On the absorbing-state phase transition in the one-dimensional triplet creation model

J. Stat. Mech. (2009) P08024

(http://iopscience.iop.org/1742-5468/2009/08/P08024)

Journal of Statistical Mechanics: Theory and Experiment
An IOP and SISSA journal

On the absorbing-state phase transition in the one-dimensional triplet creation model

Géza Ódor[1] **and Ronald Dickman**[2]

[1] MTA-MFA Research Institute for Technical Physics and Materials Science, PO Box 49, H-1525 Budapest, Hungary
[2] Departamento de Fisica and National Institute of Science and Technology of Complex Systems, ICEx, Universidade Federal de Minas Gerais, Caixa Postal 702, 30161-970, Belo Horizonte-Minas Gerais, Brazil
E-mail: odor@mfa.kfki.hu and dickman@fisica.ufmg.br

Received 2 July 2009
Accepted 3 August 2009
Published 27 August 2009

Online at stacks.iop.org/JSTAT/2009/P08024
doi:10.1088/1742-5468/2009/08/P08024

Abstract. We study the lattice reaction–diffusion model 3A $\rightarrow$ 4A, A $\rightarrow \emptyset$ ('triplet creation') using numerical simulations and n-site approximations. The simulation results suggest that the phase transition is discontinuous at high diffusion rates. In this regime the order parameter appears to be a discontinuous function of the creation rate; no evidence of a stable interface between active and absorbing phases is found. Based on an effective mapping to a modified compact directed percolation process, we shall nevertheless argue that the transition is *continuous*, despite the seemingly discontinuous phase transition suggested by studies of finite systems.

Keywords: classical Monte Carlo simulations, classical phase transitions (theory), other numerical approaches, phase transitions into absorbing states (theory)

ArXiv ePrint: 0907.0112

1742-5468/09/P08024+19$30.00

Contents

1. Introduction

The exploration of phase transitions in simple, one-component nonequilibrium models has attracted considerable interest [1]–[4], and important progress towards identifying the related universality classes has been made [5, 6]. In nonequilibrium models phase transitions may occur even in one-dimensional systems: the well known arguments due to Landau and to van Hove [7] against phase transitions in one-dimensional systems with short-range interactions do not apply in the absence of detailed balance. However, in low dimensions the effect of fluctuations is stronger, making continuous phase transitions more common. (A familiar example is the three-state Potts model, which exhibits a continuous transition in two dimensions, and a discontinuous one for $d > 2$.)

In one dimension, discontinuous phase transitions have been found in models with long-range interactions [8], or a conserved density [9, 10], and in multi-component systems [11]–[14]. Compact directed percolation (CDP) has a discontinuous transition between a pair of absorbing states (all sites full or all empty) [15, 16]; a similar transition between absorbing states is found in the one-dimensional Ziff–Gulari–Barshad model [17]. A discontinuous transition between and active phase and an absorbing one in a single-component model was claimed for the triplet creation model (TCM) [18], which does not possess a conservation law or long-range interactions. This model features particle reactions $3A \to 4A$, $A \to \emptyset$ and explicit diffusion (hopping)[3]. On increasing the diffusion probability, a crossover from a continuous to a discontinuous phase transition was detected

[3] By *explicit* diffusion we mean a particle hopping or exchange process, in contrast to *implicit* diffusion, generated by the dynamics of particle annihilation and creation at neighboring sites. Thus the coarse-grained description of the contact process, and many other models, includes a diffusion term, despite the absence of explicit diffusion.

J. Stat. Mech. (2009) P08024

in simulations and cluster mean-field approximations. Similar behavior was also reported in a stochastic cellular automaton [8].

Subsequently, Hinrichsen argued that in one dimension discontinuous transitions between an active and an absorbing state cannot exist in models like the TCM [19, 20]. The original findings for the TCM [18] were nevertheless confirmed in spreading simulations by Cardoso and Fontanari [21] and in fixed order parameter simulations by Fiore and de Oliveira [22]. The spreading exponents are shown in [21] to be those of compact directed percolation (CDP) [15, 16]; a tricritical point is suggested for a diffusion probability $D \simeq 0.95$. Very recently Park [23] reported simulation results that again support a continuous phase transition, belonging to the directed percolation (DP) universality class, at high diffusion rates.

Recently, a field theoretic analysis of bosonic reaction–diffusion (RD) models led to a hypothesis [5] based on a general phase transition classification scheme: bosonic, one-component RD systems with n-particle creation and m-particle annihilation always exhibit a first-order transition if $n > m$. This is indeed the case above the upper critical dimension (see [24]). However, in bosonic models one has to introduce a higher-order coagulation term $m'\mathrm{A} \to (m' - l)\mathrm{A}$ with $(m' > n)$, to avoid an infinite particle density in the active phase. Furthermore the topological phase space method used in [5] deals with the reactions (creation and annihilation) but does not take into account the effect of diffusion, which turns out to be relevant in some cases, when different reactions compete [25]–[27].

In this work we study the TCM in an effort to determine whether multi-particle creation, combined with rapid diffusion, can overcome fluctuations and generate a discontinuous phase transition in one dimension. This is a problem of longstanding interest in nonequilibrium statistical physics, and is related to the existence of first-order depinning transition in nonequilibrium wetting (i.e. in a system with multiplicative noise, with an attractive wall) [28].

The remainder of this paper is organized as follows. In section 2 we define the model, and review applicable simulation methods and previous results regarding the nature of the phase transition. Section 3 is devoted to a discussion of n-site approximations, and section 4 to our simulation results. In section 5 we use these results to motivate a simplified description of the model in the high diffusion rate regime, and discuss the nature of the transition using this mapping. Finally, in section 6, we summarize our findings.

2. The triplet creation model

The TCM is defined on a lattice, with each site either vacant or occupied by a particle; multiple occupancy is forbidden [18]. In the one-dimensional TCM, a particle (A) attempts diffusion at rate $D \leq 1$, creation ($3\mathrm{A} \to 4\mathrm{A}$) at rate $\lambda(1 - D)/(1 + \lambda)$, and is annihilated ($\mathrm{A} \to \emptyset$) at rate $(1 - D)/(1 + \lambda)$. In a diffusion attempt, one of the nearest-neighbor (NN) sites of the particle is chosen at random, and the particle jumps to this site if it is empty. If the target site is occupied, the configuration remains the same. In a creation attempt, if both NN sites of the particle are occupied, then one of the second-neighbor sites of the central particle is chosen at random, and if this site is empty, a new particle is placed there. If the conditions of two occupied NN sites and an empty target site are not fulfilled, the configuration does not change. Annihilation occurs independently of the states of neighboring sites. The configuration with all sites empty is absorbing. Since the sum of these transition rates is unity, the total transition rate in a system with N particles

J. Stat. Mech. (2009) P08024

is simply N. In simulations, the time increment associated with each attempted event (whether accepted or not) is $\Delta t = 1/N$, and one Monte Carlo step (MCS) corresponds to an accumulated time increment of unity.

In [18] the one-dimensional TCM was shown to exhibit a phase transition between the active and absorbing states; the transition was found to be continuous (and in the DP universality class) for smaller diffusion rates, but discontinuous for large D. By a discontinuous transition we mean one in which the order parameter is a discontinuous function of the relevant control parameter(s), in the infinite-size limit. In the TCM the order parameter is the particle density ρ, and the control parameters are λ and D. Since one of the phases is absorbing, at a discontinuous transition ρ should jump between zero and a finite value.

The characterization of a transition as continuous or discontinuous in numerical simulations is fraught with difficulties: finite-size rounding can mask the discontinuity, and any finite system must eventually become trapped in the absorbing state. To circumvent these problems, a number of strategies have been proposed.

