

Competitive nucleation in reversible probabilistic cellular automata

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(Received 26 May 2008; published 1 October 2008)

The problem of competitive nucleation in the framework of probabilistic cellular automata is studied from the dynamical point of view. The dependence of the metastability scenario on the self-interaction is discussed. An intermediate metastable phase, made of two flip-flopping chessboard configurations, shows up depending on the ratio between the magnetic field and the self-interaction. A behavior similar to the one of the stochastic Blume-Capel model with Glauber dynamics is found.

DOI: 10.1103/PhysRevE.78.040601

PACS number(s): 64.60.qe, 64.60.My, 05.50.+q, 05.70.Ln

Metastable states are common in nature; they show up in connection with first-order phase transitions. Well-known examples are supercooled and superheated liquids. Their statistical mechanics description revealed to be a challenging task. An approach based on equilibrium states has been developed via analytic continuation techniques [1] and via the introduction of equilibrium systems on suitably restricted sets of configurations [2–4]. The purely dynamical point of view, dating back to Ref. [5], has been developed via the pathwise technique [6] and the potential theoretical approach [7].

We shall stick to the dynamical description to investigate competing metastable states. This situation arises in many physical processes, such as the crystallization of proteins [8,9] and their approach to equilibrium [10]. The extreme situation is represented by glasses, in which the presence of a huge number of minima of the energy landscape prevents the system from reaching equilibrium [11]. The study of these systems is difficult, since the minima of the energy and the decay pathways between them change when the control parameters are varied. It is then of interest the study of models in which a complete control of the variations induced on the energy landscape by changes in the parameters is possible.

In this perspective, the analysis of the Blume-Capel model in Refs. [12,13] and that of the Potts model in Ref. [14] are of great interest. In the Blume-Capel model the sites of the lattice can be either empty or occupied by a 1/2-spin particle. The interaction favors the presence of neighboring aligned spins; the chemical potential λ controls the tendency to have particles or lacunas on the lattice and the magnetic field h , depending on its sign, favors either the pluses or the minuses. Depending on the parameters, in the zero temperature limit the stable state is the one with all the spins up (\mathbf{u}) or all the spins down (\mathbf{d}) or no particle at all ($\mathbf{0}$). Let $h, \lambda > 0$, so that the unique stable state is \mathbf{u} , and set $a = h/\lambda$. For $a < 1$ the transition from the metastable state \mathbf{d} to \mathbf{u} is achieved via a sequence of increasing plus square droplets in the sea of minuses. For $1 < a < 2$ and h small, the transition from \mathbf{d} to \mathbf{u} is realized via increasing squared frames in which the internal pluses are separated by the external minuses by a large one zero frame. For $a > 2$ and h small, the system started at \mathbf{d} visits the state $\mathbf{0}$ before reaching \mathbf{u} ; the transition from \mathbf{d} to $\mathbf{0}$ is achieved via increasing zero square

droplets in the sea of minuses, while the transition from $\mathbf{0}$ to \mathbf{u} is realized via increasing plus square droplets in the sea of zeros.

We study, here, metastability for a probabilistic cellular automaton [15] with self-interaction κ , focusing on the dependence of the metastability scenario on such a parameter. The model interpolates those studied in Ref. [16] ($\kappa=0$) and [17,18] ($\kappa=1$). For $\kappa=0$ each spin interacts only with its nearest neighbors; for $\kappa=1$ the self-interaction has the same strength as the nearest-neighbor coupling. In the absence of self-interaction an intermediate metastable state shows up; it is proven that the intermediate state is visited during the transition from the metastable to the stable state. The role played by the intermediate state changes as the self-interaction κ is varied. Quite surprisingly, results similar to those found in Ref. [12] for the Blume-Capel model are obtained.

Consider the two-dimensional torus $\Lambda = \{0, \dots, L-1\}^2$, with L even, endowed with the Euclidean metric; $x, y \in \Lambda$ are nearest neighbors if and only if their mutual distance is equal to 1. Associate a variable $\sigma(x) = \pm 1$ with each site $x \in \Lambda$ and let $\mathcal{S} = \{-1, +1\}^\Lambda$ be the configuration space. Let $\beta > 0$ and $\kappa, h \in [0, 1]$. Consider the Markov chain σ_n , with $n = 0, 1, \dots$, on \mathcal{S} with transition matrix

