Phase transition in a one-dimensional Ising ferromagnet at zero temperature using Glauber dynamics with a synchronous updating mode

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In the past decade low-temperature Glauber dynamics for the one-dimensional Ising system has been several times observed experimentally and occurred to be one of the most important theoretical approaches in a field of molecular nanomagnets. On the other hand, it has been shown recently that Glauber dynamics with the Metropolis flipping probability for the zero-temperature Ising ferromagnet under synchronous updating can lead surprisingly to the antiferromagnetic steady state. In this paper the generalized class of Glauber dynamics at zero temperature will be considered and the relaxation into the ground state, after a quench from high temperature, will be investigated. Using Monte Carlo simulations and a mean field approach, discontinuous phase transition between ferromagnetic and antiferromagnetic phases for a one-dimensional ferromagnet will be shown.

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I. INTRODUCTION

Glauber dynamics for the Ising spin chain has been known for almost 50 years [1], but only recently it became a really hot topic, not only from a fundamental, but also an applicative point of view [2–8]. It is well known that a purely one-dimensional (1D) system exhibits long-range ordering only at zero temperature $T=0$ K. Nevertheless, in some situations long relaxation times for the magnetization reversal with decreasing temperature can be observed, and finally at significantly low temperatures, the material can behave as a magnet. The phenomenon of slow magnetic relaxation is considered as one of the most important achievements of molecular magnetism, opening exciting new perspectives including that of storing information [9,10]. Slow relaxation of the magnetization, predicted in the 1960s by Glauber in a chain of ferromagnetically coupled Ising spins [1], in materials composed of magnetically isolated chains was observed for the first time in 2001 [2]. In 2002, this new class of nanomagnets was named single-chain magnets (SCM) [3] (for a recent review see [8]) and the Glauber dynamics for the one-dimensional Ising spins system became one of the most important theoretical approaches for SCM.

Within the Glauber dynamics for Ising spins with a spin $s=1/2$, in a broad sense, each spin is flipped $S_i(t)\rightarrow -S_i(t+1)$ with a rate $W(\delta E)$ per unit time and this rate is assumed to depend only on the energy difference implied in the flip. In this paper we consider the generalize class of zero-temperature dynamics defined as

$$W(\delta E)=\begin{cases}1 & \text{if } \delta E<0,\\ W_0 & \text{if } \delta E=0,\\ 0 & \text{if } \delta E>0,\end{cases} \tag{1}$$

which occurred to be very interesting not only from an applicative perspective, but also from a theoretical point of view as an example of nonequilibrium dynamical systems with many attractors [11]. The zero-temperature limits of the original Glauber dynamics [1] and Metropolis rates [12] (two the most popular choices) are respectively $W_0^G=1/2$ and $W_0^M=1$.

Glauber dynamics was originally introduced as a sequential updating (SU) process [1]. Also Monte Carlo method, used frequently for various models in statistical physics, as proposed originally by Metropolis *et al.* [12], is essentially SU process. Evolution under dynamics defined by Eq. (1) with random sequential updating is already well known in a case of one-dimensional system and can be derived analytically [11]. For any nonzero value of the rate W_0 ferromagnetic steady state is reached and the dynamics belongs to the universality class of the zero-temperature Glauber model [1]. The particular value $W_0=0$ corresponds to the constrained zero-temperature Glauber dynamics ([11] and references therein). In the constrained zero-temperature Glauber dynamics, the only possible moves are flips of isolated spins and therefore the system eventually reaches a blocked configuration, where there is no isolated spin [11], i.e., for $W_0=0$ the relaxation time to the ferromagnetic steady state is infinite.

The case of the synchronous updating, in which all units of the system are updated at the same time, is much more interesting. Moreover, clear evidence of a relaxation mechanism which involves the simultaneous reversal of spins has been shown experimentally for magnetic chains at low temperatures [15].

