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Critical discontinuous phase transition in the threshold contact process

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Abstract

We analyze a threshold contact process on a square lattice in which particles are created on empty sites with at least two neighboring particles and are annihilated spontaneously. We show by means of Monte Carlo simulations that the process undergoes a discontinuous phase transition at a definite value of the annihilation parameter, in accordance with the Gibbs phase rule, and that the discontinuous transition exhibits critical behavior. The simulations were performed by using boundary conditions in which the sites of the border of the lattice are permanently occupied by particles.

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1. Introduction

According to the Gibbs phase rule [1], the coexistence of k thermodynamic phases occurs within a subspace of codimension $k-1$ of the whole thermodynamic phase space, the space spanned by the thermodynamic fields. In particular, the coexistence of two phases occurs in a subspace of codimension 1. In a one-dimensional thermodynamic phase space or along an arbitrary line within a thermodynamic phase space of any dimension, the coexistence of two phases must occur at a definite point on the line. The coexistence over an interval of the line, called generic phase coexistence [2, 3], is therefore ruled out. Since discontinuous phase transitions are associated with phase coexistence, along the line, the discontinuous phase transition occurs at the point of coexistence. The simplest example of a model exhibiting this behavior is the Ising model in the presence of a field. If one varies the field, at a constant low temperature, the system undergoes a discontinuous phase transition at zero field, the coexistence of phase occurring precisely at zero field.

This picture of a discontinuous phase transition, a direct consequence of the Gibbs phase rule, is valid for systems in thermodynamic equilibrium. Whether it can be extended to include phase transitions in nonequilibrium systems at the stationary state is an open question. The

anisotropic contact process, known as Toom's NEC model, as well as some nonequilibrium models for the depinning of a bound interface has been shown to display coexistence over a finite interval of the external parameter [2–5]. Numerical simulations performed on a version of the threshold contact process in two dimensions have been used to show that this model also exhibits generic phase coexistence [6–8]. In all these examples, the asymmetry of the dynamic rules or the orientation dependence of the moving interface plays a crucial role for the appearance of the generic phase coexistence [3, 6]. First-order transition has also been found to occur in several related models [9–12].

In this paper, we analyze another version of the threshold contact process on a square lattice and show that the discontinuous phase transition occurs at a definite value of the annihilation parameter in accordance with the Gibbs phase rule. In addition, we show that it displays critical behavior in the neighborhood of the discontinuous transition, similar to the critical behavior of a continuous transition except that the exponent related to the order parameter equals zero. Another example of a model with absorbing states and critical discontinuous phase transition is the one studied by Lipowski [13]. The present threshold contact process as well as other versions of the threshold contact process [14–16] belong to a class of nonequilibrium models defined on a lattice whose dynamics is governed by a master equation. The nonequilibrium character is evinced by the absence of detailed balance in the stationary state.

In the version of the threshold process that we analyze here, particles are annihilated spontaneously and are created on empty sites that have at least two nearest-neighbor sites occupied by particles. According to these rules the empty lattice is an absorbing state. In a finite lattice this state will eventually be reached for any initial condition if we wait enough time. The situation is different on a infinite lattice. In this case the system may not reach the absorbing state and may remain in the active state characterized by a nonzero density of particles. However, even in an infinite lattice, if we start with a finite number of particles they will eventually disappear even if the creation rate is large. The growth may continue until a maximal rectangular cluster is reached. Beyond this point, the growth is not allowed because the rules forbid the creation of particles on the boundary of a rectangular cluster. This result is in contrast with the ordinary contact process for which a cluster may be grown from a single particle if the creation rate is large enough.

We remark that in one dimension the threshold contact process is trivial in the sense that in the stationary regime it displays only the absorbing state. In one dimension the creation is possible only on empty sites having the two nearest-neighbor sites occupied. As a consequence, a cluster of empty sites with two of more sites will not shrink. It will grow and eventually take the whole lattice.

