Nonequilibrium Model for the Contact Process in an Ensemble of Constant Particle Number

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We introduce and analyze numerically a nonequilibrium model with a conserved dynamics which is a realization of the contact process in an ensemble of constant particle number. The model possesses just one process in which particles jump around landing only on empty sites next to an existing particle. Particles are not allowed to land on a vacant site surrounded by empty sites. In contrast with the ordinary contact process, the present model does not have an absorbing state. In spite of lacking an absorbing state, the model displays properties that, in the thermodynamic limit, are identical to those of the ordinary contact process.

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According to equilibrium statistical mechanics, if distinct Gibbs ensembles are used to calculate a thermodynamic property of a system in equilibrium, the results will be the same [1–3]. In the thermodynamic limit, the Gibbs ensembles are equivalent, even for a system that exhibits a phase transition. A standard procedure exists for passing from one ensemble to another, the main feature being that a quantity that functions as a parameter (a conserved quantity) in one ensemble becomes a fluctuating variable in the other. For nonequilibrium systems, on the other hand, there is no general procedure. However, the possibility of using distinct ensembles in nonequilibrium models has been shown by Ziff and Brosilow [4] when they employed a constant coverage ensemble to analyze an irreversible surface-reaction model originally defined in a constant rate ensemble.

In this Letter, we introduce and analyze a nonequilibrium model with a conserved dynamics that shall be identified as the contact process in an ensemble of constant particle number. As is well known, the ordinary contact process does not conserve the number of particles, which is a fluctuating quantity. As a consequence of the conservation of particles, the present model does not have an absorbing state, in contrast with the ordinary contact process. In spite of lacking an absorbing state, the model displays properties that, in the thermodynamic limit, are identical to those of the ordinary contact process, including universal as well as nonuniversal quantities.

The ordinary contact process, proposed by Harris [5], is the simplest nonequilibrium model displaying a phase transition and critical behavior [6–18]. Because of its relevance in understanding the active-absorbing transition it has been regarded as the "Ising model" of absorbing state transitions [18]. It exhibits a continuous phase transition from an active state to an absorbing state even in one dimension and belongs to the universality class of directed percolation [19,20].

The ordinary contact process is composed of two subprocesses: a catalytic creation and a spontaneous annihilation of particles. In the basic ordinary contact process [9,16,18], particles are created on the empty sites of a regular lattice with a rate $\lambda n_{\rm nn}/z$, where $n_{\rm nn}$ is the number of occupied nearest neighbors and z the lattice coordination number. Particles are annihilated spontaneously with rate 1. Here, we use a definition in which the creation rate is fixed to be $n_{\rm nn}/z$ so that the annihilation rate becomes $\alpha = 1/\lambda$.

Empty sites surrounded by at least one particle, which we call active empty sites, play an important role in the contact process since particles are created only on those sites. A quantity that measures the number of such sites is the effective number of active empty sites $n_{\rm ac}$ defined as

$$n_{\rm ac} = \sum_i \frac{n_{\rm nn}^{(i)}}{z}, \tag{1}$$

where the sum is over all active empty sites and $n_{\rm nn}^{(i)}$ is the number of occupied nearest neighbors of site i. The catalytic creation implies that the increase in the mean number of particles $\langle n_{\rm p}\rangle$ per unit time equals the mean effective number of active sites $\langle n_{\rm ac}\rangle$. Since the decrease in the mean number of particles per unit time, due to the spontaneous annihilation, equals $\alpha\langle n_{\rm p}\rangle$, the stationary condition gives

$$\langle n_{\rm ac}\rangle = \alpha\langle n_{\rm p}\rangle. \tag{2}$$

The contact process in an ensemble of constant particle number is defined as follows. An empty site becomes occupied in a way similar to the catalytic creation. But instead of creating a new particle (and thus increasing the number of particles), one particle of the system itself, chosen at random, leaves its place and jumps to the empty site. Thus, both the processes of creation and annihilation of particles of the ordinary contact process are replaced by just a jumping process. However, this is not an unrestricted jumping because particles are not allowed to jump to a vacant site surrounded by empty sites; at least one neighbor site must be occupied. The model conserves the number of particles n and will be called *conserved contact process* (CCP). It has no parameter, except, of course, the number of particles n.

