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Inhomogeneous mean-field approximation for phase transitions in probabilistic cellular automata: an example

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Abstract. A stochastic cellular automata rule obtained by adding two rule components with probabilities $1-c1$ and $1-c4$ to Conway's 'Life' is studied both by computer simulation and theoretically. A line of phase transitions from an ordered domain-structured phase to a disordered one is observed and explained by introducing an inhomogeneous mean-field approximation which incorporates important correlations.

1. Introduction

Probabilistic cellular automata (CA) have been widely investigated in recent years (see Wolfram (1986) for a selection of articles). The CA rules can be made stochastic in several ways. Grassberger *et al* (1984) studied two elementary one-dimensional CA with very specific added noise and obtained a phase transition from class 2 (separated periodic structures) to class 3 (chaotic) behaviour (using the classification of Wolfram (1984)) via instability of kinks between ordered states. For a more general class of stochastic 1D CA, using transfer-matrix scaling, phase diagrams and critical properties of transitions between class 1 (homogeneous final states) and class 2 and between class 2 and class 3 deterministic behaviour have been calculated and compared with numerical experiments (Kinzel 1985).

In two dimensions, studies of phase transitions in a large class of simple stochastic CA have been given more recently (Kaneko and Akutsu 1986). These authors have used the simplest way to include noise, namely at each time step the value obtained by application of the deterministic rule has been reversed with a probability p. In the study of a stochastic version of Conway's 'Life' rule the noise term introduced by Schulman and Seiden (1978), called 'temperature', was defined similarly except for weighting it with the average density at each time step. By starting from an approximation akin to the mean-field approximation (MFA) of statistical physics and calculating pair correlations to first order, Schulman and Seiden (1978) arrived at a phase transition between phases of strongly differing average densities upon changing the 'temperature'. This calculation was aimed at explaining the transition they observed experimentally in the computer simulation of the rule, from an equilibrium state with average density $\langle\rho\rangle = 0$ to a disordered state setting in at some critical 'temperature'.

The rules investigated in the present paper are also defined from Conway's 'Life' rule. Two specific noise components are added with probabilities $1-c1$ and $1-c4$, which will be allowed to vary between 0 and 1 with the restriction $c1+c4 \leqslant 1$ (§ 2). The observed phase diagram in the $(c1, c4)$ plane shows a line of phase transitions

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from a disordered phase into an ordered one with domain structure made up of four phases (vertical and horizontal stripes on even and odd sites) (§ 3).

With the aim of allowing for the most important CA correlations in this structured phase, we propose here a generalised MFA which works, in general, with four sublattice densities of which two agree pairwise when considering a fixed phase (say, stripes in even rows). The analogy with ferromagnets suggests the definition of an order parameter proportional to the difference of densities in even and odd rows. The phase transition line is obtained qualitatively correctly; the transition is predicted to be first order (§ 4).

Finally, a short discussion of the results and problems is presented (§ 5).

2. The model system

For an eight-neighbour outer totalistic 2D CA the value $a_{i,j}$ of a site at position (i, j) evolves according to the rule:

$$a_{i,j}(t+1) \equiv a'_{i,j} = f(a_{i,j}, a_{i,j+1} + a_{i,j-1} + a_{i+1,j} + a_{i-1,j} + a_{i-1,j-1} + a_{i-1,j+1} + a_{i+1,j-1} + a_{i+1,j+1}). \tag{1}$$

Packard and Wolfram (1985) conveniently specified such rules by a code

$$\tilde{C} = \sum_{n=0}^{8} f(a, n) k^{k \cdot n + a} \tag{2}$$

where a denotes the state of the centre cell and n stands for the possible values of the sum over the eight neighbours. In the family of automata investigated below, $k = 2$ and $a_{i,j}$ takes the values of 0 and 1.

We shall consider the following probabilistic CA rules:

$$\begin{aligned} &f(0,3) = f(1,2) = f(1,3) = 1 \\ &f(1,1) = 1 \qquad \text{with probability } 1 - c1 \\ &f(1,1) = 0 \qquad \text{with probability } c1 \\ &f(1,4) = 1 \qquad \text{with probability } 1 - c4 \\ &f(1,4) = 0 \qquad \text{with probability } c4 \\ &f(a,n) = 0 \qquad \text{otherwise.} \end{aligned} \tag{3}$$

For $c1 = c4 = 1$, Conway's 'Life' rule results ($\tilde{C} = 224$). The other three limiting deterministic automata rules are as follows.