Our main purpose here is to determine the stationary properties of the threshold model in the thermodynamic limit and show that in this limit the discontinuous phase transition occurs at a definite value of the external parameter, in accordance with the Gibbs phase rule. To this end we study the model on finite lattices of several sizes and obtain the thermodynamic properties by means of numerical extrapolation. To circumvent the peculiarities of the threshold contact process, namely the fall into the absorbing state and the shrinking of finite clusters, we use a boundary condition in which the sites of the border of a finite square lattice are permanently occupied by particles. Using this expedient the creation of particles is always possible even if the lattice is empty because particles can be created in the corners of the lattice.

We have also studied the threshold process by means of an ensemble in which the number of particles is held fixed and by the use of the same boundary conditions. Although the change of ensemble in equilibrium statistical mechanics is well established, this is not the case of nonequilibrium models defined by stochastic rules. However, in some cases it is possible to change from a constant rate ensemble to a constant number of particle ensemble [17–20], as

happens with the present model. As in the case of thermodynamic equilibrium, the ensembles are equivalent only in the thermodynamic limit. Numerical simulations performed on the ensemble with constant particle number give the same properties as the original constant rate ensemble if the size of the system is sufficient large.

The properties of the threshold contact process have also been obtained by means of mean-field approximations, which predicts a discontinuous transition. However, as usually happens with mean-field approaches, the discontinuous transition occurs along a certain range of the parameters, in disagreement with the Gibbs phase rule. The situation here is similar to mean-field approaches used in equilibrium cases in the sense that for a certain range of the parameter-two states can be reached. However, in the equilibrium case the free energy can always be used to decide which of the phases is more stable.

2. Model and mean-field approximation

The threshold contact process studied here is defined as follows. Each site of a square lattice can be in two states: occupied by a particle or empty. At each time step a site is chosen at random. If it is occupied by a particle, then it becomes empty with probability α. If the chosen site is empty, then it is occupied with probability 1 if the number of nearest-neighbor occupied sites is equal to or greater than 2; otherwise it remains empty. In the stationary regime, this model displays a phase transition from an active state with a nonzero density of particles ρ, occurring at small values of α, to an absorbing state characterized by a vanishing density of particles. As we see, at the transition point $\alpha = \alpha_c$, the density of particles, which plays the role of the order parameter, jumps from a nonzero value to a zero value. In the remaining of this section we make use simple and pair mean-field approximations to obtain the properties of the model.

For convenience we associate a stochastic variable η_i with each site i of the lattice that takes the values 0 or 1, according to whether the site is empty or occupied. From the dynamic rules we may establish the evolution equation for the one-site probability $P(\eta_i)$. This equation involves the joint probability of a cluster of five sites, the site i itself and its four nearest neighbors. In the simple mean-field approximation the stochastic variables η_i and η_j are treated as independent so that the probability of the five-site cluster is approximated by the product $P(\eta_i)\prod_j P(\eta_j)$ where j runs over the nearest-neighbor sites of the site i. This leads us to the following evolution equation for the density of particles $\rho = P(1)$:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = 6\rho^2(1-\rho)^3 + 4\rho^3(1-\rho)^2 + \rho^4(1-\rho) - \alpha\rho. \tag{1}$$

The first three terms on the right-hand side correspond to creation of particles by pairs, triplets and quadruplets, respectively, and the last to the spontaneous annihilation. In the stationary state, the density of the active phase is given by

$$\alpha = (1-\rho)\rho(6 - 8\rho + 3\rho^2). \tag{2}$$

In figure 1 we have plotted ρ versus α. For $\alpha > \alpha_0 = 0.815\,423$, the only stable phase is the absorbing state, $\rho = 0$. For $\alpha \leqslant \alpha_0$, there is also an active state, characterized by $\rho \neq 0$, given by the upper branch of the curve defined by (2). Depending on the initial condition one approaches one or the other state.

