Two versions of the threshold contact model in two dimensions

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A R T I C L E   I N F O

A B S T R A C T

Two versions of the threshold contact process – ordinary and conservative – are studied on a square lattice. In the first, particles are created on active sites, those having at least two nearest neighbor sites occupied, and are annihilated spontaneously. In the conservative version, a particle jumps from its site to an active site. Mean-field analysis suggests the existence of a first-order phase transition, which is confirmed by Monte Carlo simulations. In the thermodynamic limit, the two versions are found to give the same results.

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1. Introduction

The contact process [1] is recognized as one of the simplest models in nonequilibrium statistical mechanics which presents a phase transition. It is characterized by the competition between a spontaneous particle annihilation process and a catalytic particle creation process. The creation occurs on sites having at least one nearest neighbor site occupied by a particle. In a finite lattice, the number of particles inevitably falls to zero, if we wait long enough, and the empty lattice constitutes an absorbing state. In an infinite lattice, however, an active state may be sustained if the annihilation rate α is smaller than a certain critical value α_c. The phase transition is continuous: the particle density ρ decays continuously to zero as α increases towards its critical value α_c. Many other models also present a continuous phase transition to a nondegenerate absorbing state and similar sets of critical exponents, such as Schlögl's first and second models for autocatalytic chemical reactions [2–4], and the directed percolation models [5], forming the DP universality class.

A possible variation of the contact process is the threshold contact process [6]. In this model, the spontaneous annihilation process competes with a creation process that happens in more restrictive conditions: there must have at least n, $n > 1$, occupied sites near an empty site. We can ask if the model still presents an active stationary state and, if the answer is yes, if the phase transition still is continuous.

It is easy to show that there is no active stationary state in one dimension if $n \geq 2$. Indeed, if a sequence of at least two empty sites is formed, it is impossible to reintroduce particles in them.

In two or more dimensions, each site has more nearest neighbors, and the creation process is less restrictive. Liu, Guo, and Evans [7–9], studying a version of the threshold contact process, have shown that the transition phase is no longer continuous, and that it does not occur for a specific value of α, but it does depend on the boundary and initial conditions. They also have studied how the existence of a initial spatial pattern can affect the phase transition.

Here, we study a threshold contact model on a square lattice in which a particle is created on a site having at least two nearest neighbor sites occupied, as shown in Fig. 1. In a previous article [10], we have shown that, for a similar threshold contact model, the characterization of the active phase may depend on the boundary conditions. If this model is simulated using periodic boundary conditions, the active cluster cannot grow and the active phase cannot be reached. This problem was avoided by changing the boundary condition, surrounding the lattice by permanent particles. In the present case, we used the same procedure, which leads to a well-defined transition point α_c.

Another issue that we consider here is the possibility of defining nonequilibrium models in distinct ensembles. This technique is traditionally used in equilibrium statistical mechanics, where the ensemble change implies a change in the thermodynamic variables. A variable that functions as a parameter in one ensemble becomes a stochastic variable in the other ensemble. It has been shown [11–14] that it is possible to define alternative ensembles for nonequilibrium models, like the contact process: if the original model is characterized by fixed rate and varying density, the alternative model is characterized by fixed density and varying rate, and both models show similar behavior as the lattice size increases and become identical in the thermodynamic limit. Here, we show how to define the threshold contact process in a conservative ensemble. Monte Carlo simulations are performed in both ensembles.

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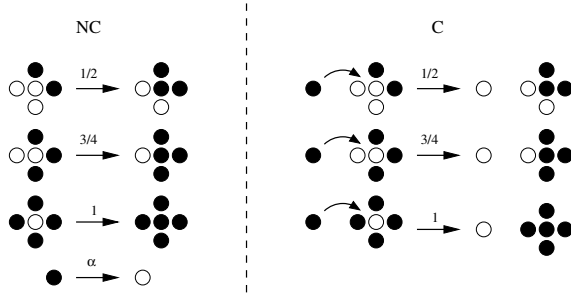*E-mail address:* efsilva@if.usp.br (E.F. da Silva).

Fig. 1. Transition rates for the NC model (left) and the C model (right). White circles are empty sites and black circles are occupied sites.

2. NC model and C model – definitions

We define two versions of the threshold contact model, designated as NC (nonconservative ensemble) and C (conservative ensemble). Both models are staged in a square lattice of length L. Each site can be occupied by a particle or can be empty, and a configuration of the lattice is given as the set of L^2 variables $\{\eta_i\}$, $\eta_i = 0, 1$. The number of particles N in a configuration is given by $N = \sum_{i=1}^{L^2} \eta_i$.

