Simulational study for the crossover in the generalized contact process with diffusion

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Abstract. In a recent work, Dantas and Stilck studied a model that generalizes the contact process model with diffusion [1]. Our approach, based on the supercritical expansion, showed that for a weak diffusion regime the crossover exponent between the directed percolation and compact directed percolation universality classes was $\phi \approx 2$. However this approach did not work for reduced diffusion rates higher than $D \approx 0.3$, where $0 \leq D \leq 1$ and $D = 1$ corresponds to an infinite diffusion rate. Thus, in the present work we estimate this crossover exponent for higher diffusion rates using a numerical simulation approach.

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1. Introduction

Recently, Takeuchi et. al, using an experiment based on turbulent liquid crystal, measured the critical exponents of the directed percolation (DP) universality class \[2\]. This work meant a conquest for an area whose research has been a growing interest in the three last decades, but which still was missing a clear experimental realization. Indeed, the study of systems with absorbing states tries to provide a scenario still poor in the understanding about the phase transitions in the nonequilibrium regime, where no general theory is available, in opposition to what occurs in the equilibrium regime with the Gibbs ensembles theory.

Using particular models to investigate general patterns, one hopes to get an insight of a possible general theory for these nonequilibrium phase transitions. The most studied model in this area is the contact process (CP), introduced by Harris as a toy model for the spreading of an epidemics \[3\]. Generally defined in a lattice, the CP consists of sites that may be occupied by particles (sick individuals) or empty (healthy individuals). An empty site becomes occupied with a transition rate proportional to the number of occupied nearest neighbor sites, and an occupied site may become empty with a unitary rate. The competition between the dynamical rules for creation and annihilation of particles generates a phase transition between a state called absorbing that is devoid of particles and an active phase, where some particles may survive. The presence of an absorbing state prevents detailed balance and, because of that, this model is intrinsically a nonequilibrium model. An interesting feature of the CP model is that even in the one-dimensional case a phase transition appears, this does not happen in equilibrium cases for models with short range interactions. Besides, this phase transition is characterized by critical exponents that belong to the directed percolation (DP) universality class, and there is a conjecture that all models with a phase transition between absorbing and active states, with a scalar order parameter, short range interactions and no conservation laws do belong to this class \[4, 5\].

To determine the universality class for a particular model is an endeavor in this research area and this may be accomplished using numerical or analytical tools that allow us to obtain, as precisely as possible, the critical exponents. Although the most usual of this techniques are numerical simulations, semi-analytical approaches as series expansions are successful in some cases, furnishing a good precision to critical exponents values. Supercritical series expansion, according the prescription by Dickman and Jensen \[6\] were used by us in past works to study critical exponents, particularly the crossover exponent between different universality classes in models that generalize the CP. In a first work \[7\], we determined the crossover exponent between the DP and Compact Directed Percolation (CDP) classes with a good precision, using PDA approximants \[8\] in order to analyze numerically the series in two variables. On the other hand, we also studied how this crossover exponent could be affected by the presence of diffusion in the model \[1\]. However, this approach only works for values of the diffusion rate up to \[D = 0.3\], where \(0 \leq D \leq 1\), \(D = 1\) being equivalent to the infinite diffusion regime.
The failure of the series expansion method for higher diffusion rates probably occurred because in order to obtain a definite series expansion we were forced to include the diffusion term in the part of the evolution operator which is treated as a perturbation.

In the present paper we extend the results obtained in a preliminary work [9], where we intended to obtain the behavior of this crossover exponent for larger values of the diffusion rate using a numerical simulational approach to determine the critical line as a function of this rate. This numerical simulational approach follows the algorithm proposed by Grassberger and De La Torre [10] to explore the time evolution of the system from an initial condition where a unique seed is present in the system. Besides the crossover between CP and CDP classes, now we also analyze the model in the neighborhood of the mean-field limit, but not very close to the previous multicritical point, determining another crossover exponent, characterized by the behavior of the critical line close to the infinite diffusion rate limit.

The paper is organized as follows: in the section 2 we present the model, its characteristics and the previous results obtained in the past works [1, 7]. In the section 3 we discuss the numerical simulation approach and the results for the crossover exponents - between CP and CDP and CP and the mean field regime. Finally, the conclusions may be found in section 4.

