E11-2011-60

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ON MODELING OF STATISTICAL PROPERTIES OF CLASSICAL 3D SPIN GLASSES

Submitted to «Journal of Physics A: Mathematics and General»

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О моделировании статистических свойств классических 3D спин-стекол

Исследуются статистические свойства классического 3D спин-стекольного слоя определенной ширины и бесконечной длины. 3D спиновое стекло представляется в виде ансамбля неупорядоченных 1D пространственных спин-цепей (ПСЦ), где взаимодействия между спин-цепями являются случайными (неидеальный ансамбль 1D ПСЦ). Доказано, что в пределе выполнения эргодической гипотезы Биркгофа 3D спин-стекло может быть генерировано вспомогательным гамильтонианом неупорядоченной 1D ПСЦ со случайным окружением. Неупорядоченный 1D ПСЦ определяется на регулярной решетке, где в каждом узле решетки помещается один случайно ориентированный спин. Также предполагается, что каждый спин случайно взаимодействует с шестью ближайшими соседними спинами (два спина на решетке и четыре в окружении). В узлах решетки спин-цепочки получены рекуррентные трансцендентные уравнения. Эти уравнения совместно с условиями Сильвестра позволяют шаг за шагом построить спин-цепочку в основном состоянии энергии, где все спины находятся в минимальной энергии классического гамильтониана. На основе этих уравнений разработан оригинальный высокопроизводительный параллельный алгоритм для моделирования 3D спинового стекла. Рассчитаны распределения различных параметров невозмущенного спинового стекла. В частности, аналитически доказано и численными расчетами показано, что распределение константы спин-спинового взаимодействия в модельном гамильтониане ближайших соседей Гейзенберга, в отличие от широко используемого распределения Гаусса–Эдвардса–Андерсона, удовлетворяет закону альфа-устойчивого распределения Леви, который не имеет дисперсии. Предложена новая формула для построения статистической суммы в виде одномерного интеграла от распределения энергии ансамбля 1D ПСЦ.

Работа выполнена в Лаборатории информационных технологий ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна, 2011

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On Modeling of Statistical Properties of Classical 3D Spin Glasses

We study statistical properties of 3D classical spin glass layer of certain width and infinite length. The 3D spin glass is represented as an ensemble of disordered 1D spatial spin chains (SSC) where interactions are random between spin chains (nonideal ensemble of 1D SSCs). It is proved that in the limit of Birkhoff's ergodic hypothesis performance, 3D spin glasses can be generated by Hamiltonian of disordered 1D SSC with random environment. Disordered 1D SSC is defined on a regular lattice where one randomly oriented spin is put on each node of lattice. Also, it is supposed that each spin randomly interacts with six nearest-neighboring spins (two spins on lattice and four in the environment). The recurrent transcendental equations are obtained on the nodes of spin-chain lattice. These equations, combined with the Silvester conditions, allow step-by-step construction of spin chain in the ground state of energy where all spins are in minimal energy of classical Hamiltonian. On the basis of these equations an original high-performance parallel algorithm is developed for 3D spin glasses simulation. Distributions of different parameters of unperturbed spin glass are calculated. In particular, it is analytically proved and numerical calculations show that the distribution of spin–spin interaction constant in Heisenberg nearest-neighboring Hamiltonian model, as opposed to widely used Gauss–Edwards–Anderson distribution, satisfies Lévy alpha-stable distribution law which does not have variance. A new formula is proposed for construction of partition function in the form of one-dimensional integral on energy distribution of 1D SSCs.

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

Preprint of the Joint Institute for Nuclear Research. Dubna, 2011

1. INTRODUCTION

The wide class of phenomena and structures in physics, chemistry, material science, biology, nanoscience, evolution, organization dynamics, hard-optimization, environmental and social structures, human logic systems, financial mathematics, etc. are mathematically well described in the framework of spin glass models [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 coupling 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 requires invention of sophisticated schemes of replica-symmetry breaking [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. It has been pointed out in the works [14–16], however, this feature retains an important physical aspect of true spin glasses, viz. they are random with respect to the positions of magnetic impurities.

