in the case that D is not too large.) The controversy arises because the best available estimate of D_t is too close to 1 (the original estimate by Dickman and Tomé was $D_t \approx 0.85$ [13]) and so any systematic error due to the strong crossover effects that appear for

large D (see [5]) may drive D_t to the boundary of phase diagram, as in the case of the Domany–Kinzel cellular automaton [23]. On top of this, there is the argument by Hinrichsen [3] which posits that a first-order transition cannot occur in fluctuating one-dimensional systems such as the triplet-creation model (see also [21, 22]). The present analysis reveals that this class of models poses a difficult challenge to mean-field approximation schemes as well, producing unsettled issues even within this more limited framework.

Acknowledgments

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