$$p(\sigma, \eta) = \prod_{x \in \Lambda} p_{x, \sigma}(\eta(x)) \quad \forall \sigma, \eta \in \mathcal{S}, \quad (1)$$

where, for $x \in \Lambda$ and $\sigma \in \mathcal{S}$, $p_{x, \sigma}(\cdot)$ is the probability measure on $\{-1, +1\}$ defined as $p_{x, \sigma}(s) = 1 / (1 + \exp\{-2\beta s[S_\sigma(x) + h]\})$ with $s \in \{-1, +1\}$ and $S_\sigma(x) = \sum_{y \in \Lambda} K(x-y)\sigma(y)$ where $K(x-y)$ is 0 if $|x-y| \geq 2$, 1 if $|x-y|=1$, and κ if $|x-y|=0$. The probability $p_{x, \sigma}(s)$ for the spin $\sigma(x)$ to be equal to s depends only on the values of the spins of σ in the five-site cross centered at x . The metastable behavior of model (1) has been studied in Ref. [16] for $\kappa=0$ and in Refs. [17,18] for $\kappa=1$.

The Markov chain (1) is probabilistic cellular automata; the chain σ_n , with $n=0, 1, \dots$, updates all the spins simultaneously and independently at any time. The chain is reversible, see Ref. [15], with respect to the Gibbs measure $\mu(\sigma) = \exp[-\beta H(\sigma)]/Z$ with $Z = \sum_{\eta \in \mathcal{S}} \exp[-\beta H(\eta)]$ and

$$H(\sigma) = -h \sum_{x \in \Lambda} \sigma(x) - \frac{1}{\beta} \sum_{x \in \Lambda} \ln \cosh\{\beta[S_\sigma(x) + h]\} \quad (2)$$

that is detailed balance $p(\sigma, \eta)e^{-\beta H(\sigma)} = p(\eta, \sigma)e^{-\beta H(\eta)}$ holds for $\sigma, \eta \in \mathcal{S}$; hence, μ is stationary. We refer to $1/\beta$ as to the temperature and to h as to the magnetic field; the interaction is short range and it is possible to extract the potentials as described in Ref. [18].

Although the dynamics is reversible with respect to the Gibbs measure associated to the Hamiltonian (2), the probability $p(\sigma, \eta)$ cannot be expressed in terms of $H(\sigma) - H(\eta)$, as usually happens for Glauber dynamics. Given $\sigma, \eta \in \mathcal{S}$, we define the energy cost

$$\Delta(\sigma, \eta) = - \lim_{\beta \rightarrow \infty} \frac{\ln p(\sigma, \eta)}{\beta} = \sum_{\substack{x \in \Lambda: \\ \eta(x)[S_\sigma(x) + h] < 0}} 2|S_\sigma(x) + h|. \quad (3)$$

Note that $\Delta(\sigma, \eta) \geq 0$ and $\Delta(\sigma, \eta)$ is not necessarily equal to $\Delta(\eta, \sigma)$; it can be proven, see [17], Sec. 2.6, that

$$e^{-\beta \Delta(\sigma, \eta) - \beta \gamma(\beta)} \leq p(\sigma, \eta) \leq e^{-\beta \Delta(\sigma, \eta) + \beta \gamma(\beta)} \quad (4)$$

with $\gamma(\beta) \rightarrow 0$ in the zero temperature limit $\beta \rightarrow \infty$. Hence, Δ can be interpreted as the cost of the transition from σ to η and plays the role that, in the context of Glauber dynamics, is played by the difference of energy.

To pose the problem of metastability it is necessary to understand the structure of the ground states; since the Hamiltonian depends on β , their definition deserves some thinking. The ground states are those configurations on which the Gibbs measure μ concentrates when $\beta \rightarrow \infty$; hence, they can be defined as the minima of the energy

$$E(\sigma) = \lim_{\beta \rightarrow \infty} H(\sigma) = -h \sum_{x \in \Lambda} \sigma(x) - \sum_{x \in \Lambda} |S_\sigma(x) + h|. \quad (5)$$

