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LETTER TO THE EDITOR

Monte Carlo study of a 2-species contact process

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Abstract. We performed Monte Carlo simulations of one-dimensional (1D) models of a contact process with two kinds of absorbing particles. For the model with hard-core repulsion between domains of opposite species the critical behaviour is the same as that of some other models with two absorbing states. However, without this repulsion the model presumably does not have the critical point and the active phase exists for any absorption rate.

Recently, a number of non-equilibrium models of adsorbing particles has been intensively studied. These studies are partially motivated by experiments, namely by the oxidation processes [1]. Another motivation is the hope that such simple, although still usually unsolvable, models might stimulate the theory and classification of non-equilibrium phase transitions, which are far more complicated than the equilibrium ones.

There is some numerical evidence [2–4] that certain models of adsorbing particles exhibit the same critical behaviour and constitute the so-called directed percolation universality class. This universality has been related to the fact that these models possess a single absorbing state [5]. We should also mention that there are also other models in this universality class, for example, the Reggeon field theory [6] or the contact process [7]. The contact process is particularly interesting due to its simplicity which enables its rigorous analysis.

The natural candidates for another universality class seem to be models with a multiple absorbing state. This is similar to the equilibrium models, where the number of ground states is an important parameter determining the universality class of the model. And indeed, there is some numerical evidence that models with a double-degenerate absorbing state belong to another universality class. Among such models one should mention the interacting monomer–dimer model [8], which is a generalization of the model introduced by Ziff *et al* [2]. Other models which presumably belong to the same universality class are probabilistic cellular automata studied by Grassberger *et al* [9].

In the present letter we introduce two 1D models of adsorbing particles with a double-degenerate absorbing state. These models are generalizations of the contact process with two kinds of particles. The introduced models differ in the interaction rules between neighbouring domains of particles of different kinds. In the first model adjacent domains of particles of different kinds are forbidden. Such domains have to be separated by at least one empty site. This hard-core model will be referred as an H-model. In the second model, refered as the S-model (soft), there is no such restriction.

Our Monte Carlo simulations suggest that although these two models have the same double-degenerate absorbing state their behaviour is entirely different. Only the H-model has a critical point and the anticipated values of the critical exponents while the S-model

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presumably does not have the critical point at all. This means that specifying the number of absorbing states is not sufficient to predict the behaviour of a given model.

Let us assume that each site of a chain can be empty or occupied by a $+$ or $-$ particle. The dynamical rules are as follows. Empty sites become occupied by particles at the rate λ. The type of adsorbing particle is chosen at random. However, in the H-model, adsorption attempts which would result in adjacent domains of particles of different kinds are rejected. The desorbing rules are the same in both models: particles of a given type desorb at a rate equal to the fraction of neigbouring sites being empty or occupied by particles of another type (the last condition is relevant only for the S-model). This means that a given particle surrounded only by particles of its own type cannot desorb. Moreover, one can see that when a certain part of the chain is occupied by particles of only one type then the dynamical rules in that part (for any of these models) are exactly the same as that of the contact process.

One expects that for small λ both models will be in the active phase with the density of particles $\rho_{\mathrm{H,S}} < 1$. With the increase of λ, the density of particles will also increase and one might expect that at certain λ_{C}, probably different for each model, we will have a transition into one of the two absorbing states; i.e. with all sites occupied by + or – particles. To check these predictions we performed Monte Carlo simulations and our results are presented in figures 1–4.

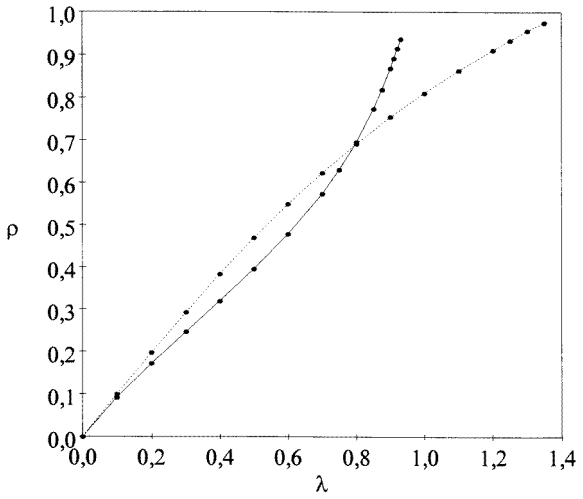

Figure 1. The density of particles ρ as a function of adsorption rate λ for the H-model (——) and the S-model (- - - -). The statistical errors are smaller than the size of the plotting symbols.