2. The model

In a one-dimensional lattice with periodic boundary condition each site may be empty or occupied by a single particle, with a occupation variable $\eta_i$, assuming values 0 or 1 if site $i$ is empty or occupied, respectively. Thus, a configuration of the system at time $t$ is expressed by the vector $|\eta\rangle = \otimes|\eta_i\rangle$. In a continuos time sense, the dynamical rules of this model are:

(i) We choose randomly a site $i$.

(ii) If this site is empty, it becomes occupied with a transition rate equal to $p_a n_{occ}/2$, where $n_{occ}$ is the number of particles in the first neighbor sites.

(iii) Otherwise, if this site is occupied, it may become empty by two processes:

(a) By a contact process with first neighbor empty sites with a transition rate $p_b n_{emp}/2$, where $n_{emp}$ is the number of holes in the first neighbor sites.

(b) Spontaneously, with a rate $p_c$.

(iv) Also a diffusive process takes place with a transition rate $\tilde{D}$.

The parameters $p_a, p_b$ and $p_c$ are positive numbers and obey the relation $p_a + p_b + p_c = 1$ and $0 \leq \tilde{D} < \infty$. For convenience, we will discuss this model in the parameter space $(p_a, p_c, \tilde{D})$. For $p_b = 0$ this model is equivalent to the CP with diffusion and if $p_c = 0, p_a = p_b$, and $\tilde{D} = 0$ it corresponds to the linear Glauber model (or voter model) [11]. In the last case, the critical exponents belong to the CDP universality class and when $p_c \neq 0$, DP exponents are expected. Therefore, we have a crossover between
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these two classes in the neighborhood of $p_c = 0$ and a generic density $g$ in this region should have the following scaling form

$$g(\Delta p_a, \Delta p_c, \tilde{D}) \sim \Delta p_a^{e_g(\tilde{D})} F\left(\frac{\Delta p_c}{|\Delta p_a|^{e_g(\tilde{D})}}\right), \quad (1)$$

where $\Delta p_a = p_a - 1/2$, $\Delta p_c = p_c$, $e_g(\tilde{D})$ is a critical exponent related with the density $g$ and $\phi(\tilde{D})$ is the crossover exponent. Besides, the scaling function $F(z)$ is singular at a value $z_0(\tilde{D})$ of its argument, which corresponds to the critical line for a certain diffusion rate value, $\tilde{D}$. Using the scaling (1), we have that the critical line is asymptotically given by $p_c = z_0(\tilde{D}) \Delta p_a^{e_g(\tilde{D})}$.

On the other hand, for a nonzero value of $p_c$ and with diffusion rate $\tilde{D} \to \infty$, the critical behavior of the model tends to the one predicted by the mean-field approximation. An asymptotic form to the critical line for the region of very high diffusion rate would therefore be given by the scaling relation

$$(p_a - p_a^c) = f_0(D - D_c)^{\phi_{MF-DP}}, \quad (2)$$

where $\phi_{MF-DP}$ is the crossover exponent between the DP and mean-field critical behavior and $D = \tilde{D}/(1 + \tilde{D})$. This relation is valid for constant $p_b$. When $p_b = 0$ we have a known result obtained by Konno [12] and verified by us and Messer and Hinrichsen [13, 14], with $\phi_{MF-DP} = 3$.

Using a mean-field cluster approximation (three-site level), we have shown that the crossover exponent has the value $\phi = 2$ in the weak diffusion regime [1], while a slight deviation to smaller values appears in an intermediate regime, converging to $\phi = 1$ in the strong diffusion limit. On the other hand, the crossover exponent $\phi_{MF-DP}$ value is unitary, being determined by two-site level approximation which furnishes the following relation for the critical line

$$(1 - D_{eff}) = \frac{(1 - \alpha)(1 + \alpha)}{1 - \alpha[1 - \xi \alpha + \alpha^2(1 - \xi)]}, \quad (3)$$

where $\alpha = (1 - p_a)/p_a$, $D_{eff} = \alpha \tilde{D}/(1 + \alpha \tilde{D})$ and $\xi = 1 - p_b$.

The results obtained using series expansions [1] have shown that, at least up to $D = 0.3$, where $D = \tilde{D}/(1 + \tilde{D})$, the crossover exponent is $\phi = 2$. Unfortunately, we were not able to study larger values of the diffusion rate probably because, to derive a well defined series, the diffusive term of the temporal operator must be treated as a perturbation, limiting the values of the diffusive transition rate that can be analyzed with reasonable precision.