In [20] more general form of zero-temperature Glauber dynamics has been investigated than one defined by Eq. (1). They have studied a model with two parameters Γ and δ, which can be presented at $T=0$ analogously to Eq. (1) as

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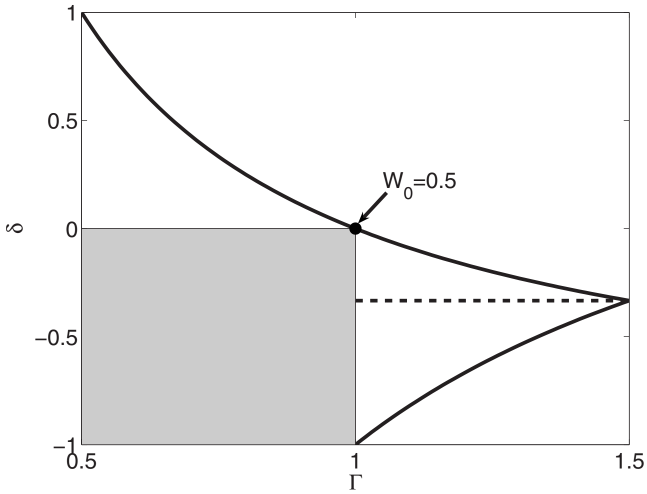

FIG. 1. Thick lines correspond to equations $\delta=(1-\Gamma)/\Gamma$ and $\delta=(\Gamma-2)/\Gamma$. The region between these two lines corresponds to the condition $W(\delta E)\in[0,1]$ (see Eq. (2)). In [20] the region denoted by the gray color has been investigated (i.e., $\delta<0$, $\Gamma\in(0,1)$). In this paper we consider one-parameter model defined by Eq. (1) and therefore we are able to investigate only upper bold line defined by Eq. (4).

$$W(\delta E)=\begin{cases}\Gamma(1+\delta) & \text{if } \delta E<0,\\ \dfrac{\Gamma}{2}(1-\delta) & \text{if } \delta E=0,\\ 0 & \text{if } \delta E>0,\end{cases} \tag{2}$$

where again $W(\delta E)$ denotes the flipping rate per unit time. To fulfill the condition $W(\delta E)\in[0,1]$, as seen from Eq. (2), the following relations have to be satisfied,

$$-1\le\delta\le\frac{1-\Gamma}{\Gamma},$$

$$\frac{\Gamma-2}{\Gamma}\le\delta\le 1. \tag{3}$$

Above relations correspond to the region between thick lines in Fig. 1. In [20] the region denoted by the gray color in Fig. 1 has been investigated [i.e., $\delta<0$, $\Gamma\in(0,1)$]. Comparing Eqs. (1) and (2) we can easily derive the following relations:

$$\Gamma=W_0+\frac{1}{2},$$

$$\delta=\frac{1/2-W_0}{1/2+W_0}, \tag{4}$$

which are parametric expression of the upper bold line of Fig. 1. In this paper we consider one-parameter model defined by Eq. (1) with $W_0\in[0,1]$ and therefore we are able to investigate only upper bold line of Fig. 1 defined by Eq. (4).

II. SIMULATION AND MEAN FIELD RESULTS

We consider the chain of L Ising spins $\sigma_i=\pm 1$ $(i=1,2,\ldots L)$ with the periodic boundary conditions. In the initial state each lattice site is occupied independently by a randomly chosen value +1 or −1, both equally probable (high temperature situation). In every time step all spins are considered simultaneously, but each spin is flipped independently with probability $W(\delta E)$ defined by Eq. (1). It occurs that for all $W_0\in(0,1)$ system eventually reaches one of the two final states—ferromagnetic steady state or antiferromagnetic limit cycle. If we measure the density of active bonds (bond is active if connects two sites with opposite spins):

