On the critical behaviour of cellular automata models of nonequilibrium phase transitions

1990 J. Phys. A: Math. Gen. 23 3353

(http://iopscience.iop.org/0305-4470/23/14/031)

J. Phys. A: Math. Gen. **23** (1990) 3353-3359. Printed in the UK

On the critical behaviour of cellular automata models of non-equilibrium phase transitions

Philippe Beney, Michel Droz and Laurent Frachebourg

Department of Theoretical Physics, University of Geneva, 1211 Geneva 4, Switzerland

Received 13 February 1990

Abstract. Two cellular automata models of non-equilibrium phase transitions with one adsorbing state are studied in one and two dimensions. New evidence is found against the conjecture according to which all the one-component models with a single adsorbing state belong to the universality class of Reggeon field theory or directed percolation.

1. Introduction

There are some close analogies between the behaviour of equilibrium and non-equilibrium systems. For example, the diagram of steady states of a non-equilibrium system is similar to the phase diagram of an equilibrium one. In both cases, one can go from one phase to another by varying a control parameter. The phase transitions can often be described in terms of an order parameter, varying continuously or not at the transition.

On the other hand, there are also some important differences between the equilibrium and non-equilibrium situations [1]. As a result of the lack of a first principle formalism for the non-equilibrium case, many fundamental aspects are not understood yet. One of them is the critical behaviour in the vicinity of a second-order phase transition. In the framework of equilibrium phase transitions, a good understanding of this question has been obtained thanks to the renormalisation group approach [2]. The critical exponents describing the behaviour of the physical quantities in the vicinity of a second-order phase transition belong to universality classes characterised by a few parameters (dimensionality of the system, number of components of the order parameter). It is a legitimate question to ask if similar universality classes can be defined for the non-equilibrium case and what are their characteristics.

The first attempt in this direction has been made for a class of models called interacting particle systems [3] and having the following characteristics. They are Markov processes on a lattice. The sites can have two states (vacant or occupied). The enumeration of the state of occupancy of all the lattice sites defines the configuration or the state of the system. Transitions between different configurations occur via elementary processes, related to creation, annihilation or hopping of particles. These models have one adsorbing state for which the lattice is completely empty (or full). Models such as contact process [4], Schlögl's first model [5], directed percolation [6] and Reggeon field theory [7] belonging to this class, have been studied both by Monte Carlo simulation [8] and series analysis [9].

0305-4470/90/143353+07$03.50

The dynamics usually considered were *sequential* dynamics for which at most one elementary process occurs per unit of time. However, *simultaneous* or *parallel* dynamics was also considered for directed percolation in one dimension [10].

These studies revealed that all the above models belong to the same universality class, leading Grassberger [11] and Janssen [12] to the conjecture that all one-component models with a single adsorbing state belong to the universality class of Reggeon field theory.

Some doubts about the above conjecture were raised by the work of Chopard and Droz [13]. They studied a cellular automata version of a surface reaction model proposed by Ziff *et al* [14]. They found, that the order parameter exponents associated with the two second-order transitions present in the model were respectively $\beta = 0.55 \pm 0.05$ and 0.45 ± 0.05. These results are not quite compatible with those of directed percolation. Note, however, that this model possesses two adsorbing states.

Moreover, Bidaux *et al* [15], have recently investigated a class of probabilistic cellular automata having two possible states per site and one adsorbing phase. The results obtained in one and two dimensions showed significant discrepancies with the critical behaviour of directed percolation.

Thus, the problem of the definition of universality classes remains open. This was the motivation for studying the cellular automata versions of two models studied by Dickman for sequential dynamics.

The paper is organised as follows. In section 2, the models and their cellular automata versions are defined. In section 3, analytical results in the mean-field approximation as well as results of numerical simulations in one and two dimensions are discussed. Finally, in section 4, these results are compared with the ones obtained by other authors and conclusions are made about the universality classes.

2. The models

We shall consider two different models, the so-called A model (or AM) and contact process model (or CPM).

2.1. The A model

This model has been introduced by Dickman and Burschka [16] as a simple model describing poisoning transitions similar to the ones observed on catalytic surfaces. One considers a d-dimensional substratum covered 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 speaking, one expects that if p is large enough, an initially empty substratum will be after some time completely covered by A particles. This is the poisoned phase or the adsorbing state. But, if p is small enough, the desorbing 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 terms of the critical exponent β:

$$1 - X_A(p) \sim (p_c - p)^{\beta}. \tag{2.1}$$

The cellular automata version of this model is straightforward. 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 cellular automata probabilistic rules are as follows.

