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MULTI SPIN-FLIP DYNAMICS: A SOLUTION OF THE ONE-DIMENSIONAL ISING MODEL

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The Glauber dynamics of interacting Ising spins (the single spin-flip dynamics) is generalized to the *p spin-flip dynamics* with a simultaneous flip of up to p spins in a single configuration move. We study *p spin-flip dynamics* of the one-dimensional Ising model with uniform nearst-neighbour interaction. The time-dependent magnetization is given exactly in this case. We have found one can evade a critical slowing down in this model when *p spin-flip dynamics* with $p > 2$ is considered.

I. INTRODUCTION

By the Monte Carlo simulations one can study statistical of systems in thermal equilibrium [1]. On the other hand, the Monte Carlo simulation by itself is a dynamical process, which can be constructed in correspondence with real dynamics. In this way also kinetic properties of systems far from an equilibrium can be investigated [1]. Thus the Monte Carlo method is *in principle* a very suitable tool for theoretical study and understanding of both equilibrium phase transitions and nonequilibrium phenomena. In practice for many systems the Monte Carlo simulation results of both the statics and the dynamics are of qualitative charcter only: 1) for equilibrium simulations in a vicinity of a phase transition the *critical slowing down* emerges [2], 2) in the case of disordered systems (e.g. the spin glasses) the spectrum of *relaxation times steadily broadens* upon lowering the temperature already far above freezing temperature, and very close to freezing temperature thermal equilibrium is not fully attainable. In both cases there are serious practical limits to the accuracy of Monte Carlo simulation results. To overcome this drawback of the Monte Carlo method, various simulation techniques accelerating relaxation to the equilibrium were prosed [4—6].

An accelerated relaxation to the equilibrium is important in Monte Carlo computations of lattice gauge theories [7, 8]. Euclidean quantum field theory of

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the lattice with dynamical fermions yields a system with many degrees of freedom and with nonlocal interaction. An accurate measurement of the thermal equilibrium averages in Monte Carlo simulations of these systems is practically not to be attained, with today's computers (basically because of the long relaxation times), even though there are already several powerful multiprocessor systems operating to solve this task [9]. Considerable effort has been devoted to the development of the accelerated Monte Carlo techniques in lattice gauge theory computations [10—14].

In this paper we investigate an accelerated dynamics of the Ising model. An analytic solution of the proposed *p spin-flip dynamics* is given for the one-dimensional Ising model with uniform nearest-neighbour interaction and periodic boundary conditions.

The paper is organized as follows. In the next section the standard single spin-flip dynamics (the Glauber dynamics [15]) is generalized to the dynamics with simultaneous flip of not more than p spins in one configuration move (the *p spin-flip dynamic*). The master equation for the *p spin-flip dynamics* is postulated. In Sect. 3 equations of motion for time-dependent local magnetizations in the one-dimensional Ising model are derived — the solution of these equations and temperature behaviour of the largest relaxation time are given.

2. FORMULATION OF THE p SPIN-FLIP DYNAMICS

In this section we formulate the *p spin-flip dynamics* for systems with the Ising spin degrees of freedom. Hereafter $\{s\}$ is used to describe the configuration of the system $\{s\} \equiv (s_1, s_2, \ldots, s_N)$, $s_i = \pm 1$, and $\mathscr{H}(\{s\})$ is its Hamiltonian. The time development is given as a stochastic process described by the master equation for the probability $P(\{s\}, t)$ that the system is in the configuration $\{s\}$ at time t

$$\frac{dP(\{s\}, t)}{dt} = \sum_{\{s'\} \neq \{s\}} W(\{s'\} \to \{s\})P(\{s'\}, t) - W(\{s\} \to \{s'\})P(\{s\}, t) \qquad (1)$$

$W(\{s\} \to \{s'\})$ is the transition probability per unit time for the move from the configuration $\{s\}$ to the configuration $\{s'\}$.