Note that all the mentioned investigations as a rule are conducted at equilibrium's conditions of medium. This fact plays a key role in both analytical and numerical simulation by Monte Carlo method.

Recently, as authors have shown [17], some type of dielectrics can be studied by model of quantum 3D spin glass. In particular, it was proved that the initial 3D quantum problem on scales of space-time periods of an external field can be reduced to two conditionally separable 1D problems where one of them describes an ensemble of disordered 1D spatial spin-chains between which are random interactions (further will be called *nonideal ensemble*).

In this paper we discuss in detail statistical properties of classical 3D spin glass with suggestion that interactions between spins have short-range character. We prove that nonideal ensemble of 1D SSCs exactly describes the statistical properties of classical 3D spin glasses in the limit of Birkhoff's ergodic hypothesis performance. In the work a new high-performance algorithm for simulation of this traditionally difficult calculated problem is developed.

In Section 2 the classical spin glass problem on 3D lattice is formulated. Equations for stationary points and corresponding Silvester conditions are ob-

tained for definition of energy minimum on lattice nodes (local minimum of energy). The formula for computation of different parameters distributions of spin glass is defined.

In Section 3 a theorem on reduction of 3D spin glass problem to the problem of nonideal ensemble of 1D SSCs is proved.

In Section 4 numerical experiments are adduced for unperturbed 1D SSCs ensemble with spin chain's length $10^3 d_0$. In particular, distributions of energy, polarization and spin–spin interaction constants of nonideal ensemble are investigated in detail.

In Section 5 partition function is investigated in detail in the configuration integral's representation. A new representation is suggested for partition function in the form of one-dimensional integral on energy distribution of nonideal ensemble.

In Section 6 the obtained theoretical and computational results are analyzed. It is very important to note that it has been proved that in the framework of the developed method it is always possible to exactly compute the ground-state energy of 3D spin glasses.

2. FORMULATION OF PROBLEM

The objects of our investigation are solid-state dielectrics, type of SiO_2 glass (amorphous silicon dioxide). According to the numerical $ab\ initio$ simulations [7], the structure of this type compound can be well described by 3D random network (Fig. 1, *a*). The red and brown lattice points on this figure correspond to different atoms, while the links between them correspond to covalent bounds. As a result of charges redistribution in outer electronic shells, atoms of Si acquire the positive charge and atoms of O correspondingly the negative charge. Thus, we can consider compounds of this type as a disordered 3D system of similar rigid dipoles (hereinafter termed as a system of 3D disordered spins, Fig. 1, *b*). Let us remind that under the similar rigid dipoles are meant the dipoles for which the absolute values are equal ($|\mathbf{p}_i| = |\mathbf{p}_j| = p^0$, where $\mathbf{p}_i$ and $\mathbf{p}_j$ are two arbitrary dipoles), and they do not vary under the influence of an external field.

The Hamiltonian of 3D classical spin glass system reads

$$H(\{\mathbf{r}\}) = -\sum_{<i\,j>} J_{i\,j}\mathbf{S}_i\mathbf{S}_j, \quad \{\mathbf{r}\} \equiv \mathbf{r}_1, \mathbf{r}_2, \ldots,$$

where indices i and j run over all nodes of 3D lattice, $\mathbf{r}_i$ correspondingly denotes the coordinates of ith spin (see Fig. 1, *b*). For further investigation we will consider a spin glass layer of certain width L_x and infinite length (see Fig. 2).