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

$$|\Psi_j\rangle(t+1) = \begin{cases} |0\rangle & \text{with probability } (1-p) \\ |A\rangle & \text{with probability } p. \end{cases} \tag{2.2}$$

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

$$|\Psi_j\rangle(t+1) = \begin{cases} |A\rangle & \text{with probability } p \text{ if the site } j \text{ has one nearest neighbour empty} \\ |A\rangle & \text{with probability 1, if all the neighbours are occupied} \\ |0\rangle & \text{with probability } (1-p) \text{ if the site } j \text{ has one nearest neighbour empty.} \end{cases} \tag{2.3}$$

2.2. The contact process model

The contact process model is in many respects similar to the A model. However, the desorption mechanism is more subtle. In the A model, there is an equiprobable desorption each time that not all the nearest neighbours of a cell are occupied. In the CPM, the probability of desorption decreases when the number of nearest neighbours increases. The cellular automata version of this model is defined by the following rules.

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

$$|\Psi_j\rangle(t+1) = \begin{cases} |0\rangle & \text{with probability } (1-p) \\ |A\rangle & \text{with probability } p. \end{cases} \tag{2.4}$$

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

$$|\Psi_j\rangle(t+1) = \begin{cases} |A\rangle & \text{with probability } q(1-n_j/z) \\ |0\rangle & \text{with probability } 1-q(1-n_j/z) \end{cases} \tag{2.5}$$

where n_j is the number of occupied nearest-neighbour cells of the cell j, and z the coordination number of the lattice ($z = 2d$ for a d-dimensional hypercubic lattice). As before, we shall restrict ourselves to the case $q = (1-p)$.

3. Results

These models have been investigated in one and two dimensions. No exact analytical solutions have been found yet, even in one dimension. However, mean-field-like approximations can be obtained. These models have also been studied numerically both on special purpose cellular automata machine (CAM-6) [17], as well as on a traditional computer. It turns out that the results obtained on the CAM-6 were somehow biased due to the cellular automata algorithm used to generate random numbers for each cell in a parallel way. Accordingly, the results quoted below are those obtained on an Apollo workstation using a reliable random number generator.

3.1. The one-dimensional case

3.1.1. The A model. Several mean-field-like approximations can be considered for such non-equilibrium models [18]. The simplest is the one-site approximation in which one writes down the evolution equation for the probability that one cell is in a given state at a given time. More elaborated approximations take into account the correlations between cells and, for example, one can write the evolution equation for the joint probability that two nearest-neighbour sites assume a given state. Applied to the rules (2.2) and (2.3) in one dimension, one finds [19] a second-order phase transition for, respectively, $p = 0.667$ and $p = 0.580$. In both cases, the order parameter critical exponent is $\beta = 1.0$.

Numerical simulations have been performed for chains of lengths L between 30 and 65 536. The results obtained by finite-size scaling analysis coincide with those obtained for the chains of length 65 536. The corresponding phase diagram and the mean-field predictions are drawn on figure 1. A second-order phase transition is obtained at $p_c = 0.365$. The order parameter critical exponent β extracted by fitting the data with the relation (2.1) over the range $0.001 \leqslant (p_c - p) \leqslant 0.02$ is $\beta = 0.280 \pm 0.010$.

Thus if mean-field-like approximations gives a qualitatively reasonable phase diagram, they overestimate the critical probability p_c and give a poor exponent β.

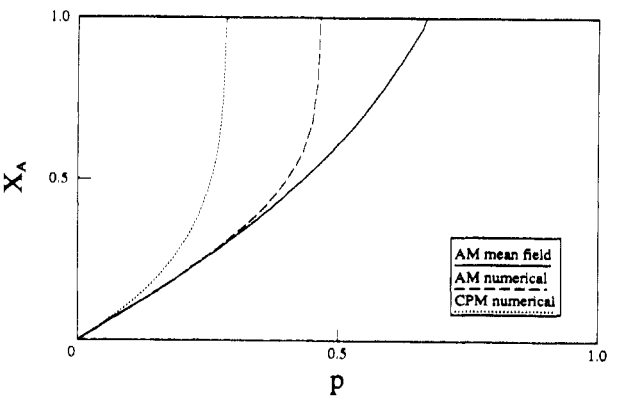

Figure 1. Phase diagram obtained by simulation for the one-dimensional A (AM) and contact process (CPM) models. The mean-field results for the A model is a one-site approximation. X_A is the steady-state coverage fraction of A and p is the adsorption probability.

