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A NEW PARALLEL ALGORITHM FOR SIMULATION OF A SPIN-GLASS SYSTEM ON SCALES OF SPACE-TIME PERIODS OF AN EXTERNAL FIELD

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Новый параллельный алгоритм для моделирования системы «спин–стекло»
на масштабах периодов пространства-времени внешнего поля

Исследованы статистические свойства ансамбля неупорядоченных 1D-пространственных спин-цепочек (ПСЦ) определенной длины во внешнем поле. В узлах решетки спиновой цепочки получены рекуррентные уравнения с минимальной энергией классического гамильтониана. С использованием этих уравнений разработан оригинальный высокопроизводительный параллельный алгоритм для моделирования 1D-спинового стекла. Рассчитаны распределения различных параметров невозмущенного спинового стекла. В частности, аналитически доказано и численными расчетами показано, что распределение спин-спинового взаимодействия в модельном гамильтониане ближайших соседей Гейзенберга, в отличие от широко используемого распределения Гаусса–Эдвардса–Андерсона, удовлетворяет закону альфа-устойчивого распределения Леви, которое не имеет дисперсии. Мы изучили критические свойства спинового стекла в зависимости от величины амплитуды внешнего поля и показали, что даже при слабых внешних полях в системе возникают сильно выраженные фрустрации. Установлено, что фрустрации имеют фрактальный характер, они самоподобны и не исчезают при уменьшении масштаба области вычислений. После усреднения по фрактальным структурам получены средние значения поляризации спинового стекла на масштабах пространственно-временных периодов внешнего поля. Аналогичным образом вычислен параметр порядка Эдвардса–Андерсона в зависимости от амплитуды внешнего поля. Показано, что средние значения поляризации и параметра порядка в зависимости от внешнего поля демонстрируют фазовые переходы первого рода.

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Gevorkyan A. S., Abajyan H. G., Sukiasyan H. S. E5-2011-29
A New Parallel Algorithm for Simulation of a Spin-Glass System
on Scales of Space-Time Periods of an External Field

We study the statistical properties of an ensemble of disordered 1D spatial spin chains (SSCs) of certain length in the external field. On nodes of spin-chain lattice the recurrent equations and corresponding inequality conditions are obtained for calculation of local minimum of a classical Hamiltonian. Using these equations for simulation of a model of 1D spin glass an original high-performance parallel algorithm is developed. Distributions of different parameters of unperturbed spin glass are calculated. It is analytically proved and shown by numerical calculations that the distribution of the spin–spin interaction constant in the Heisenberg nearest-neighboring Hamiltonian model as opposed to the widely used Gauss–Edwards–Anderson distribution satisfies the Lévy alpha-stable distribution law which does not have variance. We have studied critical properties of spin glass depending on the external field amplitude and have shown that even at weak external fields in the system strong frustrations arise. It is shown that frustrations have a fractal character, they are self-similar and do not disappear at decreasing of calculations area scale. After averaging over the fractal structures the mean values of polarizations of the spin glass on the scales of external field's space-time periods are obtained. Similarly, Edwards–Anderson's ordering parameter depending on the external field amplitude is calculated. It is shown that the mean values of polarizations and the ordering parameter depending on the external field demonstrate phase transitions of first order.

The investigation has been performed at the Laboratory of Information Technologies, JINR.

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INTRODUCTION

Spin glasses are prototypical models for disordered systems which provide a rich source for investigations of a number of important and difficult applied problems of physics, chemistry, material science, biology, nanoscience, evolution, organization dynamics, hard optimization, environmental and social structures, human logic systems, financial mathematics, etc. (see, for example, [1–9]). The considered mean-field models of spin glasses as a rule are divided into two types. The first consists of the true random-bond models, where the couplings between interacting spins are taken to be independent random variables [10–12]. The solution of these models is obtained by n-replica trick [10, 12] and the invention of sophisticated schemes of replica-symmetry breaking is required [12, 13]. In the models of second type, the bond randomness is expressed in terms of some underlining hidden site randomness and is thus of a superficial nature. However, it has been pointed out in the works [14–16] that this feature retains an important physical aspect of true spin glasses, viz. that they are random with respect to the positions of magnetic impurities.

As recently shown by authors [17], some type of dielectrics can be treated as the model of quantum 3D spin glass. In particular, it was proved that the initial 3D quantum problem on space-time scales of an external field in the direction of wave's propagation can be reduced to two conditionally separable 1D problems, where one of them describes the classical 1D spin-glass problem with the random environment.

In this paper we discuss in detail statistical properties of the spin-glass short-range interaction model which describes an ensemble of 1D spatial spin chains of certain length L_x while taking into account the influence of an external field. Recall that each spin chain from itself represents 1D lattice, where on every node of lattice one random-orientated $O(3)$ spin is located.

In section 1 the spin-glass problem on 1D lattice is formulated. Equations for stationary points and corresponding conditions for definition of energy minimum on lattice nodes (local minimum of energy) are obtained. The formula for distributions' computation for different parameters of spin-glass system are derived.

In section 2 the exact solutions of recurrent equations for angles of $(i+1)$th spin depending on ith and $(i+1)$th spin–spin interaction constant are obtained. The scheme of parallel simulation of statistical parameters of system is suggested and the corresponding pseudo-code is adduced.

In section 3 the numerical experiments for unperturbed 1D spin-glass system are adduced, including distributions of energy, polarization and spin–spin interaction constant.