Hysteresis with a weak source. A characteristic feature of discontinuous phase transitions is hysteresis. If one of the phases is absorbing; however, hysteresis cannot be observed simply by varying a control parameter, since the absorbing phase allows no escape. Bideaux *et al* [29] showed that when the transition is discontinuous, adding a weak source of activity changes the absorbing and active phases to *low-activity* and *high-activity* phases, respectively. One may then observe a hysteresis loop between these phases, on varying the control parameter. This approach was used in [29] to demonstrate a discontinuous phase transition in a probabilistic cellular automaton, and was applied to the TCM in [18], yielding a hysteresis loop. Below, we shall revisit the question of scaling under a weak source.

Conserved order parameter simulations. In conserved order parameter simulations [30], particles are neither created nor destroyed. Changes in configuration occur through particle jumps, which can be of any size up to that of the entire system, in a manner that respects the local rules of the process. The simulation yields an estimate for the control parameter value corresponding to the chosen order parameter density. Using this method, Fiore and de Oliveira found evidence for a discontinuous transition in both the TCM and the related pair creation model (with creation reaction $2\mathrm{A} \to 3\mathrm{A}$) at high diffusion rates [22].

Quasistationary (QS) simulation. As in conserved order parameter simulations, QS simulation removes the absorbing state from the dynamics, but in a manner that samples the quasistationary probability distribution (i.e. conditioned on survival) [31]. A study of the TCM using this method [14] showed that as the system size tends to infinity, the QS order parameter appears to develop a discontinuity between zero and a positive value, as λ is varied at a high diffusion rate, $D = 0.98$. (For a finite system the discontinuity is of course rounded.) A study of the TCM with biased diffusion (hopping in one direction only) yielded evidence of a sharp discontinuity [32].

Spreading simulations. Studies of the spread of activity, starting from a seed at the origin, have long been employed to characterize continuous phase transitions to an absorbing state [1, 33]. At the critical point, the survival probability $P(t)$, mean number of active sites $n(t)$, and mean-square distance $R^2(t)$ of active sites from the origin all follow power

J. Stat. Mech. (2009) P08024

laws. At a discontinuous transition, there is in principle no reason to expect scale-invariant spreading dynamics. Nevertheless, in the case of the TCM, Cardoso and Fontanari [21] demonstrated power-law spreading at the transition point, λ_c, for $D = 0.98$. The scaling exponents were identified as those of CDP, which, as noted above, suffers a discontinuous transition between a pair of symmetric absorbing states.

Interface motion. Suppose we prepare the system with all sites occupied, allow it to relax to the QS state, and then remove all particles from half of the lattice. In the subsequent evolution, the interface between active and inactive regions broadens due to diffusion, and in general drifts toward one region or the other. Below we report studies showing that the drift velocity is proportional to $\lambda - \lambda_c$. In a related analysis, we initialize the system with all sites in the region $1, \ldots, M$ occupied, and sites $M + 1, \ldots, L$ empty, and study the long-time survival probability $P(M)$. At the transition, the dependence of $P(M)$ on M is consistent with independent, randomly diffusing interfaces, as in CDP. This result supports the existence of two phases, one absorbing, the other active, separated by a large gap in density. The two phases do not coexist: the fluctuating interfaces eventually meet, and one of the phases is lost from the system.

Summarizing, the above mentioned studies, some from the recent literature and others to be reported below, provide evidence for a discontinuity in the QS order parameter, for hysteresis, and for a connection between the TCM at high diffusion rate and compact directed percolation.

2.1. Hinrichsen's objection

Some years ago, Hinrichsen presented an argument to the effect that discontinuous phase transitions between an active and an absorbing state are impossible in one-dimensional systems with local interactions, and without additional conservation laws, special boundary conditions, or macroscopic currents [19, 20]. The argument is based on the observation that the effective surface tension of interfaces in such systems does not depend on the size of the domains they delimit. Hinrichsen's argument prohibits the presence of fixed, stable boundaries between coexisting phases; as noted, no such boundaries have been observed in simulations. But this in itself does not appear to imply that the dependence of the order parameter on growth rate must be continuous at the transition. The one-dimensional totally asymmetric exclusion process (TASEP), for example, exhibits a discontinuous phase transition in a certain region of parameter space, even though the position of the boundary between high- and low-density phases fluctuates over the entire system [34, 35].

Hinrichsen [19] also reported simulation results supporting a continuous transition in the TCM at diffusion rate $D = 0.9$, that is, above the estimate for D_t given in [18]. It is now generally acknowledged that $D_t > 0.9$ in the TCM.

In a recent study [23], Park reported simulation results that support DP-like scaling in the TCM at diffusion rates of 0.95 and 0.98. Specifically, the order parameter (starting from a filled lattice) appears to decay at long times as $\rho(t) \sim t^{-\delta}$, with δ taking its DP value, over about two decades in time. We note, however, that the decay exponent is very sensitive to the choice of the time interval used for analysis and of the control parameter λ. Analyzing simulation results for $D = 0.98$ in studies extending to 10^9 MCS, we obtain local decay exponents δ_{eff} between 0.1 and 0.2, varying λ in a very narrow

J. Stat. Mech. (2009) P08024

range. A crossover between a long supercritical plateau for $t \leq 10^7$ and a rapid decay to an inactive state cannot be ruled out. For $D = 0.98$, the regime during which DP-like scaling is found in [23] (i.e. $10^7 \leq t \leq 10^9$) corresponds to overall particle densities in the range 0.67–0.32. While scaling behavior can be observed at such densities in the contact process [1], definitive results for the decay exponent would require studying systems with substantially smaller values of ρ. Finally, three or more critical exponents would have to be determined to demonstrate convincingly that the transition falls in the DP class.

Although the results of Hinrichsen and of Park do not appear to rule out rigorously a discontinuous transition in the TCM, we believe that they are fundamentally correct. This conclusion is based not on simulation results but rather on a mapping to a modified CDP process, to be developed in section 5. Analysis of this mapping leads to the conclusion that the transition is in fact continuous, despite abundant numerical evidence to the contrary.

3. n-site approximations

One of the most common theoretical approaches to Markov processes with spatial structure is a truncation of the master equation known as an n-site approximation [36]. Such approximations have been applied to the TCM in efforts to determine the order of the transition; in this section we review and extend these results.

The simplest method in this family is dynamic mean-field theory or the *one-site approximation*, in which the probability of an m-site configuration is factored into a product of m single-site probabilities, so that, for example, $P(\bullet\bullet\bullet\circ) \simeq \rho^3(1-\rho)$, where $\bullet$ ($\circ$) denotes an occupied (vacant) site and ρ is the fraction of occupied sites. The resulting equation for $\mathrm{d}\rho/\mathrm{d}t$ yields rather poor predictions for the TCM; better results are obtained using larger clusters. In the n-site approximation, the equations that govern the probability distribution for clusters of n sites are truncated by expressing the probabilities of $n+1$ site (or larger) clusters in terms of the n-site distribution. In the three-site approximation, for example, we write $P(\bullet\bullet\bullet\circ) \simeq P(\bullet\bullet\bullet)P(\bullet\bullet\circ)/P(\bullet\bullet)$. As n grows, the number and complexity of the equations increases rapidly, but it is possible to generate the equations, and integrate them numerically, via a computational algorithm [37].

