

Phase Transitions of Cellular Automata

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Cellular automata (CA) are simple mathematical models of the dynamics of discrete variables in discrete space and time, with applications in nonequilibrium physics, chemical reactions, population dynamics and parallel computers. Phase transitions of stochastic CA with absorbing states are investigated. Using transfermatrix scaling the phase diagrams, critical properties and the entropy of one-dimensional CA are calculated. The corners of the phase diagrams reduce to deterministic CA discussed by Wolfram (Rev. Mod. Phys. **55**, 601 (1983)). Three-state models are introduced and, for special cases, exactly mapped onto two-state CA. The critical behaviour of other three-state models with one or two absorbing states and with immunization is investigated. Finally CA with competing reactions and/or with disorder are studied.

I. Introduction

Discrete lattice models like Ising, Potts or lattice gas models [1] have been very useful to understand cooperative phenomena in thermal equilibrium. For these models a dynamics may be defined by changing the discrete local variable according to the local Boltzmann weight [2]. Then also the relaxation into thermal equilibrium can be studied. Since such models are well suited for numerical simulations their applications to more complicated systems like disordered materials or incommensurable structures are still extensively investigated [3].

There is a very similar class of discrete models which are called cellular automata (CA) and which find wide and general applications in mathematics, physics, chemistry, biology and computer science [4]. As before these models have a finite set of variables on a lattice. The dynamics is defined in discrete time steps with rules depending on the local neighbourhood only. However now the dynamics is not restricted to the usual Boltzmann weight and detailed balance. Therefore it can model for instance chemical reactions, population changes or other nonlinear processes far from thermal equilibrium.

The local rules of CA may be stochastic or deterministic. In the latter case even one-dimensional CA show a complex interesting behaviour [5, 6].

Starting from a disordered state the system iterates into stationary patterns which appear to fall into four classes [6]:

- 1) Evolution leads to a homogeneous state
- 2) Evolution leads to a set of separated simple stable or periodic structures
- 3) Evolution leads to a chaotic pattern
- 4) Evolution leads to complex localized structures.

Thus simple local rules lead to a kind of selforganization. Even simple kinds of selfreproduction of local patterns are observed. Hence the investigation of CA may contribute to our understanding of spontaneous pattern formation [10].

The evolution of the states of CA may be considered as processing of information. If, as in Refs. [5] and [6], all variables are updated at the same time CA may be considered as parallel computers the general theory of which may be useful for constructing new computer generations. Wolfram [6] suggests that local rules of class 4 are capable of universal computation. This means, if the initial state is considered as a program and initial data the CA is capable of evaluating any (computable) function.

If the local rules of CA are stochastic then again

new complex behaviour is observed [7]. In contrast to equilibrium dynamics even one-dimensional CA show continuous phase transitions with universal critical exponents and scaling laws [7, 8]. At least some of these transitions are in the same universality class as those directed percolation and Reggeon field theory [9].

Although D -dimensional CA describe processes far from thermal equilibrium they can be mapped on to $D+1$ -dimensional statistical mechanics [11–13]. However, in the interesting case of absorbing states the configuration space is very restricted [12].

In this paper the phase transitions of stochastic one-dimensional CA are investigated in more detail. In Sect. II the models are defined and duality relations derived. Using transfermatrix scaling [14] phase diagrams, critical properties and the entropy are calculated in Sects. III, IV and V. In particular the transitions between deterministic CA of different classes are investigated. The question of universality of CA transitions is addressed in the two following sections. Although increasing the number of local variables should not change the universality class [15], new kinds of transitions were recently reported for reactions with immunization [16] and reactions with two absorbing states [17]. Therefore 3-state CA are introduced in Sect. VI and exact mappings to 2-state CA are derived. Section VII investigates universality. CA with competing and random reaction rates are shortly discussed in Sects. VIII and IX. Finally the summary is presented in the last section. Details of the numerical method may be found in the appendix.

II. Definition of the Model

Consider an one-dimensional chain of N lattice sites. Each site may be in one of the k -states $S_v = 0, 1, 2, \dots, k-1$. Thus the whole chain has k^N states. In the following a given state (S_1, S_2, \dots, S_N) is labelled by the integer

$$i = \sum_{v=1}^N S_v k^{v-1}. \quad (1)$$

Now consider an ensemble of such states where each state i occurs with the probability P_i . This probability $P_i(t)$ evolves in discrete time steps $t=0, 1, 2, 3, \dots$ according to some transition probabilities T_{ij}

$$P_i(t) = \sum_{j=0}^{k^N-1} T_{ij} P_j(t-1). \quad (2)$$

Thus the transfermatrix T_{ij} is the probability to get a state i if the system is in state j one time step before.

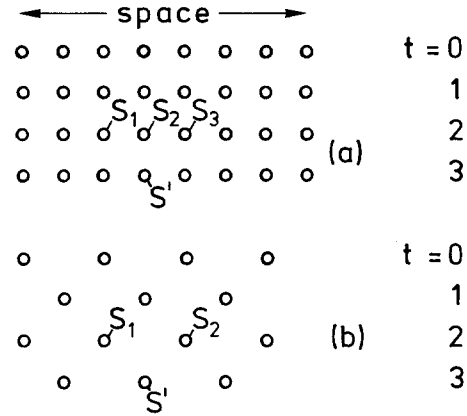


Fig. 1a and b. Geometries of one-dimensional CA studied in this paper. The probability to find variable S' at time $t=3$ depends only on the local neighbourhood S_1, S_2, S_3 (or S_1, S_2) at time $t=2$

In CA T_{ij} is defined by local rules:

$$T_{ij} = \prod_{v=1}^N p(S_{v-1}^j, S_v^j, S_{v+1}^j | S_v^i) \quad (3)$$

where S_v^j and S_v^i are the site variables of states j and i , respectively. Thus the transition of the variable S_v^j depends only on its nearest neighbours and on itself (compare with Fig. 1a). The generalizations to more neighbours is straightforward. The whole time evolution is defined by the k^3 by k matrix \underline{p} . Since the variable S_v^j has to go in one of the k possibilities S_v^i in the next time step, the matrix \underline{p} has only $k-1$ independent elements per row. If left-right symmetry is used or in addition \underline{p} depends only on the sum $S_{v-1}^j + S_v^j + S_{v+1}^j$ (totalistic rules [6]) then the number of elements of \underline{p} is reduced even more. Note that with rule (3) each site is updated simultaneously, while in usual Monte-Carlo-dynamics only one site is updated per time step [3].

In the deterministic limit the elements of \underline{p} are only one or zero, therefore each state i has a unique path as a function of time. In this case the local rules $p(S_1 S_2 S_3 | S')$ are defined by a single integer number n [5]

$$n = \sum_{\alpha=0}^{k^3-1} S'(\alpha) k^\alpha \quad (4)$$

where $\alpha = S_1 k^2 + S_2 k + S_3$ denotes the neighbourhood of the variable S_2 and $S'(\alpha)$ is the variable S' which the system takes at time $t+1$ if the system is in state (S_1, S_2, S_3) at time t (compare with Fig. 1(a)). For example, if for $k=2$ the deterministic rule table reads

$$\begin{array}{cccccccc} 111 & 110 & 101 & 100 & 011 & 010 & 001 & 000 \\ \hline 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 \end{array}$$

then one gets rule $n = (00010110)_2 = 22$, etc.

Note that the example above is a totalistic rule; in this case the rule can be denoted by another integer m

$$m = \sum_{\alpha=0}^{3(k-1)} S'(\alpha) k^\alpha \quad (5)$$

where $\alpha = S_1 + S_2 + S_3$ and $S'(\alpha)$ is again the new variable S' given (S_1, S_2, S_3) in the preceding time step. In the example above one has $m = (0, 0, 1, 0)_2 = 2$. In Refs. [5] and [6] only symmetric CA with absorbing state 0 ($p(000|0) = 1$) are considered, thus for $k=2$ there remain 32 general and 8 totalistic rules which fall into the first three classes mentioned in the Introduction. In Sects. III and IV phase transitions between these rules are investigated.

Note that $p(S_1, S_2, S_3|S')$ may be written as $\exp[-\mathcal{H}(S_1, S_2, S_3, S')/k_B T]$. Therefore T_{ij} may be considered as a row-to-row transfermatrix of a two-dimensional k -state model of equilibrium statistical mechanics [12, 13]. In general \mathcal{H} contains all kinds of interactions between S_1, S_2, S_3 and S' . The interesting case of an absorbing state, i.e. $p(000|0) = 1$ transforms into infinitely strong couplings in \mathcal{H} or, equivalently, to a restricted phase space in the partition sum [12].

Consider a $k=2$ reaction on the lattice of Fig. 1(b), which is equivalent to an alternating odd-even reaction on the process of Fig. 1(a) [12]. In this case the matrix $p(S_1 S_2|S')$ is a 4 by 2 matrix, only. For special reaction rates this process is equivalent to two-dimensional directed percolation [7, 14]. In this case $S_v = 1(0)$ means that the site v can (cannot) be reached by a directed path from the top of the system (or from a seed point at $t=0$). If the bond and site probabilities are given by p_b and p_s , respectively, one has

$$\begin{aligned} p(11|1) &= p_s p_b (2 - p_b) \\ p(01|1) &= p(10|1) = p_s p_b \\ p(00|1) &= 0. \end{aligned} \quad (5)$$

Also the case of different left-right-probabilities $p(01|1) \neq p(10|1)$ has been studied which for $p(01|1) = p(11|1) = 1$ was solved exactly [18].