For the NC model, after setting a random configuration as the initial state, the system evolves by losing (annihilation process) or gaining (creation process) particles. The annihilation process is spontaneous and occurs with rate α. The creation process is catalytic: an empty site gains a particle with rate $n/4$, where n is the number of nearest occupied sites, and $n \geq 2$. There is no particle creation if $n \leq 1$. An empty site with $n \geq 2$ is called an empty active site. Process rates for the NC model are shown in Fig. 1.

In a finite lattice, the NC model presents only one real stationary state: the absorbing state, which contains no particles. If we take as initial condition a state with any number of particles, and the system evolves for a long time, eventually the fluctuation in the number of particles can be sufficiently large that the system reaches the state with no particles and freezes. An active state is observed if α is sufficiently small, since in this situation the mean time needed for a fluctuation that carries the system to the absorbing state is exponentially big. In an infinite lattice, the metastable active state becomes a real active state, with a finite mean particle density $\langle \rho \rangle = \langle N \rangle / L^2$, and there is a phase transition to the absorbing state at $\alpha = \alpha_c$.

In Sections 3 and 4, it will be shown that the phase transition is discontinuous for the NC model, separating regions with high and low particle density. As the control parameter is the annihilation rate α, we cannot access states with ρ between those two values. Following [11], we can define a conservative version of the NC model, whose control parameter is ρ, by tuning the rates of the creation and annihilation processes so that the number of particles remains constant, and then substitute the two processes for a jumping process.

For the C model, first we set a random configuration with a selected value of ρ as the initial state. At each time step, two sites are randomly selected: if the first site contains a particle and the second site is an empty active site, the particle jumps from the first site to the second site with rate $n/4$. The rates associated to each possible move are shown in Fig. 1. We define the parameter α^* as the ratio between the density of active empty sites and the particle density.

The C model cannot present an absorbing state, because the number of particles is constant. However, if we take the limit $L \to \infty$, keeping N constant, the density vanishes, and we may identify this state with the absorbing state of the NC model. In the limit

$L \to \infty$, the C model also presents a phase transition from a state with $\rho = 0$ to a state with $\rho \geq \rho_c \neq 0$, identified with the active state of the NC model. For $0 < \rho < \rho_c$, the active and absorbing phases are both present, and α^* is approximately constant.

Comparing the two models in the thermodynamical limit, we see that the C and NC models are realizations of the same dynamics in different ensembles. A proof of this affirmation can be built following the steps used by Hilhorst and van Wijland in [12] to show the equivalence between the contact process and the conservative contact process.

3. Mean-field analysis

From the rules stated above, we set up equations for the time evolution of the density of particles $\rho = P(1)$ and the density of empty–occupied pairs of sites $\sigma = P(01)$. They are

$$\frac{d\rho}{dt} = 2P(01100) + P(01010) \\ + 3P(01110) + P(01111) - \alpha P(1) \tag{1}$$

$$\frac{d\sigma}{dt} = -6P(01110) - 4P(01111) + 4\alpha P(11) - 4\alpha P(01). \tag{2}$$

The symbol $P(\eta_0, \eta_1, \eta_2, \eta_3, \eta_4)$ denotes the probability of finding a site in the state η_0, and its nearest neighbors in the states η_1, η_2, η_3, and η_4, in directions East, North, West, and South, respectively.

We use two levels of mean-field approximations. In the simple mean field, we use the approximation

$$P(\eta_0, \eta_1, \eta_2, \eta_3, \eta_4) = P(\eta_0)P(\eta_1)P(\eta_2)P(\eta_3)P(\eta_4). \tag{3}$$

In this case, it suffices to use the Eq. (1), which becomes

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

In the stationary state, $d\rho/dt = 0$. The trivial solution is $\rho = 0$ (the absorbing state), and the other is $\rho \neq 0$ (the active state), given by

$$\alpha = 3\rho - 6\rho^2 + 4\rho^3 - \rho^4. \tag{5}$$

For $\alpha < \alpha_c$, there are two possible solutions. Only the largest value is stable, describing a system whose density is 1 when $\alpha = 0$, and decreases when α increases, until it jumps from ρ_c to 0 when $\alpha = \alpha_c$, as seen in Fig. 2, where $\alpha_c = 0.47247$ and $\rho_c = 0.37004$.