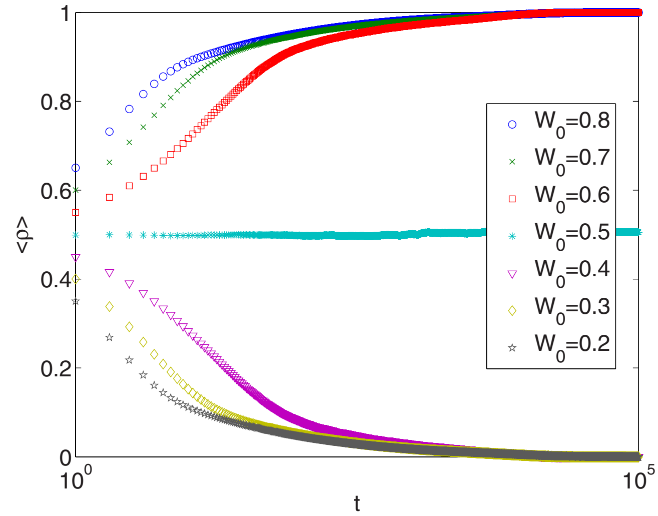

FIG. 2. (Color online) The time evolution of the mean value of the density of active bonds $\langle\rho\rangle$ measured in Monte Carlo steps for the lattice size $L=160$ is presented. Averaging was done over 10^4 samples. For $W_0<0.5$ the mean number of active bonds decreases in time to 0 (ferromagnetic steady state) and for $W_0>0.5$ increases to 1 (antiferromagnetic limit cycle).

$$\rho=\frac{1}{2L}\sum_{i=1}^{L}(1-\sigma_i\sigma_{i+1}), \tag{5}$$

we obtain in the final state $\rho_{st}=1$ (antiferromagnetic state) or $\rho_{st}=0$ (ferromagnetic state).

The time evolution of the mean value (averaged over 10^4 samples) of the density of active bonds measured in Monte Carlo steps (MCS) is presented in Fig. 2. This is seen that for $W_0<0.5$ the average number of active bonds decreases in time and eventually the system reaches the ferromagnetic steady state $[\langle\rho(\infty)\rangle=\langle\rho_{st}\rangle=0]$, while for $W_0>0.5$ it increases and eventually antiferromagnetic limit cycle is reached $[\langle\rho(\infty)\rangle=\langle\rho_{st}\rangle=1]$. Results presented in Fig. 2 show that for $W_0=0.5$ there is a phase transition between ferromagnetic and antiferromagnetic phase.

This phase transition can be predicted using the mean field approximation (MFA) analogously as it was done in [20]. In [20] the mean field equations for the density of active bonds and magnetization have been derived,

$$\frac{d\rho}{dt}=2\delta\Gamma\rho(1-3\rho+2\rho^2),$$

$$\frac{dm}{dt} = -\delta\Gamma m(m^2-1). \quad (6)$$

Using relations (4) we can easily rewrite above equations in the case of our one-parameter model,

$$\frac{d\rho}{dt} = (1-2W_0)\rho(1-3\rho+2\rho^2),$$

$$\frac{dm}{dt} = \left(W_0 - \frac{1}{2}\right)m(m^2-1). \quad (7)$$

As we see there are three types of fixed points,

$$m_{st} = \pm 1 \quad \text{and} \quad \rho_{st} = 0,$$

$$m_{st} = \pm 0 \quad \text{and} \quad \rho_{st} = 1/2,$$

$$m_{st} = \pm 0 \quad \text{and} \quad \rho_{st} = 1.$$

In [20] only two first types have been considered:

(i) ρ_{st}=0 (ferromagnetic state with m_{st}=−1,1)

(ii) ρ_{st}=1/2 (so called active phase).

However, there is a third fixed point ρ_{st}=1, m_{st}=0, which corresponds to antiferromagnetic steady state found in our computer simulations.

Let us first consider stability of the magnetization fixed points. For $W_0<0.5$ we can easily check that $|m_{st}|=1$ (ferromagnetic order) is an absorbing state, since from Eq. (7),

$$\frac{dm}{dt} < 0 \quad \text{for} \quad m \in (-1,0) \to m_{st} = -1,$$

$$\frac{dm}{dt} > 0 \quad \text{for} \quad m \in (0,1) \to m_{st} = 1. \quad (8)$$

Analogously, for $W_0>0.5$ we obtain from Eq. (7) that m_{st} =0,

$$\frac{dm}{dt} > 0 \quad \text{for} \quad m \in (-1,0) \to m_{st} = 0,$$

$$\frac{dm}{dt} < 0 \quad \text{for} \quad m \in (0,1) \to m_{st} = 0. \quad (9)$$

Therefore, MFA equation for magnetization predicts the phase transition for W_0=0.5 between ferromagnetic phase $|m_{st}|=1$ and phase with magnetization equal zero.