For the purpose of elementary transition generation we shall use operators $\hat{R}_i^{\eta}$ on the spaces of all configurations $\{s\}$, with i being an index labelling spin sites and $\boldsymbol{\eta}$ an arbitrary p-component binary vector $\boldsymbol{\eta} = (\eta_1, \eta_2, \ldots, \eta_p)$, with $\eta_q = \pm 1$. Thus there is $2^p N$ of such operators and they act in the following way

$$\hat{R}_i^{\eta}: \{s\}\ \{\hat{R}_i^{\eta} s\} = (s_1, s_2, \ldots, s_i, \eta_1 s_{i+1}, \eta_2 s_{i+2}, \ldots, \eta_p s_{i+p}, s_{i+p+1}, \ldots, s_N) \quad (2)$$

For $i > N - p$ this prescription has to be defined according to the boundary conditions. We shall use periodic boundary conditions, thus for $i + q > N$ one

has to replace the $\eta_q s_{i+q}$ by the $\eta_q s_j$, where $j = \mathrm{mod}\,(i + q, N)$. From the definition (2) we have $(\hat{R}_i^{\eta})^2 = \mathbf{1}$, thus when $\{\hat{R}_i^{\eta} s\} = \{s'\}$, then the inverse relation is $\{\hat{R}_i^{\eta} s'\} = \{s\}$. We refer to a set of all couples $(i, \boldsymbol{\eta})$ for which $\{\hat{R}_i^{\eta} s\} = \{s'\}$ as to a set of *p-transition modes between $\{s\}$ and $\{s'\}$*, which is a subset of the set of all *p-transition modes* with $2^p N$ elements.

We postulate the *p spin-flip dynamics* as the stochastic process governed by the master eq. (1) with the transition probability $W^{(p)}(\{s\} \to \{s'\})$ given in the following way

- for each *p-transition mode* of the transition $\{s\} \to \{s'\}$ the *p-transition mode transition probability* per unit time (or shortly *p-transition mode* probability is given as

$$W_i^{\eta}(\{s\}) = \alpha \frac{\exp(-\beta\mathscr{H}(\{\hat{R}_i^{\eta} s\}))}{\sum_{\{\eta\}_p} \exp(-\beta\mathscr{H}(\{\hat{R}_i^{\eta} s\}))}, \quad i = 1, 2, \ldots, N, \qquad (3)$$

where β is the inverse temperature, $\beta = 1/T$.

- the total transition probability $W^{(p)}(\{s\} \to \{s'\})$ of the *p spin-flip dynamics* is the sum of the *p-transition mode* probabilities over the set of *p-transition modes* between $\{s\}$ and $\{s'\}$.

From this definition it follows that the transition matrix $W^{(p)}(\{s\} \to \{s'\})$ for the *p spin-flip dynamics* has a nonzero transition probability between configurations which differ in not more than p spins, and the maximum distance between sites with flipped spins is less than p. The *p-transition mode* probability is a straightforward modification of heat bath algorithm transition probabilities for the single spin-flip Monte Carlo simulations. The average number of all transitions per time unit is

$$\sum_{\{\eta\}_p} \sum_{i=1}^{N} W_i^{\eta}(\{s\}) = \alpha . N \qquad (4)$$

We put $\alpha = 1$ and choose the time unit proportional to the size of the system.

The total transition probability per unit time for the transition $\{s\} \to \{s'\}$ can be writen as a sum over all *p-transition modes* in the following way

$$W^{(p)}(\{s\}\{s'\}) = \sum_{\{\eta\}_p} \sum_{i=1}^{N} \delta(\{s'\}, \{\hat{R}_i^{\eta} s\}) W_i^{\eta}(\{s\}) \qquad (5)$$

with $\delta(\{s\}, \{s'\}) \equiv \prod_{j=1}^{N} \delta_{s_j s_j'}$.

It can be directly seen that *p spin-flip dynamics* is an ergodic process and the condition of the detailed balance is satisfied

$$P_{eq}(\{s\})W(\{s\} \to \{s'\}) = P_{eq}(\{s'\})W(\{s'\} \to \{s\}), \quad (6)$$

$P_{eq}(\{s\})$ is the thermal equilibrium distribution: $P_{eq}(\{s\}) \sim \exp(-\beta\mathscr{H}(\{s\}))$. Thus according to the theory of Markov processes the thermal equilibrium distribution is the equilibrium distribution of the *p spin-flip dynamics*. The master equation (1) for the *p spin-flip dynamics* written in terms of *p-transition mode* probabilities (3) becomes

$$\frac{dP(\{s\}, t)}{dt} = \sum_{\{\eta\}_p} \sum_{i=1}^{N} W_i(\{s\})P(\{s\}, t) - W_i(\{\hat{R}_i s\})P(\{\hat{R}_i s\}, t). \quad (7)$$