For $\mathcal{T} \subset \mathcal{S}$, we set $E(\mathcal{X}) = \min_{\sigma \in \mathcal{X}} E(\sigma)$. For $h > 0$ the configuration \mathbf{u} , with $\mathbf{u}(x) = +1$ for $x \in \Lambda$, is the unique ground state; indeed each site contributes to the energy with $-h - (4 + \kappa + h)$. For $h = 0$, the ground states are the configurations such that all the sites contribute to the sum (5) with $4 + \kappa$. Hence, for $\kappa \in (0, 1]$, the sole ground states are the configurations \mathbf{u} and \mathbf{d} , with $\mathbf{d}(x) = -1$ for $x \in \Lambda$. For $\kappa = 0$, the configurations $\mathbf{c}^e, \mathbf{c}^o \in \mathcal{S}$ such that $\mathbf{c}^e(x) = (-1)^{x_1 + x_2}$ and $\mathbf{c}^o(x) = (-1)^{x_1 + x_2 + 1}$ for $x = (x_1, x_2) \in \Lambda$ are ground states, as well. Notice that \mathbf{c}^e and \mathbf{c}^o are chessboardlike states with the pluses on the even and odd sublattices, respectively; we set $\mathbf{c} = \{\mathbf{c}^e, \mathbf{c}^o\}$. Since the side length L of the torus Λ is even, then $E(\mathbf{c}^e) = E(\mathbf{c}^o) = E(\mathbf{c})$.

We study those energies as a function of κ and h , recalling that periodic boundary conditions are considered. We have $E(\mathbf{u}) = -L^2(4 + \kappa + 2h)$, $E(\mathbf{d}) = -L^2(4 + \kappa - 2h)$, and $E(\mathbf{c}) = -L^2(4 - \kappa)$; hence $E(\mathbf{c}) > E(\mathbf{d}) > E(\mathbf{u})$ for $0 < h < \kappa \leq 1$, $E(\mathbf{c}) = E(\mathbf{d}) > E(\mathbf{u})$ for $0 < h = \kappa \leq 1$, and $E(\mathbf{d}) > E(\mathbf{c}) > E(\mathbf{u})$ for $0 < \kappa < h \leq 1$.

We can now pose the problem of metastability at finite volume and temperature tending to zero (Friedlin-Wentzel

regime). Following Ref. [6], see also the Appendix of Ref. [17], given a sequence of configurations $\omega = \omega_1, \dots, \omega_n$, with $n \geq 2$, we define the energy height along the path ω as $\Phi_\omega = \max_{i=1, \dots, | \omega | - 1} [E(\omega_i) + \Delta(\omega_i, \omega_{i+1})]$. Note that the definition does not depend on the direction in which the path ω is followed. More precisely, denoted by ω' the path $\omega_n, \omega_{n-1}, \dots, \omega_1$, since

$$E(\sigma) + \Delta(\sigma, \eta) = E(\eta) + \Delta(\eta, \sigma) \quad (6)$$

for any $\sigma, \eta \in \mathcal{S}$, it follows that $\Phi_\omega = \Phi_{\omega'}$; (6) is a consequence of the detailed balance principle. Given $A, A' \subset \mathcal{S}$, we let the communication energy between A and A' be the minimal energy height Φ_ω over the set of paths ω starting in A and ending in A' . For any $\sigma \in \mathcal{S}$, we let $\mathcal{I}_\sigma \subset \mathcal{S}$ be the set of configurations with energy strictly below $E(\sigma)$ and $V_\sigma = \Phi(\sigma, \mathcal{I}_\sigma) - E(\sigma)$ be the stability level of σ , that is, the energy barrier that, starting from σ , must be overcome to reach the set of configurations with energy smaller than $E(\sigma)$; we set $V_\sigma = \infty$ if $\mathcal{I}_\sigma = \emptyset$. We denote by \mathcal{S}^s the set of global minima of the energy (5), namely, the collection of the ground states, and suppose that the communication energy $\Gamma = \max_{\sigma \in \mathcal{S} / \mathcal{S}^s} V_\sigma$ is strictly positive. Finally, we define the set of metastable states $\mathcal{S}^m = \{\eta \in \mathcal{S} : V_\eta = \Gamma\}$. The set \mathcal{S}^m deserves its name, since it proves the following (see, e.g., Ref. [17], Theorem A.2): Pick $\sigma \in \mathcal{S}^m$, consider the chain σ_n started at $\sigma_0 = \sigma$, then the first hitting time $\tau_{\mathcal{S}^s} = \inf\{t > 0 : \sigma_t \in \mathcal{S}^s\}$ to the ground states is a random variable with mean exponentially large in β , that is,

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln \mathbb{E}_\sigma[\tau_{\mathcal{S}^s}] = \Gamma \quad (7)$$

with \mathbb{E}_σ the average on the trajectories started at σ .

