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Critical behaviour of a diffusive model with one adsorbing state

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Abstract. We study the critical behaviour of a non-equilbrium model for adsorption–desorption with diffusion. We consider a parallel updating rule of the cellular automata type. Without diffusion, it is found that the critical exponents belong to the universality class of directed percolation, as has already been shown for sequential dynamics. When diffusion is present, the critical behaviour can be described in terms of a crossover between the directed percolation regime and a dynamical mean-field regime associated with the case of arbitrarily large diffusion.

1. Introduction

Simple examples of non-equilibrium systems whose steady state displays a phase transition are lattice models where a binary variable $\Psi_i = 0, 1$ is associated with each site and where the evolution rule allows for the existence of an adsorbing state (i.e. $\Psi_i = 1$ everywhere).

Applications range from processes of adsorption–desorption of particles on a surface [1] to models of spreading of a liquid through porous medium [2]. For a given model, two types of dynamics can be considered. A *sequential dynamics*, for which one updates one site at a time, or a *parallel dynamics*, where all the sites are updated simultaneously, according to a so-called cellular automaton rule.

An interesting aspect of such models is the characterization of the critical properties at the non-equilibrium phase transition observed in the stationary states. For sequential updating, it was argued, based on the results of various numerical simulations, that the critical exponents associated with those transitions belong to the universality class of directed percolation (DP) [1]. However, some doubts were raised for the case of parallel dynamics. Indeed, numerical simulations for a cellular automata version of the A model [3] lead to noticeably different critical exponents.

Further investigations are needed to clarify this question. Moreover, it is legitimate to ask how robust the possible universality classes are to modifications in the evolution rules of the model. Those are the questions we address in this paper, which is organized as follows. In section 2, we define a cellular automaton model which is a

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generalization of the A model [1, 3]. In addition to the usual adsorption–desorption processes, the particles are allowed to diffuse on the surface. Diffusion can be efficiently included in a cellular automata dynamics by using the algorithms described in [4] and [5].

In section 3, the phase diagram and critical exponents of the system are studied as a function of a parameter ρ, characterizing the importance of the diffusion process. Extensive simulations are performed using the dynamical approach introduced by Grassberger [6] for DP. For the case without diffusion, it is found that the critical exponents are compatible with those of directed percolation, in contradiction with previous results [3]. The case with diffusion is more subtle to analyse. A coherent picture is obtained in terms of effective exponents crossing over from their DP values when $\rho = 0$, to their non-equilibrium mean-field value when $\rho \to \infty$.

2. The model

We shall consider extensions of the so-called *A model* which has been introduced by Dickman and Burschka [7] as a simple model describing poisoning transitions similar to the ones observed on catalytic surfaces. One considers a d-dimensional substratum spanned by a regular hypercubic lattice. Each site has two possible states: empty or occupied by a particle A. The first step of the dynamical process is the adsorption. The probability for a vacant site to become occupied during a short time interval δt is $p\delta t$. The second step of the process is desorption. The probability for an occupied site x to become vacant is $r\delta t$, provided that at least one of the nearest neighbours of x is vacant. During the time interval δt, one of the two processes occurs at each site. For simplicity we shall restrict ourselves to the case $r = (1 - p)$. Qualitatively, one expects that, if p is large enough, an initially empty substratum will be completely covered by A particles, after some time. This is the poisoned phase or the adsorbing state. But, if p is small enough, the desorption mechanism will be efficient enough to prevent such a poisoning. Thus, one may anticipate the existence of a threshold value p_c such that, in the stationary state, the covering fraction of A on the substratum X_A will be 1 for $p \geqslant p_c$ (poisoned phase) and smaller than 1 for $p < p_c$. If X_A varies continuously across p_c the transition will be of second order and its behaviour near the threshold will be described in term of the critical exponent β:

$$1 - X_A(p) \sim (p_c - p)^{\beta}. \tag{1}$$

The cellular automata version of this model is straightforward [3]. One considers a d-dimensional lattice. Each cell of the lattice j has two possible states: $|\Psi_j\rangle = |0\rangle$ or $|A\rangle$. The probabilistic cellular automata adsorption–desorption rules (ADR) are:

If $|\Psi_j\rangle(t) = |0\rangle$ then

$$|\Psi_j\rangle(t+1) = \begin{cases} |0\rangle & \text{with probability } (1-p) \\ |A\rangle & \text{with probability } p. \end{cases} \tag{2}$$