The resulting equation of motion for a time-dependent averaged value $A(t) \equiv \langle A(\{s\})\rangle_t = \sum_{\{s\}} A(\{s\})P(\{s\}, t)$ is

$$\frac{dA(t)}{dt} = \sum_{\{s\}} \sum_{\{\eta\}_p} \sum_{i=1}^{N} [A(\{\hat{R}_i s\}) - A(\{s\})W_i(\{s\})P(\{s\}, t). \quad (8)$$

3. MULTI SPIN-FLIP DYNAMICS OF THE ONE-DIMENSIONAL ISING MODEL

In this section we deal with the one-dimensional Ising model with nearest--neighbour interaction and with periodic boundary conditions. The Hamiltonian of this model is

$$\mathscr{H}(\{s\}) - \sum_{i=1}^{N} J_i s_i s_{i+1}, \quad s_{N+1} = s_1: \quad (9)$$

For $p = 1$ the *p spin-flip dynamics* of this model becomes the usual single spin-flip dynamics (the Glauber model), the exact solution of which is well known [15—17]. Here we solve the *p spin-flip dynamics* in the case of the uniform ferromagnetic interaction $J_i = J > 0$. One obtains from (9) for the *p-transition mode* probabilites (3)

$$W_i^{\eta}(\{s\}) = \frac{\exp\left(\sum_{r=0}^{p} \beta J \eta_r \eta_{r+1} s_{i+r} s_{i+r+1}\right)}{\sum_{\{\eta\}_p} \exp\left(\sum_{r=0}^{p} \beta J \eta_r \eta_{r+1} s_{i+r} s_{i+r+1}\right)}, \quad i = 1, 2, \ldots, N \quad (10)$$

where $\eta_0 = \eta_{p+1} = 1$. In (10) and also throughout the rest of this section, all spin site indices have to be implicitly interpreted with respect to the periodic boundary conditions, i.e. if $i \neq N$, then $i \to \mathrm{mod}(i, N)$.

We proceed to the derivation of the equation of motion for the local time-dependent magnetization. Defining the local time-dependent averaged magnetization as $m_k(t) \equiv \langle s_k \rangle_t = \Sigma_{\{s\}} s_k P(\{s\}, t)$ and using the *p-transition mode* operator $\hat{R}_i^{\eta}$ definition (2) written for the individual spins $\hat{R}_i s_k = s_k + s_k \Sigma_{q=1}^{p} (\eta_q - 1)\, \delta_{i+q,k}$, one obtains from (7) the following expression for the local magnetization equation of motion

$$\frac{dm_k(t)}{dt} = \sum_{\{s\}} \sum_{\{\eta\}_p} \sum_{i=1}^{N} \sum_{q=1}^{p} \delta_{i+q,k}(\eta_q - 1) s_k W_i^{\eta}(\{s\})P(\{s\}, t) \quad k = 1, 2, \ldots, N. \quad (11)$$

We utilize the relation (10) for $W_i^{\eta}(\{s\})$ in (11) rewritten with help of identity $e^{sx} = \coth x + s \sinh x$, $s = \pm 1$. One finds the expression multilinear in the η's

$$W_i(\{s\}) = \frac{(1 - \gamma^{p+1} s_i s_{i+p+1})}{2^p(1 - \gamma^{2p+2})} \prod_{r=0}^{p} (1 + \gamma \eta_r \eta_{r+1} s_{i+r} s_{i+r+1}) \quad i = 1, 2, \ldots, N, \quad (12)$$

where $\gamma = \mathrm{than}\,(\beta J)$. Thus the sum over all possible η's in (11) can be aesily done and one recovers a closed set of equations for the local time-dependent magnetizations $m_k(t)$

$$\frac{dm_k(t)}{dt} = -pm_k(t) + \mu_1^{(p)}(m_{k-1}(t) + m_{k+1}(t)) + \mu_p^{(p)}(m_{k-p}(t) + m_{k+p}(t)) \quad (13a)$$

where

$$\mu_q^{(p)} = \frac{\gamma^q(1 - \gamma^{2p+2-2q})}{1 - \gamma^{2p+2}}, \quad q = 1, p \quad \text{and} \quad \gamma = \tanh(\beta J). \quad (13b)$$

In the case of $p = 1$ just a single term appears in (13a), $\mu_1^{(1)} = \gamma/(1 + \gamma^2) = \frac{1}{2}\tanh(2\beta J)$, i.e. (13.a) gives eqs. of the Glauber model [15].

