STUDY OF CONTINUOUS PHASE TRANSITION WITH TOOM CELLULAR AUTOMATA

DANUTA MAKOWIEC

Institute of Theoretical Physics and Astrophysics,
Gdansk University,
Wita Stwosza 57, 80–952 Gdansk, Poland
fizdm@univ.gda.pl

(Received 22 November 1999)

Abstract: The heuristic proof, since based on computer simulation investigations, is presented that though stationary Toom cellular automata exhibit many features which are characteristic for an equilibrium system (e.g. rapid change in the order parameter, when noise is fine tuned, or slow decay of the two point correlation function), the stationary state is not a Gibbsian one. It means that it is impossible to define energy on the microscopic level in such a way that the dynamic system becomes representative to some equilibrium lattice model. Moreover, properties on the coarse–grained level: fluctuations, seem to be distinct from the corresponding ones of the Ising model.

Keywords: equilibrium lattice systems, critical exponents, Gibbsian measures, Ising model

1. Introduction

The goal of this presentation is, firstly, to explain in a consistent way a piece of machinery used in equilibrium statistical mechanics to study phase transitions in lattice models, and secondly, to observe this machinery working in a system of probabilistic cellular automata with Toom rule responsible for microscopic interactions. The system considered by us differs from a standard one examined by equilibrium statistical mechanics by the following properties:

— dynamics in probabilistic cellular automata is discrete in time (cellular automata are synchronized);
— a rule implemented, i.e., Toom rule, is not reversible.

In general a stationary system governed by an irreversible rule cannot mimic an equilibrium thermodynamic system, because it is not known how to introduce a notion of energy in such a system. However, in the case of Toom cellular automata there is a strong belief that the Hamiltonian for this rule exists. In Section 2 we present arguments for this hypothesis. In Section 3 the results of computer simulations aimed at verifying the hypothesis are collected. The final conclusion is that the thermodynamic system which arises from Toom cellular automata is not an equilibrium one. The stationary measure does not fulfil necessary conditions to be a Gibbsian one. Moreover, on the macroscopic scale of fluctuations the system behaves differently from the expected system of the Ising type. However, the agreement between numerical values of critical exponents observed by us and values obtained in a deterministic system of a lattice of diffusively coupled chaotic maps [1] proves, as in the case of equilibrium systems, that there are scaling laws which are insensitive to macroscopic details of models mentioned and therefore they form a common universality class.

1.1 Phase transitions in lattice systems

When physicists talk about phase transitions they have in mind some discontinuity, or at least nonanalycity, of thermodynamic functions which describe the state of the system (say, the density for the liquid–gas transition) as a function of external parameters (temperature, pressure). The goal, and the basic difficulty, is to describe these effects starting from the microscopic level.

The simplest model featuring phase transitions is the Ising model. In the Ising model we deal with random variables σ_i (called spins) labeled by sites of a d–dimensional lattice, $i \in Z^d$. Spins can attain only one of the two values +1 or −1.

If the system considered is in equilibrium, then the probability distribution $\mu(\sigma)$ for any configuration $\sigma = \{\sigma_i\}$ is given by the Boltzmann–Gibbs weights (see [2] and references there in):

$$\mu(\sigma) = \frac{e^{-\beta H(\sigma)}}{\mathcal{Z}}, \tag{1}$$

which are determined by:

— Hamiltonian H, i.e. energy carried by a configuration. In case of Ising system the energy calculates as follows:

$$H(\sigma) = -J \sum_{<i,j>} \sigma_i \sigma_j - h \sum_i \sigma_i . \tag{2}$$

The first sum is taken over pairs of nearest neighbors;

— partition function, the normalizing term $\mathcal{Z}$ being a sum over all possible configurations of a system:

$$\mathcal{Z} = \sum_\sigma e^{-\beta H(\sigma)} ; \tag{3}$$

— β and h the external parameters: the inverse temperature and external magnetic field, respectively.

However, all these formulas have the meaning denoting that we can calculate the energy, find the partition function (3) and finally get the probability distribution (1) only if we operate on finite lattices, i.e., the configurations are considered on some finite sets Λ of Z^d. Of course, there is no singularity at all if we only consider finite sets Λ. To really "see phase transitions" we have to go to the infinite volume. This operation is called the thermodynamic limit.