A better solution can be obtained by using the pair mean-field approximation. In this case, we use

$$P(\eta_0, \eta_1, \eta_2, \eta_3, \eta_4) = \frac{P(\eta_0, \eta_1)P(\eta_0, \eta_2)P(\eta_0, \eta_3)P(\eta_0, \eta_4)}{P(\eta_0)}. \tag{6}$$

In this approximation, n-site probabilities ($n > 2$) are rewritten as products of two-site and one-site probabilities. Let us take $y = P(01)/P(0) = \sigma/(1-\rho)$. At the stationary state, and using the pair mean-field approximation, Eqs. (1) and (2) take the form

$$\frac{d\rho}{dt} = (1 - \rho)y^2 \left[3(1 - y)^2 + 3y(1 - y) + y^2\right] - \alpha\rho = 0 \tag{7}$$

$$\frac{d\sigma}{dt} = -(1 - \rho)y^3 \left[6(1 - y) + 4y\right] + 4\alpha \left[\rho - 2(1 - \rho)y\right] = 0. \tag{8}$$

One solution is $\rho = y = 0$ (absorbing state). The other solution (active state) is given by the set of equations

$$\alpha = \frac{3y}{4}(2 - 3y + y^2) \tag{9}$$

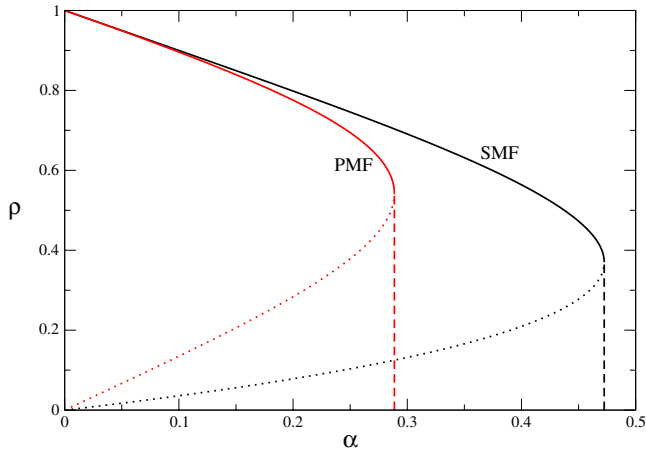$$\rho = \frac{4y(3 - 3y + y^2)}{6 + 3y - 9y^2 + 4y^3}. \tag{10}$$

Fig. 2. Particle density ρ as a function of annihilation rate α, from simple mean-field (SMF) and pair mean-field (PMF) approximations. Full lines represent the active state, dashed lines the transition to an absorbing state, and dotted lines the unstable section.
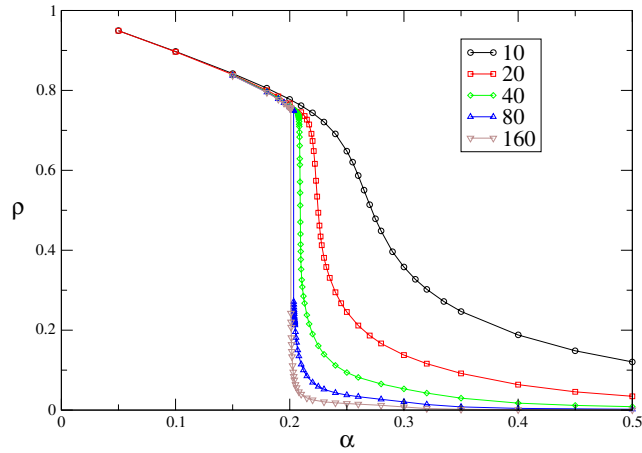

Fig. 3. Density ρ as a function of α from numerical simulations of the NC model for several values of the linear system size L.

From this solution, we get ρ versus α, as shown in Fig. 2. The critical values in the pair mean-field approximation are

$$\alpha_c = \frac{1}{2\sqrt{3}} = 0.28868 \tag{11}$$

$$\rho_c = \frac{4}{65}\left(14 - 3\sqrt{3}\right) = 0.54178. \tag{12}$$

Again, we have a jump in density describing a first-order phase transition.

4. Numerical simulation of the NC model

In order to study the transition to the absorbing phase, we have made numerical simulations of the NC model in square lattices of $L \times L$ sites, with L ranging from 10 to 160. We choose a fixed boundary condition such that the border of the lattice is fully occupied by particles that cannot be removed. Using this condition, at any moment, there are at least four empty active sites, and the system cannot reach the absorbing state. However, as the lattice size increases, the density is allowed to vanish.