$c1 = 1$, $c4 = 0$ ($\tilde{C} = 736$). This rule has been discussed in detail by Packard and Wolfram (1985). When starting from a random initial configuration it leads to a class 2 final state with domain structure made up of four phases: two with horizontal stripes (stripes either on odd or on even rows) and two with vertical stripes (on odd or on even columns). Regions formed of one of these phases are invariant under the CA rule. Starting from a disordered configuration different phases evolve on different parts of the lattice and are separated by domain walls.

$c1 = 0$, $c4 = 1$ ($\tilde{C} = 232$). This CA shows no structure when starting from a random initial state; its behaviour is chaotic.

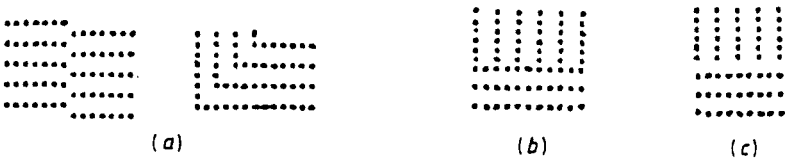

Figure 1. Sections of typical domain walls between two of the four phases: (*a*) domain walls which remain (if infinitely extended) even if $c1 = c4 = 1$; (*b*) and (*c*) are typical domain walls near the $c1 = c4 = 0$ corner of the phase diagram.

$c1 = c4 = 0$ ($\tilde{C} = 744$). Out of a random start this automaton evolves into a stable final state, similar to the one with $\tilde{C} = 736$. Nevertheless, there are important differences which become more apparent when departing somewhat from the deterministic limit, e.g. along $c1 = c4$ (see later). The most important effect brought about by $f(1, 1) = 1$ is that lines of ones when formed in one or the other of the four striped structures will not be shortened at their loose ends in consecutive time steps, thus favouring, in a spectacular way, the formation of large domains of the four phases.

The striped structure is also invariant under the 'Life' rule but its formation is extremely improbable. The four striped phases are separated by domain walls. Also some of the domain walls are stable for 'Life', see, e.g., figure 1(*a*). Such domain walls will be called invariant in the following as they do not change upon changing the strength of noise. There are some domain walls, however, which arise due to the finite probability of $f(1, 1) = 1$ and $f(1, 4) = 1$ like the ones shown in figure 1(*b*, *c*).

3. Results of computer simulation

Now allowing $c1$ and $c4$ to vary in the interval (0, 1) with the restriction $c1 + c4 \leqslant 1$, in the computer simulation of rules (3) for lattices of sizes up to 200×200 with periodic boundary conditions a line of phase transitions has been observed between a disordered and an ordered phase (figure 2). The latter is made up of the four striped structures mentioned earlier. Snapshots of the distribution of ones at large times for certain

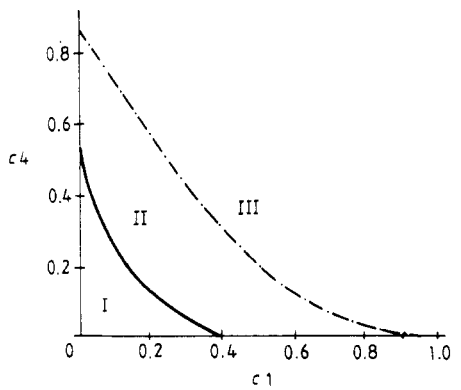

Figure 2. Phase diagram in the ($c1$, $c4$) plane. The chain curve has been drawn along experimental results obtained with an IBM PC on lattices of sizes varying from 32×32 to 80×80. Because of the poor statistics 5-10% deviations are possible. The full curve is the result of the inhomogeneous MFA explained later in the text.

characteristic values of the probability c along the diagonal $c1 = c4$ of the phase diagram are shown in figure 3.