Now we can check stability of the MFA equation for active bonds. For $W_0<0.5$ we obtain from Eq. (7) that ρ_{st} =1/2 is the stable point (active phase [20]):

$$\frac{d\rho}{dt} > 0 \quad \text{for} \quad \rho \in (0,1/2) \to \rho_{st} = 1/2,$$

$$\frac{d\rho}{dt} < 0 \quad \text{for} \quad \rho \in (1/2,1) \to \rho_{st} = 1/2. \quad (10)$$

Analogously, for $W_0>0.5$ we can easily check that

$$\frac{d\rho}{dt} < 0 \quad \text{for} \quad \rho \in (0,1/2) \to \rho_{st} = 0,$$

$$\frac{d\rho}{dt} > 0 \quad \text{for} \quad \rho \in (1/2,1) \to \rho_{st} = 1. \quad (11)$$

As we see there is a contradiction in a simple MFA equations. Considering only equation for m one can easily check that for $W_0<0.5$ there is a ferromagnetic absorbing state $|m_{st}|=1$, while for $W_0>0.5$ we obtain m_{st}=0, which might be associated with antiferromagnetic phase (if simultaneously ρ_{st}=1) or active phase (if simultaneously ρ_{st}=0). However, if one considers the MFA equation for ρ it occurs that for W_0 <0.5 ρ_{st}=0.5 (active phase), while for $W_0>0.5$ ρ_{st}=0 in a case of ρ between 0 and 0.5 (ferromagnetic phase) or ρ_{st} =1 in a case of ρ between 0.5 and 1 (antiferromagnetic phase).

Inconsistency in equations is clearly visible for $W_0<0.5$, in which $|m_{st}|=1$ and simultaneously ρ_{st}=0.5 (instead of ρ_{st} =0, which is valid for ferromagnetic phase). For $W_0>0.5$ MFA results are more reasonable, since m_{st}=0 and ρ_{st}=0 or 1. Of course only the second possibility is consistent and corresponds to antiferromagnetic phase. Contradiction which is present in MFA equations follows from MFA equation for the density of active bonds. This is understandable since, due to the Eq. (5), correlations between neighboring sites (which are not considered in a simple MFA) are essential for ρ.

Nevertheless, summing up above considerations, MFA equations suggest discontinuous phase transition for W_0 =0.5 between ferromagnetic and antiferromagnetic phase. This should be noticed that the transition value W_0=0.5 corresponds to the original Glauber dynamics [1].

In the case of discontinuous phase transition one would expect the phase coexistence. We have provided computer simulations to confirm this mean field result and indeed coexistence of ferro- and antiferromagnetic phases can be observed near the transition point W_0=0.5 (see Fig. 3). For W_0=0.5 both types of clusters (ferro- and antiferromagnetic) are nearly the same size and after a long-time competition between them eventually one of two possible steady states is reached. Because for W_0=0.5 both of them are equally probable we see the constant value of the average density of active bonds in Fig. 2. Let us now investigate the phase transition more quantitatively using Monte Carlo simulations.

Following [14,20], we use as an order parameter the mean value of the density of active bonds. We provide Monte Carlo simulations and wait until the system reaches the final stationary state. Dependence between order parameter in the stationary state $\langle\rho_{st}\rangle$ and the flipping probability W_0 is presented in Fig. 4, showing again clearly discontinuous phase transition for W_0=0.5 in agreement with the mean field result. In the case of $W_0<0.5$ the ferromagnetic steady state is obtained with probability 1 (for the infinite system $L=\infty$). For $W_0>0.5$ the antiferromagnetic state is always reached, i.e., the stationary states losses any remnants of the ferromagnetic Ising interactions.

One of the most important issues connected with the coarsening is the relaxation time τ, i.e., time needed to reach the ground state. In this paper we measure the relaxation time starting from the random initial conditions and counting how many Monte Carlo steps is needed to reach the steady state (ρ=1 or ρ=0). We average over $N=10^4$ samples and calculate the mean relaxation time,