There is a simple symmetry relation from permutating the notations of the variables S_v . For instance for $k=2$ this “duality” relation maps a CA with rule p to the same one with rule p' given by

$$p'(S_1 S_2 S_3|S') = 1 - p(\bar{S}_1 \bar{S}_2 \bar{S}_3|S') \quad (6)$$

where $\bar{S} = (S+1)$ modulo 2. As shown below for some special cases critical points can be obtained from selfdual points $p = p'$.

III. Phase Diagrams

In this section phase boundaries of one-dimensional two-state ($k=2$) CA are calculated by transfermatrix scaling (see Appendix). In Fig. 2 the phase diagram of the reaction process of Fig. 1(b) is shown for $p_1 = p(01|1) = p(10|1)$, $p_2 = p(11|1)$ and $p_0 = p(00|1) = 0$ [19].

For a finite system of N lattice sites and for any values of $p_1 < 1$ and $p_2 < 1$ any initial state $P_i(t=0)$ decays exponentially fast to the stationary state $P_0(t=\infty) = 1$ and $P_i(t=\infty) = 0$ for $i \neq 0$. This is shown in the following:

- (i) With $p_0 = 0$ one has $T_{00} = 1$ and $T_{0j} = 0 (j \neq 0)$
- (ii) From this one obtains the eigenvector $\varphi_0 = 1$ and $\varphi_i = 0 (i \neq 0)$ for the largest eigenvector $\lambda_0 = 1$.

- (iii) Then one has $P(t) = \underline{T}^t \cdot P(0) \sim \lambda_0^t \cdot \varphi \left[1 + 0 \left(\frac{\lambda_v}{\lambda_0} \right)^t \right]$

where the last equation holds asymptotically for large t . Since all other eigenvalues λ_v are smaller than $\lambda_0 = 1$ (which follows from Frobenius [20]) one obtains the desired result with the relaxation time τ given by the second largest eigenvalue $\lambda_1: \tau = (-\ln \lambda_1)^{-1}$.

In the thermodynamic limit $N \rightarrow \infty$ the situation changes: Then for p_1 and p_2 large enough λ_0 is degenerate with λ_1 and the system has two stationary states $(\varphi_i^0)_i$ as above and $(\varphi_i^1)_i$, where all states $P_i(t=0)$ (except φ_i^0) decay exponentially fast to the state $P_0(t=\infty) = 0$ and $P_i(t=\infty) = -\varphi_i^1/\varphi_1^1$. Thus in the left part of Fig. 2 (=absorbing phase) the variable 1 always dies out, while in the right part (in the active phase) the stationary state has a nonzero fraction of variable 1. In between there is a sharp phase transition whose properties are discussed in the following section. Note that according to (5) directed bond ($p_s = 1$), site ($p_b = 1$) and mixed ($p_s = p_b$) percolation are single lines shown in Fig. 2.

The corners of the phase diagram, Fig. 2, are deterministic CA. The three corners $(p_1, p_2) = (0, 0)$, $(0, 1)$ and $(1, 1)$ (rules $m=0, 4$ and 6) belong the class-1 CA. In the first two cases an initial disordered state decays to the state $i=0 = (000 \dots 00)_2$. For the rule $m=6$ the initial state decays to $i=2^N - 1 = (111 \dots 11)_2$. The CA $(p_1, p_2) = (1, 0)$ (rule $m=2$) belongs to class 3. Since in this case $S' = S_1 + S_2$ (modulo two) it behaves like the rule 90 of [5]:

A single occupied site creates a Pascal's triangle modulo two, as shown in Fig. 3. It is a selfsimilar structure with fractal dimension $\log_2 3 \simeq 1.5850$. If the initial state is disordered then one still obtains triangles on all length scales although the pattern is not selfsimilar.

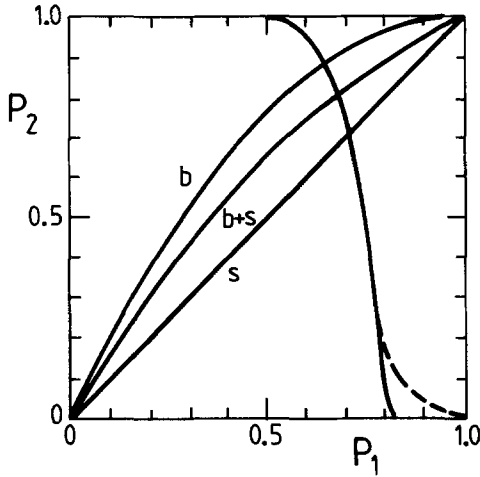


Fig. 2. Phase diagram of a 1-dim. 2-state CA constructed from Fig. 1(b). The full line is the result from scaling systems with 10, 9 and 8 sites. The expected result is indicated by the dashed line. The lines b , $b+s$ and s mark the subspaces of directed bond, mixed bond-site and site percolation, respectively

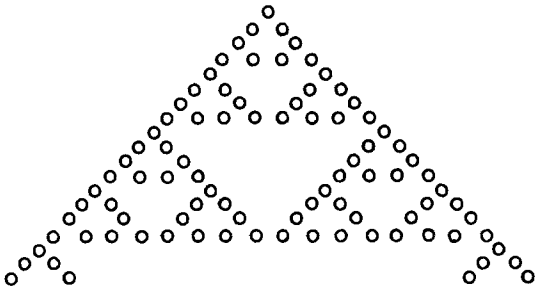


Fig. 3. Pattern created from a 1-dimensional CA (Fig. 1(b)) with deterministic rule $m=2$. The circles show the variable $S=1$ while the empty sites belong to $S=0$. The structure is a Pascal's triangle modulo two, it is selfsimilar with a fractal dimension $\log_2 3 \approx 1.586$ [5]

For finite chains with N sites the class-3 system evolves into periodic structures which sensitively depend on N . It is presumably for this reason that finite-size scaling does not work close to the deterministic CA with rule $m=2$, (note that one has to compare correlation lengths of strips with $N-2$, $N-1$, and N to get the critical point). For some triple of strips one gets a transition on the $p_2=0$ boundary of Fig. 2 while for other triples the phase boundary bends up again. Presumably the ordered state of Fig. 3 is not dense enough to support a transition away from the deterministic limit, and the phase boundary behaves as shown by the dashed line in Fig. 2. However, this has still to be shown, may be by Monte Carlo simulations on larger systems [8].

The line $p_2=1$ of Fig. 2, is mapped to itself by the duality transformation Eqs. (6), in particular one has

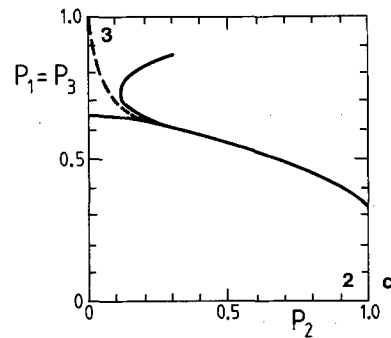
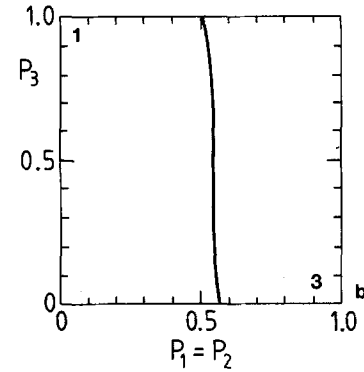
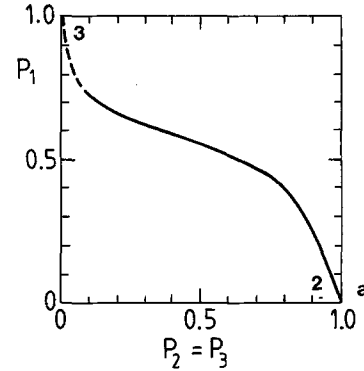


Fig. 4a-c. Phase diagram of a 1-dim. CA (Fig. 1(a)) with totalistic rules and one absorbing state ($p_0=0$). The full lines show the results from transfermatrix-scaling ($N \leq 15$), the error estimate is less than the thickness of the lines. The splitted line of c shows the results from $N=9$ and $N=8$, showing that the method fails close to class-3 CA. The expected extrapolations are indicated by dashed lines. The corners of the phase diagrams are deterministic CA which belong to different classes [6], the class number is shown in the figure and in Table 1

$p'_1 = 1 - p_1$. Thus the phase boundary has to end at the point $p_{1c} = 1/2$. In fact this upper boundary has two absorbing states $i=0$ and $i=2^k-1 = (111 \dots 11)_2$. An initial state decays into domains of $i=0$ and $i=2^k-1$. The domain walls diffuse with a drift given by $p_1 - 0.5$. For zero drift ($p_1 = 1/2$) the

Table 1. Deterministic corners of the (p_2, p_1, p_0) -cube of a 2-state CA with totalistic rules and one absorbing state. The partition into several classes is taken from Ref. 6

p_3	p_2	p_1	p_0	Rule numbers		Class
				m	n	
0	0	0	0	0	0	1
0	0	1	0	2	22	3
0	1	0	0	4	104	2
0	1	1	0	6	126	3
1	0	0	0	8	128	1
1	0	1	0	10	150	3
1	1	0	0	12	232	2
1	1	1	0	14	254	1

walls move like an annihilating random walk. On the average it takes a time $t \sim l^2$ before two walls with a distance l meet and annihilate [12, 21].