To obtain the pair mean-field approximations [21–23], in addition to the equation for the one-site probability, we also consider the evolution equation for the two-site probability $P(\eta_i, \eta_j)$ where i and j are the nearest-neighbor sites. This equation also involves the joint probability of a cluster of five sites, either the site i itself and its four nearest neighbors, or the site j itself and its four nearest neighbors. In the pair mean-field approximation the probability

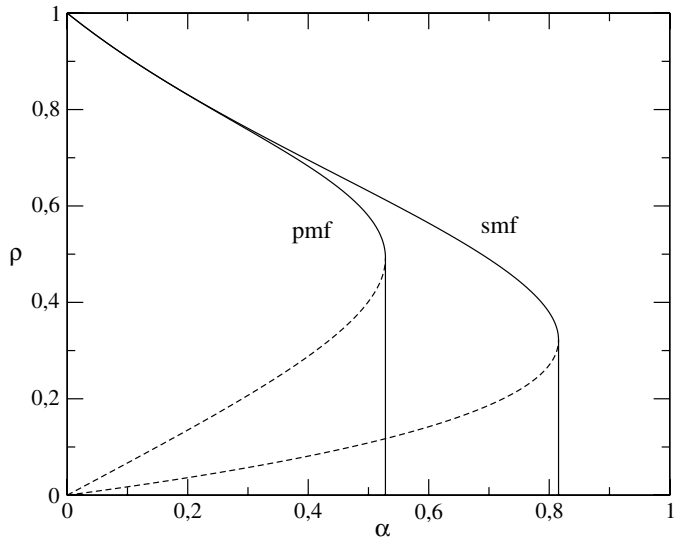

Figure 1. Density of particles ρ versus α obtained by simple mean-field (smf) and pair mean-field (pmf) approximations. Initial conditions starting above the dashed line approach the active state, $\rho \neq 0$. Below this line, the absorbing state, $\rho = 0$, is reached.

of the cluster of five sites is approximated by the product $\prod_k P(\eta_i, \eta_k)/P(\eta_i)$ where k runs over the nearest-neighbor sites of the site i. A similar factorization is used when the central site is the site j. This approximation is written in terms of $P(1) = \rho$, the probability of a site being occupied, and $P(01) = u$, the probability of a pair of nearest-neighbor sites being empty and occupied. The evolution equations for these two variables are

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \frac{3u^4}{(1-\rho)^3} - \frac{8u^3}{(1-\rho)^2} + \frac{6u^2}{1-\rho} - \alpha\rho, \tag{3}$$

$$\frac{\mathrm{d}u}{\mathrm{d}t} = \frac{u^4}{(1-\rho)^3} - \frac{2u^3}{(1-\rho)^2} - 2\alpha u + \alpha\rho. \tag{4}$$

The stationary nonzero solution for ρ is given parametrically by

$$\rho = \frac{6\sigma - 8\sigma^2 + 3\sigma^3}{3 + \sigma - 6\sigma^2 + 3\sigma^3}, \tag{5}$$

and

$$\alpha = \sigma(\sigma - 1)(2\sigma - 3), \tag{6}$$

where $\sigma = u/(1-\rho)$. Again when $\alpha > \alpha_0 = 0.528\,153$ the only phase is the absorbing phase, $\rho = 0$. For $\alpha \leqslant \alpha_0$, there is also an active phase characterized by $\rho \neq 0$. One reaches one or the other phase depending on the initial condition.

When $\alpha \leqslant \alpha_0$, the two phases can be reached depending on the initial conditions. If we start at a point below (above) the dashed line shown in figure 1 we reach the absorbing (active) state. This is in contrast with the equilibrium situation for which the stable phase can be determined by means of the free energy. Actually, as we see by numerical simulations, the overall mean-field picture is not correct although the upper branch of ρ versus α for small values of α gives correct results.