Out of a random initial state, the formation of a pure phase is extremely improbable. A typical equilibrium state is built up of domains of the striped phases with invariant domain walls between them. The phase change can uniquely be characterised by the change in the density of non-invariant domain walls: this quantity is finite in the disordered phase while it disappears as $t \to \infty$ in the four-phase regime. A similar quantity has been used as order parameter by Grassberger *et al* (1984) in treating certain probabilistic one-dimensional CA; in their case, however, no invariant domain walls exist and thus the description is much simpler. In the framework of the presently studied 2D stochastic automata rule the formulation and measurement of the density of possible non-invariant domain walls is not feasible.

While in the 1D counterpart of the model (Grassberger *et al* 1984) the number of possible final states is two (by analogy with the Ising model), in the present case there are infinitely many invariant domain arrangements in the limit of infinite lattice size (by analogy with real magnets). In the ordered four-phase regime the system will spontaneously order in one of these as $t \to \infty$. By preparing the initial state as a monodomain containing a small amount of defects, it is possible to bring the system in a strongly 'magnetised' equilibrium state and use the analogue of magnetisation as an order parameter. For the sake of definiteness the singled-out phase will be the one with horizontal stripes with $\rho_1(0)$ ($\rho_2(0)$) being the density of ones in odd (even) rows. Let us define

$$\Delta(0) = \frac{\rho_1(0) - \rho_2(0)}{\rho_1(0) + \rho_2(0)}$$

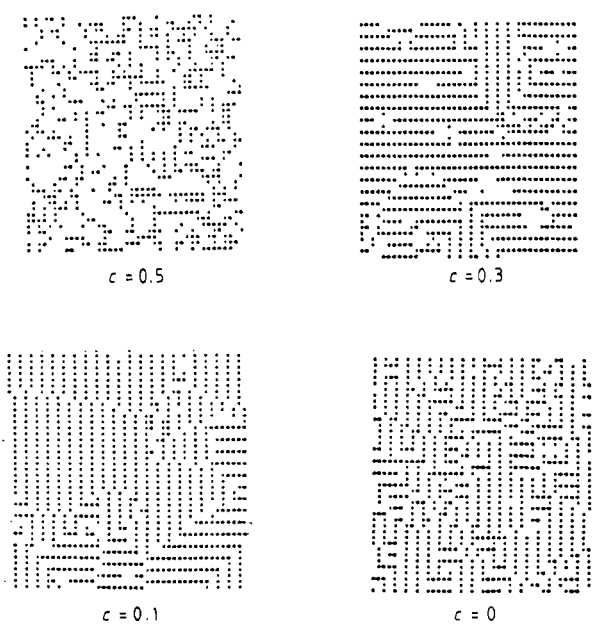

Figure 3. Snapshots of typical CA patterns after about 10^3 time steps along the diagonal $c1 = c4 = c$ of the phase diagram. Marked differences between different regimes are apparent.

to characterise the initial state. $\Delta(0)=0$ corresponds typically to a totally random initial state while $\Delta(0)=1$ characterises a striped monodomain with stripes on odd rows.

The definition of the order parameter is

$$\lim_{t\to\infty}\Delta(t)=\lim_{t\to\infty}\frac{\rho_1(t)-\rho_2(t)}{\rho_1(t)+\rho_2(t)}. \tag{4}$$

The computer experiment for measuring $\Delta(t)$ was performed on an IBM PC which ran in total for about six weeks. For the largest lattice investigated (40 000 cells) one iteration took 18 s using a program written in FORTRAN. The maximal number of iterations run was 2×10^5. Because of the long computing times needed in the vicinity of the transition, detailed study of $\Delta(t)$ could be performed only along the line $c1=c4=c$ of the phase diagram. The results for the 200×200 lattice are depicted in figure 4. The initial value of the 'magnetisation' was chosen to be 0.78. The critical value of c was found to be $c_{cr}=0.31\pm0.02$. For $c>c_{cr}$, $\Delta(t)$ exhibits an exponential