In this regime the description of metastability is reduced to the computation of \mathcal{S}^s , Γ , and \mathcal{S}^m . We choose the parameters of the model (1) in such a way that $0 < h < 1$, $h \neq \kappa$, and $2/h$, $2/(h - \kappa)$, $2/(h + \kappa)$, and $(2 + \kappa - h)/h$ are not integers. The configuration \mathbf{u} is then the unique ground state, i.e., $\mathcal{S}^s = \{\mathbf{u}\}$. Two candidates for metastability are \mathbf{d} and \mathbf{c} ; to find \mathcal{S}^m , one should compute Γ and prove that either $V_{\mathbf{d}}$ or $V_{\mathbf{c}}$ is equal to Γ . This is a difficult task, indeed all the paths ω connecting \mathbf{d} and \mathbf{c} to \mathbf{u} must be taken into account and the related energy heights Φ_ω computed. Since at each time step all the spins of the lattice can be updated, the structure of the trajectories is highly complicated. This is why the study of the energy landscape of probabilistic cellular automata is very difficult [17], Theorem 2.3; such a task is simpler for serial Glauber dynamics, where a general approach can be developed [6], Sec. 7.6.

We develop a heuristic argument to compute Γ . Recall (3) and note that κ and h have been chosen so that $S_\sigma(x) + h \neq 0$. Thus, it follows that, given $\sigma \in \mathcal{S}$, there exists a unique $\eta \in \mathcal{S}$ such that $\Delta(\sigma, \eta) = 0$; the configuration η is such that $\eta(x)[S_\sigma(x) + h] > 0$ for all $x \in \Lambda$ and is the unique configuration to which the system can jump, starting from σ , with probability tending to one in the limit $\beta \rightarrow \infty$ [see (4)]. We say that $\sigma \in \mathcal{S}$ is a local minimum of the energy if and only if $\Delta(\sigma, \sigma) = 0$; starting from a local minimum, transitions to different configurations have strictly positive energy cost and

thus happen with negligible probability in the zero temperature limit. It is immediate that \mathbf{d} and \mathbf{u} are local minima of the energy, while \mathbf{c}^e and \mathbf{c}^o are not; indeed $\mathbf{c}^e(x)[S_{\mathbf{c}^e}(x)+h] < 0$ and $\mathbf{c}^o(x)[S_{\mathbf{c}^o}(x)+h] < 0$ for all $x \in \Lambda$. We also have that $\Delta(\mathbf{c}^e, \mathbf{c}^o) = \Delta(\mathbf{c}^o, \mathbf{c}^e) = 0$; hence, at very low temperature, the system started in \mathbf{c}^o is trapped in a continuous flip-flop between \mathbf{c}^o and \mathbf{c}^e . A peculiarity of parallel dynamics is the existence of pairs $\sigma, \eta \in \mathcal{S}$ in which the chain is trapped since $\Delta(\sigma, \eta) = \Delta(\eta, \sigma) = 0$; the probability to exit such a pair is exponentially small in β .

We characterize, now, the local minima and the trapping pairs. For what concerns the local minima, we consider a configuration σ and study the sign of $S_\sigma(x)+h$. Suppose, first, $h < \kappa$ and recall $\kappa \leq 1$; the sign of $S_\sigma(x)+h$ equals the sign of the majority of the spins in the five-site cross centered at x . Hence, σ is a local minimum if and only if for each site x there exist at least two nearest neighbors such that the associated spins are equal to $\sigma(x)$. Suppose, now, $h > \kappa \geq 0$; the sign of $S_\sigma(x)+h$ is negative if and only if at least three among the spins associated to neighboring sites of x are minus. Hence, σ is a local minimum if and only if for each site x such that $\sigma(x) = -1$ there exist at least three negative minus neighbors and for each site x such that $\sigma(x) = +1$ there exist at least two positive neighbors. In conclusion, for $h > \kappa$ the local minima of the energy are those configurations in which all the pluses, if any, are precisely those associated with the sites inside a rectangle (plus-minus droplets). For $h < \kappa$ the local minima are all the configurations that can be drawn adding pluses to \mathbf{d} so that each plus (minus) has at least (at most) two neighboring pluses. Plus-minus rectangular droplets are local minima also in this case. For what concerns the trapping pairs, consider a configuration σ with a rectangle of chessboard plunged in the sea of minuses (chessboard-minus droplet) and let η be the configuration obtained flipping all the spins associated with sites in the chessboard rectangle. The configuration σ, η form a trapping pair only for $h > \kappa$. Indeed, it is immediate to show that all the spins of the chessboard tend to flip, some thinking is necessary only for the minus corners. Let x be the corner site with $\sigma(x) = -1$, since $S_\sigma(x)+h = -\kappa+h$, we have that $S_\sigma(x)+h > 0$ for $h > \kappa$ and $S_\sigma(x)+h < 0$ for $h < \kappa$. Thus, the spin tends to flip in the former case and not in the latter.