In addition this point is an endpoint of a disorder line of an exactly solved two dimensional Ising model on a triangular lattice [12]. Therefore this model can be solved exactly on the line $p_2=1$ and on a special line in the (p_0, p_1, p_2) -cube. However, phase transitions occur only for $p_0=0$, i.e. if the system has absorbing states [8]. p_0 may be considered as a source of particles ($S=1$) or as a ghost field in percolation [12, 22] which destroys the phase transition like an external field in ferromagnets.

Now we consider the CA on the geometry of Fig. 1(a). Some cuts of the phase diagrams are shown in Fig. 4. Only totalistic rules are considered, thus one has only 4 independent reaction probabilities $p_0=p(000|1)$,

$$p_1=p(100|1)=p(010|1)=p(001|1),$$

$$p_2=p(011|1)=p(101|1)=p(110|1)$$

and

$$p_3=p(111|1).$$

The eight possible deterministic CA (with absorbing state, $p_0=0$) are shown in Table 1 and have extensively been discussed by Wolfram [5]. His numerical investigations suggest that these CA belong to one of the first three classes mentioned in the Introduction (to get class 4 one needs $k \geq 3$ or more than nearest neighbours [6]). These classes are indicated in Table 1 and in Fig. 4. Figure 4 shows that there is always a phase boundary between rule $m=0$ ($p_1=p_2=p_3=0$) and $m=14$ ($p_1=p_2=p_3=1$), i.e. between a completely absorbing phase $(0, 0, 0, \dots)$ and active phase with a nonzero fraction of variable $S_v=1$. However, even the qualitative behaviour of the phase boundary cannot be related to the class of the deterministic corners. Thus Fig. 4(b) shows a phase

transition to a CA of class 3 while in Figs. 4(a) and 4(b) the phase boundaries seem to end at the class-3 CA [23]. In Fig. 4(a) the transition ends at a class-2 CA while in Fig. 4(c) one has only an absorbing stationary state close to the class-2 corner. Note that in Fig. 4(b) the transition ends exactly at $p_3=1$, $p_1=p_2=1/2$ due to duality, Eq. (6).

A simple mean field approximation is obtained by stirring the system at every time step before the next reaction occurs [7]. From this the fraction x_t of sites with variable $S_v=1$ evolves as a function of time t like a discrete cubic map

$$x_{t+1} = 3p_1 x_t (1-x_t)^2 + 3p_2 x_t^2 (1-x_t) + p_3 x_t^3 \quad (7)$$

This maps gives a continuous phase transition for $p_1=1/3$ independent of p_2 and p_3 . Figure 4 shows that spatial fluctuations change the mean field phase boundary drastically.

The corners of Figs. 2 and 4 which belong to a class-3 deterministic CA show a certain structure [5, 6]. For finite chains this behaviour is reflected in the occurrence of periodic patterns, which shows up in the degeneracy of eigenvalues of the transfermatrix T_{ij} . However, at least for one-dimensional CA such structures are destroyed by stochastic rules, as already noted in Ref. [5]. We have confirmed this by calculating the correlation times of the oscillating parts given by the eigenvalue $\lambda_2, \lambda_3, \dots$ of the transfermatrix T_{ij} , Eq. (3). While the correlation of the monotonic decay $\tau_1 = -(\ln \lambda_1)^{-1}$ is large and grows exponentially with N in the active phase, all other correlation times τ_i are very small (although all approach infinity at the deterministic limits) and we could not detect any scaling behaviour. It would be interesting to see whether such structures are stable in high spatial dimensions.

IV. Critical Properties

The phase transitions of stochastic CA with one absorbing state are continuous transitions. As in critical phase transitions of equilibrium systems [24] observable quantities have a singular part which obeys power laws with universal critical exponents and scaling relations [7, 8, 15, 25]. Below $D=4$ space dimensions these exponents differ from their mean field values [9, 25].

For $D=1$ the critical exponents and reaction rates can be determined from transfermatrix-scaling (see Appendix) [14]. The correlation time $\tau(p-p_c, p_0, \frac{1}{N})$ of a system of N sites scales asymptotically for large N as (for any scale factor b)

$$\tau\left(\varepsilon, p_0, \frac{1}{N}\right) = b^z \tau\left(b^{1/\nu_1} \varepsilon, b^{\omega/\nu_1} p_0, \frac{b}{N}\right). \quad (8)$$

Here ε means some deviation from the critical surface in the $p_0=0$ space. In addition it is assumed that the source p_0 of $S=1$ states is the scaling field in the “magnetic” space. This is similar to usual percolation where p_0 is the probability to percolate to a “ghost site” [22]. $z=v_{\parallel}/v_{\perp}$ is the dynamic exponent which relates a change of length scale to a change of time scale. v_{\parallel} and v_{\perp} describe how the correlation time τ , the correlation length ξ and reaction velocity v behave at the critical surface; one has

$$\begin{aligned}\tau(\varepsilon) &\sim \varepsilon^{-v_{\parallel}} \\ \xi(\varepsilon) &\sim \varepsilon^{-v_{\perp}} \\ v(\varepsilon) &\sim \varepsilon^{v_{\parallel}-v_{\perp}}.\end{aligned}\quad (9)$$

The number $c(\varepsilon)$ of “active” sites $S=1$ and the probability $P(t)$ of having an active site $S_v=1$ at time t if one has $S_v=1$ at $t=0$ is described by the exponent β :

$$\begin{aligned}c(\varepsilon) &\sim \varepsilon^{\beta} \\ P(t) &\sim t^{\beta/v_{\parallel}} \quad (\text{at criticality } \varepsilon=0).\end{aligned}\quad (10)$$

Using the usual scaling relations [7, 24] β is related to the “magnetic” scaling power ω by

$$\beta = v_{\parallel} + v_{\perp} - \omega. \quad (11)$$

The exponents z , v_{\parallel} and v_{\perp} have been calculated from (8) in [14] for the three cases of directed percolation in Fig. 2. One obtains

$$\begin{aligned}v_{\parallel} &= 1.734 \pm 0.002, \\ v_{\perp} &= 1.100 \pm 0.005, \\ z &= 1.582 \pm 0.001.\end{aligned}\quad (12)$$

Table 2 shows the results for $z+\omega/v_{\perp}$ obtained from (8) for $p_1=p_2=0.7058$ in Fig. 2 [14], and the resulting β calculated from Eqs. (11) and (12). The extrapolated result agrees with the value of β collected from other methods [7]:

$$0.273 \pm 0.002 \quad (13)$$

Due to universality these critical exponents are expected to describe the critical properties along all phase boundaries in Figs. 2 and 4. In fact, for the three percolation points on the transition line of Fig. 2 the numerical results are consistent with the values of (12) [7, 14]. Figure 5 shows the exponent z calculated from chains with $N-1$, N and $N+1$ sites for three other examples of the reaction process shown in Fig. 4: (i) all diagonals on Fig. 4, $p_1=p_2=p_3=p$ with a critical point $p_c=0.5385 \pm 0.0005$, (ii) the bottom line of Fig. 4(b) $p_1=p_2=p$, $p_3=0$ with $p_c=0.573$

Table 2. Estimate for the critical exponent $z+\omega/v_{\perp}$ obtained from transformmatrix-scaling of the $k=2$ state CA of Fig. 2 with $p_1=p_2$. β is given by the scaling relation Eq. (11) and the exponents z and v_{\perp} taken from Ref. 14

$N-1/N/N+1$	$z+\frac{\omega}{v_{\perp}}$	β
3/4/5	3.787	0.415
4/5/6	3.801	0.399
5/6/7	3.830	0.367
6/7/8	3.845	0.351
7/8/9	3.851	0.344
8/9/10	3.865	0.329
9/10/11	3.872	0.321
10/11/12	3.878	0.315
11/12/13	3.883	0.309
12/13/14	3.887	0.304
13/14/15	3.898	0.293

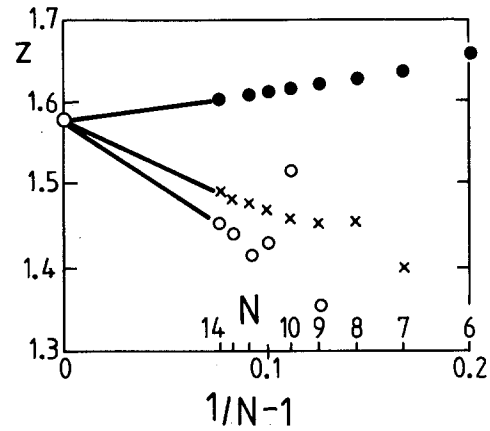


Fig. 5. Estimates z_N for the dynamical critical exponent z as a function of system size N for $p_1=p_2=p_3$ (dots); $p_1=p_2$, $p_3=0$ (crosses); $p_1=p_3$, $p_2=1$ (circles) of the model Fig. 4

± 0.005 and (iii) the right endpoint of Fig. 4(b), $p_2=1$, $p_1=p_3=p$ with $p_c=0.333 \pm 0.002$. Although there is still a strong and sometimes a nonmonotonic N -dependence, the results are consistent with the value of z in (12) and thus consistent with universality.

However, at the selfdual endpoints with two absorbing states there is a different critical behaviour given by an annihilating random walk: In Fig. 2 for $p_2=1$, $p_1=1/2$ the exact solution gives $v_{\parallel}=1$, $v_{\perp}=1/2$, $z=2$ [12]; in Fig. 4(b) for $p_3=1$ and $p_1=p_2=1/2$ we have calculated the exponent z from (8), the results are consistent with $z=2$.