In [18], the four-site approximation for the TCM was found to predict a continuous phase transition for diffusion rates $D < D_\mathrm{t}$ and a discontinuous one for $D > D_\mathrm{t}$. The predicted value for the tricritical diffusion rate D_t, however, is much smaller than that reported in simulations ($D_\mathrm{t} \simeq 0.95$). Since the phase diagram predicted by the n-site approximation generally converges to the correct one as $n \to \infty$, it is of interest to study the results for larger n. In certain cases, predictions based on a sequence of n-site approximations behave in a consistent manner, and can be extrapolated to provide estimates of the transition point and critical exponents, via the coherent anomaly method [37, 38].

For small n, the position of D_t varies considerably. For example, the $n \leq 3$ approximations yield a discontinuous transition even for $D = 0$, but for $n \geq 4$ there is a tricritical point at some $D_\mathrm{t} > 0$. The estimates for D_t increase gradually with n; for $n = 8$, one finds $D_\mathrm{t} > 0.5$, for example. On the other hand, for a fixed, large diffusion rate, the transition remains discontinuous, with a large jump in the order parameter, which does not diminish appreciably with increasing n. For $D = 0.98$, for example, figure 1 shows that all the approximations studied ($n \leq 18$) yield a discontinuous transition.

J. Stat. Mech. (2009) P08024

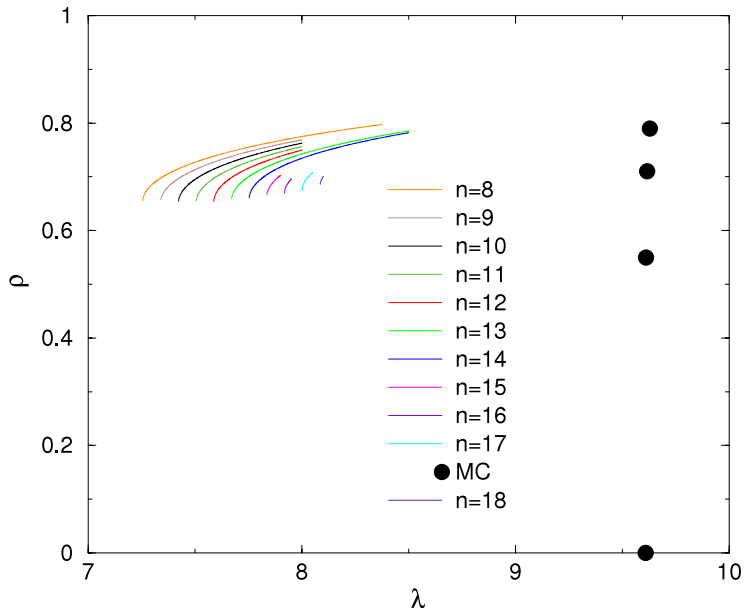

Figure 1. Order parameter versus creation rate in the one-dimensional TCM with $D = 0.98$, in the n-site approximation with $n = 8, \ldots, 18$. Points show the simulation.

Recently, Ferreira and Fontanari published results casting doubt on the utility of n-site approximations for the TCM [39]. They show, for example, that for $D = 0$, the values of λ_c veer *away* from the simulation value as n is increased from 11 to 18; our studies confirm this observation. (We note that a nonmonotonic approach to the critical point is observed in a stochastic cellular automaton in which at least three particles are required for particle generation or survival [8].) Moreover, the values of the tricritical reproduction rate $\lambda_t(n)$ (for $n \leq 14$) appear to converge to an unphysical (negative) value as $n \to \infty$ [39].

Thus if the n-site approximations converge to the correct values, they do so in a nonmonotonic fashion, such that for the cluster sizes accessible with present technology ($n \leq 20$ or so), quantitative results for λ_c cannot be obtained for the TCM. Although our n-site approximations show stable nonvanishing gap sizes at $D = 0.98$ for $n \leq 18$ (figure 1), we find that for a given level ($n = 13$, say), $\lambda_c(D)$ is not a monotonic function of D, and the location of the tricritical point is rather uncertain. Figure 2 shows that on increasing the diffusion rate from $D = 0.6$ to 0.66, the critical point shifts to higher values, but for $D > 0.66$ this tendency reverses. On the other hand, there is no evidence of a discontinuous transition for $0.67 \leq D \leq 0.71$. Our analysis provides a higher λ_t estimate for $n = 13$ than found in [39]; the reason for this difference is not known, since our result for $\lambda_t(n = 4)$ agrees with that reported in the latter work. We observe a similar behavior for $n = 14$ and 15; our tricritical point estimates do not fall on the extrapolation line given in [39].

For the cluster sizes studied, $\lambda_t(n)$ cannot be fitted with a linear function of $1/n$, so that the $n \to \infty$ limiting value cannot be estimated with confidence. It seems likely that $\lambda_t(n)$ exhibits an oscillatory convergence with n; if so, the question of whether

J. Stat. Mech. (2009) P08024

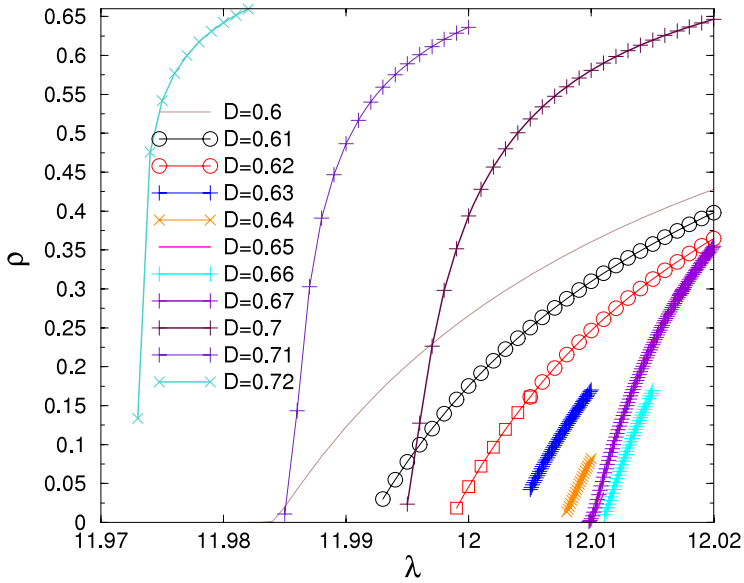

Figure 2. Order parameter versus creation rate in the one-dimensional TCM in the 13-site approximation.

$\lim_{n\to\infty} D_t(n) < 1$ (that is, the existence of a discontinuous transition) cannot be resolved using the available n-site approximation results.

4. Simulation results

We study the TCM via Monte Carlo simulation, using several approaches that complement earlier analyses: dependence on the initial value of the order parameter, interface dynamics, scaling in the presence of a weak source of activity, and scaling of the quasistationary order parameter. While some of the results would seem to provide good evidence of a discontinuous transition, we shall defer our conclusion until section 5.