The most straightforward statement about the existence of the phase transition is based on considering free energy function:

$$f(\beta,h) = -\frac{1}{\beta}\lim_{\Lambda\to Z^d}\frac{1}{|\Lambda|}\log \mathcal{Z}_\Lambda. \tag{4}$$

In case of the two–dimensional Ising model it appears that the first derivative of the free energy function with respect to the external magnetic field $\partial f/\partial h$ has a discontinuity when crossing the line $h = 0$ at $T < T_c$. Since it is the first derivative that is discontinuous we speak about the first order phase transition. At the point $(T_c, 0)$, the first derivatives are continuous, and the singularity is revealed by higher derivatives — we speak about the continuous transition.

1.2 Gibbs states

A convenient mathematically rigorous way of formulating the existence of phase transitions is in terms of Gibbs states. Sticking to the Ising model, let us consider the conditional probability of a configuration σ_Λ on any finite window of a lattice $\Lambda \subset Z^2$ if some fixed boundary condition $\tilde{\sigma}_{\Lambda^c}$ is chosen as:

$$\mu(\sigma_\Lambda | \tilde{\sigma}_{\Lambda^c}) = \frac{1}{\mathcal{Z}_\Lambda(\tilde{\sigma}_{\Lambda^c})} e^{-\beta H_\Lambda(\sigma_\Lambda \otimes \tilde{\sigma}_{\Lambda^c})}. \tag{5}$$

The energy

$$H_\Lambda(\sigma_\Lambda \otimes \tilde{\sigma}_{\Lambda^c}) = H(\sigma_\Lambda) + H_{\text{Int}}(\sigma_\Lambda), \tag{6}$$

consists of two parts: the internal energy associated with a configuration σ_Λ – $H(\sigma_\Lambda)$ and the energy of the interaction of σ_Λ spins with the fixed outside configuration — $H_{\text{Int}}(\sigma_\Lambda)$.

Hence, by changing Λ — the windows size and position on the infinite lattice Z^2, we observe properties of the infinite configurations. We say that we study a thermodynamic system through "cylindrical events" [2].

By a state we mean a probability measure defined on a probability space of all possible configurations and the σ–algebra of cylindrical events. A measure is a Gibbsian one with respect to the Hamiltonian (6) if for all configurations σ_{Λ^c} outside any finite Λ, the conditional probability for a configuration σ_Λ inside Λ is given by (5). Thus, equations (5) express the requirement that each finite volume is in equilibrium with the whole, where the equilibrium is described by μ.

We say that a system undergoes a first order phase transition for a particular value of external parameters (β, h) if there is more than 1 Gibbs state which arises from the interactions. The fact that the Gibbs state is not unique means that there is a certain instability with respect to boundary conditions — a small change on the boundary may lead to a dramatical change in the limiting measure. At high temperatures, random variables σ_i are "almost independent" and, as a result, there is a unique limit — the unique Gibbs state. We say the system is ergodic. Hence, the first order phase transition corresponds to a change in the number of ergodic equilibrium measures (physicists used to say: a change in the number of pure phases).

The continuous transition does not necessarily change the number of pure phases. It corresponds to much more subtle phenomena — slow decay of correlation. In a system the large homogeneous areas, fluctuations, appear and propagate over the macroscopic scale. The divergence of coherence time and length scales observed at the transition point are responsible for one of the most spectacular property of the second–order phase transition: universality. The occurrence of fluctuations on all scales translates quantitatively into scaling laws, which govern the behavior of macroscopic quantities close to the transition. Second–order transitions can then be classified according to the values of the corresponding exponents. Thanks to a diverging correlation length, numerical values of these critical exponents are insensitive to many details of underlying physics, as expressed by a microscopic Hamiltonian function. Universality classes, or sets of transitions possessing the same critical exponents, gather physical phenomena of seemingly different nature, provided that a small number of macroscopic constraints are respected. Static exponents of second–order transitions in equilibrium, locally interacting systems depend only on the type of symmetry broken by the ordered phase and on the space dimension d, [3]. The points in parameter space where the continuous phase transitions take place are customarily called critical points in analogy to the critical point of liquid–gas system, which was the earliest known example of this phenomena.

1.3 Spinflip dynamics

In the time of computers physicists discovered an extraordinary tool to examine lattice systems. This tool named Monte Carlo method allows to evaluate multi–dimensional integrals which occur when one calculates the partition function (3) and then finds the free energy function and other thermodynamic quantities, see [4, 3]. The process of integration is a kind of a walk in the configuration space done according to some Markov stochastic prescription. In this way the static equilibrium system description moves into the field of dynamic systems with stochastic rules.