3.1.2. The contact process model. Similar simulations have been made for the CPM. The phase diagram obtained for chains of length 40 000 is also drawn in figure 1. A second-order phase transition occurs at $p_c = 0.281$ and the order parameter critical exponent (fitted in the same range than for the AM) is $\beta = 0.260 \pm 0.020$.

3.2. The two-dimensional case

3.2.1. The A model. One-site and pair-mean-field approximations predict in two dimensions a second-order phase transition for, respectively, $p_c = 0.800$ and 0.785. As for the one-dimensional case, the critical exponent is $\beta = 1$.

More interesting are the numerical simulations on this model. The simulations have been made for square lattices of sizes $L \times L$, with $L = 16$, 32, 64, 128 and 256. The resulting phase diagram is shown in figure 2. The critical probability is $p_c = 0.747$. The order parameter critical exponent β extracted by fitting the data with the relation (2.1) over the range $0.001 \leqslant (p_c - p) \leqslant 0.02$ is $\beta = 0.52 \pm 0.01$. The fit is given in figure 3.

One can note some oscillations of the transition line as a function of p. We are presently not able to explain the reasons for such behaviour.

3.2.2. The contact process model. For the CPM, simulations similar to those described in subsubsection 3.2.1 above leads to the phase diagram drawn in figure 2. The second-order phase transition occurs at $p_c = 0.438$ and the order parameter critical exponent β extracted by fitting the data with the relation (2.1) over the range $0.001 \leqslant (p_c - p) \leqslant 0.020$ is $\beta = 0.52 \pm 0.03$.

For all the above cases, the measurement procedure was typically the following. Starting from an initial configuration (empty substratum) we did from 10 000 to 50 000

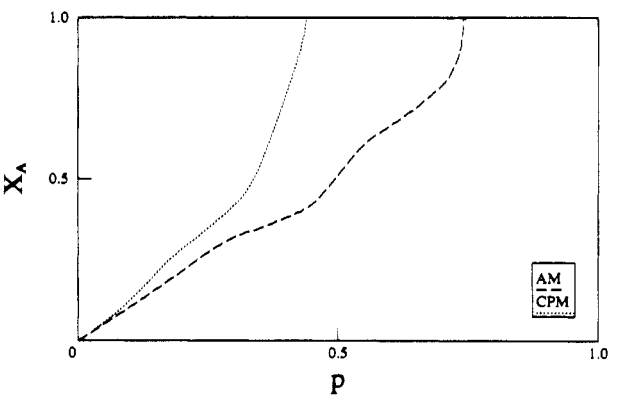

Figure 2. Phase diagram obtained by simulation for the two-dimensional A (AM) and contact process (CPM) models. X_A is the steady-state coverage fraction of A and p is the adsorption probability.

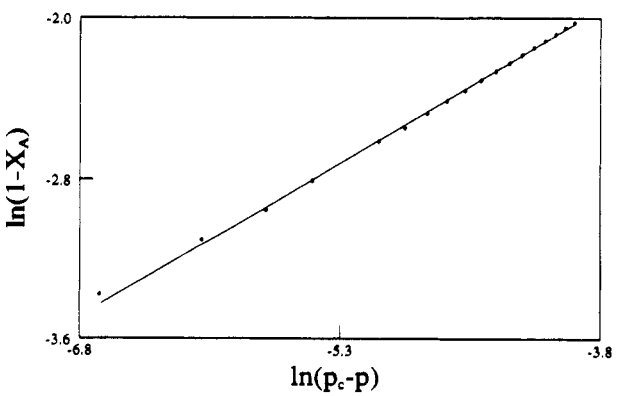

Figure 3. Logarithm of the order parameter $(1 - X_A)$ as a function of the logarithm of the deviation from criticality for model A. The slope gives for the critical exponent $\beta = 0.52 \pm 0.01$.

iterations to reach the stationary state. Obviously, the greatest number of iterations was made near p_c. Then a stationary average was taken by averaging over 500 points, two successive points being separated by 100 iteration steps.