In section 4 the statistical properties of spin glass, on the scales of space-time periods of external field are investigated in detail. The distribution of average polarization on different coordinates and Edwards–Anderson-type ordering parameter of spin-glass system in external field are investigated.

In Conclusion the obtained theoretical and computational results are analyzed.

1. FORMULATION OF THE PROBLEM

We consider a classical ensemble of disordered 1D spatial spin chains (SSC) of length L_x (Fig. 1), where for simplicity is supposed that the interactions between spin chains are absent. A specificity of a problem is such that statistical properties of a system on very short time intervals δt at which system cannot be thermally relaxed are of interest to us. Let us note that for a problem the following time correspondences take place $\tau \ll \delta t < \Omega^{-1} \ll \tau_T \ll 1$, where Ω is a frequency of an external field, τ is a relaxation time of spin in an external field and τ_T is the time of thermal relaxation. In other words, we suppose that the spin-glass system is frozen and nonsusceptible to thermal evolution.

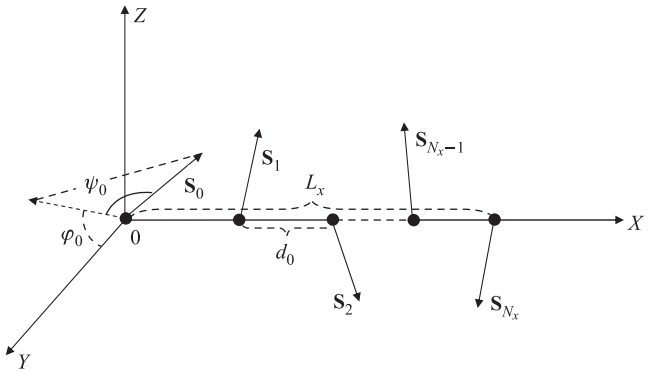

Fig. 1. A stable 1D spatial spin chain with random interactions and the length of $L_x = d_0 N_x$, where d_0 is a distance between nearest-neighboring spins, N_x designates the number of spins in chain. The spherical angles φ_0 and ψ_0 describe the spatial orientation of $\mathbf{S_0}$ spin, the pair of angles (φ_i, ψ_i) defines the spatial orientation of the spin $\mathbf{S}_i$

Mathematically such a type of spin glass can be described by 1D Heisenberg spin-glass Hamiltonian [1–3]:

$$H(N_x) = -\sum_{i=0}^{N_x-1} J_{i\,i+1}\mathbf{S}_i\mathbf{S}_{i+1} - \sum_{i=0}^{N_x-1} \mathbf{h}_i\mathbf{S}_i, \tag{1}$$

where $\mathbf{S}_i$ describes the ith spin which is the unit length vector and has a random orientation, $\mathbf{h}_i$ describes the external field which is orientated along the axis x:

$$h_i = h_0 \cos(k_x x_i), \quad x_i = i \cdot d_0, \quad k_x = 2\pi/L_x, \tag{2}$$

where h_0 is the amplitude of the external field. In addition, in expression (1) J_{ii+1} characterizes a random interaction constant between ith and $(i+1)$th spins which can have positive as well as negative values (see [1, 18]). The distribution of spin–spin interaction constant will be found by way of calculations of classical Hamiltonian problem.

For further investigations, Eq. (1) is convenient to write in spherical coordinates (see Fig. 1):

$$H(N_x) = -\sum_{i=0}^{N_x-1} \{J_{i\,i+1}[\cos\psi_i \cos\psi_{i+1} \cos(\varphi_i - \varphi_{i+1}) + \\ + \sin\psi_i \sin\psi_{i+1}] + h_i \sin\psi_i\}. \tag{3}$$

For the consecutive calculations of problem the equations of stationary points of Hamiltonian will play a central role:

$$\frac{\partial H}{\partial \psi_i} = 0, \quad \frac{\partial H}{\partial \varphi_i} = 0, \tag{4}$$

where $\Theta_i = (\psi_i, \varphi_i)$ are the angles of ith spin in the spherical coordinate system (ψ_i is a polar angle and φ_i is an azimuthal one).

Using expression (3) and equations (4) it is easy to find the following system of trigonometrical equations:

$$\begin{gathered} \sum_{\nu=i-1;\nu\neq i}^{i+1} J_{\nu i}[\sin\psi_\nu - \tan\psi_i \cos\psi_\nu \cos(\varphi_i - \varphi_\nu)] + h_i = 0, \\ \sum_{\nu=i-1;\nu\neq i}^{i+1} J_{\nu i} \cos\psi_\nu \sin(\varphi_i - \varphi_\nu) = 0, \quad J_{\nu i} \equiv J_{i\nu}. \end{gathered} \tag{5}$$