V. Entropy, Coverage and Kink-Density

As discussed in Sect. III, the ($k=2$) stochastic CA of Figs. 2 and 4 have a transition from an absorbing phase which has only the absorbing state

$i=(0,0,0,\dots)$ to an active phase with a nonzero coverage c defined by

$$c = \sum_{i=0}^{2^N-1} \frac{c_i}{N} P_i^0 \quad (14)$$

where $P_i^0 = P_i(t=\infty)$ is the stationary probability to find state i and $c_i = \sum_{v=1}^N S_v^i$ is the number of active sites $S_v^i = 1$. As a measure for the amount of order in the active phase one may define an entropy S by (measure or metric entropy in Ref. 6)

$$S = - \sum_{i=0}^{2^N-1} P_i^0 \ln P_i^0. \quad (15)$$

Another quantity of interest may be the average number n of 01 or 10 “kinks” on the chain given by

$$n = \sum_{i=0}^{2^N-1} n_i P_i^0 \quad (16)$$

where n_i is the fraction of kinks of state i .

All of these quantities c , S and n may be considered as order parameters since they are zero in the absorbing phase; there only the state $i=0$ is occupied. In particular they are zero in *finite* systems of N sites since an active phase appears in the thermodynamic limit only (compare with Sect. III).

This is similar to a ferromagnet where a spontaneous magnetization can occur in the thermodynamic limit only. Nevertheless there is a possibility to get the order parameter from the eigenvectors of the transfermatrix [26]. Here we use a similar method to get c , S and n from the eigenvector (φ_i^1) of the second largest eigenvector λ_1 of the matrix T_{ij} , Eq. (3).

Any initial distribution $P_i(t=0)$ may be expanded in (right) eigenvectors φ_i^v and eigenvalues λ_v of the transfermatrix T_{ij}

$$P_i(t=0) = \sum_v a_v \varphi_i^v. \quad (17)$$

Then the stationary state is given by

$$P_i^0 = \lim_{t \rightarrow \infty} \sum_v \lambda_v^t a_v \varphi_i^v = a_0 \varphi_i^0 + a_1 \varphi_i^1. \quad (18)$$

The last equation holds in the active phase only since there one has $\lambda_0 = \lambda_1 = 1$. Since $\varphi_i^0 = 0$ for $i \neq 0$ (compare with Sect. III) the stationary distribution is proportional to φ_i^1 for $i \neq 0$. Taking $P_0(t=0) = 0$ one has $P_0^0 = 0$ since $T_{i0} = 0$ for $i \neq 0$. Thus

$$P_i^0 = \begin{cases} 0 & i=0 \\ -\varphi_i^1/\varphi_0^1 & i \neq 0 \end{cases} \quad (19)$$

The normalization factor follows from that fact that $\varphi_i^0 = 1$ is the left eigenvector of λ_0 , therefore $\sum_i \varphi_i^1 = 0$.

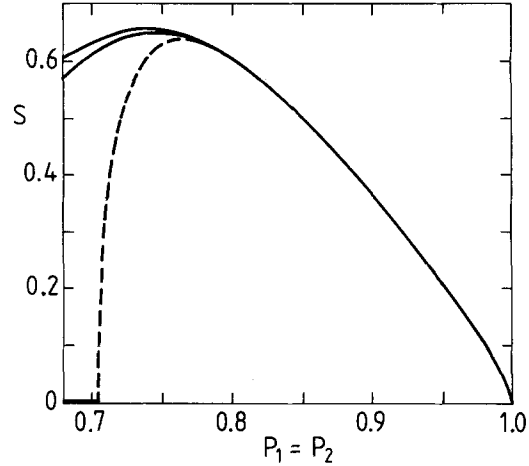


Fig. 6. Entropy S on the line s of Fig. 2 for $N=8$ (upper) and $N=10$ (lower full line). The dashed line sketches the law $S \sim (p - p_c)^\beta$ obtained from finite size scaling ($p_c = 0.7058 \pm 0.0001$ [7])

The situation here is different from the one of usual statistical mechanics like in ferromagnets where a symmetry is broken spontaneously. There φ_i^0 still describes the disordered phase since states with positive and negative magnetization have the same coefficients. But in the ordered phase one needs both φ_i^0 and φ_i^1 in (18) to get the statistical weight for states with only positive magnetization and therewith the magnetization.

We have used Eq. (19) for a *finite* system to calculate c , S and n approximately for the *infinite* system with Eqs. (14), (15) and (16). Figure 6 shows the result for the entropy S as a function of $p = p_1 = p_2$ of the CA of Fig. 2. Close to $p = p_c$ S has its maximum which is close to the entropy of the completely disordered case, $S = \ln 2 = 0.6931\dots$. In the infinite system, $N = \infty$, one has $S = 0$ below the critical point $p_c = 0.7058 \pm 0.0001$ [14]. However, for $N=8$ and 10 S is still very large below p_c but slowly decreases with increasing N . We have tried to estimate the critical behaviour from the N -dependence at $p = p_c$. Following the theory of finite size scaling [27] one has for $N \rightarrow \infty$, neglecting corrections to scaling and the regular part

$$\begin{aligned} S(p_c, N) &\sim N^{-x/\nu_1} \\ c(p_c, N) &\sim N^{-\beta/\nu_1} \\ n(p_c, N) &\sim N^{-y/\nu_1} \end{aligned} \quad (20)$$

where the exponents, x , β and y describe the critical behaviour in the infinite system for $p \gtrless p_c$

$$\begin{aligned} S(p, \infty) &\sim (p - p_c)^x \\ c(p, \infty) &\sim (p - p_c)^\beta \\ n(p, \infty) &\sim (p - p_c)^y. \end{aligned} \quad (21)$$

Table 3. Entropy S , coverage c and kink density n of the $k=2$ state CA of Fig. 2 at the critical point $p_1=p_2=0.7508$ for different sizes N

N	S	c	n
6	0.6587	0.5597	0.4162
7	0.6503	0.5261	0.3977
8	0.6407	0.5206	0.3822
9	0.6309	0.4981	0.3690
10	0.6231	0.4921	0.3575
11	0.6120	0.4757	0.3475
12	0.6032	0.4700	0.3386
13	0.5948	0.4573	0.3306
14	0.5869	0.4521	0.3235
15	0.5794	0.4419	0.3170

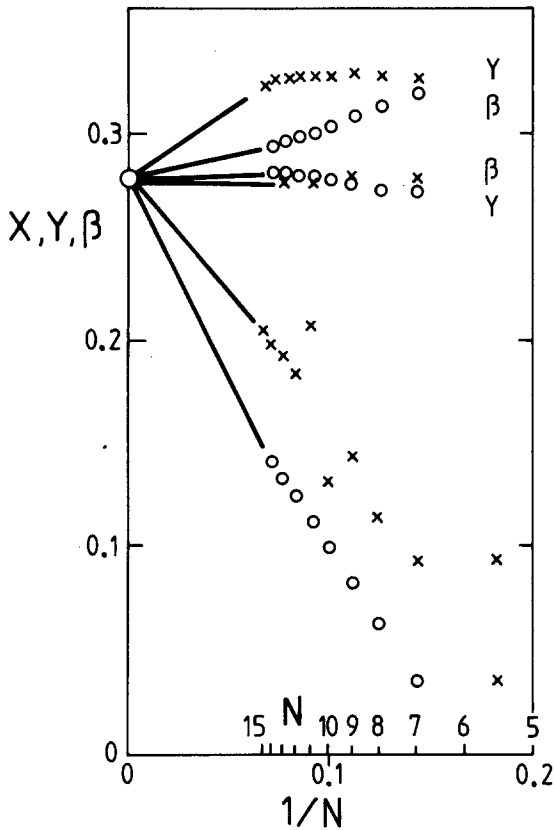


Fig. 7. Estimates of the critical exponents x, y and β of entropy, kink density and coverage, respectively obtained from scaling systems with sizes N and $N-1$ at the critical point. The crosses are from the $k=2$ CA of Fig. 2 with $p_1=p_2=0.7508$ and absorbing boundary condition, the circles are from the $k=2$ CA of Fig. 4 with $p_1=p_2=p_3=0.5385$ and periodic boundary conditions

If the influence of correlations can be neglected then one has $S \sim c \ln c$ and $n \sim c$, in this case one gets $y = x = \beta$.

Table 3 and Fig. 7 show the results for two different models. In fact all exponents seem to converge for $N \rightarrow \infty$ to the value of β of (13). The slow converge of $x(N)$ seems to be due to the logarithmic cor-

rections. Hence the coverage, the entropy and the kink density decay to zero at p_c with the critical exponent β . Note that β is determined from the properties of zero source $p_0=0$ while in Table 2 the scaling of p_0 was used to derive β .

VI. Three State Models: Exact Mappings to Two State Processes

In this section we investigate $k=3$ state stochastic CA for two reasons: (i) those models may have applications on multicomponent reactions (ii) the problem of universality of the phase transitions of those models is considered in the following section. Here we show that special $k=3$ processes can be mapped onto $k=2$ CA.