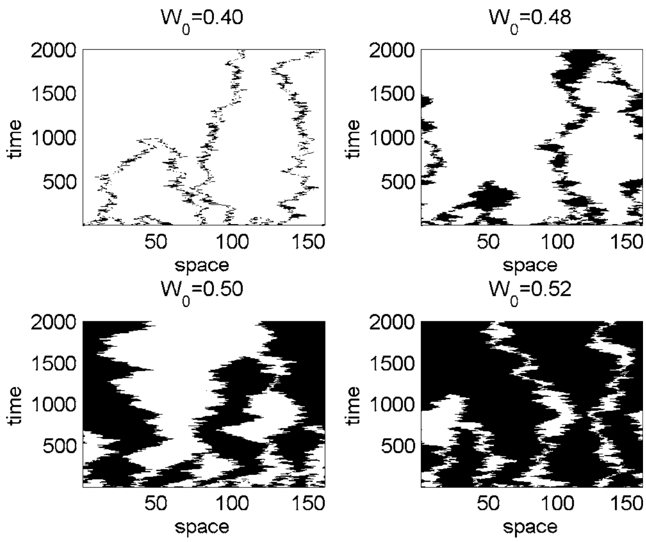

FIG. 3. The time evolution of the Ising spins chain of the length $L=160$ is presented. Black points represent active bonds and thus black regions correspond to antiferromagnetic and white to ferromagnetic clusters. Coexistence of both types of clusters is visible for $W_0 \approx 0.5$. For $W_0=0.5$ both types of clusters are nearly the same size and there is a long-time competition between them leading eventually to one of two possible steady states (ferromagnetic or antiferromagnetic)

$$\langle \tau \rangle = \frac{1}{N}\sum_{i=1}^{N} \tau_i, \qquad (12)$$

where τ_i is the relaxation time of ith sample. In Fig. 5 $\langle \tau \rangle$ divided by the square of the lattice size L as a function of the flipping probability W_0 is shown. This is seen that for W_0

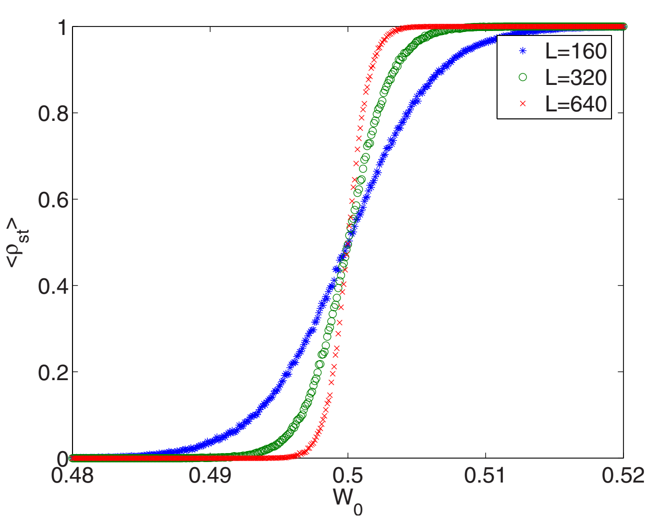

FIG. 4. (Color online) Density of active bonds ρ_{st} in stationary state as a function of flipping probability W_0 (so called exit probability) averaged over 10^4 samples. In the thermodynamical limit $L \to \infty$ for $W_0 < 0.5$ ferromagnetic steady state is reached with probability one ($\rho_{st}=0$) and for $W_0 > 0.5$ antiferromagnetic steady state is reached with probability one ($\rho_{st}=1$). Note that, the transition value $W_0=0.5$ corresponds to the original Glauber dynamics.

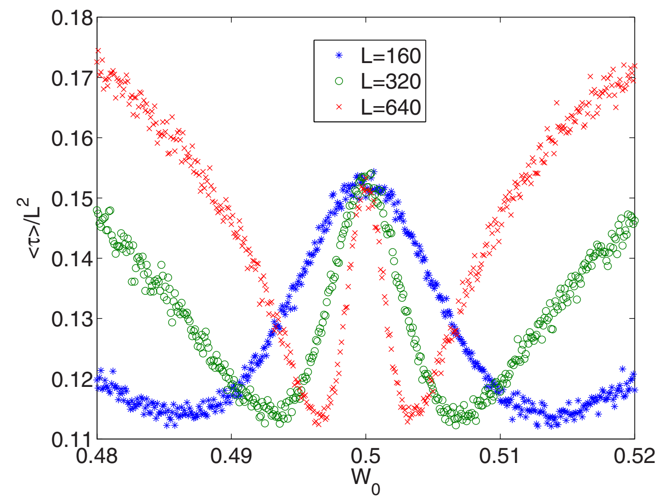

FIG. 5. (Color online) The mean relaxation times $\langle \tau \rangle$ divided by the square of lattice size L as a function of flipping probability $W_0 \in [0.48, 0.52]$. Averaging was done over 10^4 samples. Note that for $W_0=0.5$ relaxation time scales with the system size as $\langle \tau \rangle \sim L^2$. However, for $W_0 \neq 0.5$ scaling exponent differs from known value $\alpha=2$ (see Fig. 6).