4. Conclusions

From the above results, we can draw the following conclusions. For the A model in one dimension, both the critical probability p_c and the critical exponent β are similar in the cellular automata approach (i.e. a parallel updating) and the sequential updating approach $\beta = 0.277$ [9].

However, for the CPM, the critical probability for the cellular automata model $p_c = 0.281$ is larger than that estimated for the sequential updating approach $p_c = 0.233$ [9]. The critical exponent β are compatible in both approaches and also compatible with the value for the two-dimensional directed percolation $\beta = 0.276$ [6].

Thus, one sees in the above examples that changing the dynamics from sequential to parallel may affect the position of the phase transition, but does not affect (within the precision of the simulation) the critical exponent β. These observations support the conjecture of Grassberger and Janssen.

Let us now analyse the two-dimensional situation. There are, to our knowledge, no results about the critical probabilities for these models with sequential updating. Therefore, we have nothing with which to compare our values of p_c.

More interesting are the values obtained for the critical exponent β. The values for the two models, respectively $\beta = 0.52 \pm 0.01$ and $\beta = 0.52 \pm 0.03$ are not compatible with the best estimate for the three-dimensional directed percolation, namely $\beta = 0.586$ [6]. However, the results obtained are compatible with previous simulations on a cellular automata model of the Ziff model [13].

One could argue that this discrepancy is due to one of the two following reasons. First, the critical domain is very small and we do not see the true critical exponent. However, the range of values of $p_c - p$ used is similar to the one-dimensional case and comparable with the range used by other authors. Moreover, if one is out of the critical region, one would expect the effective critical exponent to be in between its true value and the mean-field prediction. This is not the case here.

A second reason could be the fact that we were not yet in a steady state. We have checked this point for the two-dimensional CPM. Increasing the number of iterations before the steady state was reached by a factor thirty did not change the results in a significant manner.

Thus we conclude that our two-dimensional models give some other evidence that the conjecture of Grassberger and Janssen may not be correct for cellular automata models as already noticed on different models by Bidaux *et al* [15]. We believe that using a fully parallel dynamics instead of a sequential one is a relevant difference and thus that the type of dynamics used may be one parameter characterising the universality classes for non-equilibrium phase transitions.

Acknowledgment

This work was supported by the Swiss National Science Foundation.

References

[1] Droz M and Chopard B 1988 *Chaos and Complexity* ed R Livi, S Ruffo, S Ciliberto and M Buiatti (Singapore: World Scientific) p 307
[2] Ma S K 1976 *Modern Theory of Critical Phenomena* (New York: Benjamin)
[3] Liggett T M 1985 *Interacting Particle Systems* (Berlin: Springer)
[4] Harris T E 1974 *Ann. Prob.* **2** 969
[5] Schlögl F 1972 *Z. Phys.* B **253** 147
[6] Kinzel W 1983 *Percolation Structures and Processes* ed G Deutscher and J Adler
[7] Grassberger P and de la Torre A 1979 *Ann. Phys. (NY)* **122** 373
[8] Dickman R 1989 *Phys. Rev.* B **40** 7005
[9] Dickman R 1989 *J. Stat. Phys.* **55** 997
[10] Kinzel W 1985 *Z. Phys.* B **58** 229
[11] Grassberger P 1982 *Z. Phys.* B **47** 365
[12] Janssen H K 1981 *Z. Phys.* B **42** 151
[13] Chopard B and Droz M 1988 *J. Phys. A: Math. Gen.* **21** 205
[14] Ziff R M, Gulari E and Barshad Y 1986 *Phys. Rev. Lett.* **56** 2553
[15] Bidaux R, Boccara N and Chaté H 1989 *Phys. Rev.* A **39** 3094; 1990 *Cellular Automata and Modeling of Complex Systems* ed P Maneville *et al* (Berlin: Springer) p 73
[16] Dickman R and Burschka 1988 *Phys. Lett.* **127A** 132
[17] Toffoli T and Margolus N 1987 *Cellular Automata Machine: A New Environment for Modeling* (Boston, MA: MIT Press)
[18] Dickman R 1986 *Phys. Rev.* A **34** 4246
[19] Beney Ph 1989 *Diploma Thesis* University of Geneva