By spinflip dynamics we mean a stochastic evolution for infinite configurations of spins on a lattice in which every individual spin flips with a certain rate or a certain probability according to the configuration of spins nearby. This stochastic dynamics is designed in such a way that the, so–called, detailed balance condition it satisfied. It effects in that all stationary states of such systems are Gibbs states, and microdynamics is time reversible with respect to these Gibbs measure. Such systems are named kinetic Ising models. However, why not to consider such a spin-flip dynamics, in which the detailed balance condition is not satisfied. For such systems in general very little is known about their stationary states [2, 5]. Could it be that there is still some Hamiltonian out there for which the stationary states are

Gibbsian? If the answer to this question was "yes" then the following would make sense:

$$\ln \mu(\sigma_\Lambda) \to H_\Lambda(\sigma) \quad \text{for } |\Lambda| < \infty .$$

Thus, from the measure we would gain the notion of energy. It is known that the general answer to this question is "no". There are non–trivial examples like voter model in 3 dimensions for which non–Gibbsianness of the stationary measures has been proved [6].

2. Toom probabilistic cellular automata

In the kinetic Ising models the updating rule is designed in such a way that the dynamics mimics the continuous time. When we switch to a discrete time, by for example, demanding synchronization of the updating rule, we land in the area of discrete time interacting particle systems modeled by probabilistic cellular automata [7].

In the reversible case, i.e., when the local PCA rule is reversible (which implies that PCA satisfy the detailed balance condition with respect to some Gibbs measure for some local energy) then all translation invariant stationary measures are precisely all Gibbs measures for this local energy [8]. In the non–reversible case, practically nothing is known about the nature of stationary measures in the regime where there is more than one stationary measure. A basic example of non–reversible PCA for which it has been conjectured that the stationary measures at low noise could be Gibbsian is the Toom model [2, 7, 9].

The simplest version of the Toom model is PCA which can be seen as North–East–Center majority vote model on a square lattice. That is

$$\begin{array}{ccccccc}
* & - & * & - & * & - & * \\
| & & | & & | & & | \\
* & - & N_i & - & * & - & * \\
| & & | & & | & & | \\
* & - & C_i = \sigma_i & - & E_i & - & * \\
| & & | & & | & & | \\
* & - & * & - & * & - & *
\end{array}$$

and the following updating rule is applied at each time step t and at each lattice site i:

$$(N_i, E_i, C_i) \longrightarrow \Sigma_i = N_i + E_i + C_i,$$

$$\sigma_i(t+1) = \begin{cases} \operatorname{sgn}(\Sigma_i) & \text{with probability } \frac{1}{2}(1+\varepsilon) \\ -\operatorname{sgn}(\Sigma_i) & \text{with probability } \frac{1}{2}(1-\varepsilon), \end{cases}$$

i.e. the parameter ε mimics the temperature effects. The deterministic dynamics, case when $\varepsilon = 1$, has two configurations: $\sigma = 1$ and $\sigma = -1$ as stationary states. Moreover, these states are stable against finite excitations of an opposite sign. One characteristic feature of the evolution observed in the simulations is that typical excitations of one phase are triangular islands of the other phase, namely:

North

+ + + + + + + + +
+ − + + + + + + +
+ − − + + + + + +
+ − − − + + + + +
West + − − − − + + + + **East**
+ − − − − − + + +
+ − − − − − − + +
+ − − − − − − − +
+ + + + + + + + +

South

In the deterministic model, the southern and western boundaries of these islands are stationary, and the northeast boundary moves southwest with unit speed, so the islands disappear in a time proportional to its linear size. As noise is introduced, the southern and western boundaries acquire a drift to the south and west, respectively, and the speed of the northeast boundary decreases; islands shrink more slowly. Suppose that we continue to increase the noise. At some value of a noise these two motions: the drift of southern and western boundaries and the walk of northeast boundary, balance each other in a sense that large islands of one phase start to live for a long time. Such a behavior is a fundamental feature of Gibbs states in the regime of the phase transition. Therefore there is an expectation that Toom stationary states model some thermodynamic system of the Ising type [7, 8, 5].