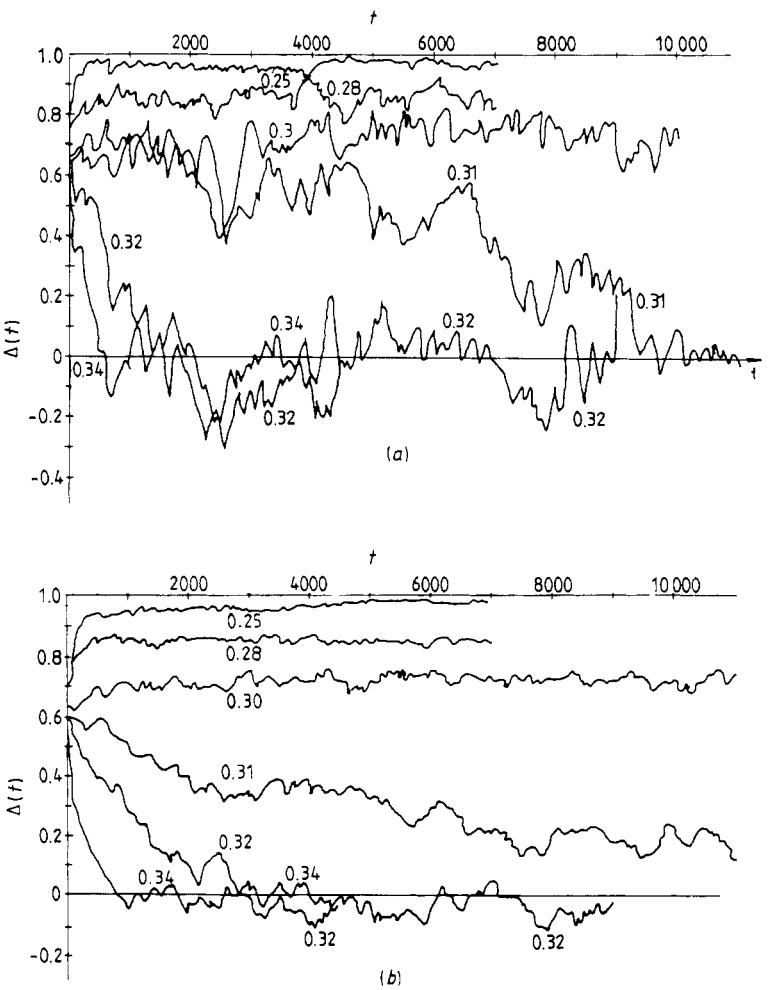

Figure 4. Time development of $\Delta(t)$ for different values of the probability c ($c1=c4\equiv c$) showing averages over the preceding 50 time steps at each point to wash out part of the fluctuations. (*a*) Lattice size 64×64, (*b*) 200×200.

decay for small values of t with relaxation time τ, which increases as c approaches c_{cr}; the exponential interval is followed by a fluctuating one: $\Delta(t)$ fluctuates around zero, the amplitude of fluctuations again growing with decreasing $c - c_{cr}$. All these features are very much reminiscent of the corresponding ones found in Monte Carlo studies of spin systems, especially of Ising systems (Binder 1979, Binder and Stauffer 1984 and references therein). At $c = 0.31$ the longest run (2×10^5) was insufficient to reach zero average 'magnetisation' for the largest lattice.

With decreasing $c < c_{cr}$, the average value of $\Delta(t)$ for large times increases steadily. Whether there is a jump of $\Delta(\infty)$ at c_{cr} or the transition is continuous, could not be decided from the computer simulation. The difficulties of deciding the order of transition in the Monte Carlo experiment for spin systems have been stressed and explained in detail by Binder (1979). Applying similar considerations here, a clear indication of metastability (i.e. a two-step $\Delta(t)$ curve for $c < c_{cr}$) could not be observed in the present runs.

As a phase transition cannot occur in finite systems, examination of the size dependence of our results is crucial. The computer experiment has been run for four different lattice sizes (with periodic boundary conditions) $L = 32$, 64, 128 and 200; no qualitative change in the features of the results has been spotted. Concerning the dependence on L, again strong similarities with the results of Monte Carlo experiments for the Ising model have been found: (i) the amplitude of the fluctuations grows with decreasing L, roughly as $1/L$; (ii) the relaxation time increases with increasing L; (iii) the mean value of the 'magnetisation' has, on average, been found to be higher for smaller lattices. For illustration see figure 4(a) where the lattice size is $L = 64$.