To see this consider the transfermatrix T_{ij} of (2) with $S_v^i \in \{0, 1, 2\}$. In the following the CA is restricted to processes which see the configurations of variable $S_v^i=0$, only, independent of the distribution of $S_v^i=1$ and $S_v^i=2$. For example for the local rule $p(S_1, S_2 | S')$ of the geometry, Fig. 1(b) one has

$$\begin{aligned} p(11|0) &= p(12|0) = p(22|0) = \tilde{p}(11|0) \\ p(01|0) &= p(02|0) = \tilde{p}(01|0). \end{aligned} \quad (22)$$

Now all $k=3$ states $\alpha = (S_1, S_2, \dots, S_N)$ are mapped to $k=2$ states $\tilde{\alpha}$ by changing the variable $S_v=2$ to $\tilde{S}_v=1$, for example if $\alpha = (0, 1, 0, 2)$ then $\tilde{\alpha} = (0, 1, 0, 1)$. Thus a whole class of states α is mapped into a single state $\tilde{\alpha}$. This mapping defines a transfermatrix $\tilde{T}_{\tilde{\alpha}\tilde{\beta}}$ of a $k=2$ CA as follows

$$\tilde{T}_{\tilde{\alpha}\tilde{\beta}} = \sum_{\alpha \in \tilde{\alpha}} T_{\alpha\beta} \quad (23)$$

where the sum runs over all states α of class $\tilde{\alpha}$ and β is a state of class $\tilde{\beta}$. Equation (23) is a valid definition since the right side does not depend on the state β of class $\tilde{\beta}$. Namely one has with (3)

$$\tilde{T}_{\tilde{\alpha}\tilde{\beta}} = \sum_{\alpha \in \tilde{\alpha}} \prod_v p(S_v^\beta S_{v+1}^\beta | S_v^\alpha) \quad (24)$$

which may be written as a single product of terms $p(S_v^\beta S_{v+1}^\beta | 0)$ if $S_v^\alpha=0$ or

$$[p(S_v^\beta S_{v+1}^\beta | 1) + p(S_v^\beta S_{v+1}^\beta | 2)] = [1 - p(S_v^\beta S_{v+1}^\beta | 0)]$$

if $S_v^\alpha \neq 0$. In both cases, by the restriction (22), the expressions depend on the configuration of zero's only, that is they depend on $\tilde{\beta}$, only. Therefore (23) and (24) do not depend on the special state β but only on $\tilde{\beta}$.

Now let λ be an eigenvalue of $T_{\alpha\beta}$ with right eigenvector $(\varphi_\alpha)_\alpha$. Then one has with Eq. (23)

$$\begin{aligned}
\sum_{\beta} T_{\alpha\beta} \varphi_{\beta} &= \lambda \varphi_{\alpha} \\
\Rightarrow \sum_{\alpha \in \tilde{\alpha}} \sum_{\beta} T_{\alpha\beta} \varphi_{\beta} &= \lambda \sum_{\alpha \in \tilde{\alpha}} \varphi_{\alpha} \\
\Rightarrow \sum_{\beta} \sum_{\tilde{\beta} \in \tilde{\alpha}} T_{\tilde{\alpha}\tilde{\beta}} \varphi_{\beta} &= \lambda \sum_{\alpha \in \tilde{\alpha}} \varphi_{\alpha} \\
\Rightarrow \sum_{\beta} \tilde{T}_{\tilde{\alpha}\tilde{\beta}} \tilde{\varphi}_{\tilde{\beta}} &= \lambda \tilde{\varphi}_{\tilde{\alpha}}, \quad \tilde{\varphi}_{\tilde{\alpha}} = \sum_{\alpha \in \tilde{\alpha}} \varphi_{\alpha}.
\end{aligned} \tag{25}$$

Therefore, if $\tilde{\varphi}_{\tilde{\alpha}} \neq 0$, λ is an eigenvalue of \tilde{T} with eigenvector $\tilde{\varphi}$. From this it follows, that these special $k=3$ CA are equivalent to $k=2$ CA with local rules \tilde{p} defined in Eq. (22).

VII. Universality Classes

Critical phase transitions in thermal equilibrium have universal properties like critical exponents and scaling functions which do not depend on microscopic details of the system [24]. In particular they do not depend on the kind of the lattice nor the range of the interactions, but e.g. for Potts models they depend on the number of variables per site [1].

Field theoretic investigations indicate [15] that for nonequilibrium phase transitions with absorbing states the critical properties do *not* depend on the number k of local variables, in contrast to equilibrium statistical mechanics. On the other side, for CA with two absorbing states [17] and CA with long time memory [16] new universality classes were reported. Here we study these problems for one-dimensional CA.

a) $k=3$ CA with one Absorbing State

First consider a $k=3$ state CA with one absorbing state $i=0$. For simplicity we use the geometry of Fig. 1(b), thus the reaction rate is given by a 9×3 matrix $p(S_1 S_2 | S')$, Eq. (3). Using the symmetries between left and right and between variables $S_v^i=1$ and $S_v^i=2$ [e.g. $p(12|1)=p(12|2)$] only five independent transition probabilities are left:

$$\begin{aligned}
p(12|1) &= p_1, & p(01|1) &= p_2, & p(02|1) &= p_3, \\
p(11|1) &= p_4, & p(22|1) &= p_5.
\end{aligned} \tag{26}$$

In this five dimensional parameter set there is a subspace which can be mapped onto a $k=2$ state CA. Namely, according to Sect. VI, the $k=3$ CA has the same critical behaviour of the CA of Fig. 2 (with \tilde{p}_1 and \tilde{p}_2) if

$$2p_1 = p_4 + p_5. \tag{27}$$

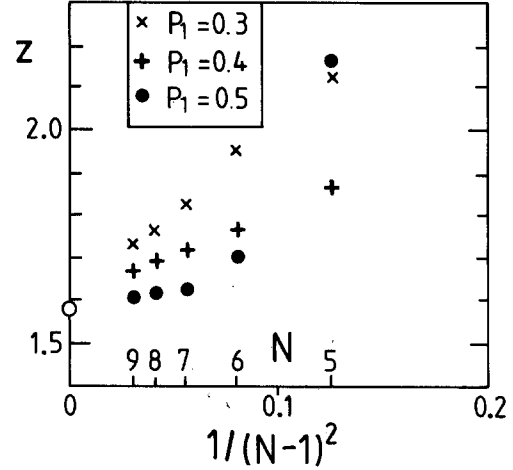


Fig. 8. Estimates of the dynamical critical exponent z from scaling systems with sizes $N, N-1$ and $N-2$ with periodic boundary conditions. The model is the $k=3$ state CA of Fig. 1(b) with one absorbing state and $p_2=p_3=p_4=p_5$ [see (26)]. The results for different values of p_1 are shown. The circle shows the value of z for $k=2$ CA

In this case, according to (22), the rules of the $k=2$ CA are given by

$$\begin{aligned}
\tilde{p}_1 &= p_2 + p_3, \\
\tilde{p}_2 &= 2p_1 = p_4 + p_5.
\end{aligned} \tag{28}$$

Hence still a four dimensional parameter subspace can be mapped to the $k=2$ CA of Fig. 2, in particular for $p_1=p_2=p_3=p_4=p_5=p$ this problem has the same critical behaviour as directed site percolation with $p_c = p_c^D/2$ where $p_c^D = 0.7058 \pm 0.0001$ is the percolation threshold.

If the parameters do not obey (28), i.e. if the dynamics of the variable $S_v^i=0$ sees the structure of the dynamics of variables $S_v^i=1$ and $S_v^i=2$ one has to apply numerical methods to check universality. For the case $p=p_2=p_3=p_4=p_5$ we have calculated the exponent z for different probabilities p_1 using transfermatrix scaling (Note that the size of the matrix is $3^{N+1} \times 3^{N+1}$, thus we could use only strips with $N \leq 9$). Figure 8 shows the results. In all cases the values of $z(N)$ seem to converge to the known result $z=1.581$ [7], confirming the field theoretic predictions [15].

b) CA with Two Absorbing States

The problem with two absorbing states [17] is more difficult to handle by numerical methods. In the absorbing phase an initial state decays to a state which consists of domains of both of the absorbing states. Since the domain walls move like a random walk and annihilate when two of them meet this

state decays algebraically to the stationary state which consists of one of the absorbing states. Thus the whole absorbing phase behaves like a critical point with power law decay of correlations. From the random walk behaviour one obtains $z=2$.

In Ref. [17] the kink density n (16) was investigated by Monte Carlo methods for a $k=2$ CA with two absorbing states $(0, 1, 0, 1, \dots)$ and $(1, 0, 1, 0, 1, \dots)$. In the absorbing phase n decays with time like $n \sim t^{-1/2}$. At the critical point p_c one finds $n \sim t^{-\alpha}$ with $\alpha=0.27 \pm 0.08$ and an exponent $\beta=0.6 \pm 0.2$ which obviously differs much from the value of (13). However, as can be seen from Fig. 4 of Ref. [17], the determination of the critical behaviour is difficult due to fluctuations, finite site effects and the presence of algebraic decay in the absorbing phase, thus an alternative way of deriving critical properties would be useful.