After setting the initial configuration (all sites are occupied), we let the system evolve by randomly choosing at each step a site in the lattice, and then change its state according to the rules defined previously. The time is then increased by $1/L^2$. After discarding
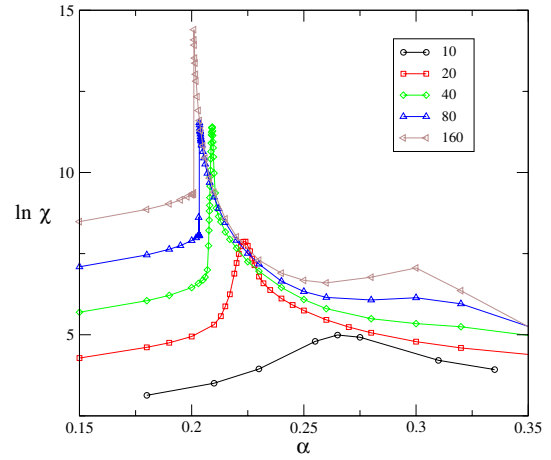

Fig. 4. $\ln \chi$ as a function of α from the numerical simulation of the NC model for several values of the linear system size L.
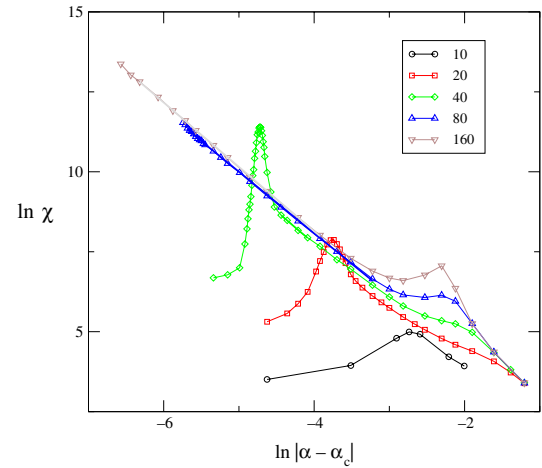

Fig. 5. $\ln \chi$ as a function of $\ln |\alpha - \alpha_c|$ from the numerical simulation of the NC model, for $\alpha_c = 0.2002$ and several values of the linear system size L.

some initial configurations, we calculate the mean density and the second moment $m = \langle \rho^2 \rangle$ from the remaining configurations. We use a number of Monte Carlo steps ranging from 10^5 to 4×10^7. Fig. 3 shows ρ as a function of α for several values of the linear system size L. As L grows, the density presents a jump, as can be seen in Fig. 3. The transition point is estimated as $\alpha_c = 0.201$.

A better estimate of the transition point can be obtained by calculating the variance of the particle number $\chi = \langle N^2 \rangle - \langle N \rangle^2 = L^2(m - \rho^2)$ in the subcritical regime. The NC model presents a discontinuous phase transition, which can be seen as a special case of a critical phase transition, where the exponent β, related to the order parameter ρ, is null. However, there still is a divergence in the correlation length; therefore, the variance must show the behavior

$$\chi \sim |\alpha - \alpha_c|^{-\gamma} \tag{13}$$

near the transition point.

In Fig. 4, we plot $\ln \chi$ as a function of α. We note that each curve has a peak which moves to the left when L increases and determines α_c at the limit $L \to \infty$.

In order to determine α_c and γ, we plot $\ln \alpha$ as a function of $\ln |\alpha - \alpha_c|$ for some values of α_c, choose the value that produces the smallest deviation from a straight line and estimate its standard deviation. From this procedure, we get the value $\alpha_c = 0.2002(4)$ and the exponent $\gamma = 1.96(6)$, as seen in Fig. 5.

In Fig. 5, comparing the graphs obtained for $L = 10, 20, 40$, on the one hand, and $L = 80, 160$, on the other, we also observe the formation of a peak in the first three graphs. This peak results from transitions from the high-density phase to the low-density phase, which can be observed when the lattice is sufficiently small. Therefore, the maximum value of $\chi(L)$ obeys the scaling rule $\chi_{max} \approx L^d$ for $L = 10, 20, 40$. We believe that it would be needed a exceedingly long simulation time in order to observe peaks like these for the other lattice lengths.

5. Numerical simulation of the C model

In this section, we perform simulations of the stationary state of the C model, obtaining the mean value of α^* for different values of ρ. The results obtained can be compared with the results for the NC model if we make the correspondence $\alpha^* \to \alpha$, as the local rules for particle addition and extraction are the same and, using Eq. (1) to obtain α as a function of the stationary state of the NC model, we get

$$\alpha = \frac{2P(01100) + P(01010) + 3P(01110) + P(01111)}{P(1)}. \quad (14)$$

From this point, in order to simplify the notation, we will use the same symbol for α^* and α.