In figure 1 we have shown the density of particles ρ as a function of the adsorption rate λ. We present our results for the active phase and only for those values of λ for which we could reach satisfactory accuracy. Despite the apparent similarity to the contact process, the numerical calculations are much more difficult, especially for large λ. For $\lambda = 0.9$–0.93 for the H-model and for $\lambda = 1.20$–1.35 for the S-model, we simulated chains of length up to 10^4 and performed several independent runs of up to 5×10^6 Monte Carlo steps. Such extensive simulations were neccessary because for large λ the dynamics has a very large relaxation time. The reason is that in this case the chain is occupied by large neighbouring domains (separated in the H-model by some empty sites) which might change their configurations only through flips at the boundaries (since their interiors are inactive).

The results presented in figure 1 require some comments. First, let us notice that for any configuration of particles the number of sites where the adsorbtion attempt would be successful is larger for the S-model than for the H-model. This suggests that $\rho_S > \rho_H$. Our simulations show that this prediction is true, but only for $\lambda < 0.8$.

Why do we have $\rho_S < \rho_H$ for $\lambda > 0.8$? The explanation of such, contradictory at first, behaviour is as follows. Increasing λ, we increase the number of adsorbtion attempts. In the small λ regime this leads to the almost linear increase of the density ρ in both models. However, when λ is large enough a new mechanism comes into play in the H-model. Namely, due to the hard-core repulsion between domains, when the density is large it is difficult to put more particles into the steady state. There is, however, one way in which the H-model can increase the density, namely it has to eliminate small domains. In such a way, the number of sites which separate domains of opposite particles will decrease and the density will increase. We would like to emphasize that this coarsening is related to the competition of two absorbing states which cannot be adjacent. The increase of the domain size with increasing λ also takes place in the S-model but here, due to the absence of the repulsion, there is no competition: the particles can adsorb at any empty site and as a result the increase of ρ is not singular.

Assuming that in the vicinity of the critical point λ_C the density has the power-law behaviour $1 - \rho_H \sim (\lambda_C - \lambda)^\beta$ and using the values of ρ_H in the range $\lambda = 0.875$–0.93, we estimate that $\lambda_C \approx 0.954$ and $\beta \approx 0.89$. The estimation of β strongly suggests that the H-model belongs to the same universality class as some other models with a double-degenerate absorbing state for which very similar values of β have been reported [8, 10].

The concave shape of the density, even for large λ, in the S-model suggests that there is no phase transition in this model and this seems to us more likely than the possibility that the S-model has a critical point with $\beta > 1$ (to our knowledge there is no model of this kind with $\beta > 1$).

We also performed so-called dynamic Monte Carlo simulations to determine some other properties of these models. However, our calculations are not aimed at the most precise estimations of the critical properties but rather at their qualitative examination.

An important quantity in such non-equlibrium models is the characteristic time τ defined for the finite systems as the averaged time needed for entering the absorbing state. At the critical point one expects that this quantity increases in a power-law way with the system size, $\tau \sim L^\phi$. Kim and Park's estimation of ϕ for the interacting monomer–dimer model gives $\phi = 1.734$ [8].

In figure 2 we plotted on a logarithmic scale the characteristic time τ for the H-model as a function of the system size L for several values of λ. Each point has been obtained by averaging over at least 2000 measurements; the initial configurations have had all sites empty. The increasing slope for $\lambda = 0.8 < \lambda_C$ confirms that the system is in the active phase with τ increasing exponentially with the system size. From the slope estimated from the results obtained for the three largest L for $\lambda = \lambda_C$, we obtain $\phi \approx 1.75$. This result is in very good agreement with Kim and Park's result, which gives further support to our claim that the H-model belongs to the same universality class as their interacting monomer–dimer model.

For $\lambda > \lambda_C$ we have $\tau \sim L^2$ with very good accuracy; the case $\lambda = 1.5$ is shown in figure 2. Such dependence can be easily understood. For $\lambda > \lambda_C$ the empty chain quickly becomes filled with domains separated by narrow holes (holes between neighbouring domains of the same kind of particles quickly become filled with particles; slowly evolving configurations consist of neighbouring domains of different particles). Further dynamics leads to the elimination of the smallest domains and to the enlargement of the remaining