The mean effective number of active sites per particle, denoted by $\overline{\alpha}$, is given by

$$\overline{\alpha} = \frac{\langle n_{\rm ac} \rangle_n}{n}, \tag{3}$$

where $\langle \cdots \rangle_n$ denotes an average in the ensemble with a constant particle number. Evidence for the equivalence between the n-constant and α-constant ensembles will be given by showing that, for sufficiently large systems, $\overline{\alpha} = \alpha$ whenever $n = \langle n_{\rm p} \rangle$. In particular, we will show that the critical value $\overline{\alpha}_c$ of the CCP coincides with the critical value α_c of the ordinary contact process. Moreover we show that the critical exponent β and the fractal dimension d_F at the critical point are the same for both models.

Because of the fact that the dynamics conserve the number of particles, the CCP does not have an absorbing state, with the exception of the trivial case $n = 0$. This conservation law allows us to carry out numerical simulations without the danger of falling into the absorbing state as happens in the ordinary contact process. Thus, the quasistationary states [18] observed in the ordinary contact process, in the subcritical regime, become genuine stationary states in the CCP. We have simulated the CCP on a one-dimensional lattice with N sites. For a given number of particles n the mean effective number of active sites per particle $\overline{\alpha}$ was obtained through (3). The results are shown in Fig. 1 where $\overline{\alpha}$ is plotted against the particle density $\rho = n/N$ for values of N ranging from 10 to 10^4.

The graph of Fig. 1 becomes sharper as one increases the system size N developing a singularity at $\rho = 0$ in the limit $N \to \infty$. The value of $\overline{\alpha}$ at the singularity point defines $\overline{\alpha}_c$. In the thermodynamic limit, states with nonzero densities are such that $\overline{\alpha} < \overline{\alpha}_c$, that is, the effective number of active sites per particle is always smaller than $\overline{\alpha}_c$. Numerically, we estimate $\overline{\alpha}_c$ by studying the properties of the model in the subcritical regime ($\overline{\alpha} > \overline{\alpha}_c$), which will be done further on. Using the value $\overline{\alpha}_c = 0.303\,23$, given below, we show, in Fig. 2, a log-log plot of $\varepsilon = \overline{\alpha} - \overline{\alpha}_c$ versus ρ for several values of the system size N. The critical exponent β is estimated as the inverse of the slope of the tangent straight line fitted to the data points since β is defined through $\rho \sim |\varepsilon|^{\beta}$. The best fit gives $\beta = 0.277(1)$ which is in agreement with the value $\beta = 0.276\,49(4)$ for the basic ordinary contact process in one dimension [17].

We have also simulated the ordinary contact process in one dimension to compare it with the CCP. For a given value of the parameter α we have calculated the mean number of particles $\langle n_{\rm p} \rangle$. The first and second columns of Table I show α and $\overline{\rho} = \langle n_{\rm p} \rangle / N$ for the basic ordinary contact process with $N = 10^4$ sites. The third and fourth columns show $\rho = n/N$ and $\overline{\alpha}$ for the CCP. We have chosen the values of n to be the same as that of $\langle n_{\rm p} \rangle$. The last column, which gives $\overline{\alpha}$ for the CCP, is in agreement with the first column, which gives α for the ordinary contact process. The small discrepancies between $\overline{\alpha}$ and α are expected since the system is not infinite, although large.

The critical value $\overline{\alpha}_c$ of the mean effective number of active sites per particle in the CCP can be evaluated by carrying out a simulation of an infinite system with a finite number of particles. Since n is finite and the system is infinite, the density vanishes, $\rho = 0$. No matter how large n is, the system remains in the subcritical regime. This is indeed what happens as can be seen in Table II which shows the value of the mean effective number of active sites $\overline{\alpha}$ for several values of the number of particles n. When $n \to \infty$ the quantity $\overline{\alpha}$ accumulates into the critical value $\overline{\alpha}_c$. A linear extrapolation gives $\overline{\alpha}_c = 0.303\,23(4)$ which agrees very well with the critical value of $\alpha_c = 0.303\,228(2)$ for the basic ordinary contact process [15].