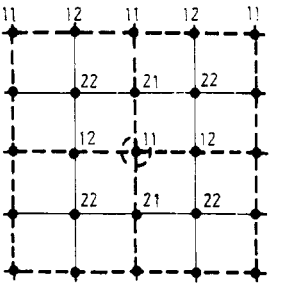

Figure 5. According to the evenness or oddness of the coordinates of a given site, each site belongs to one of four sublattices 11, 12, 21 or 22. 1 stands for odd and 2 for even. Shown is a section of the 11 sublattice and the neighbourhood of a site on it.

4. Theory

Here we propose to treat the transition from chaos to four-phase regime in the framework of a generalised inhomogeneous MFA as follows.

Let us introduce four sublattices as shown in figure 5 and four average densities corresponding to the sites on the respective sublattices. These densities will be denoted by ρ_{11} (odd-odd), ρ_{12} (odd-even), ρ_{21} (even-odd) and ρ_{22} (even-even). A cell, say, on the 11 sublattice has four 22, two 21 and two 12 neighbours.

A straightforward generalisation of the standard homogeneous MFA for CA (Schulman and Seiden 1978) to the case of the above inhomogeneous neighbourhood yields four coupled equations for the densities $\rho_{\kappa l}$ ($\kappa, l = 1, 2$) at time step $t+1$ as a function of the densities at time step t and of the probabilities $c1$ and $c4$ in the following form:

$$\begin{aligned}
\rho'_{11} &\equiv \rho_{11}(t+1) = S(\rho_{11}(t), c1, c4, \boldsymbol{N}(\rho_{22}(t)), \boldsymbol{M}(\rho_{12}(t), \rho_{21}(t))) \\
\rho'_{12} &= S(\rho_{12}, c1, c4, \boldsymbol{N}(\rho_{21}), \boldsymbol{M}(\rho_{11}, \rho_{22})) \\
\rho'_{21} &= S(\rho_{21}, c1, c4, \boldsymbol{N}(\rho_{12}), \boldsymbol{M}(\rho_{11}, \rho_{22})) \\
\rho'_{22} &= S(\rho_{22}, c1, c4, \boldsymbol{N}(\rho_{11}), \boldsymbol{M}(\rho_{12}, \rho_{21}))
\end{aligned} \tag{5}$$

where ($\tilde{\rho} \equiv 1 - \rho$)

$$\boldsymbol{N} = (N_0, \ldots, N_4) \qquad \boldsymbol{M} = (M_0, \ldots, M_4)$$

$$N_i(\rho) = \binom{4}{i} \tilde{\rho}^{4-i} \rho^i$$

$$M_0(\rho_1, \rho_2) = \tilde{\rho}_1^2 \tilde{\rho}_2^2 \qquad M_4(\rho_1, \rho_2) = M_0(\rho_1 \leftrightarrow \tilde{\rho}_1, \rho_2 \leftrightarrow \tilde{\rho}_2)$$

$$M_1(\rho_1, \rho_2) = \sum_{j=0}^{1} \binom{2}{j} \binom{2}{j+1} \rho_1^j \tilde{\rho}_1^{2-j} \rho_2^{1-j} \tilde{\rho}_2^{1+j}$$

$$M_2(\rho_1, \rho_2) = \sum_{j=0}^{2} \binom{2}{j}^2 \rho_1^{2-j} \tilde{\rho}_1^j \rho_2^j \tilde{\rho}_2^{2-j} \qquad M_3(\rho_1, \rho_2) = M_1(\rho_1 \leftrightarrow \tilde{\rho}_1, \rho_2 \leftrightarrow \tilde{\rho}_2)$$

$$\boldsymbol{M}(\rho_1, \rho_2) = \boldsymbol{M}(\rho_2, \rho_1)$$

and

$$\begin{aligned}
&S(\rho_{11}, c1, c4, \boldsymbol{N}(\rho_{22}), \boldsymbol{M}(\rho_{12}, \rho_{21})) \\
&\quad = \sum_{j=0}^{n} N_j(\rho_{22}) M_{n-j}(\rho_{12}, \rho_{21})(\delta_{n,3} + \rho_{11}(\delta_{n,2} + \tilde{c}1\delta_{n,1} + \tilde{c}4\delta_{n,4})).
\end{aligned} \tag{6}$$

Here $\tilde{c}1 = 1 - c1$ and $\tilde{c}4 = 1 - c4$.