Cellular automata belong to the so–called complex systems. Dealing with complex systems one has to be prepared for emerging of new phenomena. It is said sometimes, that complex systems exist on the, so–called, edge of order and chaos [10] and because of this it is quite impossible to predict what kind of phenomena would arise in a system if one shifted a little the system parameters. For example, the deterministic TCA exhibit strong chaotic properties, in the sense of unpredictability, when the initial state randomly prepared at some Bernoulli parameter p arrives at $p = 1/2$ [11]. At some level of the stochastic perturbation the mentioned chaotic behavior is observed in the stochastic TCA. Studying the complex system of Toom cellular automata we feel like taking a walk on the edge of chaos.

In simulations we examine properties of stationary Toom probabilistic cellular automata in a critical regime. The first goal is to answer the question whether the stationary measures are Gibbsian or not. This is done by verifying two necessary conditions for a measure to be a Gibbsian one: the quasilocality of interactions and proper features of the least probable events. The second goal is to find physics in this phase transition [9, 12]. There exists a heuristic statement that all stochastic systems which preserve the up–down spin symmetry belong to the same universality class of Ising model [12]. We ask whether the singularities of thermodynamics functions have the same power low behavior with respect to the tuning parameter: noise ε, (temperature in thermodynamic systems) as systems belonging to the Ising universality class. If the answer is "yes" then it means that microscopic differences are irrelevant close to the transition point, and there exists a level: coarse–grained level , where these two systems: Toom and Ising, are equivalent to each other. Hence we would have the notion of energy for the coarse–grained Toom cellular automata.

3. Computer experiments and results

The first problem to be solved is how to mimic the thermodynamic limit since the phase transitions appear only in the limit of the infinite size of a lattice. The solution is not easy. One of the simplest ways is to implement periodic boundary conditions. In this way we immediately deal with an infinite lattice, however the system built consists of the infinite number of large identical squares. Therefore we have to remember that the limiting system is different from the original one.

Our basic experiments go as follows [13]:

We start with a lattice configuration of all spins *up*: $\sigma = 1$. Then we switch on the Toom probabilistic evolution with a given noise level ε. The evolving system is given after some time T_0 to reach the stationary state:

$$\{\sigma(0)=1\}\ \xrightarrow[\text{to reach stationarity}]{\text{Toom rule at }\varepsilon\ (T_0\text{ times})}\ \sigma(t)\in<\sigma>,$$

where $<\sigma>$ means the set of typical configurations of a stationary measure. What we measure is the mean magnetization, namely, we calculate consecutively the average over a configuration and along the trajectory:

$$<m(\sigma)>=\frac{1}{T}\sum_{t=T_0}^{T_0+T}\frac{1}{L^2}\sum_{i=1}^{L^2}\sigma_i(t)\,. \tag{8}$$

Typically $T_0 = 100L$ for $L < 100$ and $T = 10\ 000$. Few independent runs are performed to avoid possible metastable states.

3.1 Microscopic Hamiltonian search

On Figure 1 we present the decay of the magnetization (8) when the value of noise changes. For comparison we draw the decay of the magnetization in Domany system which is the equilibrium system that is the closest one to the Toom system [7]. Notice the large difference between these two models when one compares