We have investigated the same model with the transfermatrix method. Unfortunately, in the active phase the closeness of a class 3 deterministic CA lead to irregular behaviour of $\tau(N)$ and did not allow any conclusions to be drawn from finite size scaling; similar effects have been discussed in Sect. III. Therefore we have studied this problem for a different model, namely a $k=3$ CA with two absorbing states $i_1=(1, 1, 1, \dots, 1)$ and $i_2=(2, 2, 2, \dots, 2)$ on the geometry of Fig. 1(b). Again, by using symmetries of left-right and variables $S_v^i=1$ and $S_v^i=2$ only four parameters of the 9×3 matrix $p(S_1 S_2 | S')$ are left:

$$\begin{aligned} p_1 &= p(12 | 1), \\ p_2 &= p(01 | 1), \\ p_3 &= p(02 | 1), \\ p_4 &= p(00 | 1). \end{aligned} \quad (29)$$

Note that $p(11 | 1) = p(22 | 2) = 1$ to get the two absorbing states $i_1 = (3^N - 1)/2$ and $i_2 = 3^N - 1$. As before there is a subspace of probabilities for which the model can be mapped onto the $k=2$ process of Fig. 2. Namely if one has $p_1 = 1/2$ then, with Eq. (22), the dynamics of variable $S_v^i = 0$ does not see the difference between $S_v = 1$ and $S_v = 2$, and the system is mapped onto the $k=2$ CA of Fig. 2 with one absorbing state $\tilde{p}_0 = 0$ and

$$\begin{aligned} \tilde{p}_1 &= 1 - p_2 - p_3, \\ \tilde{p}_2 &= 1 - 2p_4. \end{aligned} \quad (30)$$

In particular the problem with $p_1 = 1/2$ and $p_2 = p_3 = p_4 = p$ is again equivalent to directed site percolation with $p_c = (1 - p_c^p)/2 \simeq 0.148$.

Hence at least for this subspace of CA with two absorbing states one has the same critical behaviour as for usual $k=2$ CA.

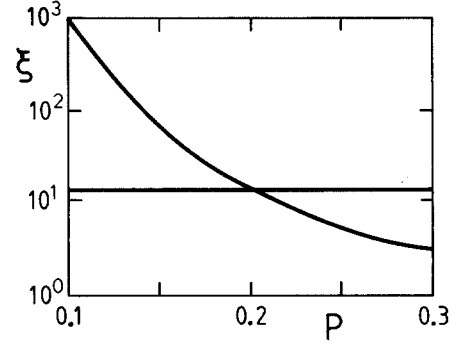


Fig. 9. Correlation times ξ for a $k=3$ state CA with two absorbing state ($N=6$, $p_1=1/2$, $p_2=p_3=p_4=p$)

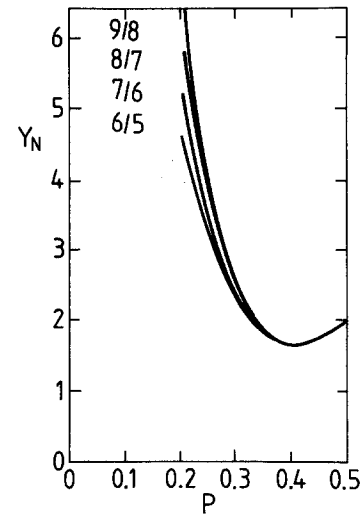


Fig. 10. Logarithmic ratio Y_N of correlation times, Eq. (A.9) as a function of $p=p_1=p_2=p_3=p_4$ for a $k=3$ state CA with two absorbing states. This figure indicates a transition at $p \approx 0.35$

Although this subspace with two absorbing states can be mapped onto a problem with one absorbing state the mechanism of randomly moving and annihilating domain walls is still present. In the absorbing phase $p > p_c$ there is still an algebraic decay of correlations. In a finite system there is an eigenvalue λ_2 and an correlation time $\tau_2 = -(\ln \lambda_2)^{-1}$ corresponding to this mechanism. This eigenvalue λ_2 cannot be mapped onto the $k=2$ CA described in Sect. VI, since $\tilde{\phi}_x = 0$ as easily can be shown. However λ_2 can be obtained from a submatrix of $T_{\alpha\beta}$ which corresponds to a different $k=2$ CA. Therefore one has two independent correlation times as shown in Fig. 9: τ_1 for the decay of variable $S_v^i = 0$ and τ_2 for the domain wall annihilation. In the active phase τ_1 increases exponentially with strip width N while τ_2 increases like N^2 .

In the case $p_1 < 1/2$ the domain walls create the state $S_v^i = 0$. Therefore the decoupling mentioned above and the mapping onto $k=2$ CA does not hold any

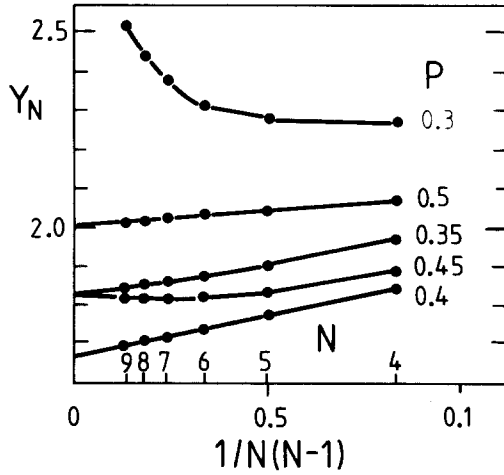


Fig. 11. Y_N as in Fig. 10 as a function of system size N . The extrapolated value $\lim_{N \rightarrow \infty} Y_N$ is the dynamical exponent z in the absorbing phase

more. We have studied this problem for $p_1 = p_2 = p_3 = p_4 = p$ numerically with transfermatrix scaling. In Fig. 10 $Y_N = \ln[\tau(p, N)/\tau(p, N-1)]/\ln(N/N-1)$ (compare with Eq. (A.9)) is shown as a function of p . For $p \lesssim 0.3$ the results are consistent with $Y_N \sim N$ indicating an active phase. For $p \gtrsim 0.35$ Y_N seems to converge to a constant $z = \lim_{N \rightarrow \infty} Y_N < \infty$ indicating a

phase with algebraic decay of correlations due to the motion of domain walls of the two absorbing states. However, as shown in Fig. 11, the value of z seems to depend on p . For $p = 1/2$ one gets $z = 2$ since one has an annihilating random walk. But for $p < 1/2$, the variable $S_v^i = 0$ is created and annihilated at the domain walls. Figure 11 indicates that for this case one gets different nonuniversal critical behaviour with $z < 2$. At the transition point p_c , which from Fig. 11 is estimated to have the value $p_c = 0.33 \pm 0.03$, the value of z seems to be much larger than $z = 1.581$ from (12). However this was also the case for the problem which could be mapped onto a $k=2$ CA, thus this does not necessarily mean new critical behaviour. Therefore we cannot determine the critical properties at the transition from the present method.

c) Infection with Immunization

Cardy recently investigated the following epidemic process [16]: (i) Infected sites infect their neighbours with probability p in the next time step and become immun. (ii) Immun sites have the probability $p-q$ of being reinfected by infected neighbours. A field theory was developed for this process and it was shown that for $q \neq 0$ one gets new critical properties.

Table 4. Transition probabilities $p(S_1 S_2 S_3 | S')$ of a $k=3$ state CA which describes an infection with immunization. The values not shown are given by symmetries

$S_1 S_2 S_3 S'$	0	1	2
000	1	0	0
001	$1-p_1$	p_1	0
002	1	0	0
010	0	p_1	$1-p_1$
011	0	p_1	$1-p_1$
012	0	p_1	$1-p_1$
020	0	0	1
021	0	p_2	$1-p_2$
022	0	0	1
100	—	—	—
101	$1-p_1$	p_1	0
102	$1-p_1$	p_1	0
110	—	—	—
111	0	p_1	$1-p_1$
112	0	p_1	$1-p_1$
120	—	—	—
121	0	p_2	$1-p_2$
122	0	p_2	$1-p_2$
200	—	—	—
201	—	—	—
202	1	0	0
210	—	—	—
211	—	—	—
212	0	p_1	$1-p_1$
220	—	—	—
221	—	—	—
222	0	0	1

Here we study such a process for an one-dimensional CA on the geometry of Fig. 1(a). The system consists of normal $S_v^i = 0$ and of infected, $S_v^i = 1$ states. To describe immunization we introduce a third variable $S_v^i = 2$ of immune states. Thus the memory effect of the $k=2$ state process is equivalent to a $k=3$ state CA. The rules $p(S_1, S_2, S_3 | S')$ are defined in Table 4. We have used two probabilities $p_1 = p$ and $p_2 = p - q$ with the meaning described above. Note that one has infinitely many absorbing states, since by definition all states which do not have infected sites do not change with time.

If j is a state without normal sites and i is a state with normal sites, $S_v^i = 0$, then one has $T_{ij} = 0$. That means that there is no transition from states without to states with normal sites. Therefore the matrix T_{ij} has all the eigenvalues of the corresponding $k=2$ CA with infected and immune states, only. If the other eigenvalues are not larger then the model has the same critical behaviour as the $k=2$ CA investigated in the previous sections. In fact we have checked numerically for different values of p and q that the correlation time of the $k=2$ CA is exactly the one of the $k=3$ model.

We expect the same behaviour for any such immunization process described above, at least in the active

phase: After a transient time all sites will be either infected or immune, therefore the asymptotic behaviour is a usual process with infection probability $p-q$. This argument and the results above for the one dimensional model are at variance with the field theory of Ref. [16].

VIII. Competing Reactions

In this section we are interested in the problem whether stochastic CA may show any structure in time direction. The mean field equation of (7) and Ref. [7] are iterations of simple nonlinear maps which may have oscillations with any period and even may show chaotic motion [28]. However, for all cases of $k=2$ and $k=3$ CA we have studied so far we have found time independent stationary states, only.