4.1. Initial density dependence

If a phase transition is discontinuous the evolution of the system should depend strongly on the initial condition, while at a continuous transition the evolution is toward the same QS state regardless of the initial condition. In [40], simulations of the TCM at a diffusion rate $D = 0.98$ are reported, showing that at the transition ($\lambda_c \simeq 9.60$) the value of the order parameter at long times depends on its initial value. For initial particle densities $\rho(0)$ between 0.3 and unity the system evolves to the active state, while for $\rho(0) \leq 0.3$ it rapidly approaches the absorbing state. (In studies using $\rho(0) < 1$, the initially occupied sites are chosen at random, uniformly over the lattice.) These results demonstrate that an active phase, characterized by a high value of the order parameter, is accessible starting from a high density but not from a low one. The findings for a high diffusion rate are in sharp contrast to those found for $D = 0$, for which the critical reproduction rate is $\lambda_c = 12.015$. In this case, the particle density attains the same QS value, starting from very different initial values.

doi:10.1088/1742-5468/2009/08/P08024

J. Stat. Mech. (2009) P08024

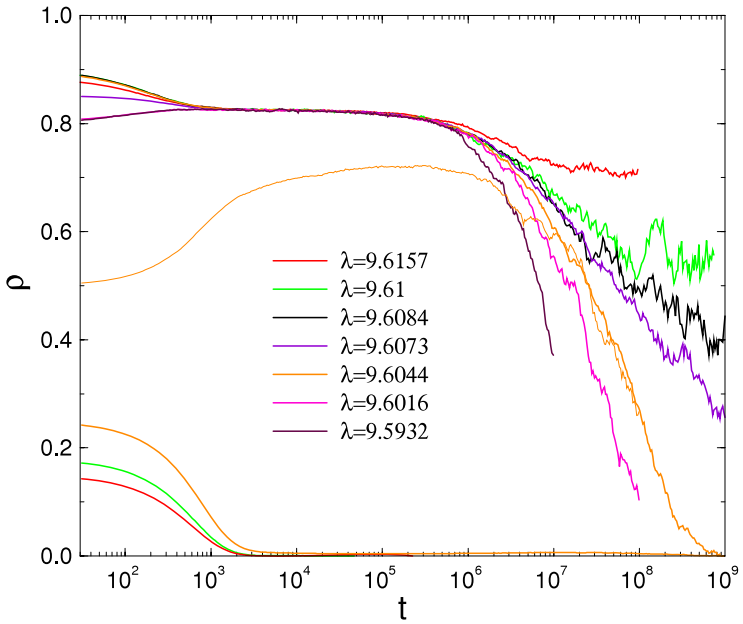

Figure 3. TCM: $\rho(t)$ for $D = 0.98$, using various initial particle densities, and creation rates near the transition value, as indicated.

Here we extend the simulations of [40] to much larger systems. We follow the evolution of the order parameter $\rho(t)$ in systems of $L = 2 \times 10^5$ sites (with periodic boundary conditions) for times of up to 10^9 MCS, averaging over 5–20 realizations. For $D = 0.98$, we find that for low initial values ($\rho(0) \leq 0.25$), the density falls exponentially for $\lambda \leq 9.616$ (see figure 3).

For the same reproduction rates, using $\rho(0) > 0.25$, the order parameter $\rho(t)$ exhibits a long plateau ($10^3 < t < 10^5$ MCS) at a high density. At longer times $\rho(t)$ decays, as expected in a finite system. For $D = 0.5$, by contrast, the order parameter curves $\rho(t)$, starting from high and low initial values, attain a common value at long times (see figure 4).

4.2. Fluctuating boundary studies

In these studies the initial configuration consists of two blocks—one, of n_0 sites, fully occupied, and the other, of $L - n_0$ sites, completely empty. For $D = 0.98$ and $\lambda = 9.60$, one finds that in the initially occupied region, the particle density quickly relaxes to its QS value of about $\rho_{\rm QS} \simeq 0.83$. The ensuing evolution is characterized by the drift of the boundaries between active and empty regions. A given realization stops either when it attains the absorbing state or when the number of particles indicates that the active phase has filled the entire system (we use a particle number of $N_{\rm stop} = 0.84L$ as the criterion for this event). Figure 5 shows a typical history for $L = 2000$ and $n_0 = 1500$. (The graph shows the mean density in blocks of 50 sites, with time increasing downward, in steps of 10 000 time units between each density profile.) The boundaries between active and inactive regions appear to follow independent, unbiased random walks.

If the boundaries can be represented by independent, unbiased random walkers, then the number $N(t)$ of particles (which is approximated by $\rho_{\rm QS}$ times the size of the active

J. Stat. Mech. (2009) P08024

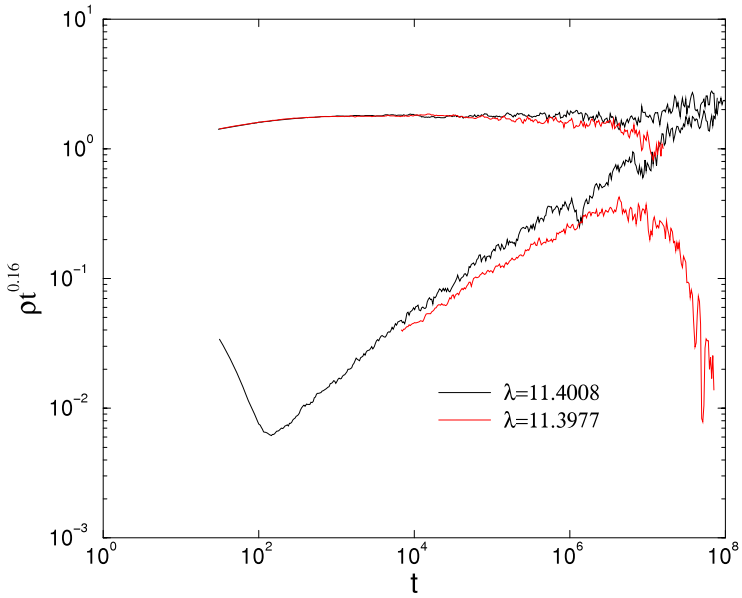

Figure 4. $\rho(t)$ as in figure 3, but for $D = 0.5$.

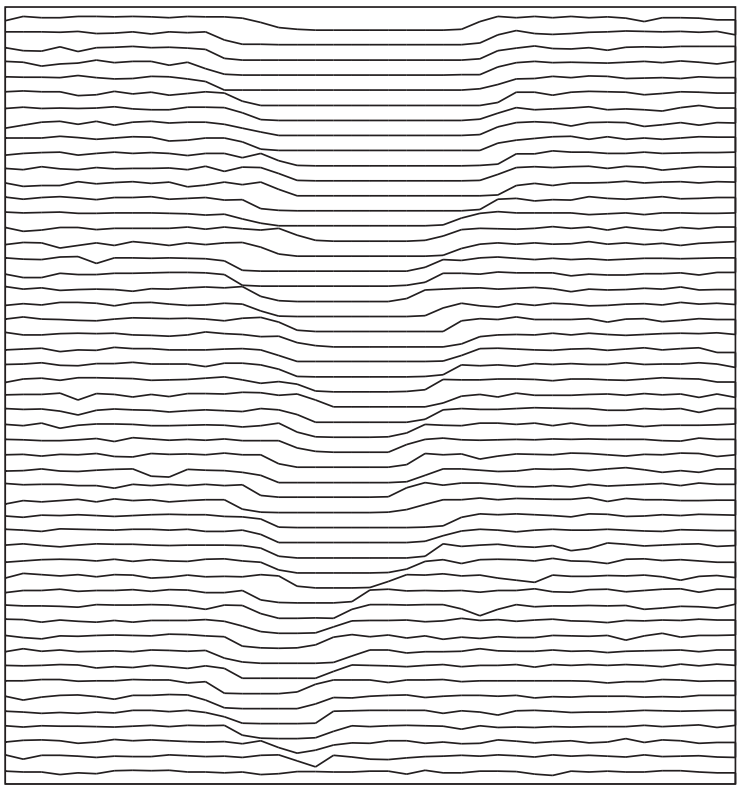

Figure 5. Space–time evolution of particle density for $D = 0.98$, $\lambda = 9.60$, and $L = 2000$, starting from a fully occupied region of 1500 sites with the remainder empty. Time increases downward, with each sweep (at intervals of 10 000 time units) showing the density profile averaged over blocks of 50 sites.