In the case when all interaction constants between ith spin with its nearest-neighboring spins J_{i-1i}, J_{ii+1} and angles $(\psi_{i-1}, \varphi_{i-1})$, (ψ_i, φ_i) are known, it is

possible to explicitly calculate the pair of angles $(\psi_{i+1}, \varphi_{i+1})$. Correspondingly, the ith spin will be in the ground state (in the state of minimum energy) if in the stationary point $\Theta_i^0 = (\psi_i^0, \varphi_i^0)$ the following conditions are satisfied:

$$A_{\psi_i\psi_i}(\Theta_i^0) > 0, \quad A_{\psi_i\psi_i}(\Theta_i^0)A_{\varphi_i\varphi_i}(\Theta_i^0) - A^2_{\psi_i\phi_i}(\Theta_i^0) > 0, \tag{6}$$

where $A_{\alpha_i\alpha_i}(\Theta_i^0) = \partial^2 H_0/\partial\alpha_i^2$, $A_{\alpha_i\beta_i}(\Theta_i^0) = A_{\beta_i\alpha_i}(\Theta_i^0) = \partial^2 H_0/\partial\alpha_i\partial\beta_i$, in addition:

$$\begin{aligned} A_{\psi_i\psi_i}(\Theta_i^0) = \Bigg\{ \sum_{\nu=i-1;\nu\neq i}^{i+1} J_{\nu i}[\cos\psi_\nu \cos(\varphi_\nu - \varphi_i^0) + \\ + \tan\psi_i^0 \sin\psi_\nu] + h_i \tan\psi_i^0 \Big\} \cos\psi_i^0, \end{aligned} \tag{7}$$

$$A_{\varphi_i\varphi_i}(\Theta_i^0) = \sum_{\nu=i-1;\nu\neq i}^{i+1} J_{\nu i} \cos\psi_\nu \cos(\varphi_\nu - \varphi_i^0) \cos\psi_i^0, \quad A_{\psi_i\varphi_i}(\Theta_i^0) = 0.$$

Evidently by equations (5) and conditions (6) we can calculate a huge number of stable 1D SSCs which will allow one to investigate the statistical properties of 1D SSCs ensemble. It is supposed that the average polarization (magnetization) of 1D SSCs ensemble (polarizability of 1D SSC) at absence of external field is equal to zero.

Now we can construct the distribution function of energy of 1D SCCs ensemble. To this effect it is useful to divide the nondimensional energy axis $\varepsilon = \epsilon/\delta\epsilon$ into regions $0 > \varepsilon_0 > \ldots > \varepsilon_n$, where $n \gg 1$ and ϵ is a real energy axis. The number of stable 1D SSC configurations with length of L_x in the range of energy $[\varepsilon - \delta\varepsilon, \varepsilon + \delta\varepsilon]$ will be denoted by $M_{L_x}(\varepsilon)$ while the number of all stable 1D SSC configurations — correspondingly by symbol $M_{L_x}^{\text{full}} = \sum_{j=1}^{n} M_{L_x}(\varepsilon_j)$. Accordingly, the energy distribution function of ensemble may be defined by the expressions [19]:

$$\begin{gathered} F_{L_x}(\varepsilon; d_0(T)) = M_{L_x}(\varepsilon)/M_{L_x}^{\text{full}}, \\ \lim_{n\to\infty} \sum_{j=1}^{n} F_{L_x}(\varepsilon_j; d_0(T))\delta\varepsilon_j = \int_{-\infty}^{0} F_{L_x}(\varepsilon; d_0(T))d\varepsilon = 1, \end{gathered} \tag{8}$$

where the second expression shows normalization condition of distribution function to unit. In a similar way we can also define distributions of polarization and spin–spin interaction constant.

2. SIMULATION ALGORITHM

Using the following notation:

$$\xi_{i+1} = \cos\psi_{i+1}, \quad \eta_{i+1} = \sin(\varphi_i - \varphi_{i+1}), \tag{9}$$

equations system (5) may be transformed to the following form:

$$C_1 + J_{ii+1}\left[\sqrt{1-\xi_{i+1}^2} - \tan\psi_i \xi_{i+1}\sqrt{1-\eta_{i+1}^2}\right] = 0, \quad C_2 + J_{ii+1}\xi_{i+1}\eta_{i+1} = 0, \tag{10}$$

where parameters C_1 and C_2 are defined by the expressions:

$$\begin{aligned} C_1 &= J_{i-1i}[\sin\psi_{i-1} - \tan\psi_i \cos\psi_{i-1}\cos(\varphi_i - \varphi_{i-1})] + h_i\cos\psi_i, \\ C_2 &= J_{i-1\,i}\cos\psi_{i-1}\sin(\varphi_i - \varphi_{i-1}). \end{aligned} \tag{11}$$

From the system (11) we can find the equation for the unknown variable η_{i+1}:

$$C_1\eta_{i+1} + C_2\sqrt{1-\eta_{i+1}^2}\tan\psi_i + \sqrt{J_{ii+1}^2\eta_{i+1}^2 - C_2^2} = 0. \tag{12}$$

We can transform equation (12) to the following equation of the fourth order:

$$[A^2 + 4C_1^2C_2^2\sin\psi_i]\eta_{i+1}^4 - 2[AC_2^2 + 2C_1C_2^2\sin^2\psi_i]\eta_{i+1}^2 + C_2^4 = 0, \tag{13}$$

where

$$A = J_{i\,i+1}^2\cos^2\psi_i - C_1^2 + C_2^2\sin^2\psi_i. \tag{14}$$

Discriminant of equation (13) is equal to

$$\begin{aligned} D = C_2^4(A + 2C_1\sin^2\psi_i)^2 - C_2^4(A^2 + 4C_1^2C_2^2\sin^2\psi_i) = \\ = 4C_2^4C_1^2\sin^2\psi_i(A + C_1^2\sin^2\psi_i - C_2^2). \end{aligned}$$