The local minima and the trapping pairs can be used to construct the optimal paths connecting \mathbf{d} and \mathbf{c} to the ground state \mathbf{u} . We distinguish two cases.

Case $h > \kappa \geq 0$. Although \mathbf{c}^e and \mathbf{c}^o are not local minima of the energy, the system started in \mathbf{c} is trapped in a continuous flip-flop between \mathbf{c}^o and \mathbf{c}^e . This trapping persists even if a rectangle of pluses is inserted in the chessboard background (plus-chessboard droplet); a path from \mathbf{c} to \mathbf{u} can be constructed with a sequence of such droplets. The difference of energy between two plus-chessboard droplets with side lengths, respectively, given by $\ell, m \geq 2$ and $\ell, m+1$ is equal to $4-2(\kappa+h)\ell$. It then follows that the energy of a such a droplet is increased by adding an ℓ -long slice if and only if $\ell \geq [2/(\kappa+h)]+1 = \lambda_c^u$ ($[x]$ denotes the largest integer smaller than the real x). The length λ_c^u is called the critical length.

It is reasonable that the energy barrier V_c is given by the difference of energy between the smallest supercritical plus-chessboard droplet, i.e., the plus-chessboard square droplet with side length λ_c^u , and the configuration \mathbf{c} ; by using (5) we get that such a difference of energy is equal [19] to $\Gamma_c^u = 8/(\kappa+h)$.

A path from \mathbf{d} to \mathbf{u} can be constructed with a sequence of plus-minus droplets. By using (5) we get that the difference of energy between two plus-minus droplets with side lengths, respectively, given by $\ell, m \geq 2$ and $\ell, m+1$ is $4(2-h\ell)$. It then follows that the energy of a plus-minus droplet is increased by adding an ℓ -long slice if and only if $\ell \geq [2/h]+1 = \lambda_d^u$. The length λ_d^u is the critical length for the plus-minus droplets; by using (5) we get that the difference of energy between the smallest supercritical plus-minus droplet and \mathbf{d} is equal to $\Gamma_d^u = 16/h$.

An alternative path from \mathbf{d} to \mathbf{u} can be constructed via a sequence of frames with the internal rectangle of pluses separated by the external minuses by a large one chessboard stripe. These are peculiar trapping pairs in which the flip-flopping spins are those associated with the sites in the stripe of chessboard. We can prove that the difference of energy between two frames with internal (rectangle of pluses) side lengths, respectively, given by $\ell, m \geq 2$ and $\ell, m+1$ is equal to $8-4(h-\kappa)-4h\ell$, so that the critical length for those frames is given by $\lambda_d^f = [(2-h+\kappa)/h]+1$ and the difference of energy between the smallest supercritical frame and \mathbf{d} is equal to $\Gamma_d^f = 16[1-(h-\kappa)/2]^2/h$.

A path from \mathbf{d} to \mathbf{c} can be constructed with a sequence of chessboard-minus droplets. By using (5) we get that the difference of energy between two chessboard-minus droplets with side lengths, respectively, given by $\ell, m \geq 2$ and $\ell, m+1$ is equal to $4-2(h-\kappa)\ell$. It then follows that the energy of a chessboard-minus droplet is increased by adding an ℓ -long slice if and only if $\ell \geq [2/(h-\kappa)]+1 = \lambda_d^c$. The length λ_d^c is the critical length for the chessboard-minus droplets; the energy difference of energy between the smallest supercritical chessboard-minus droplet and \mathbf{d} is equal to $\Gamma_d^c = 8/(h-\kappa)$.