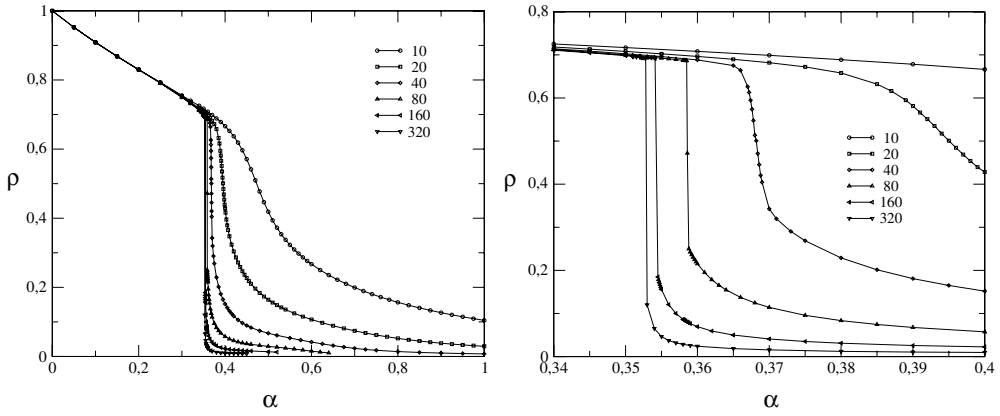

Figure 2. Density of particles ρ versus α obtained by Monte Carlo simulations on a square lattice for several values of L. The plot on the right is an enlargement of the plot on the left.

3. Monte Carlo simulations

The Monte Carlo simulations were performed on a square lattice with $N = L \times L$ sites. We used a boundary condition such that the sites at the border of the lattice are permanently occupied by particles. We start with an initial condition in which the lattice is full of particles. At each time step a site is chosen at random and the time is increased by an amount equal to $1/N$. If the chosen site is occupied by a particle, then it becomes vacant with a probability α. If the chosen site is empty, then a particle is created at the site if at least two nearest-neighbor sites are occupied by particles; otherwise it remains vacant. After discarding the initial configurations the average number of particles n and the variance in the number of particles X are determined from the remaining configurations. The quantities n and X have been determined as a function of α by using a number of Monte Carlo steps ranging from 10^6 to 10^7. Figure 2 shows the density of particles $\rho = n/N$ versus α for several values of the system size L. As one increases L, the density approaches a step function at $\alpha = \alpha_c = 0.352$. Figure 3 shows the variance X versus α for some values of L. This quantity displays a maximum at a certain value of α for each value of L, which approaches α_c as one increases L. The maximum value of the variance diverges as one increases L. For sufficiently large values of L the variance diverges as

$$X \sim \varepsilon^{-2}, \tag{7}$$

where $\varepsilon = \alpha - \alpha_c$, as can be seen in the inset of figure 3.

The value of α_c can also be determined by a time-dependent Monte Carlo simulation, defined as follows. Instead of a finite square lattice we consider an infinite quadrant of a square lattice. If we denote the sites of the square lattice by (i, j) the sites of the quadrant are those with the property $i \geqslant 1$ and $j \geqslant 1$. The boundary condition is such that the sites at the border of the quadrant, $(i, 0)$ and $(0, j)$, are permanently occupied by particles. At each time step a particle among the n particles inside the quadrant is chosen at random and the time t is increased by an amount $1/n$. With probability p the site becomes empty. With the complementary probability $1 - p$ one does the following. One of the four nearest-neighbor sites is chosen at random, say site k. If the site k is empty, then a particle is placed at k with probability $1/n_k$ where n_k is the number of particles in the neighborhood of k, if $n_k \geqslant 2$.