From the condition of non-negativity of discriminant $D \geqslant 0$ we can find the following condition:

$$A + C_1^2\sin^2\psi_i - C_2^2 \geqslant 0. \tag{15}$$

Further substituting A from (14) into inequality (15), we can find the new condition to which the interaction constant between two successive spins should satisfy:

$$J_{i\,i+1}^2 \geqslant C_1^2 + C_2^2. \tag{16}$$

Now we can write the following expressions for unknown variables ξ_{i+1} and η_{i+1}:

$$\xi_{i+1}^2 = \frac{C_2^2}{J_{ii+1}^2\eta_{i+1}^2},$$

$$\eta_{i+1}^2 =$$
$$= C_2^2 \frac{J_{ii+1}^2 \cos^2\psi_i + C_3 + 2C_1^2 \sin^2\psi_i \left[1 \pm C_1^{-1} \cot\psi_i \sqrt{J_{ii+1}^2 - C_1^2 - C_2^2}\right]}{J_{ii+1}^4 \cos^4\psi_i + 2C_3 J_{ii+1}^2 \cos^2\psi_i + (C_1^2 + C_2^2 \sin^2\psi_i)^2}, \tag{17}$$

where $C_3 = -C_1^2 + C_2^2 \sin^2\psi_i$.

Finally in consideration of (9) for the calculating angles $\left(\varphi_{i+1}, \psi_{i+1}\right)$ we find:

$$0 \leqslant \xi_{i+1}^2 \leqslant 1, \quad 0 \leqslant \eta_{i+1}^2 \leqslant 1. \tag{18}$$

These conditions are very important for elaborating correct and high performance simulation algorithm. Moreover, as shown [20], the condition (16) excludes the possibility to get normal distribution for spin–spin interaction constants in the 1D Heisenberg nearest-neighboring spin-glass Hamiltonian model.

Algorithm Description. Let us note that the developed algorithm is an iterative algorithm depending on 1D SSCs nodes. The first and second nodes are initialized randomly, then ith node is obtained from $(i-2)$th and $(i-1)$th layers nodes. Every node contains the following information:

φ — polar angle,
ψ — azimuthal angle,
J — interaction coefficient.

The following parameters are initialized in the following way:
φ_0 and φ_1 — **rand()**$^*2^*\pi^*R$;
ψ_0 and ψ_1 — **acos (rand())**;
J_{01} — **rand()**,
where **rand()** function generates uniformly distributed random numbers on the interval $(0, 1)$.

The algorithm pseudo code is following:

```
for m = 1 : n   // n separate independent sets of problem
    for i = 1 : N_x
for j = 1 : R   // regenerate J_i maximum R times if needed
    for k = 1 : L_i   // go through all elements in the ith layer if conditions
                          (9) are satisfied
                  begin
                      // calculate energy on ith layer,
                      // calculate polarization on x, y and z axis
                      // calculate x_{i+1} and y_{i+1},
                      // save J_i value
                      . . . .
```

end
endfor
endfor
endfor
endfor
if ($i == N_x$) // reached the N_xth layer
begin
// save energy, polarizations values
end
endif
// construct distribution functions of energy ε, polarization p and interaction constant J
// calculate the mean value of energy $\bar{\varepsilon}$, polarization $\bar{p}$, interaction constant $\bar{J}$ and its variance $\bar{J^2}$.

3. NUMERICAL EXPERIMENTS

Let us suppose that the ensemble consists of M number of spin chains each of them with the length of $100d_0$. For realization of simulation we will use parallel algorithm the scheme of which is represented in Fig. 2 (see also [19]). The algorithm works as follows. Randomly M sets of initial parameters are generated and parallel calculations of equations (17) for unknown variables x_i and y_i transact taking into account conditions (16) and (18). However, only specifying initial conditions is not enough for the solution of these equations. Evidently, these equations can be solved after the definition of the constant J_{01}, which is also randomly generated. When the solutions of recurrent equations are found, the conditions of stability of spin on the node (7) are being checked. The process of simulation proceeds on the current node if the conditions (7) are satisfied. If conditions are not satisfied, the new constant J_{01} is randomly generated and correspondingly new solutions are found which are checked later on conditions (7). This cycle is being repeated on each node until the solutions do not satisfy conditions of the energy local minimum.

At first, we have conducted numerical simulation for definition of different statistical parameters of the ensemble which consists of $5 \cdot 10^4$ spin chains and at absence of external field (the case of unperturbed Hamiltonian). Note that during simulation we suppose that spin chains can be polarized correspondingly up to 20,

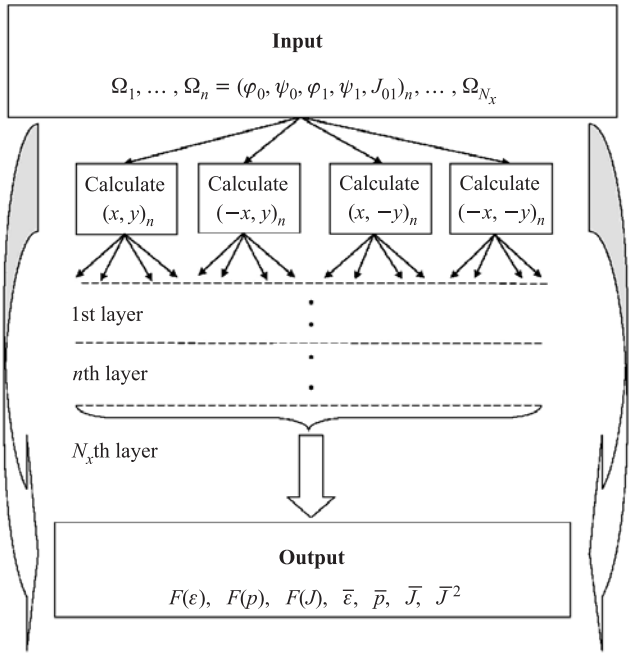

Fig. 2. The algorithm of parallel simulation of statistical parameters of 1D SSCs ideal ensemble. In the scheme the following designations are made: $F(\varepsilon), F(p)$ and $F(J)$ are distribution functions of energy, polarization and spin–spin interaction constants of 1D SSCs ensemble. In addition, $\bar{\varepsilon}, \bar{p}, \bar{J}$ and $\bar{J}^2$ designate average values of the corresponding parameters of system