The solution of the set of the homogeneous linear equations $\boldsymbol{m}(t) = \boldsymbol{\Gamma m}(t)$ is given through the eigenvectors $\boldsymbol{v}^{(n)}$ and eigenvalues λ_n of the matrix $\boldsymbol{\Gamma}$: $\boldsymbol{m}(t) = \boldsymbol{m}(t) = \Sigma_n c_n \boldsymbol{v}^{(n)} \exp(t\lambda_n)$, with c_n given by the initial conditions. In (13a) $\boldsymbol{\Gamma}^{(p)}$ is a symmetric band matrix with the bandwidth $2p + 1$

$$\Gamma_{kl}^{(p)} = -p\delta_{kl} + \sum_{q=,p} \mu_q^{(p)}(\delta_{k-q,l} + \delta_{k+q,l}) \quad k, l = 1, 2, \ldots, N \quad (14)$$

The eigenvectors and eigenvalues of the $\boldsymbol{\Gamma}^{(p)}$ are

$$v_l^{(n)} = \exp\left(\mathrm{i}\frac{2\pi}{N} nl\right), \quad (15a)$$

$$\lambda_n^{(p)} = -p + 2 \sum_{q=1,p} \mu_q^{(p)} \cos\left(\frac{2\pi}{N} nq\right), \quad n = 0, 1, \ldots, N-1. \quad (15b)$$

As before, for $p = 1$ only one of the two terms appearing in the sum should be taken. All eigenvalues $\lambda_n^{(p)}$ are nonpositive, and $\lambda_0^{(p)} > \lambda_n^{(p)}$, for $n = 1, 2, \ldots, N-1$.

We take the site averaged magnetization defined as $m(t) \equiv \Sigma_{k=1}^{N} m_k(t)$. For a given local magetization $m_k(0)$ at a time $t = 0$ we get the final solution for time-dependent magnetization

$$m(t) = \frac{1}{N} \sum_{k=1} \sum_{l=1} \sum_{n=0} m_l(0) \exp\left(i \frac{2\pi}{N} n(k-l)\right) \exp\left(-\frac{t}{\tau_n^{(p)}}\right), \qquad (16)$$

where $\tau_n^{(p)} = -(\lambda_n^{(p)})^{-1}$, $n = 0, 1, \ldots, N-1$ is the found spectrum of relaxation times of the *p spin-flip dynamics*. For homogeneous initial conditions $m_k(0) = \bar{m}$ just one mode from (15) contributes and we have $\bar{m}(t) = \bar{m}_0 \exp(-t/\tau_0^{(p)})$. Because $\tau_0^{(p)}$ is the largest relaxation time of the spectrum, the homogeneous mode has the slowest relaxation to equilibrium.

For $p = 1$ one recovers the well-known result of Glauber:

$$\tau_0^{(1)} = (1 - 2\gamma/(1+\gamma^2))^{-1} = (1 - \tanh 2\beta J)^{-1},$$

[15]. For β to inf the largest relaxation time $\tau_0^{(1)}$ diverges as $\sim \frac{1}{2} \exp(4\beta J)$.

For $p > 1$ the largest relaxation time of the one-dimensional Ising model *p spin-flip dynamics* is

$$\tau_0^{(p)} = \left[p - 2\left(\gamma - \frac{\gamma^p(1-\gamma^2)}{(1+\gamma^{p+1})}\right)\right]^{-1} \qquad (19)$$

For β to inf and $p = 2$ the $\tau_0^{(2)}$ diverges exponentially with the inverse temperature $\tau_0^{(2)} \sim \frac{1}{8} \exp(4\beta J)$ but for $p > 2$ it remains finite $\tau_0^{(p)} \sim \frac{1}{p-2}$, i.e. there is no critical slowing down at critical temperature.

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ДИНАМИКА МНОЖЕСТВЕННЫХ ИЗМЕНЕНИЙ ОРИЕНТАЦИЙ СПИНА: РЕШЕНИЕ ОДНОРАЗМЕРНОЙ ИЗИНГОВСКОЙ МОДЕЛИ

В предлагаемой работе глауберовская динамика взаимодействующих изинговских спинов (динамика одиночных изменеийй ориентаций спина) обобщается на случай динамики изменения ориентации p спинов. Изучается именение ориентации p спинов в одноразмерной изинговской модели с униформным взаимодействием оближайших соседей. В этом случае приводится точное выражение для магнетизации, зависящей от времени. Было найдено, что можно избежать критического замедления в этой модели, если взять в учет динамику изменений ориентации $p > 2$ спинов.