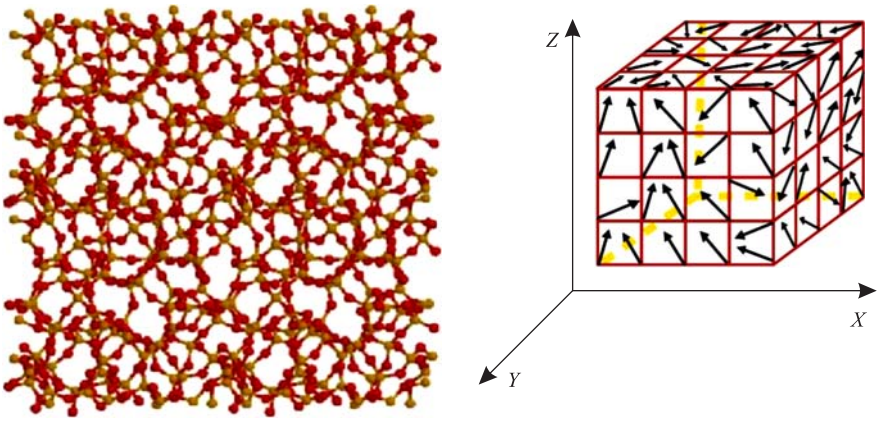

Fig. 1. The structure of amorphous silicon dioxide SiO_2 is described by 3D random network with covalent bonds. Every silicon vertex (gold sphere) has 4 edges and every oxygen vertex (red sphere) has 2 edge *

We will consider 3D compound in the framework of nearest-neighboring Hamiltonian model. Let us note that even for this relatively simple model numerical simulations of spin glasses are extremely hard to solve NP problems.

At first we will consider an auxiliary Heisenberg Hamiltonian of the form

$$H_0(\{\mathbf{r}\};\, N_x) = H_0^{(1)}(\{\mathbf{r}\};\, N_x) + H_0^{(2)}(\{\mathbf{r}\};\, N_x), \tag{1}$$

where the first term $H_0^{(1)}(\{\mathbf{r}\};\, N_x)$:

$$H_0^{(1)}(\{\mathbf{r}\};\, N_x) = -\sum_{i=0}^{N_x-1} J_{i\,i+1}\mathbf{S}_i\mathbf{S}_{i+1},$$

describes the disordered 1D *spatial spins chain* (SSC), while the second term $H_0^{(2)}(\{\mathbf{r}\};\, N_x)$:

$$H_0^{(2)}(\{\mathbf{r}\};\, N_x) = -\sum_{i=0}^{N_x-1}\sum_{\sigma=1}^{4} J_{i\,i_\sigma}\mathbf{S}_i\mathbf{S}_{i_\sigma},$$

correspondingly describes the random surroundings of 1D SSC (see Fig. 2). In (1) $J_{i\,i+1}$ and $J_{i\,i_\sigma}$ are correspondingly random interaction constants between arbitrary i and $i+1$ spins and between i and i_σ spins, $\mathbf{S}_i$, $\mathbf{S}_{i+1}$ and $\mathbf{S}_{i_\sigma}$ are spins

* The colored version of the figures of the present work is available at http://www.jinr.ru/publish