40 and 100 percent, i.e., the total value of spins sum in each chain can be within the interval of $\{-5 \leqslant p \leqslant +5\}$, $\{-10 \leqslant p \leqslant +10\}$ and $\{-100 \leqslant p \leqslant +100\}$, where p designates the polarization of spin chain. In other words, each spin chain is a vector of a certain length which is directed to coordinate x. Calculations have shown that in ensemble a full self-averaging of spin chains (the polarization vector) occurs in each of the above-mentioned scenarios in all directions. Energy distributions $F(\varepsilon)$ practically independent from simulation scenario and by one global maximum are characterized (see Fig. 3, *a*) and correspondingly the average energy for all scenarios is equal to $\bar{\varepsilon} \cong -53.084$. As for distributions of polarizations, $F(p_x), F(p_y)$, and $F(p_z)$, in considered cases, they are very symmetric on all coordinates and correspondingly the average values of polarizations $\bar{p}_\eta = \int F(p_\eta) p_\eta dp_\eta$; $\eta = \{x, y, z\}$ are close to zero on all coordinates (see Fig. 3, *b*). It is important to note that the distribution of spin–spin interaction constant is not accepted a priori as normal (Gauss–Edwards–Anderson model),

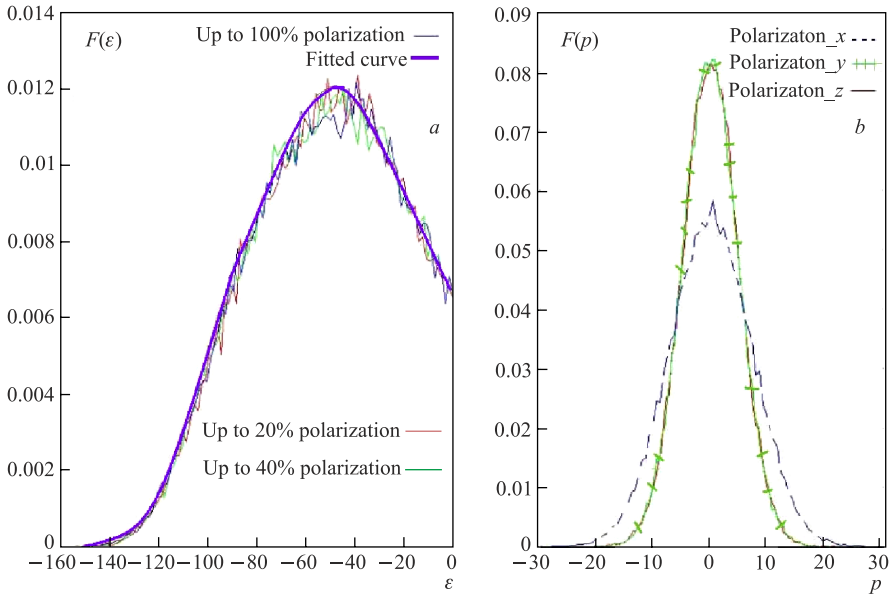

Fig. 3. *a*) The energy distributions for ensembles of 1D SSCs of the length $L_x = 100d_0$, with spin-chain polarizations correspondingly up to $20, 40$ and 100 percents. Note that all ensembles consist of $5 \cdot 10^4$ spin chains but various level of spin-chain polarizations, however their distributions are practically similar and have only one global maximum. *b*) The polarization distributions correspondingly on coordinates x, y and z are shown for scenario up to 100 percent polarized spin chains

but it is calculated from the first principles by analyzing the statistical data of simulation. As the detailed analysis of numerical data shows (in particular its asymptotes), the distribution of interaction constant can be approximated precisely by Lévy alpha-stable distribution function (see Fig. 4, *a*). For more details about Lévy distribution see [21]. Let us note that at simulation of spin chain four solutions arise on each node of 1D lattice, which satisfy equations of stationary points (5). It is possible to think that it would lead to exponentially growth of number of solutions along with increase in number of nodes or length of spin chain. However, such a scenario of solutions branching does not occur due to accounting of additional conditions (6)–(7) and also (16) (see the numerical simulation for different initial parameters in Fig. 5).

At last it is important to recall that condition (16) plays an important role during the modeling. This condition specifies the border of regions where interaction constants J are localized and thus the process of simulation is very effective (see Fig. 6).