Among the solutions of equations (5) and (6) of special importance are those three cases which reflect the symmetries of the underlying square lattice, as follows.

Case 1. $\rho_{11}(t) = \rho_{22}(t) \qquad \rho_{12}(t) = \rho_{21}(t).$ (7)

Such a solution may describe antiferromagnetic-type ordering (stripes along the square diagonal).

Case 2. $\rho_{11}(t) = \rho_{12}(t) \qquad \rho_{21}(t) = \rho_{22}(t).$ (8)

This special case can lead to stripes parallel to the horizontal edge of the square.

Case 3. $\rho_{11}(t) = \rho_{21}(t) \qquad \rho_{12}(t) = \rho_{22}(t).$ (9)

This may give vertical stripes, along the other edge of the square, perpendicular to the previous one.

A further symmetry allows the interchange of even and odd which leads to two equivalent solutions in all three cases.

For the family of rules investigated here (equation (3)) only cases 2 and 3 are of interest. They can account for the four phases observed in the computer experiment described in the previous section. It is also sufficient to restrict ourselves to, say, horizontal stripes only. So let us consider case 2 in the following. Then equations (5) and (6) reduce to ($\rho_{11} \equiv \rho_1$, $\rho_{22} \equiv \rho_2$):

$$\rho_1(t+1) = 6\rho_1^2\rho_2\tilde{\rho}_2^5 + 30\rho_1\tilde{\rho}_1\rho_2^2\tilde{\rho}_2^4 + 20\tilde{\rho}_1^2\rho_2^3\tilde{\rho}_2^3 + \rho_1[\rho_1^2\tilde{\rho}_2^6 + 12\rho_1\tilde{\rho}_1\rho_2\tilde{\rho}_2^5 + 15\tilde{\rho}_1^2\rho_2^2\tilde{\rho}_2^4 + \tilde{c}1(2\rho_1\tilde{\rho}_1\tilde{\rho}_2^6 + 6\tilde{\rho}_1^2\rho_2\tilde{\rho}_2^5) + \tilde{c}4(15\rho_1^2\rho_2^2\tilde{\rho}_2^4 + 40\rho_1\tilde{\rho}_1\rho_2^3\tilde{\rho}_2^3 + 15\tilde{\rho}_1^2\rho_2^4\tilde{\rho}_2^2)] \quad (10)$$

$$\rho_2(t+1) = [\text{the same as equation (10), but with } \rho_1 \leftrightarrow \rho_2,\ \tilde{\rho}_1 \leftrightarrow \tilde{\rho}_2]. \quad (11)$$

The fixed points of equations (10) and (11) give the equilibrium densities and are attained when

$$\rho_1(t+1) = \rho_1(t) \equiv \rho_1^* \qquad \rho_2(t+1) = \rho_2(t) \equiv \rho_2^*.$$

In addition to the trivial fixed points $\rho_{1t}^* = \rho_{2t}^* = 0$, equations (10) and (11) possess the homogeneous finite fixed point solutions

$$\rho_{1h}^* = \rho_{2h}^* = \langle\rho\rangle \quad (12)$$

which is the same as the fixed point of the standard MFA when applied to the automata (3). This solution is shown in figure 6 with a full line. Equation (12) is stable for all initial values $\rho_1(0)$, $\rho_2(0)$ for $c1$, $c4$ values lying in the regions II and III of figure 2.

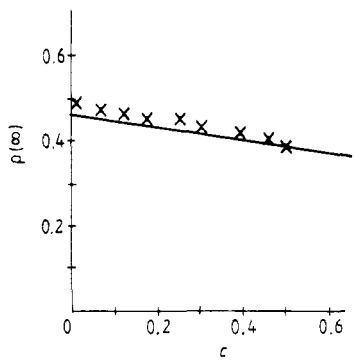

Figure 6. Average density of 1s along $c1 = c4 = c$. The full line represents the result of standard MFA; the crosses are results of computer simulation.