The simulations of the C model have been done on a square lattice of linear length L, taking a fixed boundary condition such that the border of the system is again fully occupied by particles that cannot be removed. We choose an initial configuration of density ρ, randomly occupied by particles. At each time step, we choose two sites inside the lattice. If one of the sites is occupied and the other is an active empty site, we take the particle to the empty active site with probability $n/4$, and we do not do anything with probability $1 - n/4$. We discard some initial configurations and calculate the mean value of α by the use of Eq. (14). Simulation times are much lower for the C model than for the NC model.

Fig. 6 shows ρ as a function of α for the C model. We note a strong fall of ρ when $\alpha \sim 0.2$ for the C model, which converges to a jump as L grows—as we take smaller values of ρ, an empty cluster appears and pushes the active phase to the boundaries of the lattice, and different values of ρ correspond to different ratios of the areas of the active and empty phases.

The curves for the same value of L in Figs. 3 and 6 are very similar, except for the appearance of a loop in the C model, shown in the inset of Fig. 6. We notice, however, that the size of the loop decreases when $L \to \infty$. Estimates of α_c can be obtained by making graphs $\alpha \times L^{-1}$ for several values of ρ, and extrapolating to $L \to \infty$. The best estimate using this method is $\alpha = 0.201(1)$ (taking $\rho = 0.55$).

6. Time-dependent simulation

We also simulated the time evolution of the NC model starting from an infinite empty lattice, except for one occupied site. In a time-dependent simulation, we can distinguish a supercritical phase, where the mean value of the particle number $\langle N \rangle$ grows geometrically or exponentially with time t, a subcritical phase, where $\langle N \rangle$ can grow initially, but approaches a limit value N_∞ when t increases indefinitely, and a critical transition phase, when $\langle N \rangle$ presents an algebraic behavior:

$$\langle N \rangle \approx t^\eta \quad (15)$$

as t increases indefinitely.

As we said before, it is impossible for an isolated particle to attract more particles in the NC model: the system will fall without doubt in the stationary state. We circumvent this problem by
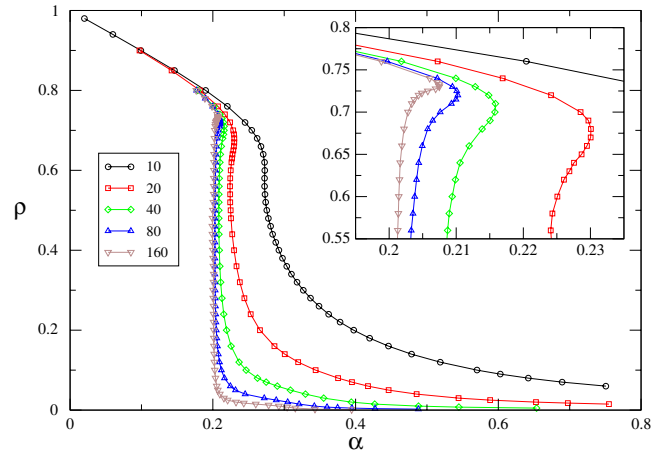

Fig. 6. Density ρ as a function of α from the numerical simulation of the C model for several values of the linear system size L. The inset shows an amplification of the region where the loops appear.
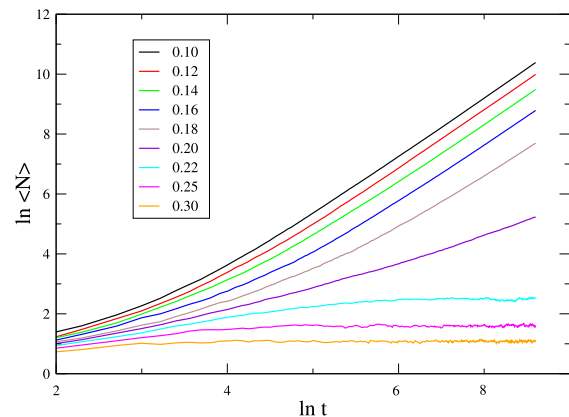

Fig. 7. The average number of particles $\langle N \rangle$ for the NC model as function of t for several values of α.

putting the initial particle in contact with two lines of particles that cannot be removed. If we associate coordinates to each site of the lattice, then the coordinates of the first particle are $(1, 1)$, the lines $x = 0$ and $y = 0$ are occupied by immovable particles, and the area of growth is the quadrant $x, y > 0$.