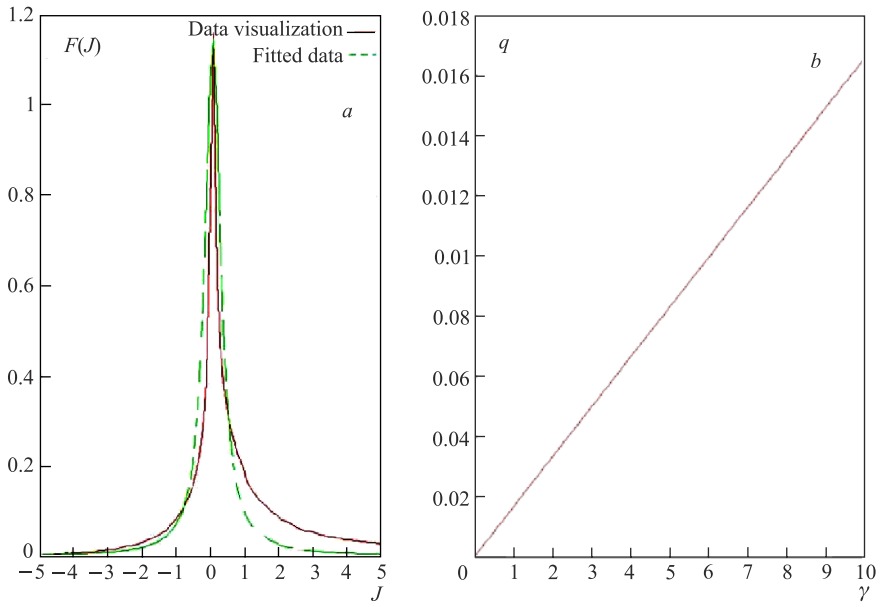

Fig. 4. *a*) The distribution of spin–spin interaction constant essentially differs from Gauss–Edwards–Anderson distribution model and corresponds to Lévy alpha-stable distributions class. The dotted curve is fitted by Cauchy function. *b*) It is obvious from the graphic that for a wide range of parameter γ there is not any phase transition in the spin-glass system depending on the amplitude of an external field. It means that under the influence of an external field the system is reconstructed so, that the average energy of spin chain practically is not being changed

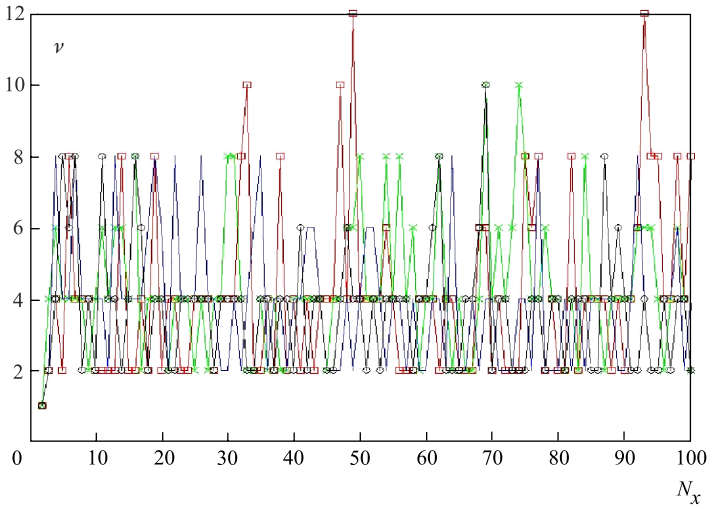

Fig. 5. The process of solutions ν branching with increase in length of 1D spin chains is shown. As one can see the number of solutions does not exceed 12 on each layer of branching for spin chains of length N_x and till the end of the spin chain it is independent from the initial angular configurations needed for the start of the simulation

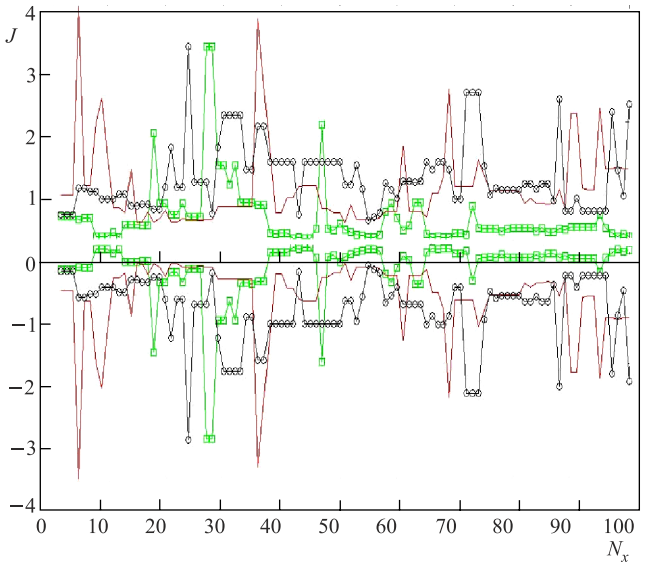

Fig. 6. Localization regions changes of the spin–spin interaction constants are shown, depending on the node sequence number of 1D lattice. Different curves correspond to different numerical experiments

4. STATISTICAL PROPERTIES OF ENSEMBLE IN EXTERNAL FIELD

Using the obvious similarity between temperature T of usual statistical ensemble and the average energy coming on one spin $\varepsilon_0 = \bar{\varepsilon}/N_x$, we can define the *partition function* as follows:

$$Z(\mathbf{g};\mathbf{J}) = \int \frac{d\Omega_1}{4\pi} \dots \int \frac{d\Omega_{N_x}}{4\pi} \exp\left\{-\frac{H(N_x;\mathbf{g})}{\varepsilon_0}\right\}, \tag{19}$$

where $\mathbf{J}$ describes the set of spin–spin interaction constants in chain.