This is not true for the decay into stationary states. An initial state may relax to the final state with an oscillatory component. In the transfermatrix T_{ij} this shows up as a complex conjugate eigenvalue pair λ_1 and λ_2 . The asymptotic decay of $P_i(t=0)$ is given by

$$P_i(t) \sim \varphi_i^0 + (\lambda_1^t + \bar{\lambda}_1^t) \varphi_i^1 \\ = \varphi_i^0 + \exp(-t/\tau) \cos(qt) \varphi_i^1 \quad (31)$$

with $\tau = -\ln|\lambda_1|^{-1}$ and $\lambda_1 = |\lambda_1| \cdot \exp(iq)$.

Similar effects occur in equilibrium statistical mechanics at “disorder lines” [29]. For instance in lattice gas models, in the disordered phase of the temperature-coverage-phase diagram there is a line where the second and third largest eigenvalues λ_1 and λ_2 merge to a complex conjugate pair yielding an oscillating and incommensurate asymptotic decay of correlations [30]. Such lines are also found in one dimensional lattice gases [31]. Only systems with competing interactions show such a behaviour.

For CA a merging of eigenvalues λ_1 and λ_2 can occur for nonzero source $p_0 = p(000|1) \neq 0$, only. Namely for $p_0=0$ the matrix T_{ij} has elements $T_{00}=1$ and $T_{j0}=0$ for $j>0$. This gives the largest eigenvalue $\lambda_0=1$, and the other eigenvalues are eigenvalues of the submatrix T'_{ij} with $i>0$ and $j>0$. Since T' has only positive elements and in general is irreducible its largest eigenvalue λ_1 is positive and nondegenerate due to the theorems of Frobenius [20].

But for $p_0>0$ transitions from monotonic to oscillating transient decay are possible. We want to demonstrate this for 0-dimensional CA but we have also found such a behaviour for finite chains by investigating T_{ij} numerically. Consider a CA on a single site with two states $S=0$ and $S=1$. With $p(0|1)=p_0$ and $p(1|1)=p_1$ the transfermatrix T_{ij} has the form

$$\begin{pmatrix} 1-p_0 & 1-p_1 \\ p_0 & p_1 \end{pmatrix} \quad (32)$$

with eigenvalue $\lambda_0=1$ and $\lambda_1=p_1-p_0$. The decay of an initial state to the stationary state $P_0^0=(1-p_1)/(1-p_1+p_0)$, $P_1^0=p_0/(1-p_1+p_0)$ is monotonic for $p_1>p_0$ and oscillating with period 2 for $p_1<p_0$, but it is always commensurate with respect to the time step. A “disorder line” does not exist for this case.

But for a $k=3$ state CA competing reactions can be introduced yielding a transition to oscillating decay. For instance consider the reaction of states $S=0, 1$ and 2 giving by the following transfermatrix T_{ij}

$$\begin{pmatrix} 1-p_0 & 1-p_1-p_3 & 1-p_1-p_2 \\ p_0 & p_1 & p_2 \\ 0 & p_3 & p_1 \end{pmatrix}. \quad (33)$$

For $p_0 p_3 \neq 0$ one obtains nondegenerate eigenvalues $\lambda_1 > \lambda_2$. This means one needs the sequence $0 \rightarrow 1 \rightarrow 2 \rightarrow 0$ competing with $0 \rightarrow 1 \rightarrow 0$ to obtain oscillating decay. The eigenvalues are given by

$$\lambda_0=1, \\ \lambda_{1/2}=p_1-p_0/2 \pm ((p_0/2)^2 + p_2 p_3 - p_3 p_0)^{1/2}. \quad (34)$$

This gives the line where λ_1 and λ_2 merge by

$$p_0^2/4 + p_2 p_3 = p_3 p_0. \quad (35)$$

The correlation time τ and the wavevector q of the oscillations are

$$\tau^{-1} = -\frac{1}{2} \ln(p_1^2 + p_0(p_3 - p_1) - p_2 p_3), \quad (36)$$

$$q = \arctg[(p_1 - p_0/2)/(p_3 p_0 - p_0/4 - p_2 p_3)^{1/2}]. \quad (37)$$

IX. Random Probabilities

So far we have studied stochastic CA with homogeneous local reaction probabilities. In this section CA are introduced which have probabilities $p_v^t(S_1 S_2 | S')$ which are randomly distributed either in space v in time t or both in space and time. If there is still an absorbing state, i.e. $p'(00|1)=0$, then we expect that these disordered CA still have a phase transition. However its critical properties may change.

For equilibrium phase transitions a heuristic argument of Harris shows for which cases the critical behaviour is changed [32]. We apply this argument to nonequilibrium critical points of disordered CA.

First consider a D -dimensional CA with reaction probabilities which are distributed in space, only. The distribution may be continuously parameterized

by x with $x=0$ being the pure system. The critical point $p_c(x)$ is assumed to be a smooth function of x . The Harris argument checks the consistency of the existence of a single typical correlation length ξ which obeys Eq. (9), i.e. $\xi \sim (p - p_c(x))^{-\nu_\perp}$. Since the system can only feel the properties within a region of size ξ , it locally sees a fluctuation δx of x with $\delta x \sim \xi^{-\frac{D}{2}}$. This gives

$$\begin{aligned} \xi^{-\frac{1}{\nu_\perp}} &\sim p - p_c(x + \delta x) = p - p_c(x) - A \xi^{-\frac{D}{2}} \\ &\sim \xi^{-\frac{1}{\nu_\perp}} (1 - A \xi^{\frac{1}{\nu_\perp} - \frac{D}{2}}). \end{aligned} \quad (38)$$

Thus for $p \rightarrow p_c(x)$, i.e. $\xi \rightarrow \infty$, Eq. (38) can only be valid if

$$2 - D\nu_\perp < 0. \quad (39)$$

In equilibrium statistical mechanics the left side is just the specific heat exponent α . According to Harris for each random system (39) is valid, in particular if the pure system $x=0$ does not obey (39) then the critical properties are changed. Renormalization group arguments indicate that also the reverse is true: If the pure system has $\alpha < 0$ then randomness is irrelevant and the critical properties are not changed [24]. From this and the values of ν_\perp of CA with one absorbing state [7] we conclude that spatial disorder does change the critical behaviour of CA in any dimension (the mean field case is just marginal).

Similar arguments hold for the other two cases of randomness, one just has to replace $D\nu_\perp$ by ν_\parallel and $D\nu_\perp + \nu_\parallel$ for randomness in time and space plus time, respectively. From this one obtains the following result: Space or time randomness is relevant while randomness in both space and time together give the same critical properties as in the pure system.

So far we have discussed the case of weak disorder. For strong disorder with competing reactions new qualitative effects occur. In this case the system acts as a filter to many different states, similar to pure class-2 CA. If the dynamics is given by a Hamiltonian with random competing interactions such a system is called "spin glass" [33]. For infinite-range interactions the system has a phase transition [34] with the consequence that even such *stochastic* CA stay infinitely long in one of the many stationary states. The number of stationary states grows exponentially with system size [35] and the states have an interesting overlap, structure ("ultrametric topology" [36]). Recently these CA found applications as models for memory [37] and prebiological evolution [38].

For short range spin glasses, at least in two dimensions there is no phase transition [39]. Nevertheless

the filter effect is seen in the slow decay of the remanent magnetization at low temperatures [40]: Due to the symmetry of the Hamiltonian this means that almost any initial state decays fast to a state with high overlap to the initial one; then this new state decays very slowly with time t . The average relaxation time τ drastically increases with decreasing temperature T like $\ln \tau \sim T^{-\nu_z}$ [41] with a large exponent ν_z (whose precise value is still not known [42]). In the context of CA this means, for any finite observation time τ there is a temperature T below which the stochastic CA behaves as an effective filter. Furthermore, for a given set of states one can construct interactions (\cong rules) such that these states are stationary ones for infinite range rules or quasi-stationary ones for short range rules [37].

X. Summary

Cellular automata (CA) are simple mathematical models for the dynamics of cooperative phenomena far from thermal equilibrium. They consist of k states on each site of a lattice reacting in discrete time steps by transition probabilities which depend on nearest neighbour states, only. Such models have been discussed in mathematics, physics, biology, ecology, chemistry and computer science.

In this paper phase transitions of such stochastic CA have been investigated. If the model has absorbing states, i.e. states which cannot be left according to the transition probabilities then CA have a sharp transition between qualitatively different stationary phases: An absorbing phase containing the absorbing states, only and an active phase containing all but the absorbing states with some probability distribution.

The phase diagrams of several one-dimensional $k=2$ CA with one absorbing state have been calculated by transfermatrix scaling. The corners of the phase diagrams are deterministic CA which belong to three different classes [6]. There does not seem to exist any connection between the topology of the phases and the class of the deterministic limits. The structures created by deterministic rules are destroyed within the active phase. Several transition points have exactly been determined by duality relations.

These phase transitions of CA with one absorbing state are continuous, i.e. for example approaching the transitions the fraction of active sites goes continuously to zero. Universal critical exponents, scaling functions and scaling relations describe the singularities of the observable quantities at the transition. In particular it has been demonstrated that

finite size scaling of the correlation time can be applied and yields three independent critical exponents from which all other ones can be calculated. The two scaling fields have been identified as the source p_0 of the active states and the reaction probability for $p_0=0$.

The critical exponents have been calculated for several points on the phase boundaries. The numerical results support universality of the critical properties. Only special points corresponding to annihilating random walks have different critical behaviour.