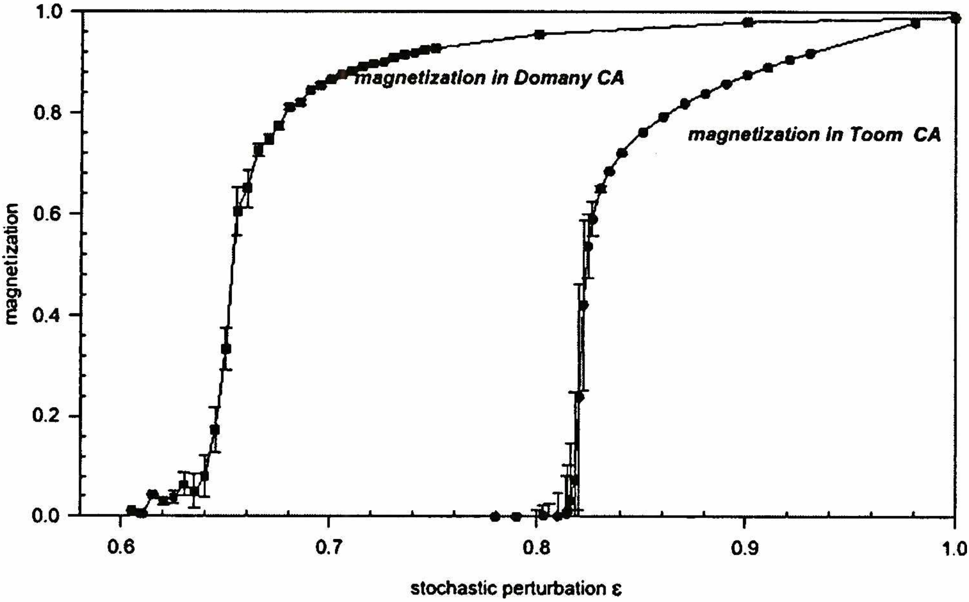

__Figure 1.__ The decay of the magnetization <m> in Toom CA (dots) and Domany CA(squares). The regimes "ferromagnetic" $< m > > 0$, and "paramagnetic" $< m > \approx 0$ are separated by the region of critical changes. Notice the increase of standard deviation errors, marked by error bars, in the region of the phase transition

standard deviation errors which accompany the plotted points. Changes on a lattice configuration at one time step are much larger under Toom dynamics than under Domany dynamics. This is the sign of chaotic properties of Toom cellular automata.

The typical configurations representative for configurations from ferromagnetic, critical and paramagnetic regimes are presented in Figure 2. Figure 3 is to show the two point correlation of magnetization between spins. Such a strong correlation appears abruptly when with ε we go down crossing a value of 0.83 . Finally, in Figure 4 one can find the way, so–called Binder method, to determine the exact value of the transition point. Having localized the transition area, we apply the Griffiths–Pearce argument [2] to verify quasilocality of Toom stationary measures. Quasilocality, i.e., continuity with respect to the product topology on Z^d, is the necessary condition for a measure to be Gibbsian.

The proof of violation of quasilocality requires [5]:

- find a special configuration such that the system has more than one phase;
- show that these two phases can be selected by the proper choice of boundaries;
- show that the selection of these phases goes despite the distance to the border.

In particular we measure the continuity of magnetization of the central point of a lattice O with respect to the evolution of the fixed surrounding state and different