doi:10.1088/1742-5468/2009/08/P08024

J. Stat. Mech. (2009) P08024

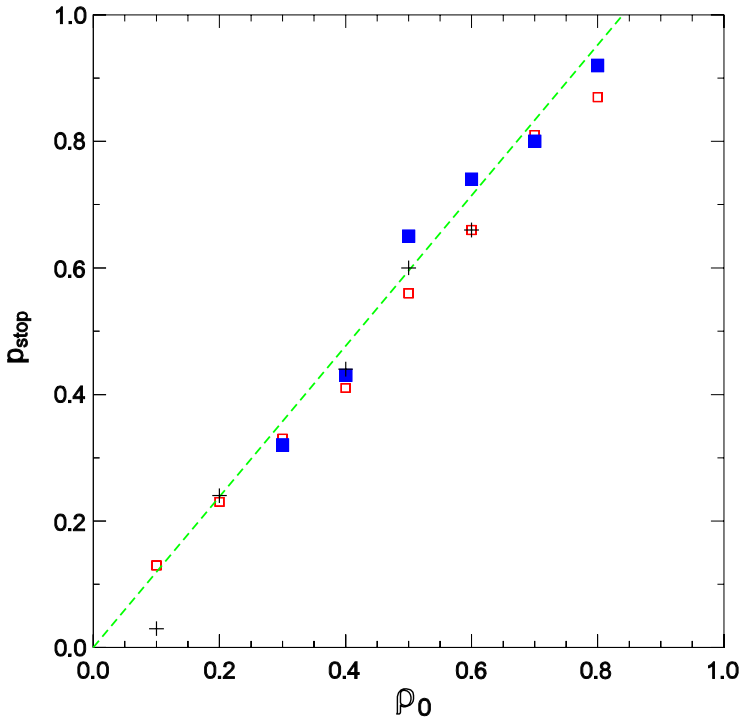

Figure 6. Probability $p_{\rm stop}$ versus $\rho_0 = n_0/L$ in the TCM with an inhomogeneous initial configuration. +, $L = 500$; open squares, $L = 1000$; filled squares, $L = 2000$. The dashed line is for $p_{\rm stop} = n_0/N_{\rm stop}$ as expected for a random walk.

region) should also follow an unbiased random walk. The walk starts at $N = n_0$ and is subject to absorbing frontiers at $N = 0$ and $N_{\rm stop}$. Well known results on random walks [41] then imply that the probability $p_{\rm stop}$ of reaching $N_{\rm stop}$ before $N = 0$ is given by $n_0/N_{\rm stop}$. We estimate $p_{\rm stop}$ in sets of 100 realizations, on rings of 500, 1000, and 2000 sites; the linear trend evident in figure 6 supports the fluctuating boundary interpretation. This in turn suggests that at high diffusion rates, the dynamics of active and inactive domains is effectively that of CDP.

Away from the phase transition, we expect the interface to drift on the average, advancing into the inactive region for $\lambda > \lambda_{\rm c}$ and vice versa. We determined the mean interface velocity for $D = 0.98$ on rings of 3000 sites, using $n_0 = 1500$. After allowing the system to relax for 50 000 MCS, we record the density profile ρ_i, and determine the interface position x_i via the criterion $\rho(x_i) = \rho_{\rm B}/2$, with $\rho_{\rm B}$ the bulk particle density at the λ value of interest. We then allow the system to evolve for an additional 20 000 MCS, and again determine the interface position. Figure 7 shows the interface drift velocity v, as determined in samples of 3×10^4 realizations, varying linearly with $\lambda - \lambda_{\rm c}$; linear regression yields $v = 0$ for $\lambda = 9.60(1)$, in agreement with other estimates of the transition point. (We verified that the interface velocity obtained using a ring of 5000 sites, and observation times of 10^5 and 2×10^5 MCS, agrees to within 2% with the value obtained using the smaller system.)

The above results show that for large D the system is divided into well defined active and empty regions. A typical configuration of a large system (2×10^4 sites) at the

J. Stat. Mech. (2009) P08024

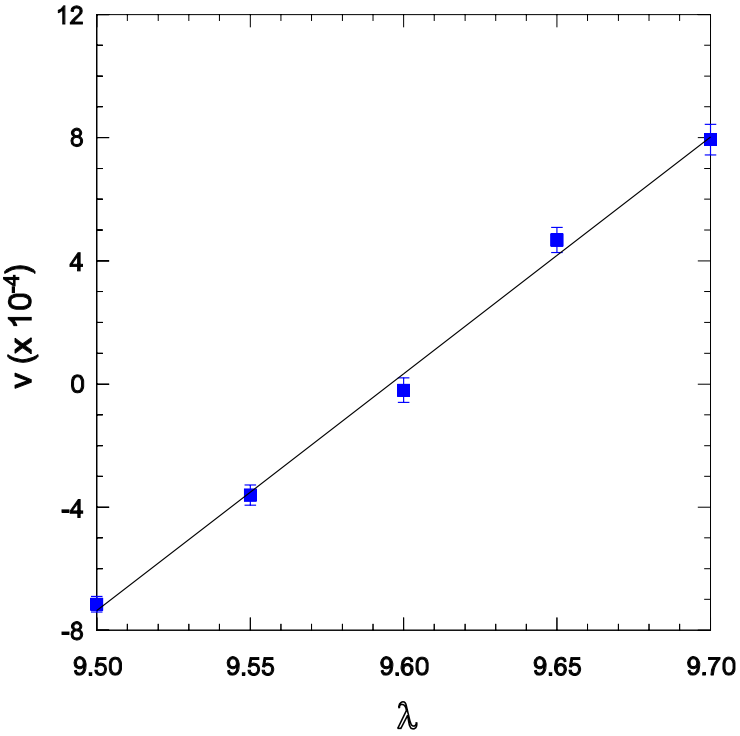

Figure 7. Interface drift velocity v versus creation rate λ, for $D = 0.98$, $L = 3000$. The straight line is a least-squares linear fit to the data.

transition ($D = 0.98$, $\lambda = 9.608$) bears this out. In order to visualize the configuration of a large system, we plot the cumulative particle number $S(x) = \sum_{i=1}^{x} \sigma_i$ versus position x, where σ_i is an indicator variable taking values of 0 and 1 at empty and occupied sites, respectively. Thus the local density $\rho(x)$ corresponds to the slope of the graph at x, with empty regions corresponding to horizontal lines. In these studies we initially occupy half the sites, randomly, so that initially the local density is $\simeq$0.5. In the initial phase of the evolution, the global density rapidly grows to about 0.8; thereafter it begins to fluctuate, as empty regions form. The configuration shown in figure 8, for a time of about 2.6×10^8 MCS (comparable to the simulation times in [23]), consists of a series active regions with density $\rho \simeq 0.845$, and empty regions, giving an overall density of 0.25. Of note is the high density in the active regions, and the similarity of the density in active regions separated by large inactive gaps. We verified that for this choice of D and λ, the density in active regions $\rho_a = 0.840(5)$, *independent of system size and of overall density*. The system reaches the absorbing state via fluctuations of the boundaries between active and inactive regions, which eventually drive the active fraction to zero, while the active region density remains constant. For comparison, in figure 8 we also show a typical configuration for $D = 0$ and $\lambda = \lambda_c(0) = 12.015$. The initial condition is the same as for $D = 0.98$, and the simulation is again halted when ρ falls to 0.25, which occurs at $t \simeq 17\,000$ MCS for these parameters. In this case the empty regions are typically much smaller than under rapid diffusion, and the local density in active regions varies considerably.