If $|\Psi_j\rangle(t) = |A\rangle$ then

$$|\Psi_j\rangle(t+1) = \begin{cases} |A\rangle & \text{with probability } p \text{ if the site } j \text{ has at least one nearest-neighbour empty} \\ |A\rangle & \text{with probability 1, if all the neighbours are occupied,} \\ |0\rangle & \text{with probability } (1-p) \text{ if the site } j \text{ has at least one nearest-neighbour empty.} \end{cases} \tag{3}$$

A new ingredient is now added to the model, namely diffusion. Once the particles have been adsorbed on the surface, they are not necessarily frozen on the surface before a possible desorption occurs; they can diffuse to nearest-neighbour empty sites. Such a diffusion can be simulated in two dimensions by the following cellular automaton rule (DIFF) [4]: one divides the two-dimensional square lattice into adjacent blocks, each of them containing 2×2 cells. These blocks are called the Margolus neighbourhood. The diffusion process is realized in two steps. First, the particles in a block are moved according to some symmetry operations conserving the number of particles in each block. Among the possible symmetry operations, one has the $\pm\pi/2$ rotations and the identity transformation. For each block on the lattice, a randomly chosen symmetry operation, belonging to the above set, is performed. Second, the block sublattice is shifted by one lattice constant in both directions x and y. This step allows the particles to move from one block to an adjacent one. The whole process is then repeated and, thus, the particles can propagate randomly through the system.

Although the motions of the particles belonging to a same block are strongly correlated, the second step of the algorithm ensures that these correlations disappear rapidly. It was shown that this algorithm reproduces the usual diffusion equation at a macroscopic scale [4]. The diffusion constant D is directly related to the probability of performing a $\pm\pi/2$ rotation. In our case we have chosen $D = a^2/4\tau$, where a is the lattice spacing and τ the iteration time of the automata.

The global evolution rule is the following: one applies the rule ADR once and the rule DIFF ρ times. For $\rho = 0$, one recovers the simple A model; for $\rho \to \infty$ the diffusion mixes all the states and one expects the behaviour of the system to be mean-field like. Qualitatively, one anticipates that the diffusion will have two effects on the phase diagram. First, the critical probability p_c should increase monotonically with ρ. Second, the values of the critical exponents should vary from those of the pure A model to their mean-field values. How this variation occurs (continuous variation of the exponents as a function of ρ or simple crossover phenomena) is not an easy question and will be discussed later on.

3. Numerical simulations

Simulations has been done for a two-dimensional system of size $L \times L$, with $L = 128$ and 256. The stationary quantities were obtained as follows. Starting from an initial state where each cell is empty, one iterates the evolution rules for 1000 steps (per site) which turns out to be sufficient to reach stationarity. The stationary values are then computed by averaging over 200 measures, each of them separated by 100 iteration steps (per site). Moreover an average was made over 20 samples.

The first quantity recorded is the density of A particles adsorbed, which is related to the order parameter of the problem. One should be very careful with the finite size effects. Indeed, if the dynamics is ergodic, a temporal average over an arbitrarily long time would lead to a vanishing order parameter for all values of p. Thus the time average performed to measure the stationary quantities should extend on a time interval large enough to guarantee stable values, but not too large to allow the system to explore a 'non-physical' ergodic component of the phase space. This remark is particularly important in the vicinity of the critical probability p_c, where critical slowing down is observed [8]. Since it is crucial to have a very precise determination of p_c to obtain the critical exponents, a different approach should be used to find p_c. We applied the method introduced by Grassberger for DP [6].

We started with a lattice filled with A particles, except for one single site and let the system evolve according to the CA rules. We measured the density of empty sites $n_0(t)$, the average square cluster size $R^2(t)$ and the survival probability $P(t)$ during the simulation. If the system is sufficiently large so that none of the clusters we simulate reaches the boundaries, our data are free of finite size effects.

At the critical probability p_c, we expect power law behaviour for these quantities, namely

$$A_i(t) \sim t^{\eta_i} \tag{4}$$

where $A_i(t)$ stands for n_0, R^2 or P. In a log–log plot of these quantities, upward (downward) curvatures indicates that the value of p is super (sub) critical. The critical probabilities obtained for different values of ρ are quoted in the second column of table 1.