The integration in expression (19) in the above-mentioned model may start from the end of the chain (see [22]). When integrating over the solid angle $d\Omega_i$ we take the direction of the vector $(J_{i\,i+1}\mathbf{S}_i + p^0\mathbf{h}_i)$ as a polar axis and it is easy to obtain the following expression:

$$\begin{gathered} Z(\mathbf{g};\mathbf{J}) = \prod_{i=0}^{N_x-1} \frac{\sinh G_i}{G_i}, \\ G_i(\mathbf{g};\bar{\varepsilon},J_{ii+1}) = \frac{1}{\varepsilon_0}\sqrt{J_{ii+1}^2 + 2p^0h_iJ_{ii+1}\cos\beta_i + (p^0h_i)^2}. \end{gathered} \tag{20}$$

Assuming that the distribution of spin $\mathbf{S}_{i+1}$ around the field $\mathbf{h}_i$ direction is isotropic, one can perform an integration over the angle β_i and after simple calculations find:

$$Z(\mathbf{g},\varepsilon_0;\mathbf{J}) = \prod_{i=0}^{N_x-1}\left[\frac{1}{2}\int_0^{\pi}\frac{\sinh G_i}{G_i}\sin\beta_i d\beta_i\right] = \prod_{i=0}^{N_x-1}\left\{\frac{1}{b_i}\Lambda_i(\mathbf{g};\varepsilon_0,J_{i\,i+1})\right\}, \tag{21}$$

where $\Lambda_i(\mathbf{g};\varepsilon_0,J_{ii+1}) = [\cosh a_i^+ - \cosh a_i^-]$, $a_i^{\pm} = \dfrac{1}{\varepsilon_0}[J_{ii+1} \pm p^0h_i]$, $b_i = \dfrac{2}{\varepsilon_0^2}J_{ii+1}p^0h_i$.

Now using expression (21) we can average the *partition function* by distribution $F(J)$:

$$\bar{Z}(\mathbf{g},\varepsilon_0) \equiv \langle Z(\mathbf{g},\varepsilon_0;J)\rangle_J = \prod_{i=0}^{N_x-1}\left\langle\frac{1}{b_{i,j}^0}\Lambda_i^0(\mathbf{g},\varepsilon_0;J)\right\rangle_J, \tag{22}$$

where $\langle\dots\rangle_J \equiv \int\dots\int\dots F(J_{01})\dots F(J_{N_x-1N_x})dJ_{01}\dots dJ_{N_x-1N_x}$.

Like in the usual thermodynamics, Helmholtz free energy for 1D SSC ensemble may be specified in the following way:

$$Q(\mathbf{g},\varepsilon_0) = \varepsilon_0\ln\bar{Z}(\mathbf{g},\varepsilon_0), \quad \varepsilon_0 < 0. \tag{23}$$

Note that all thermodynamic properties of the statistical system in this case may be obtained by means derivation of the free energy by external field parameters $\mathbf{g}$. After the derivation of the free energy by h_0, we can find:

$$q(\gamma, N_x) = \frac{\partial Q(\mathbf{g}, \varepsilon_0)}{\partial \bar{h}_0} = -\frac{1}{\gamma} \sum_{i=0}^{N_x - 1} \left\{1 - \gamma y_i \coth\left(\gamma y_i\right)\right\}, \tag{24}$$

where $\bar{h}_0 = h_0 p^0$, $\gamma = \bar{h}_0/\varepsilon_0$, $y_i = \cos\left(k_{N_x} x_i\right)$, $x_i = i d_0$, $k_{N_x} = 2\pi/N_x$.

As calculations show, the free energy derivation linearly depends on γ parameter. The last result testifies the absence of a phase transition in this parameter (see Fig. 4, *b*). Thereby a logical question arises: Are there phase transitions in considered system depending on other parameters?

To answer this question, we will investigate the behavior of the average value of polarization depending on parameter γ or the value of an external field. Using the definition (8) we can calculate the polarization distribution on coordinates $F(p_\eta, \gamma)$, where $\eta = x, y, z$. As numerical simulation shows, distributions of polarizations depending on parameter γ are strongly frustrated [23] and these frustrations do not disappear at regular dividing of computation region (see Fig. 7, *a, b, c*). Moreover, at each division a self-similar structure is conserved which testifies about its fractal character. The dimensionality of fractal structure is calculated by the simple formula:

$$D_\eta(\gamma) = \ln(n)/\ln(N), \tag{25}$$

where n is the number of partitions of the structure size, and N is the number of placing of the initial structure. The calculation particularly shows, that at value of $\gamma = 0.00425$ dimensionality $D_x \approx 1.2095$. In a similar manner, D_y and D_z can be calculated. It is obvious that at increasing γ all of them converge to 1.