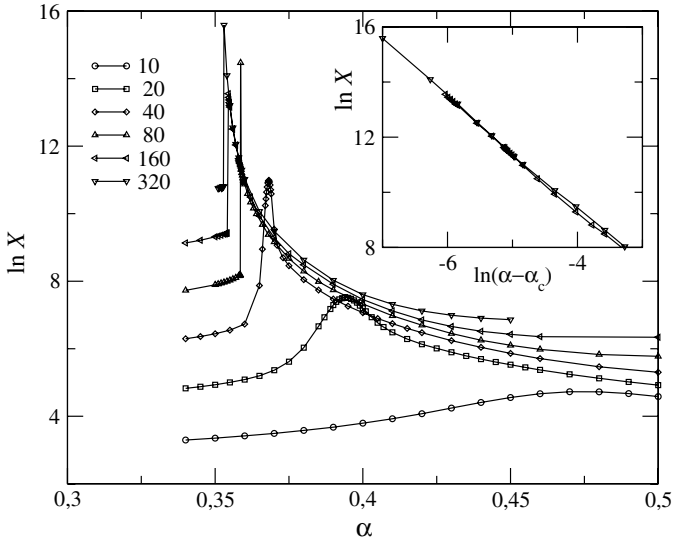

Figure 3. Variance in the number of particles X versus α obtained by Monte Carlo simulations on a square lattice for several values of L. The slope of a straight line fitted to the data points in the inset equals -2.

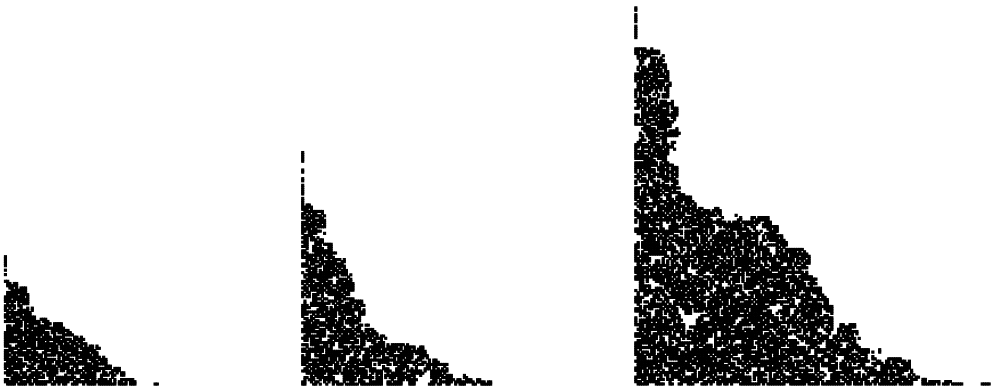

Figure 4. Snapshots taken at $t = 10\,000$, $50\,000$ and $100\,000$ mcs, from left to right, for $\alpha = 0.352$. The number of particles are, respectively, 1061, 1788 and 5585.

If $n_k \leqslant 1$, the site k remains empty. One can readily show that these transition rules are equivalent to the original rules given above as long as $p = \alpha/(4+\alpha)$.

The simulation is performed by starting with a particle at site $(1, 1)$. Figure 4 shows snapshots of the configurations taken at three instants of time obtained for $\alpha = 0.352$. The average number of particles n is determined as a function of time t by repeating the simulation several times. We have used a number of runs ranging from 100 to 1000. The supercritical regime is characterized by an unbounded increase of n with t, that is, $n \to \infty$ as $t \to \infty$. The simulations show an exponential growth of n if t is large enough:

$$n \sim \mathrm{e}^{\gamma t}, \tag{8}$$

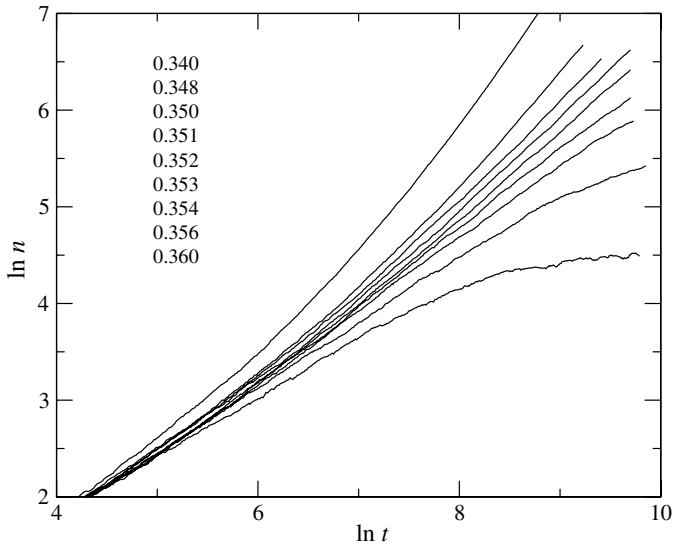

Figure 5. Number of particles n as a function of time t for several values of α.

thus diverging when $t \to \infty$. In the subcritical regime the average number of particles n is bounded and reaches a finite value when $t \to \infty$ so that $\rho = 0$ because the system is infinite. The change from one behavior to the other defines the transition point. This property is used to determine the transition point from the log–log plot of n versus t as shown in figure 5. From this plot we estimate the transition point to be $\alpha_c = 0.352(1)$. If we assume the algebraic behavior

$$n \sim t^{\zeta}, \tag{9}$$

at the critical point, we obtain from the slope of the log–log plot in figure 5 the value $\zeta = 0.93(3)$. However, one cannot reject other types of behaviors. For instance, the numerical results are also consistent with the behavior

$$n \sim \frac{t}{\ln t}, \tag{10}$$

which can be understood as the algebraic behavior (9) with an exponent $\zeta = 1$ plus logarithm corrections.

The transition point obtained by the time-dependent Monte Carlo simulations is in agreement with the abrupt decay of ρ observed in the plot of ρ versus α shown in figure 2. Indeed, the inflexion points of ρ versus α occur at $\alpha = 0.473$, 0.392, 0.368, 0.3586, 0.3542 and 0.3529 for $L = 10$, 20, 40, 80, 160 and 320, respectively. A quadratic extrapolation of α in the variable $1/L$ gives $\alpha_c = 0.3515(10)$.

4. Conservative ensemble

In this section we analyze the threshold model by means of an ensemble in which the number of particles n is held constant. The rule are as follows. At each time step a site is chosen at random, say site i. If it is empty and have at least two nearest-neighbor sites occupied, then another site of the lattice is chosen at random, say site j. If site j is occupied, then the particle at this site jumps to the site i. This procedure obviously conserves the number of particles. It

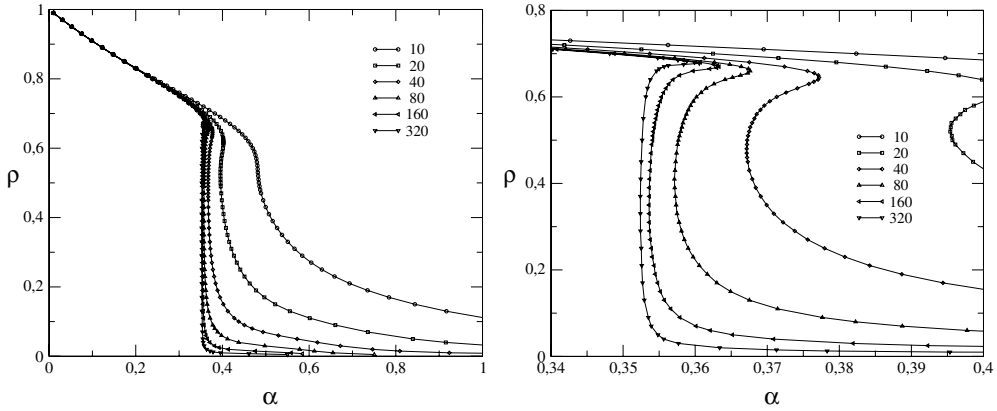

Figure 6. Density of particles ρ versus α obtained by Monte Carlo simulations on a square lattice for several values of L by using the constant particle ensemble. The plot on the right is an enlargement of the plot on the left.