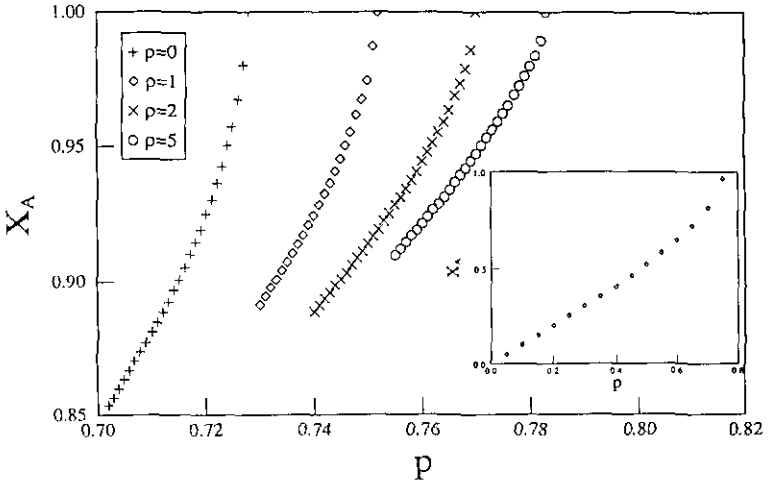

Figure 1. Phase diagram for several values of ρ. The density X_A of A particles adsorbed in the stationary state is plotted as a function of p for $\rho = 0, 1, 2, 5$.

Having a precise determination of p_c, we can now draw the phase diagrams. In figure 1, the phase diagrams are given for several values of ρ. One notices that the phase boundary behaves differently as a function of ρ as one approaches the critical probability $p_c(\rho)$. As expected, $p_c(\rho)$ is an increasing function of ρ; for large values of ρ, the phase boundary approaches the critical probability in a much more linear way than for smaller values of ρ. This is again in agreement with the interpretation of a more mean-field-like behaviour as ρ becomes large.

The order parameter critical exponent $\beta(\rho)$ as defined by (1) can be extracted from these data. In figure 2, the logarithm of $1 - X_A(p)$ is plotted as a function of the logarithm of $p_c(\rho) - p$ for the cases $\rho = 0$ and 5. The values of the critical exponent $\beta(\rho)$ are given in table 1. We note that for $\rho = 0$, the value of β is now compatible with the one of DP, in agreement with the Grassberger conjecture [9]. One notes that $\beta(\rho)$ increases linearly with ρ for the values of ρ considered.

However, these values for $\beta(\rho)$ should be interpreted carefully. Indeed, due to finite size of the lattices considered in the simulations one cannot investigate values of p arbitrary close to p_c. At best $(p_c(\rho) - p)/p_c(\rho) \sim 10^{-3}$ can be obtained. It may

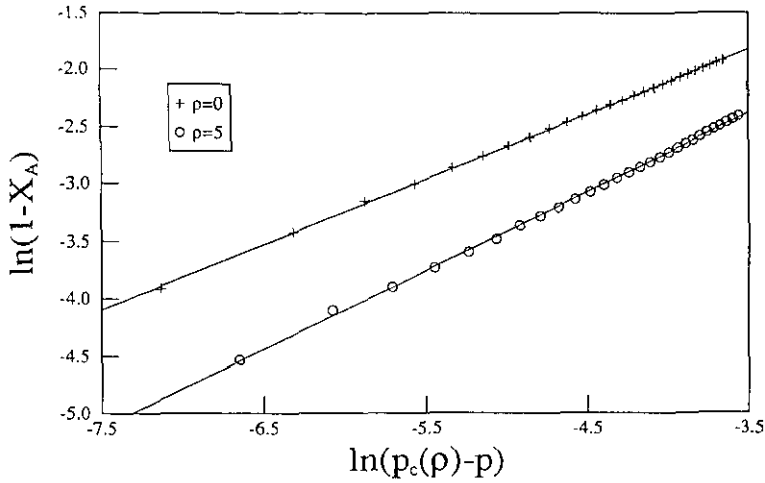

Figure 2. Logarithmic dependence of the density of empty sites $1 - X_A$ in the stationary state as a function of the logarithm of $p_c(\rho) - p$ for $\rho = 0, 5$.

Table 1. Critical probability p_c and order parameter critical exponent $\beta(\rho)$ for several values of ρ.