$=0.5$ the mean relaxation time scales as $\langle \tau \rangle \sim L^2$, which is well known result in a case of sequential updating [16,17]. The dependence between the mean relaxation time $\langle \tau \rangle$ and the flipping probability W_0 is nonmonotonical. For $W_0 \to 0$ the relaxation time grows rapidly [18,19], which can be understood recalling that $\langle \tau \rangle$ if infinite for $W_0=0$ [11]. For increasing W_0 the mean relaxation time decreases up to a certain point $W_0^{\min}(L)$. However, due to the phase transition in $W_0=0.5$, for $W_0 \in [W_0^{\min}(L), 0.5]$ it grows again, resulting nonmonotonic behavior shown in Fig. 5. The maximum peak is narrower with the growing lattice size, which is expected behavior for the phase transition. The minimal value $W_0^{\min}(L)$ depends on the system size L as $W_0^{\min}(L) = -2.5/L + 0.5$ and therefore $\lim_{L\to\infty} W_0^{\min}(L) \to 0.5$. The mean relaxation time for this minimal value scales with the system size as $\langle \tau(W_0^{\min}) \rangle \sim L^2$, i.e., with the same exponent as for the transition point $W_0=0.5$.

The most important question here is the one concerning the origin of the phase transition. As it was mentioned above, in the case of Metropolis flipping rate ($W_0=1$) the system reaches antiferromagnetic limit cycle, instead for the ferromagnetic steady state [13,14]. It can be easily understood, because for the flipping probability $W_0=1$, the case of synchronous updating is fully deterministic (see an example below):

$$\cdots\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\cdots,$$

$$\cdots\uparrow\uparrow\downarrow\uparrow\downarrow\downarrow\cdots,$$

$$\cdots\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\cdots,$$

$$\cdots\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\cdots,$$

$$\cdots\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\cdots. \qquad (13)$$

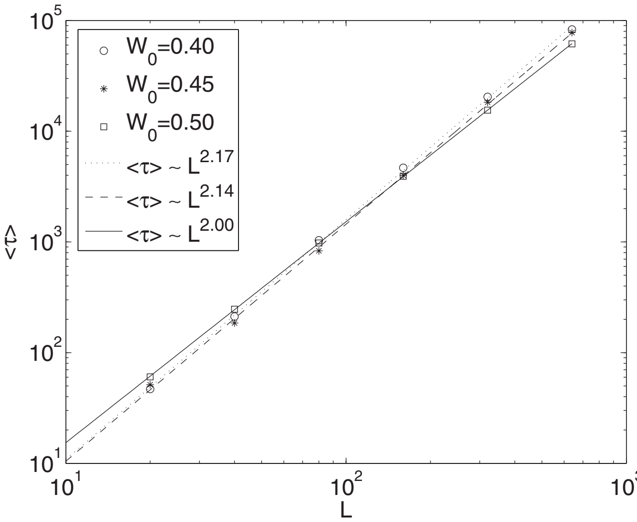

FIG. 6. The mean relaxation time $\langle\tau\rangle$ over the system size L for several values of W_0. For all values of W_0 the mean relaxation time scales with the system size nearly as $\langle\tau\rangle \sim L^{\alpha}$ with $\alpha\approx 2$. However, for different values of W_0 the scaling exponent α slightly varies. In the Fig. 7 the dependence between the scaling exponent α and parameter W_0 is presented.