can be shown [17–20] that this rule gives properties that are identical, in the thermodynamic limit, to the original rules of the model, which we call constant rate ensemble. In the constant particle number ensemble, the number of particles n, or the density of particles $\rho = n/N$, works as a parameter and the probability of the transition α becomes a function of ρ since in this ensemble the quantity α is not given *a priori*. If we define an active site as an empty site with at least two nearest-neighbor sites occupied by particles, then it can be shown [17–20] that the quantity α is related to the number of active sites n_{ac} by

$$\alpha = \frac{n_{\mathrm{ac}}}{n}. \tag{11}$$

Equation (11) allows us to determine α in simulations performed by the use of the rules of the constant particle number ensemble.

We have performed simulations on a square lattice with $N = L \times L$ sites with the same boundary conditions used previously, that is, the border of the lattice is permanently occupied by particles. For each density of particles we have determined α by using equation (11) and a number of Monte Carlo steps ranging from 10^6 to 10^7. Figure 6 shows the results obtained for several values of the system size L. Increasing L the curve ρ versus α approaches a step function at the same value α_c obtained by the constant rate ensemble.

To check that the curves of density versus α approach a step function we proceed as follows. For each value of ρ we plot α as a function of $1/L$ as shown in figure 7. All curves shown is this figure approach the same value as one increases L. Extrapolations obtained by a quadratic fitting give the same value of α_c, within the statistical errors, namely $\alpha_c = 0.3516(5)$, in excellent agreement with the constant rate ensemble result found previously.

5. Discussion and conclusion

We have shown by numerical simulations that the discontinuous phase transition occurring in the threshold contact process occurs at a definite point of the parameter α in accordance with the Gibbs phase rule. This has been accomplished by the use of two distinct ensembles and by an appropriate boundary condition that circumvent some peculiarities of the model, namely the fall into the absorbing state and the shrinking of finite clusters. The two ensembles give

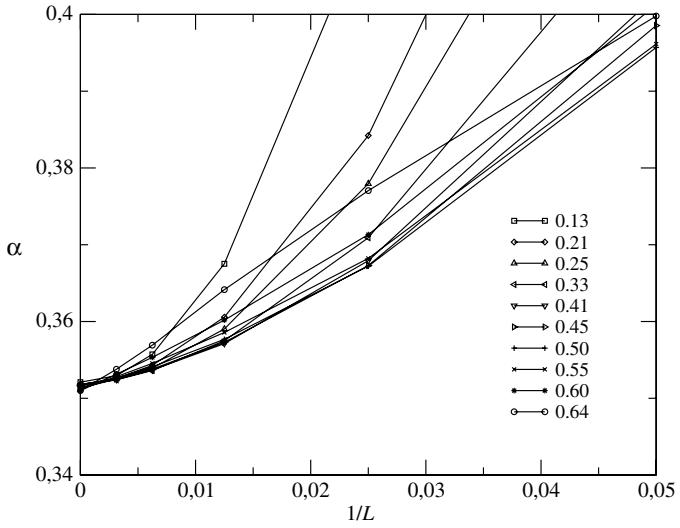

Figure 7. Plot of α as a function of the inverse of the system size L for several values of the density of particles ρ. A quadratic extrapolation in the variable $1/L$ gives results for α_c within the interval $0.3511 \leqslant \alpha_c \leqslant 0.3521$.