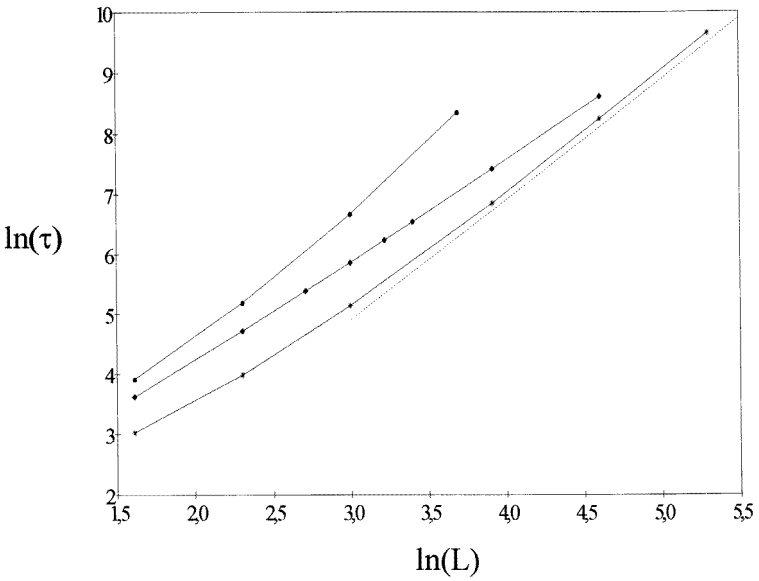

Figure 2. The logarithm of the characteristic time τ as a function of the logarithm of the system size L for the H-model for $\lambda = 0.8$ (●), $0.954(= \lambda_C)$ (♦), and 1.5 ($*$). The slope of the dashed line which is used as an eye guide is equal to two exactly.

ones. After some initial time the chain will be filled with very few domains of a size comparable to the system size. Approximately, the domain dynamics in our model can be regarded as a random walk with walkers placed in the holes between domains. This is actually an annihilating random walk since the elimination of a certain domain corresponds to the annihilation of two random walkers. Since the averaged time needed for a random walker to move along a distance of the order of L increases as L^2 thus τ will scale in the same way. The relation with the random walk will also be discussed below.

Let us emphasize that the asymptotic increase with the system size of the characterisitic time is slowest at criticality. This is in contrast, for example, to the usual contact process, where in the absorbing phase τ increases much slower than at criticality.

In figure 3 we present the same quantity for the S-model. One can see that both for $\lambda = 1.3$ and 1.35 the curves have increasing slope which for the largest L exceeds 2. We have to admit, however, that for $\lambda = 1.35$ the evidence is rather slight and simulations of larger systems would be needed to obtain convincing results.

Such increasing slope suggests that asymptotically τ in the S-model has exponential dependence and for these values of λ the system is in the active phase. This confirms the results presented in figure 1. However, to confirm that the S-model remains in the active phase even for larger λ we would need much more extensive simulations.

We also measured the time dependence of the survival probability $P(t)$. This quantity describes the probability that after time t the system did not reach the absorbing phase. The initial configuration in these simulations consists of one empty site and all the other sites occupied by particles of the same kind. One expects that at criticality $P(t)$ has a power-law decay, $P(t) \sim t^{-\delta}$.

Our results for the H-model are presented in figure 4. From the slope of the curve for $\lambda = \lambda_C$ we estimate $\delta = 0.29$. This result is again in very good agreement with estimations

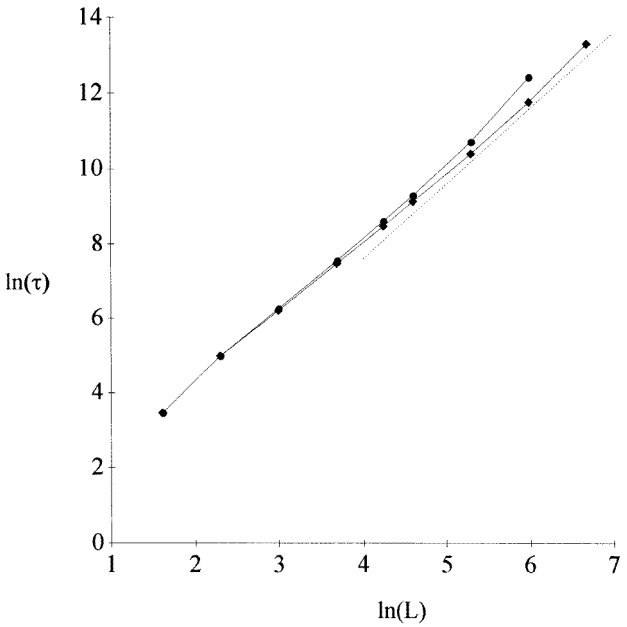

Figure 3. The logarithm of the characteristic time τ as a function of the logarithm of the system size L for the S-model for $\lambda = 1.3$ (●) and 1.35(⧫). The slope of the dashed line which is used as an eye guide is equal to two exactly.

for the interacting monomer–dimer models, as well as with some other estimations for models which presumably also belong to the same universality class [11]. We checked that for $\lambda < \lambda_C$ the slope diminishes to zero, which is the expected behaviour in the active phase.