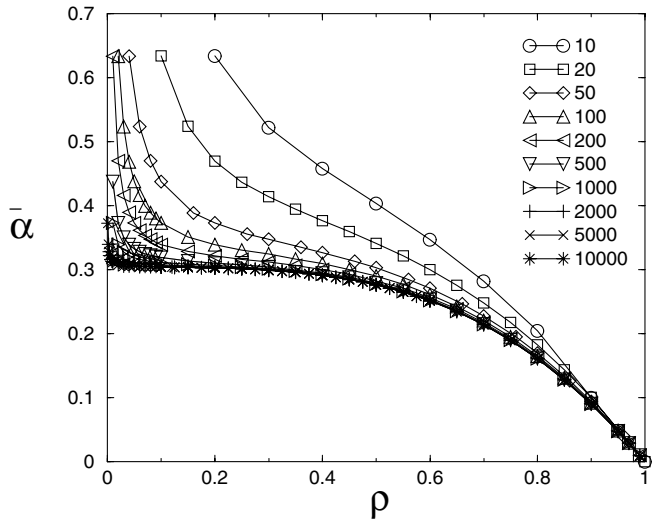

FIG. 1. The effective number of active sites per particle $\overline{\alpha}$ as a function of the particle density ρ in the one-dimensional CCP for several values of the number of sites N.

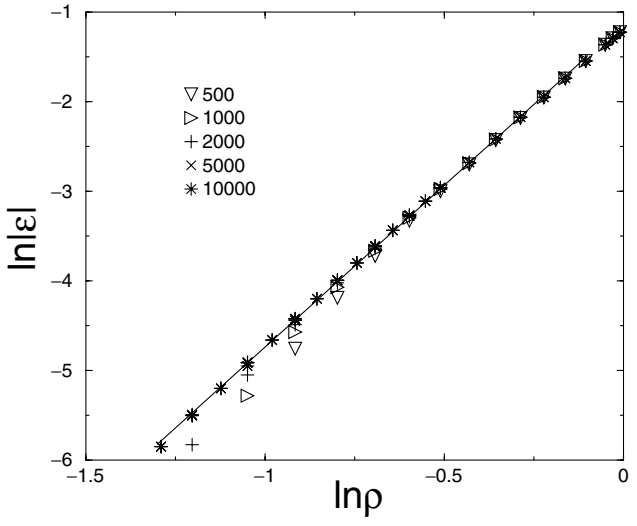

FIG. 2. A log-log plot of $\varepsilon = \overline{\alpha} - \overline{\alpha}_c$ versus ρ for the one-dimensional CCP for several values of the system size N. The slope of a tangent straight line fitted to the data points equals 3.61(1). The reciprocal of the slope gives $\beta = 0.277(1)$.

TABLE I. Results of the simulation of the one-dimensional basic ordinary contact process (first and second columns) and the one-dimensional CCP (third and fourth columns) for $N = 10\,000$.

α	$\overline{\rho}$	ρ	$\overline{\alpha}$
0.1	0.8874(1)	0.8874	0.1000(1)
0.15	0.8170(1)	0.8170	0.1501(1)
0.2	0.7289(2)	0.7289	0.2002(2)
0.25	0.6033(8)	0.6033	0.2503(2)
0.27	0.528(1)	0.528	0.2704(3)
0.28	0.477(2)	0.477	0.2804(2)
0.29	0.406(3)	0.406	0.2905(3)
0.295	0.354(5)	0.354	0.2956(4)
0.30	0.270(5)	0.270	0.3007(4)

For an infinite system with n particles, let us denote by $g(r, n)$ the pair correlation function, that is, the probability of finding a particle at position r given a particle at the origin. We assume that $g(r, n)$ obeys the following scaling relation:

$$g(r, n) = r^{-\mu} g^* \left(\frac{r}{n^\theta} \right). \tag{4}$$

Since the integral of $g(r, n)$ gives n, it follows that μ and θ are related by $\mu = d - 1/\theta$. We have calculated the pair correlation as a function of r in one dimension for several values of n ranging from $n = 2$ to $n = 1000$. Figure 3 gives a scaling plot of the data of pair correlation function according to (4). The best data collapse gives $\theta = 1.34(1)$.