J. Stat. Mech. (2009) P08024

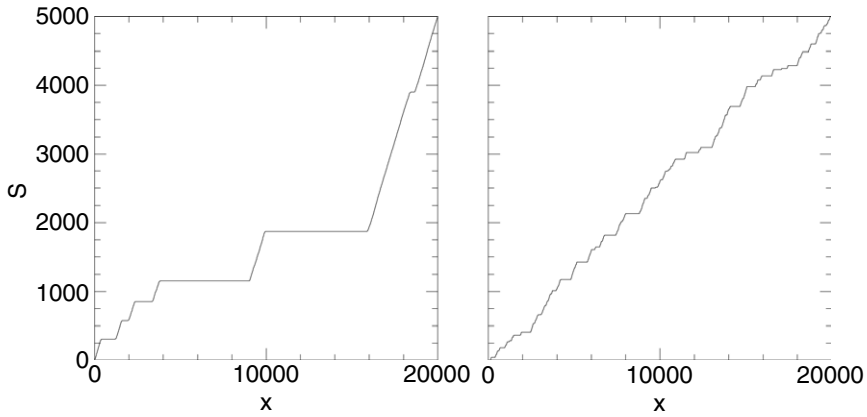

Figure 8. Cumulative particle number $S(x)$ versus position x in a typical configuration. Left, $D = 0.98$, $\lambda = 9.608$; right, $D = 0$, $\lambda = 12.015$.

4.3. Effect of a weak source

We turn next to studies of the stationary order parameter in the presence of a weak source, h, defined as the probability, per unit time and per vacant site, of inserting a particle. In [18] a weak source was used to demonstrate hysteresis; here, we consider the scaling of the order parameter as $h \to 0$ at the transition. For $D = 0$, we determine ρ at $\lambda = 12.015$, varying h between 10^{-9} and 10^{-5}. For each h value, a series of lattice sizes (from 5000 to 50 000 sites) are used to estimate the limiting infinite-size value of ρ. We verify the scaling law $\rho \propto h^{1/\delta_h}$ with $1/\delta_h = 0.109(1)$, in agreement with the value expected for directed percolation in one spatial dimension, $1/\delta_h = 0.108\,25(3)$ [1].

For $D = 0.98$ and $\lambda = 9.60$, we observe a very different scenario. For a given value of h, two values of ρ are found, depending on the initial density. For large initial densities, ρ approaches a value of about 0.815 as $h \to 0$, while for a low initial density, $\rho \propto h$ (see figure 9). The order parameter, moreover, is essentially independent of system size for $L \geq 1000$. These results are consistent with a discontinuous transition, and the absence of critical scaling, for $D = 0.98$.

4.4. Quasistationary order parameter

To close this section we report results on the QS value of the order parameter as a function of system size. In [14], estimates for the limiting ($L \to \infty$) value of $\rho_{\rm QS}$ were found to exhibit a discontinuity at the transition, for $D = 0.95$; here we focus on $D = 0.98$. We determined ρ in QS simulations of duration $t_{\rm max} = 10^7$ MCS (for $L = 100$) up to $t_{\rm max} = 2 \times 10^9$ MCS (for $L = 10^4$), allowing the initial 10% of the time for relaxation. In figure 10 we plot the QS order parameter versus $1/L$, for λ values near the transition. The curves divide into two families. One set (for $\lambda \leq 9.605$) approaches zero as $L \to \infty$, while for larger values of λ, the density approaches a nonzero limiting value. In the minute interval $9.605 < \lambda < 9.610$ the limiting ($L \to \infty$) value of the order parameter ρ jumps from zero to about 0.6. The inset shows that at the transition point, $\lambda = 9.6084$, ρ decays exponentially with system size. At a continuous transition one expects the density to decay as a power-law, $\rho_{\rm QS} \sim L^{-\beta/\nu_\perp}$.

J. Stat. Mech. (2009) P08024

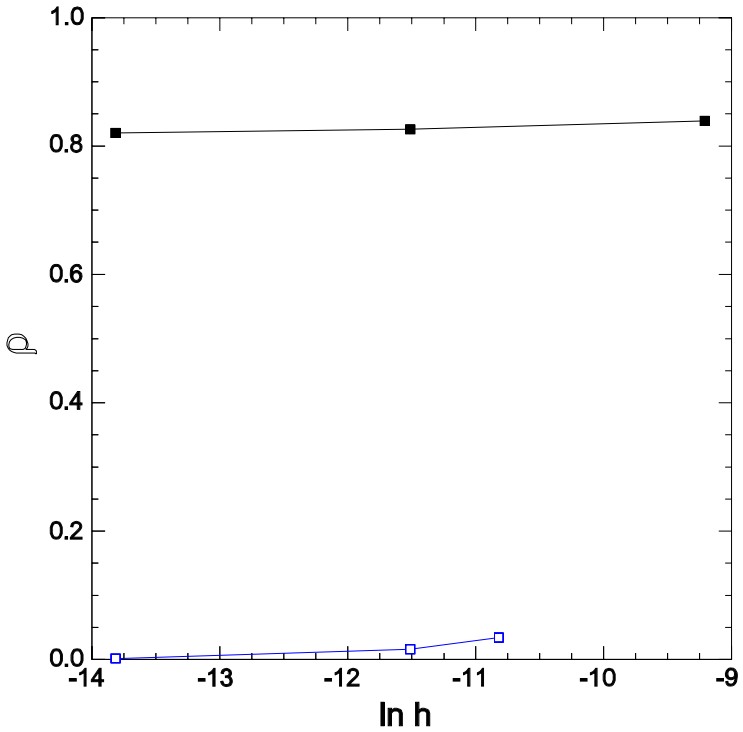

Figure 9. Order parameter versus source intensity h for $D = 0.98$, $\lambda = 9.60$, $L = 1000$. Upper curve, initial density unity; lower curve, initial density zero.

5. Why the transition is continuous, and why it appears to be discontinuous

At various points in this discussion we have drawn an analogy between the TCM at high diffusion rates and compact directed percolation. The picture that emerges from the simulations reported above, and from some of the earlier studies [21, 22], is that in this regime the system contains essentially two kinds of regions, one of high density and the other empty. The boundaries between these regions perform independent random walks, leading eventually to extinction of activity.

The above scenario corresponds to the phase transition in CDP, and suggests that we construct a reduced description in which blocks of ℓ sites in the active region (with particle density of the order of $\rho_a \approx 0.85$) correspond to sites in state 1 of the CDP, and blocks of ℓ empty sites correspond to sites in state 0 in the CDP. The dynamics of the CDP consists exclusively of random walks performed by the interfaces between strings of zeros and strings of ones. As we vary λ through its critical value in the TCM, the drift velocity of the interfaces in the corresponding CDP passes through zero, and the asymptotic density of ones jumps from 0 to 1.