In region I of figure 2, however, an additional new pair of fixed points ρ_{1i}^*, ρ_{2i}^* appear ($\rho_1^* \neq \rho_2^*$) which can be reached from 'striped' initial states $\rho_1(0)$, $\rho_2(0)$ ($\rho_1(0) \neq \rho_2(0)$) only.

This bifurcation heralds a new phase which can be identified with the striped phase and the fixed points ρ_{1i}^*, ρ_{2i}^* with asymptotic densities $\rho_1(\infty)$, $\rho_2(\infty)$ of § 3. Accordingly, the theoretical prediction for the order parameter Δ, given by equation (4), is

$$\Delta = \frac{\rho_{1i}^* - \rho_{2i}^*}{\rho_{1i}^* + \rho_{2i}^*}.$$

ρ_{1i}^*, ρ_{2i}^* depend on $c1$ and $c4$, the corresponding dependence of Δ on $c1 = c4 = c$ is shown in figure 7 with a full curve. The transition is predicted to be of first order. The MF value of the critical noise strength is 0.178 83.

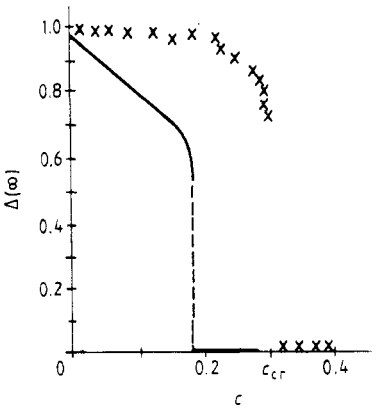

Figure 7. The order parameter Δ of the four-phase regime, defined in equation (4), as a function of the probability c ($c1 = c4 = c$). The experimental points marked by × have been obtained from 'striped' initial states with $\Delta(0) = 0.78$. The full curve is the result of inhomogeneous MFA.

5. Summary and discussion

Standard MFA for cellular automata is based on the supposition that the system is 'stirred' at each time step, the values at neighbouring sites of a centre cell are uncorrelated. For many CA rules the average density which can be calculated in such a way is near to the observed one (Wolfram 1983). This holds true also for the CA rule investigated here both in the disordered regime and in the four-phase region which follows the former upon decreasing $c1$ and $c4$. $\langle\rho\rangle$ changes continuously when crossing the phase boundary and has no relevance to the order which sets in. In the four-phase region the correlations manifest themselves mainly in stripe-forming action. It has been proposed here that the essence of these correlations can be accounted for by handling densities on, say, odd and even rows separately, in the framework of an inhomogeneous MFA. Starting with striped initial states (i.e. randomly distributed 1s in odd and even rows but with much differing probabilities) each centre cell observes a specifically correlated average neighbourhood. The time evolution of the system of equations for the two densities terminates at a strongly different pair of fixed points. The order parameter Δ (equation (4)) by which the four-phase region has been characterised is analogous to the magnetisation in a ferromagnet and the specifically prepared initial state may be thought of as if it had been produced by some instantaneous magnetic field. The same process of aligning the initial state has also been used in the computer experiment to measure the 'magnetisation'.

Naturally, a theory of such simplicity cannot be expected to give quantitatively correct results. The agreement between theory and experiment for the magnitude of Δ is within 20% (disregarding the shift in the transition point); the phase transition line in the $c1$, $c4$ plane is predicted qualitatively correctly. There is a discrepancy between theory and experiment concerning the position of this line ($\approx$40%), however, which is not surprising: order is destroyed only for higher probabilities $c1$ and $c4$ than predicted above, due to domain-structure-forming correlations which certainly cannot be accounted for in such a simple theoretical framework.

In the light of the well known success and usefulness of MFA in qualitatively predicting phase diagrams and yield order parameters (and other simple characteristics)

of ordered systems in condensed matter physics, it seems inspiring to explore the limits of the MFA effectiveness in the vast field offered by probabilistic cellular automata rules. Moreover, with its help, analogies with real physical (and other) systems may be worked out in more detail, for which the example presented in this paper might serve as an illustration.

Acknowledgments

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