As long as n is finite the pair correlation function $g(r, n)$ decays exponentially as $\exp -r/\xi$, for large values of r. From the scaling relation (4) it follows that the correlation length ξ behaves asymptotically as

$$\xi \sim n^\theta, \tag{5}$$

and diverges when $n \to \infty (\overline{\alpha} \to \overline{\alpha}_c)$. In this limit, the system loses its natural length scale; the correlation function behaves then algebraically as

$$g(r) \sim r^{-\mu}, \tag{6}$$

TABLE II. Results of the simulation of the one-dimensional CCP for an infinite system. The last row is a linear extrapolation for $n \to \infty$.

n	$\overline{\alpha}$
2	0.633 98(1)
5	0.437 48(3)
10	0.372 73(3)
20	0.339 40(1)
50	0.318 47(3)
100	0.311 15(1)
200	0.307 31(3)
500	0.304 93(2)
1000	0.304 08(1)
∞	0.303 23(4)

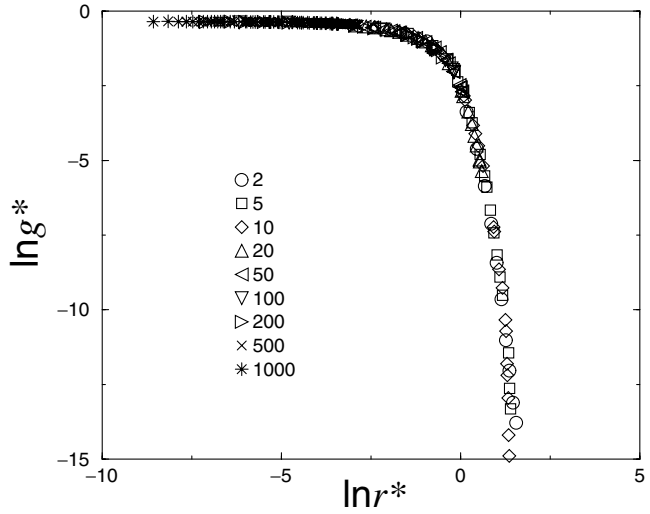

FIG. 3. Scaling plot of pair correlation function $g(r, n)$ for the one-dimensional CCP for several values of n where $g^* = g r^{1-1/\theta}$ and $r^* = r n^{-\theta}$. The best data collapse gives $\theta = 1.34(1)$.

and the system becomes a fractal, as can be seen in Fig. 4. The fractal dimension d_F is defined through $m(r) \sim r^{d_F}$, where

$$m(r) = \int_{r' \le r} g(r')\, d^d r', \tag{7}$$

which measures the quantity of particles inside a sphere of radius r. From (6) it follows that $m(r) \sim r^{d-\mu}$ so that $d_F = d - \mu = 1/\theta$. To make connection with results coming from the ordinary contact process we remember that at the critical point the ordinary contact process generates also fractal clusters [14]. According to Grassberger [11], the fractal dimension is related to the survival probability exponent δ, the mean number of

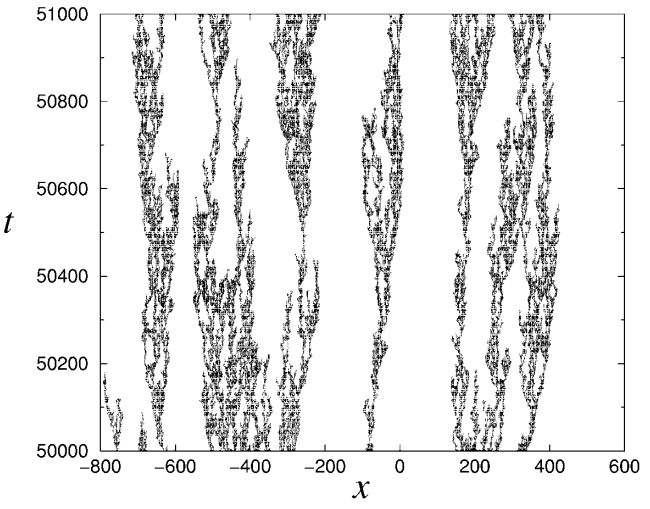

FIG. 4. Typical trial for the one-dimensional CCP with $n = 200$ particles. Each dot represents the position x of a particle at time t. A unit of time corresponds to n particle jumps. At the beginning of the process, all particles are close together. The system is large enough so that the particles do not reach the boundaries.