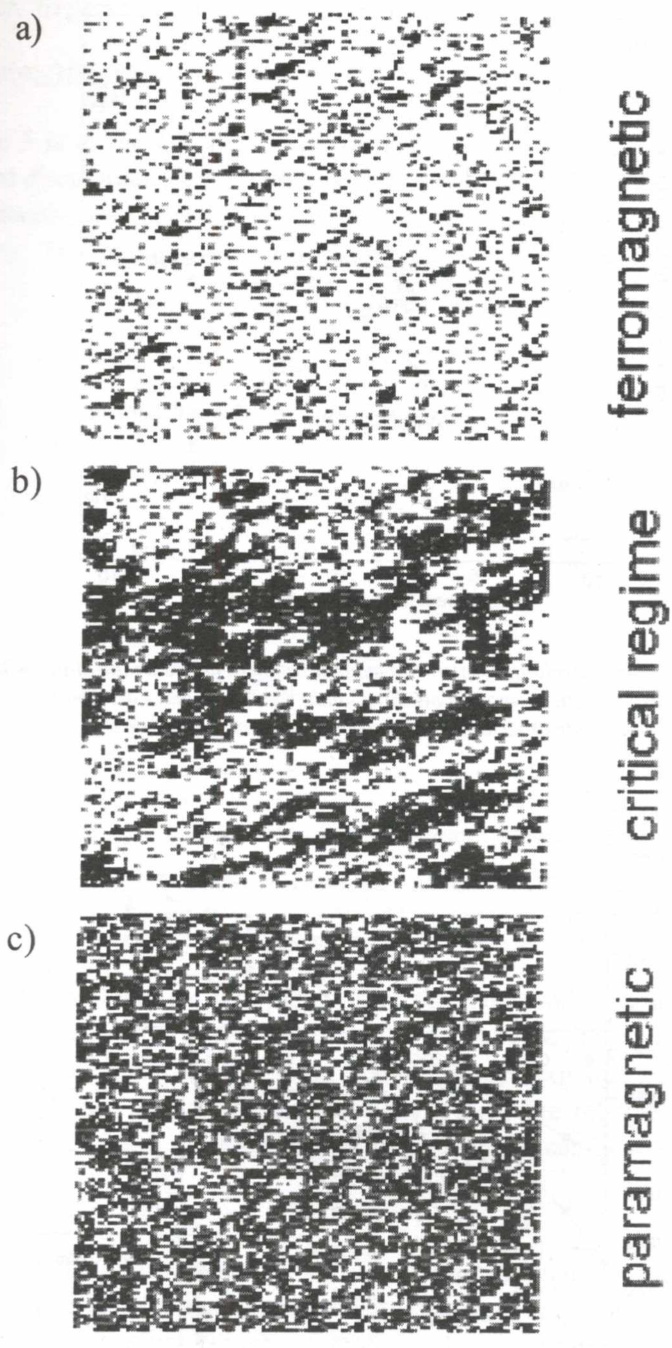

Figure 2. *Typical snapshots of TCA, in time asymptotic regions, observed for a linear size lattice $L = 200$. Up– and down– spins are represented by white and black pixels, respectively. (a) Ordered "ferromagnetic" phase $\varepsilon = 0.90$, (b) critical regime $\varepsilon = 0.82$, (c) disordered "paramagnetic" phase, $\varepsilon = 0.60$*

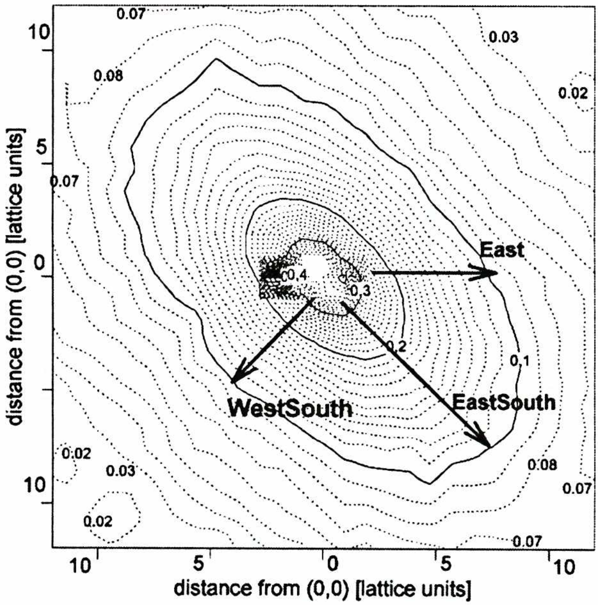

Figure 3. The two–point correlation function of magnetization obtained on the lattice with L = 200 at ε = 0.820 (the contour plot). EastSouth, WestSouth and East denote the basic three directions for the correlation dependence

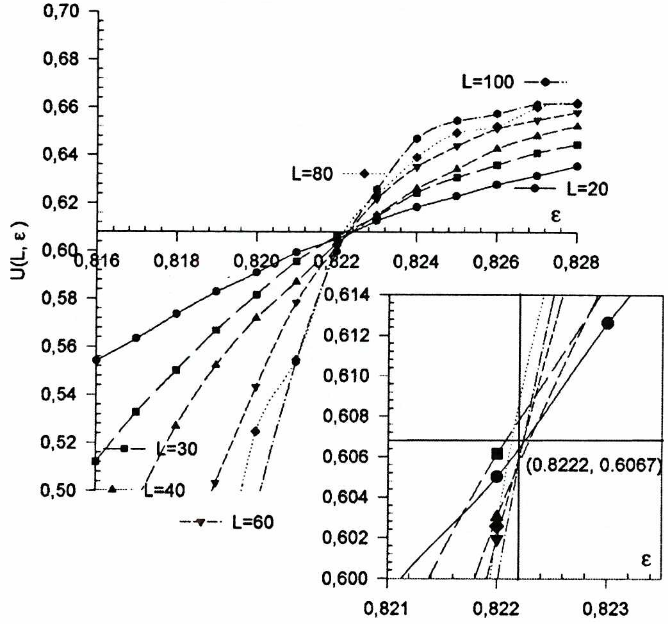

Figure 4. Estimates for ε_{cr} by Binder's method. Plots of cumulants $U(L, \varepsilon) = 1 - (\langle m^4\rangle / 3\langle m^2\rangle^2)$ versus ε are presented for system sizes: $20 \le L \le 100$. Symbols correspond to raw data, lines to spline connections of these points to determine the intersection region — the small window

boundaries. To prove discontinuity of the measured function we have to show that:

$$< m(\sigma_O) | \sigma_\Lambda(\varepsilon_{in}) \otimes +_{\sigma_\Lambda^c} > \neq < m(\sigma_O) | \sigma_\Lambda(\varepsilon_{in}) \otimes -_{\sigma_\Lambda^c} > \text{ when } \Lambda \text{ large}.$$

Figure 5 is to present $m(\sigma_0)$ at different ε_{in} and with + configuration outside. Features of discontinuity are evident for $0.80 \leq \varepsilon \leq 0.82$ if $L < 300$.