If the above caricature of the TCM as an effective compact directed percolation model were valid, a discontinuous transition would be guaranteed. There are, however, two additional processes that must be taken into account. Evidently, gaps (strings of empty sites) can arise within active regions, otherwise the TCM starting from a fully occupied lattice would never reach the absorbing state. A fundamental point is that the process of gap nucleation, while essential to the TCM dynamics, occurs at an extremely

J. Stat. Mech. (2009) P08024

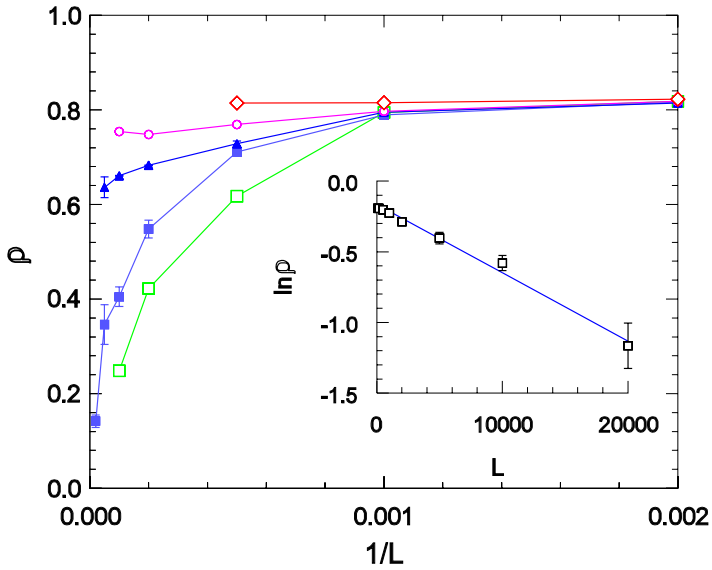

Figure 10. QS order parameter ρ versus reciprocal system size for $D = 0.98$ and (lower to upper) $\lambda = 9.60$, 9.605, 9.61, 9.62, and 9.65. Inset: semi-log plot of ρ versus L for $\lambda = 9.6084$.

small rate. By 'gap nucleation' we mean the generation of a gap large enough (of g^* sites, say) that its boundaries fluctuate independently of one another. Gaps of size $g \geq g^*$ are equally likely to grow or to shrink, whereas smaller gaps tend to shrink due to particles diffusing in from the adjacent occupied regions.

The data of figure 3 permit an order of magnitude estimate of the rate of gap nucleation: the density begins to fall appreciably from its plateau value at $t \approx 10^5$, and there are $\mathcal{O}(10^5)$ sites in the system, giving a rate of $\kappa \sim 10^{-10}$ per site. In figure 11 we plot the mean first-passage time t for the appearance of a gap of size g in a system of 10^4 sites (parameters $D = 0.98$ and $\lambda = 9.608$), starting with all sites occupied. (In these studies t is estimated using samples of $N_r = 50$–500 realizations, with smaller N_r for larger system sizes.) The first-passage time grows rapidly for smaller sizes and then crosses over to a slower growth around $g \simeq 30$, at which point $t \sim 6 \times 10^4$. Identifying this crossover size as g^* gives a nucleation rate of $\kappa \sim 10^{-9}$ per site.

It is natural to take the block size ℓ in the CDP mapping as the critical gap size g^*, so that a one-site gap in the equivalent CDP process is equally likely to grow or to shrink to zero. Since we map g^* TCM sites to a single site in the CDP, the effective gap nucleation rate in the latter is then $\kappa_{\rm eff} = g^*\kappa$. The estimates for the nucleation rate and for g^* given above yield $\kappa_{\rm eff}$ in the range 10^{-9}–10^{-7} per CDP site.

As noted above, a small gap can shrink when particles diffuse in from outside. Can a large gap be destroyed in this manner? To answer this, consider an interface (treated as fixed, for the sake of this argument) between large active and empty regions: the local density $\rho(x) = \rho_{\rm a}$ for $x < 0$ and $\rho \simeq 0$ for $x > 0$. Think of the edge of an active region as a particle source. Particles are emitted at a rate of order $s = 1 - D$, diffuse away at rate D, and decay at rate $\gamma = (1 - D)/(1 + \lambda)$. In the stationary state, a continuum diffusion

J. Stat. Mech. (2009) P08024

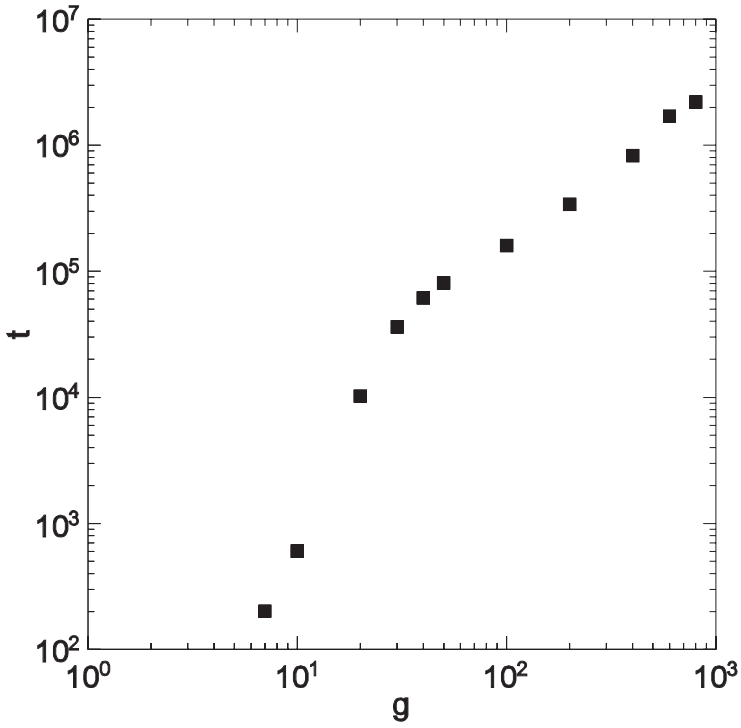

Figure 11. Mean first-passage time t for appearance of a gap of size g. Parameters: $L = 10^4$, $D = 0.98$, $\lambda = 9.608$.

analysis yields a local density for $x > 0$ of

$$\rho(x) = s \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-\gamma t} \frac{\mathrm{e}^{-x^2/4Dt}}{\sqrt{4\pi D t}} \tag{1}$$

giving $\rho(x) \simeq s e^{-x/w}$ with an interface width $w = \sqrt{D/\gamma}$. For $D = 0.98$ and $\lambda = 9.60$ this gives $w \simeq 23$; for these parameters simulation shows that near the edge of a large gap, the density decays to zero $\propto e^{-x/25}$. Nucleation of an active region inside a gap occurs at a rate of $\approx (1 - D)[\rho(x)]^3$, making the probability of nucleating activity deep within a gap negligible. For $x = 100$ and D and λ as above, for example, we find a nucleation rate of $\sim 10^{-13}$. The essential point is that $\rho(x)$ decays exponentially, so that nucleation of activity is limited to the neighborhood of the edges, whereas the nucleation of gaps can occur anywhere inside an active region.

Thus we conclude that the TCM at a high diffusion rate is equivalent to compact directed percolation with a very small, but nonzero, rate of gap formation within clusters of ones. But this process is in turn equivalent (insofar as scaling properties are concerned) to the Domany–Kinzel cellular automaton (DKCA) [15] with $p_1 \simeq 1/2$ and $p_2 = 1 - \kappa_{\mathrm{eff}}$. (Recall that in the one-dimensional DKCA, p_1 is the probability of a site taking state 1, given one neighbor in state 1, and one in state 0, at the preceding time, and that p_2 is the probability of state 1 given that both neighbors are in state 1 at the previous step.) CDP corresponds to the line $p_2 = 1$. From the work of Janssen [42] and of Lübeck [43] we know that for $p_2 = 1 - \epsilon$, the transition occurs at $p_c = 1/2 + \mathcal{O}(\sqrt{\epsilon})$.

The phase transition of the DKCA is discontinuous *only* for $p_2 = 1$; for *any* $p_2 < 1$, it is continuous and belongs to the DP universality class. We are led to the same conclusion regarding the TCM: for any $D < 1$, there is a small but finite rate of nucleating gaps within active regions, so that the effective value of p_2 is slightly less than unity.

Given the nearness of the equivalent DKCA to the line $p_2 = 1$, it is not surprising that simulations of the TCM using lattice sizes L and simulation times t_m yield an apparently discontinuous phase transition for $Lt_m < 1/\kappa$. It is only for large systems and long simulation times that the effects of gap nucleation become apparent, as in the studies of [19] and [23]. (Indeed, the results shown in figure 3 are also compatible with DP-like decay of the order parameter.) But numerical studies of the stationary order parameter can be expected to show discontinuous behavior, this near the CDP line. For similar reasons, it is not surprising that n-site approximations, using clusters of fewer than 20 sites, miss the effect of gap nucleation; much larger clusters would be needed to capture this properly.