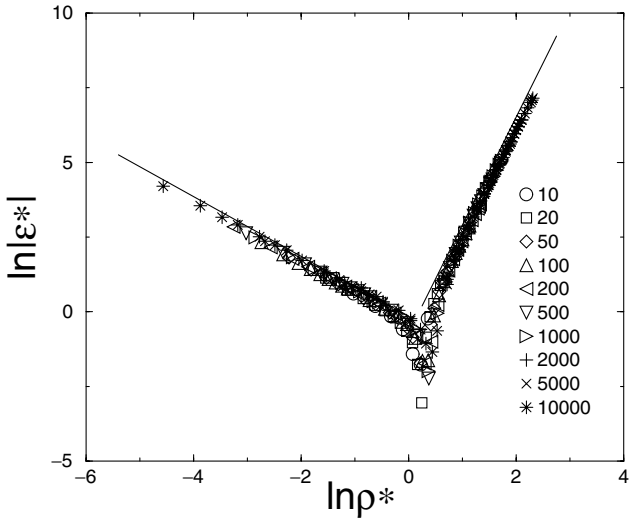

FIG. 5. Scaling plot of the data from Fig. 1 where $\rho^* = L^{\beta/\nu}\rho$ and $\varepsilon^* = L^{1/\nu}\varepsilon$, in the supercritical regime (right branch) and $\rho^* = L^{1-1/\theta}\rho$ and $\varepsilon^* = L^{1/\theta}\varepsilon$, in the subcritical regime (left branch). The data collapse was obtained using the values $\theta = 1.34$, $\beta = 0.277$, and $\nu = 1.097$ [17]. The slopes of the straight lines are 3.61 and -1.

particles exponent η, and the dynamic exponent z by $d_F = 2(\eta + \delta)/z$. Using the numerical results for these exponents [17], we get $d_F = 0.7479(1)$ so that $1/d_F = 1.3370(2)$ which agrees very well with our result $\theta = 1.34(1)$.

A finite size scaling can be set up for the density of particles. In analogy to what has been established for the ordinary contact process, we write

$$\rho = L^{-\beta/\nu} f(\varepsilon L^{1/\nu}), \tag{8}$$

where L is the linear size of the system, $\varepsilon = \overline{\alpha} - \overline{\alpha}_c$ and ν is the exponent related to the correlation length, that is, $\xi \sim |\varepsilon|^{-\nu}$. However, in the subcritical regime, $\varepsilon \sim n^{-1}$, as can be inferred from the results of Table II, which combined with the result (5) gives $\xi \sim |\varepsilon|^{-\theta}$. On the other hand, from (5) it follows that n should scale as $L^{1/\theta}$ so that ρ scales as $L^{-d+1/\theta}$. These results allow us to write the following scaling relation:

$$\rho = L^{-d+1/\theta} f(\varepsilon L^{1/\theta}) \tag{9}$$

which replaces (8) in the subcritical regime. At $\varepsilon = 0$ the consistency between the two scaling forms allows us to conclude that $\beta/\nu = d - 1/\theta$ or yet $\beta/\nu = d - d_F$. In Fig. 5 we show the scaling plot of ε versus ρ, employing the scaling forms (8) and (9).

The CCP model has a relationship with a model treated by Bröker and Grassberger [21] in the sense that these two models are conserved versions of models belonging to the directed percolation universality class, namely, the contact process and the directed percolation model, respectively. In the Bröker and Grassberger model, however, the conservation of particles is achieved in a global way by removing the excess of particles from the system. Creation and annihilation are then not spatially correlated.

An interesting feature of the CCP is that, in the subcritical regime, the increase in the number of particles makes the system approach criticality, as can be seen in Table II. As long as the system is infinite it becomes critical when the number of particles increases without bounds. In this sense it has similarities with self-organized criticality, within the interpretation advanced by Dickman and others [22], in which the successive addition of particles into the system drives it to criticality. On the other had, the models studied by Dickman *et al.* [22] and also by Rossi *et al.* [23] have infinitely many absorbing states, in contrast with the contact process, that has just one, and the CCP, that has none, placing them in a universality class [23] distinct from directed percolation.

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