ρ	$p_c(\rho)$	β_{eff}
0	0.7278 ± 0.0003	0.56 ± 0.02
1	0.7518 ± 0.0004	0.59 ± 0.03
2	0.7702 ± 0.0003	0.64 ● 0.03
5	0.7833 ± 0.0004	0.70 ± 0.03
∞	0.8000	1.00

well be that, as ρ increases, the width of the critical region decreases and that the true critical behaviour is not seen in our simulation. The critical exponents quoted in table 1 would simply be an apparent exponent characterizing how the phase boundary behaves near but not very close to the critical point. However, it is this apparent exponent which is of importance for interpreting the experimental data.

A more satisfactory way to describe the situation is to introduce, by analogy with equilibrium critical phenomena, a so-called *effective critical exponent* defined as follows [10]:

$$\beta_{eff}(\rho, \delta p(\rho)) = \delta p(\rho) \frac{d \ln[1 - X_A(\rho, \delta p(\rho))]}{d \delta p(\rho)} \tag{5}$$

with $\delta p(\rho) = p_c(\rho) - p$.

This effective exponent has been calculated for several values of ρ. The derivative in this equation is performed numerically and, as a result, the data are quite noisy. A smoothed interpolation of β_{eff} as a function of $(p_c(\rho) - p)$ for several values of ρ is given in figure 3. For $\rho = 0$, one sees that the effective exponent does not vary with p in the range investigated ($(p_c(\rho) - p) \leqslant 0.025$). For $\rho > 0$, the effective exponent is compatible (taking into account error bars) with the DP exponent when $(p_c(\rho) - p) \to 0$. It increases when $(p_c(\rho) - p)$ increases. The departure from its DP value, at fixed $\delta p(\rho)$, is larger when ρ increases, in agreement with the idea of a crossover towards a mean-field behaviour for very large values of ρ.

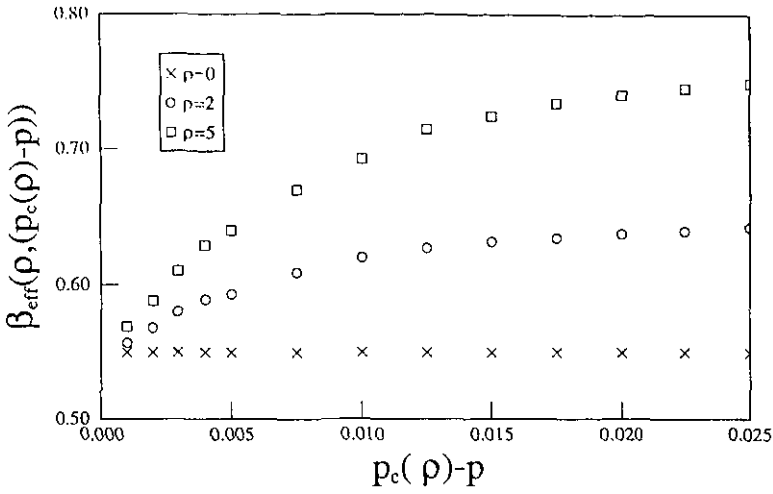

Figure 3. Effective exponent $\beta_{\text{eff}}(\rho,(p_c(\rho)-p))$ as a function of $(p_c(\rho)-p)$ for $\rho = 0, 2, 5$.

4. Conclusions

The first conclusion concerns the case without diffusion $\rho = 0$. These results lead to critical exponents in agreement with those obtained by Dickman *et al* [1], namely the critical exponents of the d-dimensional A model (the ones of DP in dimension $d+1$), independently of the type of dynamics used. The reason for the discrepancy with previous results has been traced back to unexpectedly poor properties [11] of the random generator used in [3].

As far as the case with diffusion is concerned, the results of the simulation can be explained in a fairly convincing way in terms of an effective exponent and a crossover from DP to mean-field behaviour. A similar question has been addressed by Dickman for a model with sequential dynamics [12]. However, the values of ρ used in these simulations were not large enough to see a significant deviation of the order parameter critical exponent from its DP value.

However, further work is needed to provide a more 'first principles' explanation to our findings. One important point would be to formulate a non-equilibrium version of the Ginzburg–Landau criterion [13] used in the framework of the equilibrium phase transition. One would like to know how the parameters of the model (in particular ρ) enter into the width of the critical region. A more ambitious programme would be to formulate a renormalization group approach for this non-equilibrium problem. One then would be able to decide if one has a crossover between two different fixed points, the DP one (for $\rho = 0$) and the mean-field one (for $\rho = \infty$) or if one may find a line of fixed point (parametrized by ρ) with continuously varying exponents. Both problems are currently investigated.

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