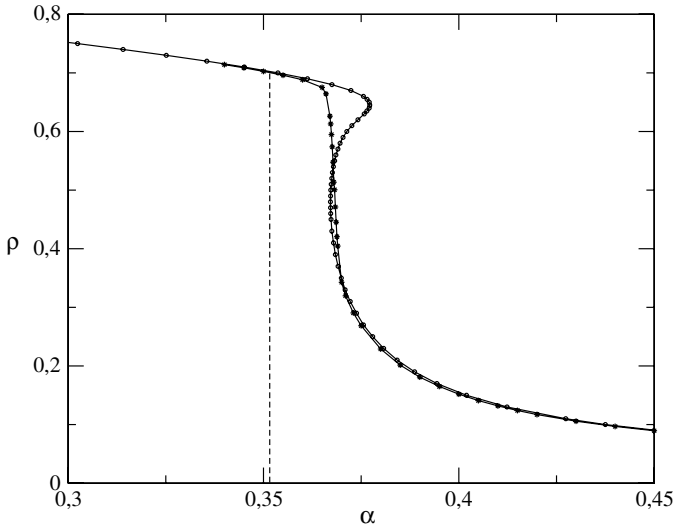

Figure 8. Density ρ versus α for the linear system size $L = 40$ obtained from the constant rate ensemble (stars) and constant particle number ensemble (circles). The vertical dashed line indicates the transition point $\alpha_c = 0.3516$.

the same properties in the thermodynamic limit, obtained here by numerical extrapolation of finite systems. It is worth comparing the results coming from the two ensembles as shown in figure 8 where the density ρ is plotted against α for the case of a lattice of linear size $L = 40$. One observes that the curves are very close to one another except around the loop appearing in the constant particle number ensemble. However, the loop disappears in the

thermodynamic limit and both curves become identical. We remark that the loop should not be confused with a van der Waals loop [24] and that it is not a peculiarity of nonequilibrium models. It has been observed previously in equilibrium models [24] in which case it is due to the surface tension contribution to the thermodynamic potentials. We remark that although hysteresis is usually expected to be present around a first order, no hysteresis has been found in simulations performed by using the constant rate ensemble. However, the loop observed in simulations performed by means of the constant particle ensemble could be identified as hysteresis although it disappears in the thermodynamic limit giving rise to a tie line.

In equilibrium systems, discontinuous phase transitions usually are not critical in the sense that the spatial and time correlation lengths are finite. The correlations diverge when the two or more phases become identical, at the critical point. Nevertheless, discontinuous phase transition with divergence of the correlation length is not impossible and has been called critical first-order phase transition [25]. Critical behavior at a discontinuous phase transition may also occur in nonequilibrium systems as is the case of the class of models belonging to the voter model [26, 27] or to the compact direct percolation as seems to be the case of the present threshold process. The critical behavior in the threshold model studied here can be seen from the behavior of ρ as a function of t, as given in equations (9) or (10), and also from the behavior or the variance X as a function of α, as given in equation (7).

If we wish to describe the critical behavior of the critical first-order transition by a set of critical exponents, then the exponent related to the order parameter should vanish, that is,

$$\beta = 0. \tag{12}$$

The relation $2\beta + \gamma = \mathrm{d}\nu_\perp$ between β and the exponents γ and $\nu_\perp$, related to the variance per site $\chi = X/L^d$ and to spatial correlation length, is therefore replaced by

$$\gamma = \mathrm{d}\nu_\perp. \tag{13}$$

Assuming the following behavior for the variance,

$$X \sim \varepsilon^{-(\gamma+\mathrm{d}\nu_\perp)}, \tag{14}$$

and taking into account the result (7), it follows that $\gamma + \mathrm{d}\nu_\perp = 2$ which combined with equation (13) leads us to the following results for the exponents γ and $\nu_\perp$:

$$\gamma = 1, \qquad \text{and} \qquad \nu_\perp = 1/2, \tag{15}$$

thus supporting the compact direct percolation critical behavior of the first-order phase transition occurring in the present two-dimensional threshold process. Since the upper critical dimension of the compact direct percolation is $d = 2$ one expects logarithm corrections in the critical behavior of some quantities. If this is the case, then the correct behavior of n versus t is given by (9) instead of (10).

Acknowledgments

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