On the other hand, only for $W_0=1$ updating is really synchronous. For decreasing W_0 only isolated spins are concerned really synchronously, since in the case of isolated spins $\delta E<0$ [see Eq. (1)] the flip is provided with the probability 1. Flipping of isolated spins leads clearly to growth of ferromagnetic domains. Let us introduce for a while a notation $L_{\delta E=0}$ for the number of spins that flipping would not change the energy and $L_{\delta E<0}$ for the number of spins that flipping would decrease the energy. The flip for $\delta E=0$ is realized with the probability W_0 and for $\delta E<0$ with the probability 1, which means that on average $L_{\delta E<0}+W_0 L_{\delta E=0}$ is flipped in a single time step. In the case of $W_0=1$, as mentioned above, the antiferromagnetic order is reached. On the other hand, for $W_0=1/L_{\delta E=0}$ on average only one not isolated spin (i.e., with $\delta E=0$) is flipped in a single time step, similarly to the case of the sequential updating for the system without isolated spins. Thus, because in the case of sequential updating ferromagnetic steady state is reached, one can expect also ferromagnetic order in the case of synchronous updating for small values of W_0. Clearly the phase transition must occur somewhere between the antiferromagnetic order, preferred by a fully synchronous updating ($W_0=1$), and the ferromagnetic steady state, preferred by sequential updating ($W_0=1/L_{\delta E=0}$).

As mentioned above, for $W_0=0.5$ and $W_0=W_0^{\min}(L)$ the mean relaxation time scales with a system size as $\sim L^2$. We have checked also the scaling for other values of W_0. For all values of W_0 the mean relaxation time scales with the system size nearly as $\langle\tau\rangle \sim L^{\alpha}$ with $\alpha\approx 2$ (see Fig. 6). However, for different values of W_0 the scaling exponent α slightly varies. The dependence between scaling exponent and the flipping probability is presented in Fig. 7. The shape of the curve $\alpha(W_0)$ mimic the shape of $\langle\tau(W_0)\rangle$.

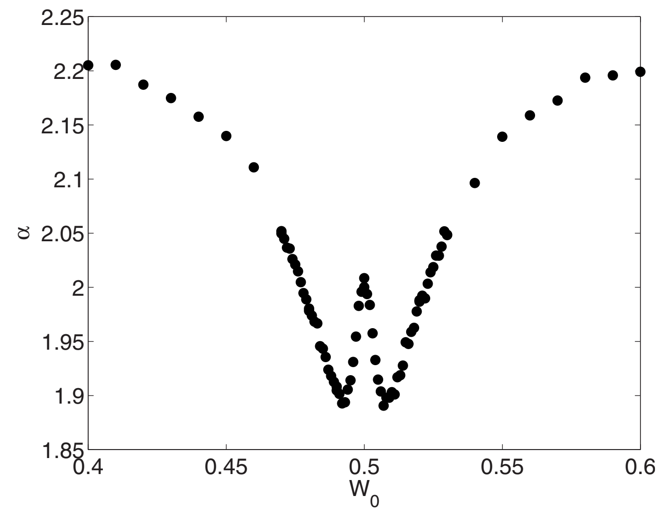

FIG. 7. The mean relaxation time $\langle\tau\rangle$ scales with the system size as $\langle\tau\rangle \sim L^{\alpha}$. For $W_0=0.5$ the scaling exponent $\alpha=2$, which is well known result in the case of sequential updating. However, in general scaling exponent depends on the flipping probability W_0, i.e., $\alpha=\alpha(W_0)$. Dependence between scaling exponent α and the flipping probability W_0 is shown. Simulations were done for the system size $L\in[20,1280]$ and averaged over 10^4 samples.

III. SUMMARY

In this paper we have been investigating the relaxation of the Ising spins chain under the generalized class of Glauber dynamics at zero-temperature. Within such a dynamics, the flipping probability in a case of conserved energy is given by arbitrary value of $W_0\in[0,1]$ (review in a case of sequential updating can be find in [11]). We have proposed to use synchronous updating for such a generalized class of zero-temperature dynamics. Our motivation for this work came from recent experiments showing slow relaxation in magnetic chains at low temperatures [2–8,15]. We have shown by Monte Carlo simulations that there is a phase transition for $W_0=0.5$, which correspond to the value originally proposed by Glauber [1]:

(i) for $W_0<0.5$ ferromagnetic fixed point ($m_{st}=\pm 1$, $\rho_{st}=0$) is stable

(ii) for $W_0>0.5$ antiferromagnetic fixed point ($m_{st}=0$, $\rho_{st}=1$) is the stable one.

Following [20] we were able to obtain the mean field result which also suggests phase transition between ferro- and antiferromagnetic phases for $W_0=0.5$.

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