An entropy S has been defined and calculated numerically. It is nonzero only in the active phase, has a maximum close at the transition and goes to zero with the power law $S \sim (p - p_c)^\beta$. The exponent β has been determined from finite size scaling demonstrating that all exponents can be calculated without using the scaling field p_0 conjugate to the order parameter. β has also been obtained from the coverage of active sites and the kink density.

The universality of such phase transitions has been explored further by introducing $k=3$ state CA. For special subspaces of the set of local reaction probabilities the $k=3$ models have exactly been mapped onto $k=2$ ones. There are $k=3$ CA with one or two absorbing states which have the same critical properties as $k=2$ CA with one absorbing state only.

For transition rates where such a mapping does not apply the critical properties have been calculated numerically. In the case of $k=3$ CA with two absorbing states a phase transition was found. In the absorbing phase the correlation decays algebraically with a critical exponent which seems to vary continuously with the model parameters. Due to this "phase of critical points" the present method did not allow a determination of the properties of the transition. In the case of CA with one absorbing state the numerical results were consistent with an universal behaviour of $k=3$ and $k=2$ CA. A simple model of an infection process with immunization was shown to have the same critical behaviour as usual $k=2$ CA. Arguments were given that this holds for all such processes, in contrast to a recent field theoretic investigation [16].

The case of competing reactions was shortly discussed. Similar to the "disorder lines" of equilibrium systems a transition from monotonic to incommensurate oscillating decay to the stationary state was found for $k=3$ CA.

If the local reaction rates are distributed randomly then CA with absorbing states still show a phase transition. Applying the Harris criterium of equilibrium systems to CA one obtains the following result: If the system is random either in space or in time then randomness changes the critical properties

in any dimension; if the system is random both in space and time then the critical properties are the same as those of the pure system.

Strong randomness with competing reaction rates leads to spin glass behaviour: Even stochastic CA may have infinitely many stationary (or for short range models very long living) states. Hence those CA filter the initial information which decays to a final state with large overlap to the initial one.

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Appendix

A.1. Transfermatrix

The transfermatrix T_{ij} , Eq. (3) of a k -state CA on a chain of N sites is a k^N by k^N matrix. The integers i and j label the k^N states as defined in (1). For the numerical evaluation of the largest eigenvalues it is convenient to write T_{ij} as a product of N sparse matrices [43]

$$\underline{T} = \underline{L} \underline{M}^{N-2} \underline{R}. \quad (\text{A.1})$$

Due to the boundaries the matrices L , M , and R differ slightly. Each matrix has only k^{N+1} elements which are nonzero, and each element is given by the local probabilities $p(S_1 S_2 S_3 | S')$ of (3). Neither \underline{T} nor \underline{L} , \underline{M} , or \underline{R} have to be stored in the computer, all what is needed is the multiplication of a vector by \underline{T} which is a few lines computer program as shown below.

T_{ij} is the probability to find state i at time $t+1$ given state j at time t . Thus T_{ij} adds a whole row (=whole time step) to the total probability. This process is split up into N steps by (A.1), each steps adding a single site only. L adds the left site, R the right one and M one site in the middle. For example, the meaning of the matrix M is illustrated in Fig. 12 for $N=5$: Given state $j=(S_6, S_5, S_4, S_3, S_2, S_1)_k$ at time $t+1$, M_{ij} is the probability to find state $i=(S'_6, S'_5, S'_4, S'_3, S'_2, S'_1)_k$ at time t . Note that at least $N+1$ variables are necessary to transfer the probability from site to site, hence M is a k^{N+1} by k^{N+1} matrix. From Fig. 12 one immediately obtains that M_{ij} is zero unless one has

$$S_v = S'_{v-1} \quad v=2, \dots, N. \quad (\text{A.2})$$

Hence, for a given row i only the variable S_6 is independent and there are only k states j_1, \dots, j_k for

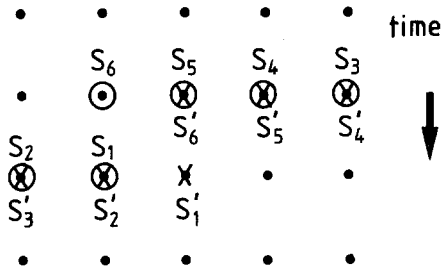


Fig. 12. States $i=(S'_v)$ and $j=(S_v)$ of the sparse transfermatrix M_{ij} as described in the text

which M_{ij} is nonzero. With Eq. (1) one obtains

$$j_\mu = [i/k] + (\mu - 1)k^N, \quad 1 \leq \mu \leq k \quad (\text{A.3})$$

where $[a]$ means the largest integer below a . From Fig. 12 and the meaning of M_{ij} it follows that the nonzero elements of M_{ij} are given by

$$M_{ij} = p(S_{N+1}, S_N, S_{N-1} | S'_1) \quad (\text{A.4})$$

with $p(S_1 S_2 S_3 | S')$ of Eq. (3). The set S_{N+1}, S_N, S_{N-1} can again be written as a single integer which is given by

$$(S_{N+1}, S_N, S_{N-1})_k = [j/k^{N-2}] \quad (\text{A.5})$$

while S'_1 is given by

$$S'_1 = (i/k) \text{ modulo } k. \quad (\text{A.6})$$

Therefore each element M_{ij} can be easily determined from the integer representation of states i and j , from simple integer operations (A.3), (A.5) and (A.6) and from the local rules $p(S_1 S_2 S_3 | S')$.

The largest eigenvalue λ_0 of T is $\lambda_0 = 1$, since $\sum_i T_{ij} = 1$ by definition. The second largest eigenvalue λ_1 determines the correlation length. In the case of absorbing states, for example for $T_{0j} = 0$ ($j \neq 0$), λ_1 is easily obtained by a simple iteration:

- (i) Start with an (almost) arbitrary vector u_i^0 ($1 \leq i \leq k^{N-1}$);
- (ii) Generate vectors \underline{u}^n by $\underline{u}^n = T \underline{u}^{n-1}$ and replacing u_0^n by $u_0^n = 0$.
- (iii) Then λ_1 is obtained from

$$\lambda_1 = \lim_{n \rightarrow \infty} \frac{u_i^{n+1}}{u_i^n}. \quad (\text{A.7})$$

In practice the iteration is stopped if the relative change of u_i^n is smaller than an given ε ; usually we have used $\varepsilon = 10^{-8}$.

If the system has more absorbing states i , their weight u_i^n has to be replaced by $u_i^n = 0$ at each iteration step. If there are no absorbing states, one has to iterate two independent vectors \underline{u} and \underline{v} keeping

them linear independent at each iteration step. In general, to obtain the m largest (in absolute value) eigenvectors one has to iterate m independent vectors $\underline{u}_1^n, \dots, \underline{u}_m^n$. The eigenvalues are given for $n \rightarrow \infty$ by the m by m matrix $u_{\nu\mu} = \langle u_\nu^n | u_\mu^n \rangle$ [44].

The iteration $\underline{u}^{n+1} = T \underline{u}^n$ is obtained from the matrix product (A.1), each term given by (A.2) to (A.6). For instance (for $k=2$) the product $\underline{v} = M \underline{u}$ is given by calling the following FORTRAN subroutine

```
SUBROUTINE MAT(U, V, P, N)
DIMENSION U(1), V(1), P(8, 2)
N1=2xx(N+1)
N2=2xxN
N3=2xx(N-2)
DO 1 I=1, N1
J1=(I-1)/2+1
J2=J1+N2
K1=(J1-1)/N3+1
K2=(J2-1)/N3+1
K3=MOD(I-1, 2)+1
1 V(I)=P(K1, K3) x U(J1)+P(K2, K3) x U(J2)
RETURN
END
```

Note that in (old) FORTRAN the indices I have to start with I=1, hence we have added an one to each index. The matrix $P(I, J)$ is the matrix $p(S_1, S_2, S_3 | S')$ of (3) which is stored once in the beginning. Of course, also the states J1 and J2 and the indices K1, K2 and K3 may be calculated for each I in the beginning and stored as a vector; depending on the architecture of the computer this may be somewhat faster.

A.2. Scaling

Following Nightingale [45] the critical properties of the infinite system are determined from scaling the correlation time τ with the size N of the system, using the asymptotic form Eq. (8). In practice one obtains τ from the eigenvalue λ_1 of the matrix T_{ij}

$$\tau = -(\ln \lambda_1)^{-1}. \quad (\text{A.8})$$

Then the quantity

$$Y_N = \ln [\tau(p, N)/\tau(p, N-1)] / \ln [N/N-1] \quad (\text{A.9})$$

is calculated for a line in the parameter space parameterized by p . If $p > p_c$ denotes the active phase then one has [44]

$$\begin{aligned} Y_N &\sim N & p > p_c \\ Y_N &= z & p = p_c \\ Y_N &\rightarrow 0 & p < p_c \end{aligned} \quad (\text{A.10})$$

where z is the dynamical critical exponent. Hence from the intersection of the functions $Y_{N+1}(p)$ and $Y_N(p)$ at the point (z_N, p_N) one obtains an estimate for z and p_c , respectively. From the N -dependence one can estimate the quality of the results, the extrapolation to $N \rightarrow \infty$ gives the final estimate. In principle one may also obtain universal irrelevant exponents from z_N and p_N , but in practice this is difficult due to cancellation effects [46].

The other exponents ν_{\parallel} and ω can be obtained from the scaling of the corresponding partial derivatives of τ , as can be seen from (8).

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Note Added in Proof

Randomness in both space and time can be integrated out to give a pure CA with averaged reaction probabilities. I thank the referee and M. Schreckenberg for pointing this out to me.