3. Numerical simulations

To simulate this model, we follow the scheme introduced by Grassberger and De La Torre [10] to determine the critical point in models with absorbing states through a numerical
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Simulation of the time evolution. We carry it out using a single seed particle as initial condition and a lattice with \( N = 10000 \) sites with periodic boundary conditions. The time is discretized and at each step we realize the following dynamical rules:

(i) A list of all sites occupied by particles is stored, and at each time step one of them is chosen randomly.

(ii) Once the site is chosen, a random number \( p \) uniformly distributed in the interval \([0, 1]\) is generated. If \( p < D = \tilde{D}/(1 + \tilde{D}) \) the particle jumps to one of the empty first neighbor sites, if possible. If both are empty, the destination site is chosen with equal probability. Otherwise, we choose a reaction: creation or annihilation. With a probability \( p_a \) an empty site, in one of the first neighbors, is occupied, if possible. Otherwise, the particle at the chosen site will be annihilated either through the spontaneous or through the auto-catalytic process.

(iii) To define the process switching a particle to a hole, another random number \( q \) is generated. If \( q < p_c/(1 - p_a) \) the change is spontaneous, otherwise it will happen with a probability proportional to the number of empty sites in first neighbors of the chosen site.

(iv) The time interval associated with the steps above is \( \delta t = 1/N_A \), where \( N_A \) is the number of sites occupied by particles before the step. The process is repeated until either a maximum number of steps \( n_{max} \) is attained or the absorbing state \( N_A = 0 \) is reached.

(v) A total of \( N_{rep} \) runs are done and mean values are calculated as functions of time.

In our simulations, we choose \( n_{max} = 2 \times 10^5 \) and \( N_{rep} = 2000 \). Thus, for a fixed value of \( D \) and \( p_c \), we estimate the the critical point of the model, \( p_c^* \), generating a sequence of critical curves as shown in the figure 1. As we can see, there is a good agreement between the simulational data and that one obtained by series expansion. Not surprisingly, in the high diffusion limit, more fluctuations are observed, preventing a precise determination for the critical point. This difficulty, in turn, is reflected in a poorer estimate of the crossover exponent.

Using this curves for different diffusion rates and the scaling form for a particular critical curve, \( p_c = z_0 \Delta p_a^\phi \), we calculate how the crossover exponent behaves as a function of the diffusion rate. This is shown in the figure 2. The results fluctuate around \( \phi = 2 \) and, starting at \( D = 0.9 \), we observe a systematic change of the mean value of the estimates, converging approximately to \( \phi = 0 \). Actually, an quadratic extrapolation results in \( \phi = 0.09 \) when \( D = 1 \), making reasonable the idea that we recover the mean-field prediction of the critical line for infinite diffusion, in accordance with the one-site level approximation result, where \( p_a = 1/2, \forall p_c \).

These critical curves may be fitted with a good agreement by the expression \( p_a - 1/2 = A(D)p_c^{1/2} + B(D)p_c^{1/2+\varphi} \), as shown in the figure 3. the values of the coefficients \( A, B \) and the exponent \( \varphi \) being given in the table 1. Notice that around \( D = 0.9 \), \( \varphi \) tends to zero and \( |A| \rightarrow |B| \), but with opposite signals. This behavior seems indicate the same tendency to \( \phi = 0 \) exhibited in the figure 1. However, we believe that the
Figure 1. Top: Phase diagrams obtained using numerical simulation approach. Bottom: Comparative picture between the numerical simulation and series expansion results to the same values of the diffusion rate.

Figure 2. Behavior of the crossover exponent as a function of the diffusion rate.
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Figure 3. Comparison between the simulational data (points) and the critical lines obtained by expression $p_a = A(D)p_c^{1/2} + B(D)p_c^{1/2+\varphi}(full lines)$.

intermediate region where $0 < \varphi < 2$ must be a numerical artifact, since in the numerical simulational approach, a discontinuous transition in numerical values is not expected, so probably we should have $\varphi = 2$, when $p_c \neq 0$ and $\varphi = 0$ otherwise.