It is perhaps worth recalling that CDP-like spreading behavior is observed in a *surface modified* version of directed percolation in one spatial dimension [44]. In this case, propagation of activity at the edges of the active region occurs with a different creation rate (λ', say) than in the bulk, which has a creation rate of λ_B. Let λ_c denote the critical creation rate for the original problem, that is, for $\lambda' = \lambda_B$. For $\lambda' < \lambda_c$, the phase transition occurs at some bulk creation rate $\lambda_B > \lambda_c$, which means that the bulk has a finite activity density even for $t \to \infty$. Thus the active cluster is compact, and the scaling behavior is that of CDP. The essential difference between this model and the TCM is that in the former case large gaps cannot be nucleated within the active region: since $\lambda_B > \lambda_c$ at the transition, gaps tend to shrink.

6. Discussion

We have presented various pieces of evidence suggesting that the order parameter is a discontinuous function of the creation rate in the TCM at high diffusion rates (our numerical studies focus on $D = 0.98$). We do not find evidence of stable coexisting active and inactive regions; the boundaries between these regions are observed to fluctuate, as asserted in [19]. The numerical evidence in favor of a discontinuous transition includes hysteresis (under a weak source), the initial density dependence of the order parameter at later times (with or without a particle source), the high particle density within active regions, the random-walk-like fluctuations of the boundaries between active and inactive regions, and the apparent absence of power-law scaling of the QS order parameter as a function of system size, at the transition point.

Despite the numerical evidence in favor of a discontinuous transition, a mapping of the TCM to a effective dynamics resembling that of compact directed percolation, but with a very small gap nucleation rate, leads to the conclusion that the transition is continuous for any $D < 1$. The studies reported above, suggesting a discontinuous transition, were performed using relatively small systems and/or limited times. For example, to see the effect of gap nucleation in those studies with a weak source of activity, the source strength h would have to be much smaller than the gap nucleation rate κ.

The failure of n-site approximations to give a clear indication of the nature of the transition may again be attributed to the very small gap nucleation rate for $D \simeq 1$. These

J. Stat. Mech. (2009) P08024

approximations, however, are problematic even for $D = 0$: the values predicted for λ_c do not converge monotonically to the correct value with increasing n [39].

The continuous nature of the transition in the one-dimensional TCM was of course asserted some time ago by Hinrichsen [19], and received further support in Park's simulations [23]. Our argument nevertheless contributes to an intuitive understanding of this result, and might provide the basis for a rigorous demonstration of the continuous nature of the transition.

Acknowledgments

We are grateful to José F Fontanari and Mário J de Oliveira for helpful discussions. Support from Hungarian research fund OTKA (grant nos T046129, T77629) is acknowledged. The authors acknowledge access to the HUNGRID, Clustergrid and the supercomputer of NIIF Budapest. RD acknowledges support from CNPq, and Fapemig, Brazil.

References

[1] Marro J and Dickman R, 1999 *Nonequilibrium Phase Transitions in Lattice Models* (Cambridge: Cambridge University Press)
[2] Hinrichsen H, 2000 *Adv. Phys.* **49** 815
[3] Ódor G, 2004 *Rev. Mod. Phys.* **76** 663
[4] Lübeck S, 2004 *Int. J. Mod. Phys.* B **18** 3977
[5] Elgart V and Kamenev A, 2006 *Phys. Rev.* E **74** 041101
[6] Ódor G, 2008 *Universality In Nonequilibrium Lattice Systems* (Singapore: World Scientific)
[7] van Hove L, 1950 *Physica* **16** 137
[8] Ódor G, Boccara N and Szabó G, 1993 *Phys. Rev.* E **48** 3168
[9] Glauber R J, 1963 *J. Math. Phys.* **4** 191
[10] Menyhárd N and Ódor G, 1998 *J. Phys. A: Math. Gen.* **31** 6771
[11] Evans M R, Kafri Y, Koduvely H M and Mukamel D, 1998 *Phys. Rev.* E **58** 2764
[12] Godrèche C, Luck J-M, Evans M R, Mukamel S S D and Speer E R, 1995 *J. Phys. A: Math. Gen.* **28** 6039
[13] Wijland F, Oerding K and Hilhorst H J, 1998 *Physica* A **251** 179
[14] Maia D S and Dickman R, 2007 *J. Phys.: Condens. Matter* **19** 065143
[15] Domany E and Kinzel W, 1984 *Phys. Rev. Lett.* **53** 311
[16] Essam J W, 1989 *Physica* A **22** 4927
[17] Ziff R, Gulari E and Barshad Y, 1986 *Phys. Rev. Lett.* **56** 2553
[18] Dickman R and Tomé T, 1991 *Phys. Rev.* A **44** 4833
[19] Hinrichsen H, 2000 arXiv:cond-mat/0006212
[20] Henkel M, Hinrichsen H and Lübeck S, 2008 *Nonequilibrium Phase Transitions* (Berlin: Springer)
[21] Cardozo G O and Fontanari J, 2006 *Eur. Phys. J.* B **51** 555
[22] Fiore C E and de Oliveira M J, 2004 *Phys. Rev.* E **70** 046131
[23] Park S-C, 2009 arXiv:0903.3436v2
[24] Ódor G, 2003 *Phys. Rev.* E **67** 056114
[25] Ódor G, 2004 *Phys. Rev.* E **70** 026119
[26] Ódor G, 2004 *Phys. Rev.* E **70** 066122
[27] Canet L and Delamotte H C B, 2004 *Phys. Rev. Lett.* **92** 255703
[28] Muñoz M A, 2004 *Advances in Condensed Matter and Statistical Mechanics* ed E Korutcheva and R Cuerno (New York: Nova Science)
[29] Bidaux R, Boccara N and Chaté H, 1989 *Phys. Rev.* A **39** 3094
[30] Tomé T and de Oliveira M J, 2001 *Phys. Rev. Lett.* **86** 5643
[31] de Oliveira M M and Dickman R, 2005 *Phys. Rev.* E **71** 4266
[32] Dickman R, 2007 unpublished
[33] Grassberger P and de la Torre A, 1979 *Ann. Phys., NY* **122** 373
[34] Derrida B, Evans M R, Hakim V and Pasquier V, 1992 *J. Phys. A: Math. Gen.* **26** 1493
[35] Schütz G M and Domany E, 1993 *J. Stat. Phys.* **72** 277
[36] ben-Avraham D and Köhler J, 1992 *Phys. Rev.* A **45** 8358

J. Stat. Mech. (2009) P08024

[37] Dickman R, 2002 *Phys. Rev.* E **66** 036122
[38] Konno N and Katori M, 1990 *J. Phys. Soc. Japan* **59** 1581
[39] Ferreira A A and Fontanari J F, 2009 *J. Phys. A: Math. Theor.* **42** 085004
[40] Dickman R and Maia D S, 2008 *J. Phys. A: Math. Theor.* **41** 405002
[41] van Kampen N G, 1992 *Stochastic Processes in Physics and Chemistry* (Amsterdam: North-Holland)
[42] Janssen H.-K, 2005 *J. Phys.: Condens. Matter* **17** S1973
[43] Lübeck S, 2006 *J. Stat. Mech.* P09009
[44] Mendes J F F, Dickman R and Herrmann H, 1996 *Phys. Rev.* E **54** R3071

J. Stat. Mech. (2009) P08024