Note that $\Gamma_d^f < \Gamma_d^u$ for h, κ small. Moreover, let $a = h/\kappa$ and remark that, provided the magnetic field h is chosen small enough as a function of a , $\Gamma_d^c < \Gamma_d^f$ for $a > 2$ and $\Gamma_d^c > \Gamma_d^f$ for $1 < a < 2$. Hence, for $a > 2$ we obtain $V_d = \Gamma_d^c$, that is the chain escapes from \mathbf{d} and reaches the state \mathbf{c} in a time that can be estimated as in (7) with $\Gamma = \Gamma_d^c$. Starting from \mathbf{c} the chain will reach \mathbf{u} by overcoming the energy barrier $V_c = \Gamma_c^u < V_d$. Note that $V_c = V_d$ in the limiting case $\kappa = 0$, hence both \mathbf{c} and \mathbf{d} are metastable states (results in [16] are recovered). For $1 < a < 2$, $V_d = \Gamma_d^f$, that is the chain escapes from \mathbf{d} and reaches the state \mathbf{u} via a sequence of increasing frames in a time estimated as in (7) with $\Gamma = \Gamma_d^f$.

Case $h < \kappa \leq 1$. By paying the smallest energy cost any local minimum can be transformed in a configuration with the pluses forming well-separated rectangles (see [18]); hence, the most relevant local minima are the plus rectangular droplets. As noted above, for this choice of the parameters the system cannot be trapped in chessboard-minus droplets. Thus, the energy barrier V_d is given by the energy

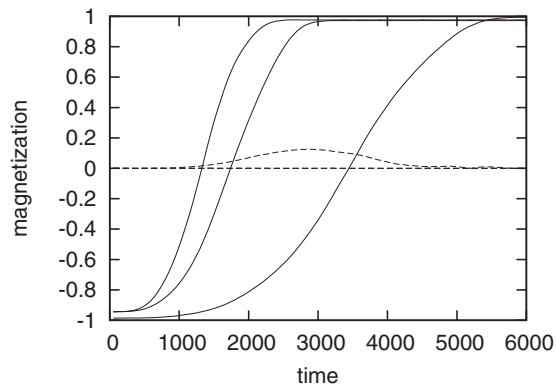


FIG. 1. The time unit is the time step of the chain. Solid lines (from the left-hand side to the right-hand side) represent the magnetization of the runs $(\kappa, \beta) = (0.15, 0.55), (0.4, 0.5), (0, 0.025, 0.7)$. Dashed lines represent the absolute value of the staggered magnetization; the non-null curve is found for $(\kappa, \beta) = (0.025, 0.7)$.

$\Gamma_{\mathbf{d}}^{\mathbf{u}}$ of the smallest supercritical plus droplet. As before, we also have $V_{\mathbf{c}} = \Gamma_{\mathbf{c}}^{\mathbf{u}}$. Since $V_{\mathbf{c}} < V_{\mathbf{d}}$, we have that \mathbf{d} is the unique metastable state, the communication energy is $\Gamma = \Gamma_{\mathbf{d}}^{\mathbf{u}}$, the tunneling time is $\exp\{\beta\Gamma_{\mathbf{d}}^{\mathbf{u}}\}$ in the sense of (7), and the zero

temperature limit transition from the metastable state \mathbf{d} to the stable state \mathbf{u} is achieved via the nucleation of a plus-minus square droplet with side length $\lambda_{\mathbf{d}}^{\mathbf{u}}$. For $\kappa=1$ the results proven in [17] are recovered.

The metastability scenario depends on the ratio between the magnetic field and the self-interaction. For $\kappa=0$ the two states \mathbf{d} and \mathbf{c} are both metastable. For $a > 2$ and h small, \mathbf{c} is crucial, although not metastable, since it is visited during the transition from the metastable state \mathbf{d} to the stable state \mathbf{u} . For $2 > a > 1$ and h small, the chessboard configuration plays no role at all and the exit from the metastable \mathbf{d} state is achieved via the direct formation of the plus phase via a sequence of increasing plus-minus droplets. The scenario is very similar to the one proven in Ref. [12] for the Blume-Capel model with Glauber (serial) dynamics; the role of the chemical potential λ is played here by the self-interaction κ . This behavior has been tested at finite temperature via a Monte Carlo simulation [20]. We have considered $L=1000$, $h=0.2$, and run the chain for $(\kappa, \beta) = (0.025, 0.7), (0.15, 0.55), (0, 4, 0.5)$. By measuring the staggered and the usual magnetization, we point out that the system visits \mathbf{c} before reaching \mathbf{u} only in the run $\kappa=0.025$ and $\beta=0.7$ (see Fig. 1), which is the only run with $a > 2$.

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