Table 1. Coefficients of the expression which fits the critical lines.

| D   | A      | B      | $\varphi$ |
|-----|--------|--------|-----------|
| 0   | 0.636  | -0.297 | 0.861     |
| 0.1 | 0.742  | -0.256 | 0.129     |
| 0.2 | 0.871  | -0.397 | 0.049     |
| 0.3 | 0.626  | -0.182 | 0.094     |
| 0.5 | 0.419  | -0.035 | 0.643     |
| 0.8 | 1.160  | -0.891 | 0.016     |
| 0.9 | -0.075 | 0.327  | 0.005     |
| 0.93| -3.478 | 3.738  | 0.004     |
| 0.95| -13.193| 13.472 | 0.003     |
| 0.97| -56.760| 56.983 | 0.001     |
| 0.99| -40.564| 40.755 | 0.001     |

On the other hand, making $p_b$ constant, we can analyze how the critical points behave in the neighborhood of the mean field regime, which corresponds to an infinite diffusion rate limit, but not so close of $p_c = 0$. This behavior for the contact process was considered exactly by Konno [12] and more recently by us [13] and Messer and Hinrichsen [14], using series and field theoretic analysis, respectively. For the CP the expected result is $\phi_{MF-DP} = 3$, but to obtain reliable estimates from simulations it is needed to obtain critical points in a region very close to the limit of infinite diffusion rate, since a secondary behavior emerges for high rate values before the asymptotic regime is
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Figure 4. Critical lines obtained for fixed values of $p_b$.

Figure 5. Crossover exponent between the DP and mean-field regime.

reached, as shown in [15], where this exponent was estimated to be $\phi_{MF-DP} = 4$. Our simulations allowed us to reach values up to $D = 0.995$ and the critical curves described in the space $(D, p_a)$ are shown in the figure 4. Finally, analyzing the behavior of these curves close to the point $(D = 1, p_a = 1/2)$, we found the crossover exponents $\phi_{MF-DP}$ exhibited in the figure 5, where CP with diffusion is a particular case that corresponds to $p_b = 0$. We observe in a region near to this point that the crossover exponent value is $\phi_{MF-DP} = 3$. However a trend to smaller values starts around $p_b = 0.2$. This tendency, in a linear extrapolation, seems result in an unitary exponent, already for $p_b = 1/2$, according the prediction of the mean-field approximation. Actually, we obtain $\phi_{MF-DP} = 1.02$ when $p_b = 1/2$ with this extrapolation.
4. Conclusions

In this paper we discuss the behavior of the two crossover exponents for a model which generalizes the contact process with diffusion. In a first moment we look for the behavior of the crossover exponent that characterizes the change of DP to CDP universality classes. This behavior is found in the neighborhood of the point \((p_a = 1/2, p_c = 0)\) for a fixed diffusion transition rate. A preliminary result for this behavior was accomplished using a perturbative series expansion method, but estimates were restricted to values below \(D = 0.3\), with \(0 \leq D < 1\) [1]. Here, using a numerical simulation of the time evolution, we obtained a strong evidence that this exponent has the same value of the case without diffusion, \(\phi = 2\), changing this value only in the extreme case in which the diffusion rate diverges. In this last case, we expected that the value of \(\phi\) should vanish, according to the mean-field approximation, where \(p_a = 1/2\), independently of \(p_c\). Besides, we speculate in a preliminary paper [13] that this numerical change was related with a possible loss of the compact clusters of particles in a high diffusion regime. Unfortunately this possibility is still a speculation, since it is restricted at this moment to a phenomenological argument. We also studied a second model with a different dynamics for the diffusion, where the particles, if possible, jump to a next nearest neighbor. Nevertheless, this version furnished results very similar to an original case, so we omit these results here.

On the other hand, the behavior of the model in a region not too near \(p_c = 0\), with \(p_b\) fixed, allowed us to estimate the crossover exponent \(\phi_{MF-\text{DP}}\), which characterizes the change of the critical exponents from a DP to a mean-field critical regime, in the limit of infinite diffusion limit. The original case for the CP with diffusion, equivalent to set \(p_b = 0\), was already exactly studied by Konno who obtained \(\phi_{MF-\text{DP}} = 3\). This value was re-obtained by us and Messer and Hinrichsen using different approaches [13, 14]. With the data originating of our simulations we concluded that this exponent maintains the same value for \(p_b \approx 0\), tending to one when \(p_b \to 1/2\), in accordance with the mean-field approach in its pair approximation. However, it should be remembered that when \(p_b = 1/2\) the model belongs to CDP regime, and this could be a reason for this tendency. Finally, it would be interesting to a more complete understanding of this model if these crossover exponents would be related by a scaling relation, since the curves used to determine these two exponents are not independent.

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