Additionaly, we verify the above presented result by considering probability of rare events. The properties of this probability are described by large deviations

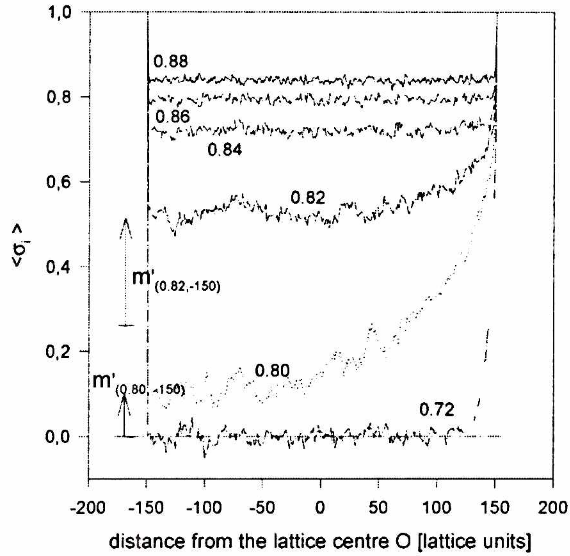

***Figure 5.** The influence of boundary spins which are all set to +. TCA evolve with different ε. The influence arrives through East and North boundaries and changes the internal lattice state. The minimal sub–ordering gained for ε = 0.800 is m' > 0.12, L = 300*

theorems [2]. The heuristic interpretation of the theory of large deviations proves that the probability, that a configurations σ taken from the probability distribution ν "looks in Λ like a typical configuration from μ" decays exponentially in the volume of the subset Λ and the rate of this decay is $i(\mu | \nu)$ the relative entropy density between measures μ and ν. Hence the following formula can be written:

$$\text{Prob}_\nu \{\sigma_\Lambda \text{ is typical for } \mu\} \sim e^{-|\Lambda| \, i(\mu|\nu)}.$$

For $i(\mu | \nu)$ it is known that if $i(\mu | \nu) = 0$ and both measures arise from the same probablistic cellular automata then both measures are Gibbsian [8]. Therefore, we search for a probability to meet a square block configuration $l \times l$ typical for (–) phase in configurations occurring at the critical regime to evaluate:

$$i_l(- | +) = \frac{1}{l^2} \ln \text{Prob}_+ \{m(\sigma_{l \times l}) < 0\}. \tag{9}$$

The result is presented in Figure 6. The zero value of $i_l(\,|\,)$ is attained when the block size l exceeds the lattice size L. Thus, the relative entropy density between the stationary measure with negative magnetization and the stationary state of critical regime is different from zero.

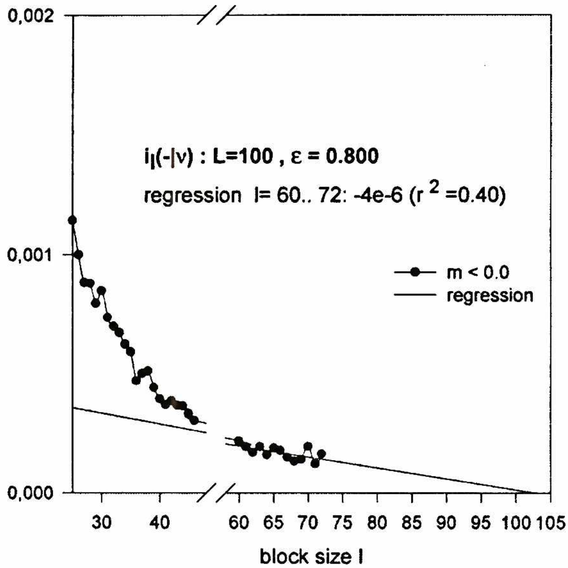

Figure 6. Density of the relative entropy between stationary measures of – phase and ν which is the measure of TCA shifted a little from the critical point. Linear regression indicates $i_l = 0$ at $l > 105$. This is impossible on the lattice of size $L = 100$. The number in () means the correlation coefficient r^2 for the linear fit