However, the behaviour for $\lambda > \lambda_C$ is somehow unexpected. Namely, from the slope in figure 4 we estimate that in the absorbing phase the survival probability also has power-law behaviour but with the exponent $\frac{1}{2}$. This is in contrast with most models of this type, where in the absorbing phase the effective exponent δ increases to infinity. Such a value of δ means that again the random walk is at work. This behaviour can be understood if we assume that the long living configurations are those which, in the initial stage, increase the empty hole and then fill it with particles of the opposite kind. The situation is shown in figure 5. Assigning random walkers at the boundary of the inner domain (this is an approximate procedure), we easily deduce [12] that indeed the survival probability of random walkers will scale in time with the exponent $\frac{1}{2}$.

We do not present results for $P(t)$ for the S-model. For small $\lambda(< 1.3)$ our results show vanishing slope which confirms that the model is in the active phase. For large $\lambda(\geqslant 1.35)$ our results are bending but the slope is still positive. Thus, from the behaviour of the survival probability we cannot confirm definitely that the S-model is in the active phase for such λ.

The main results of the present letter can be summarized as follows. Although both H- and S-models have two absorbing states, only the H-model has a critical point at a finite adsorbtion rate λ and the expected values of critical exponents. Most likely the S-model does not have the phase transition at finite λ. The factor responsible for the phase transition in

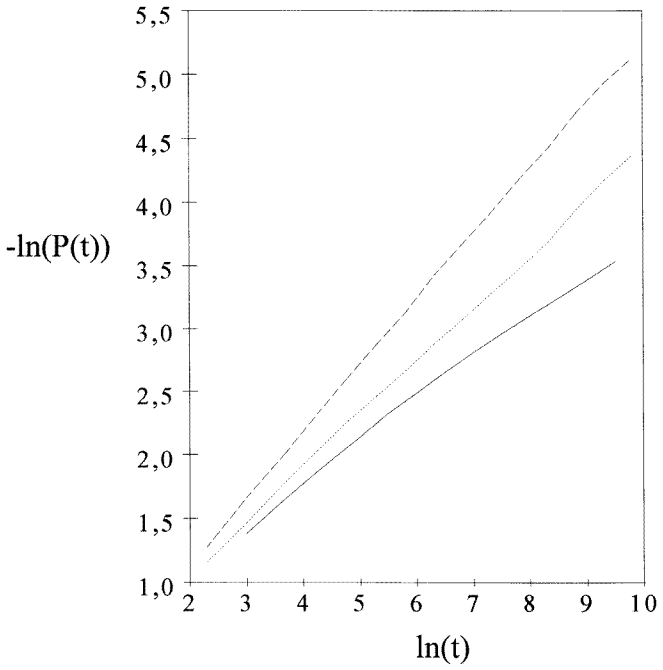

Figure 4. The logarithmic plot of the survival probability $P(t)$ as a function of t for the H-model for $\lambda = 0.954(= \lambda_C)$ (——), 1.0 (- - - -) and 1.1 (– – –).

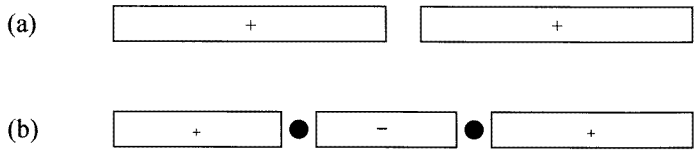

Figure 5. (a) The initial configuration used to determine $P(t)$. (b) The structure of the majority of the long living configurations. Random walkers are denoted as full circles.

the H-model is the hard-core repulsion between domains of opposite kinds of particles. This repulsion in the large-λ regime implies competition of two absorbing states and 'enforces' the coarsening of the active phase as the only way to increase the density in the H-model. Surprisingly, this repulsion is also responsible for the lower density of particles in the H-model in the small-λ regime. Since there is no such mechanism of competition in the S-model, there is thus no critical point in this model. Our simulations show that specifying merely the multiplicity of the absorbing state is not enough to determine the behaviour of a given model.

Both H- and S-models can be generalized to an arbitrary number of kinds of particles. To examine properties of such multi-species models is left as a future problem.

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