In order to save simulation time, a particle list is created at the beginning and actualized as the system evolves. At each step, a particle from the list is chosen: with probability $\alpha/(\alpha + 1)$, the particle is destroyed and the list decreases by one unit; with probability $1/(1 + \alpha)$, we choose one of the four nearest neighbor sites, check if this site is empty and, if so, we check the number n of neighbor particles of the empty site. If $n \geq 2$, a particle is put on the empty site and the list increases by one unit. Finally, the time is increased by $1/N$. If the number of particles goes to zero, another particle is created at site $(1, 1)$. As a result, after a long time, a cluster of particles is formed, with the approximate form of a right-angle triangle, in which particles are mainly added to the hypotenuse.

This sequence of steps recreates the annihilation and creation rates of model NC, except at sites located along the boundaries of the lattice, where the actual creation rate is lower than the rate of model NC. However, the difference is minor: as time goes by, the fraction of occupied sites which are in contact with the boundary decreases.

We estimate the critical rate α_c in the present time-dependent simulation by determining, for different values of α, the mean number of particles $\langle N \rangle$ and by plotting $\ln \langle N \rangle$ as a function of $\ln t$, as shown in Fig. 7.

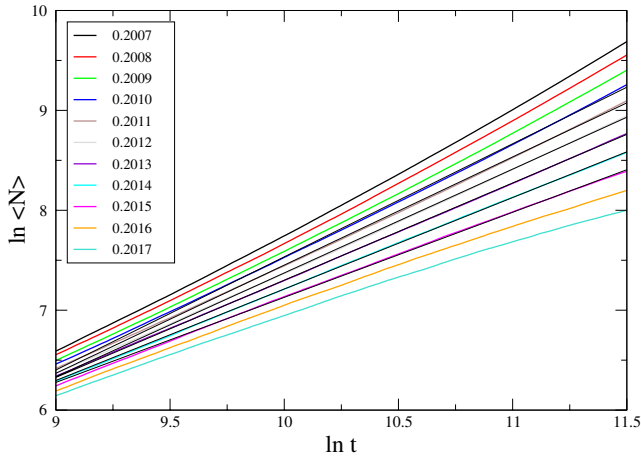**Fig. 8.** The same as Fig. 7, for further values of α around the critical point.

For $\alpha > \alpha_c$, the average number of particles increases but reaches a limiting value. For $\alpha < \alpha_c$, the average number of particles increases as t^2, as can be seen in Fig. 7. The critical value is obtained at the transition between the two behaviors. Fig. 7 also shows us that the critical point must be near $\alpha = 0.2$.

In order to obtain a better value for the critical point, we simulate the model for several values of α near 0.2 using a larger time interval, and make a graph $\ln \langle N \rangle \times \ln t$ for $9 < \ln t < 11.5$ ($8 \times 10^3 < t < 10^5$), as seen in Fig. 8. α_c is then estimated as the value of α for which the angular coefficient (the exponent η) given by linear regression has the smallest incertain. Using this method, we obtain $\alpha = 0.2013(2)$ and $\eta = 0.97(5)$.

7. Conclusion

We have presented two versions of the threshold contact model in a square lattice, characterized by a discontinuous phase transition for a specific value of the annihilation rate α_c. The two versions can be understood as distinct ensembles of the same model, that become identical in the thermodynamic limit. Taking into account the best estimates of α_c given by the two versions, the final estimate is $\alpha_c = 0.2007(6)$.

We also measured two critical exponents: the exponent η associated with the divergence of the variance of the particle number at the critical point, for which the best estimate is $\gamma = 1.96(6)$, and the exponent η associated with the algebraic growth of the mean particle number from a unitary seed, for which the best estimate is $\eta = 0.97(5)$. Working in a version of the threshold contact model in two dimensions similar to the NC model [10], we have also found $\gamma \approx 2$ and $\eta \approx 1$ (with possible logarithm corrections).

Even if the two models are equivalent in the thermodynamical limit, there are some qualitative differences between them for finite values of L. For the NC model, it is hard to obtain reliable values of ρ near the discontinuity point when we increase L. For the C model, the active region seems to terminate in a metastable spinodal point located at $\alpha_s > \alpha_c$. However, the loop decreases as L increases, ceasing to exist in the thermodynamic limit and giving origin to a tie line.

Acknowledgments

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