3.2 Coarse–grained Hamiltonian search

The three static critical exponents of Ising–like phase transition in TCA estimated by us [13]: β, γ and ν which describe the algebraic dependence on the distance to criticality of magnetization, susceptibility and correlation length, respectively, together with the corresponding values found in Ising systems and coupled map lattices (according to [1]) are as follows:

The value of the fourth critical exponent α which is responsible for free energy

	β	γ	ν	$\alpha = 2 - 2\nu$	$\alpha = 2 - 2\beta - \gamma$
TCA	0.12	1.59	0.85	0.3	0.17
Ising (*2D*)	0.125	1.75	1.0	0	0
CML	0.115	1.55	0.22	0.22	0.22

properties at criticality is calculated following scaling and hyperscaling relations valid for equilibrium thermodynamical systems [3]. The discrepancy between Ising system critical exponents and Toom cellular automata is evident. However, one can notice the similarity between Toom system and coupled map lattices. This similarity is extremely intriguing since the phase transition in CML is driven by deterministic chaos and the parameter tuning the phase transition (temperature in ordinary Ising systems or stochastic noise in Toom cellular automata) is the coupling constant between the diffusive and chaotic parts of microdynamics. The crucial feature which moves both systems into the similar critical properties is the synchronization of the updating procedure.

3.3 Closing remarks

Our proofs of both non–Gibbsianness and non–Isingness, are heuristic. They arise from Monte Carlo exploration of the extremely large configuration space. One could easily improve the quality of our estimations, if considered lattices are of large linear size (this would ensure about non–Gibbsianness) and more points are collected to fit curves which describe the singularities (this would provide critical exponents more reliable). Thus the model discussed here needs further investigations.

Acknowledgement

This work was partially supported by Gdansk University Grant: No BW –5400–5–0261–9. Some of simulations were performed in TASK — Academic Center of Computing, Gdansk, Poland.

References

[1] P. Marcq, H. Chate and P. Manneville, *Phys. Rev. Lett.* **77**, 4003, 1996
P. Marcq, H. Chate and P. Manneville, *Phys. Rev.* **E 55**, 2606, 1997

[2] A. C. D. van Enter, R. Fernandez and A. D. Sokal, *J. Stat. Phys.* **72**, 879, 1993

[3] J. J. Binney, N. J. Dowrick, A. J. Fisher and M. E. J. Newman, in *The Theory of Critical Phenomena*, Oxford University Press, Oxford, 1992

[4] *Monte Carlo Methods in statistical Physics* ed. K. Binder Springer–Verlag, Berlin–Heidelberg–NewYork, 1979
K.Binder, *Z.Phys.* **B 43**, 119, 1981

[5] R. Fernandez, *Physica* **A 263**, 117, 1999

[6] J.L.Lebowitz and R.Schonmann, *Prob.Th.Rel.Fields* **77**, 49, 1988

[7] J. L. Lebowitz, Ch. Maes and E. R. Speer, *J. Stat. Phys.* **59**, 117, 1990

[8] Ch. Maes and K. Vande Velde, *Physica* **A 206**, 587 (1994)
Ch. Maes and K. Vande Velde, *Commun.Math.Phys.* **189**, 277, 1997

[9] Ch. H. Bennett and G. Grinstein, *Phys. Rev. Lett.* **55**, 657, 1985

[10] C. G. Langton, *Physica* **D 42**, 12, 1990
H. A. Gutowitz and C. G. Langton in *Mean Field Theory of the Edge of Chaos*, Proceedings of ECAL3, Springer Verlag, New York, 1995
A. Wuensche in *Classifying Cellular Automata Automatically*, Santa Fe Institute working paper 98–02–018, 1998

[11] D.Makowiec, *Physica* **A 234**, 435, 1996

[12] G. Grinstein,C. Jayaprakash and Yu He, *Phys. Rev. Lett.* **55**, 2527, 1985
B. C. S. Grandi and W. Figueiredo, *Phys. Rev.* **E 53** 5484, 1996

[13] D. Makowiec, *Phys. Rev.* **E 55**, 6582, 1997
D. Makowiec, *Phys. Rev.* **E 56**, 5193, 1997
D. Makowiec, *Acta Phys. Pol.* **B 29**, 1599, 1998
D. Makowiec, *Phys. Rev.* **E 60**, 3787, 1999