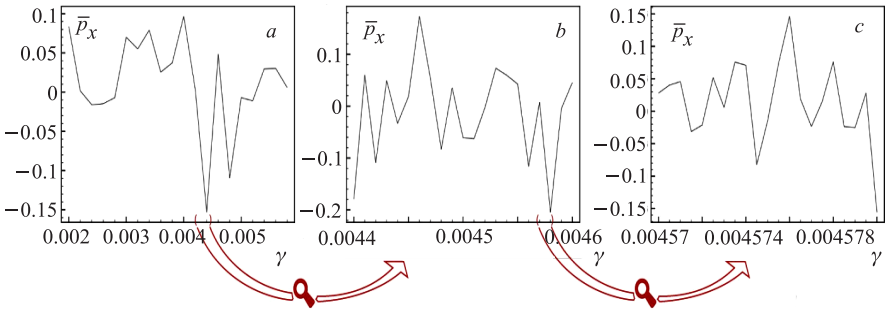

Fig. 7. The type of fractals arising at area partition of self-similar figures is visible and connected with frustrations of spin-glass medium

At last we will pass to a question on average value of polarization. Namely, how to calculate it? Taking into account above-mentioned, it is obvious that the average value of polarization (magnetization) must be calculated by the following formula:

$$\langle P_\eta(\gamma)\rangle = \lim_{M\to\infty}\left\langle \frac{1}{M}\sum_i p_i \right\rangle_f = \left\langle \int_{-\infty}^{+\infty} F(p_\eta,\gamma)p_\eta dp_\eta \right\rangle_f , \qquad (26)$$

where the slanting bracket $\langle\,.\,\rangle_f$ stands for averaging of expression by the fractal structure which itself represents an arithmetic mean. As follows from Fig. 8, *a*, after averaging on fractal structures the average value of polarization depending on γ has several phase transitions of the first order.

Finally we can introduce a parameter which can characterize the ordering process in system. Using obvious similarity between our and usual cases we can define Edwards–Anderson-type ordering parameter in the form:

$$\langle P_\eta^2(\gamma)\rangle = \lim_{M\to\infty}\left\langle \frac{1}{M}\sum_i p_i^2 \right\rangle_f = \left\langle \int_{-\infty}^{+\infty} F(p_\eta,\gamma)p_\eta^2 dp_\eta \right\rangle_f . \qquad (27)$$

As calculations show, the ordering parameter also has several phase transitions of the first order, however at increasing of γ, the system goes to the full ordering (see Fig. 8, *b*).

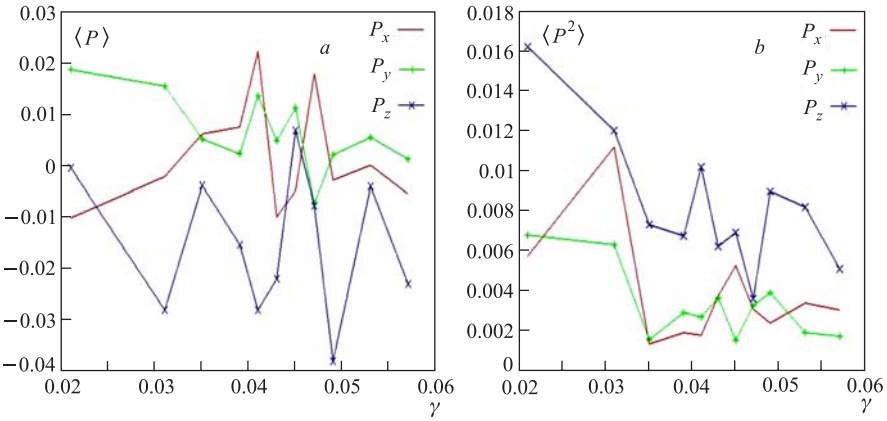

Fig. 8. *a*) The average polarization in ensemble of coordinates x, y, z is shown, where phase transitions of the first order are visible. *b*) The order parameter of Edwards–Anderson type depends on the external field. It is visible that in measure of increase of an external field, frustrations in a spin-glass system disappear and an ordering occurs in it

CONCLUSION

Using equations for stationary points of Hamiltonian (5) and conditions of energy minimum (6)–(7) on nodes of periodic lattice we have developed a new high performance parallel algorithm (see scheme in Fig. 2) for a simulation of 1D spin glass. The idea of algorithm is based on the construction of stable spin-chains of certain lengths. We have shown that the number of spin chains (the simulation number) can be considered as a «timing» parameter as in case of dynamic system and the ergodic properties of system can be studied depending on this parameter. It is shown by numerical experiments that distribution functions of different parameters of the system after $\propto N_x^2$ simulations converge to the equilibrium values. In other words, system which consists of $\propto N_x^2$ number spin chains satisfies Birkhoff's ergodicity conditions. We have shown that the distribution of spin–spin interaction constants can be found directly by way of calculations of classical equations (5) and analysis of statistical data of simulation. It is theoretically shown (see inequality (16)) that at least for the 1D spin-glass problem the distribution of the spin–spin interaction constants cannot be Gauss–Edwards–Anderson type. In particular, the analysis of numerical data of simulation shows that they obey to Lévy's alpha-stable distribution law. In other words, if we use the normal distribution in these problems, we make calculations ineffective, not to say doubtful.

As is shown, the derivative of a free energy (24) does not have a phase transition depending on the parameter of an external field's energy (see Fig. 4, *b*). The last means that under the influence of an external field the essential changes of energy does not occur in the system. The last, however, does not mean that in the system a critical phenomena cannot occur under the influence of an external field related to other parameters. Only through numerical calculations we were able to show that in the system the phase transitions of the first order occur under the influence of weak external field in the value of average polarization of spin glass in all coordinates (see Fig. 8, *a*). As calculations show, the critical phenomena can be considerable even for weak fields. For example, they can lead to formation of a superlattice of a dielectric constant in the spin-glass' medium which can have a wide applications for solutions of different applied problems.

Finally, it is important to note that the algorithm can be simply generalized for high dimensional cases and in particular for 3D case, which means that it will be a very needed instrument for numerical investigations of the above-mentioned class of problems.

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