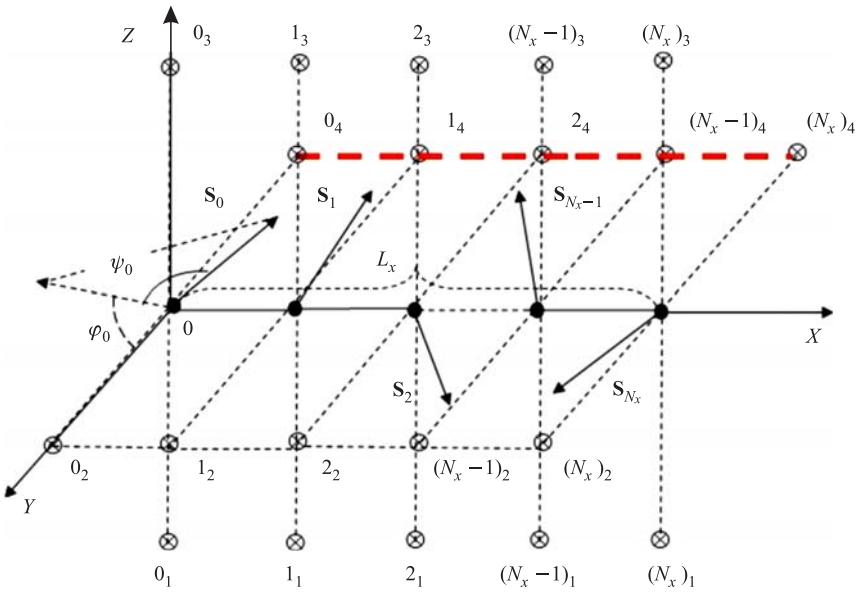

Fig. 2. 1D SSC with the random environment. Recall that each spin chain is surrounded by four spin chains which randomly interact with it. Symbols $\otimes$ designate spins from the random environment (four spin chains of surrounding)

(vectors) of unit length, which are randomly orientated in O(3) space. From the general reasons it follows that with the help of (1) Hamiltonian and by way of successive constructing we can restore the Hamiltonian of 3D problem. Recall that the meaning of the construction is as follows. On the first step the central spin chain on the x axis with its surroundings from four random spin chains is considered (see Fig. 2). On the second step as central spin chains are considered corresponding spin chains from the random surroundings, each of which are surrounded by new four neighboring spin chains. Thus, repeating this cycle periodically, we can construct the Hamiltonian of 3D problem. This idea will be rigorously proved below.

For further investigation of spin glass problem, it is useful to write the Hamiltonian (1) in spherical coordinates system:

$$H_0(\{\mathbf{r}\};N_x) = -\sum_{i=0}^{N_x-1}\Bigg\{J_{i\,i+1}\Big[\cos\psi_i\cos\psi_{i+1}\cos\left(\varphi_i-\varphi_{i+1}\right)+\sin\psi_i\sin\psi_{1+1}\Big]+ \\ +\sum_{\sigma=1}^{4}J_{i\,i_\sigma}\Big[\cos\psi_i\cos\psi_{i_\sigma}\cos\left(\varphi_i-\varphi_{i_\sigma}\right)+\sin\psi_i\sin\psi_{i_\sigma}\Big]\Bigg\}. \quad (2)$$

Now the main problem is to find the angular configurations and spin–spin interaction constants which can make the Hamiltonian minimal on each node of lattice.

Let us consider the equations of stationary point:

$$\frac{\partial H_0}{\partial \psi_i} = 0, \quad \frac{\partial H_0}{\partial \varphi_i} = 0, \tag{3}$$

where $\Theta_i = (\psi_i, \varphi_i)$ defines the orientation of ith spin (ψ_i, φ_i are correspondingly the polar and the azimuthal angles). In addition, $\mathbf{\Theta} = (\mathbf{\Theta}_1, \mathbf{\Theta}_2 \dots \mathbf{\Theta}_{N_x})$ describes the angular configuration of spin chain consisting of N_x spins.

Substituting (2) into (3), we can find the following recurrent equations:

$$\begin{aligned} & J_{i-1\,i}\Big[-\sin\psi_i\cos\psi_{i-1}\cos(\varphi_i-\varphi_{i-1})+\cos\psi_i\sin\psi_{i-1}\Big]+ \\ & \quad + J_{i\,i+1}\Big[-\sin\psi_i\cos\psi_{i+1}\cos(\varphi_i-\varphi_{i+1})+\cos\psi_i\sin\psi_{i+1}\Big]+ \\ & \quad + \sum_{\sigma=1}^{4} J_{i\,i_\sigma}\Big[-\sin\psi_i\cos\psi_{i_\sigma}\cos(\varphi_i-\varphi_{i_\sigma})+\cos\psi_i\sin\psi_{i_\sigma}\Big]=0, \end{aligned} \tag{4}$$

$$\begin{aligned} & \Big\{\Big[J_{i-1\,i}\,\cos\psi_{i-1}\sin(\varphi_i-\varphi_{i-1})+J_{i\,i+1}\,\cos\psi_{i+1}\times \\ & \quad \times\sin(\varphi_i-\varphi_{i+1})\Big]+\sum_{\sigma=1}^{4} J_{i\,i_\sigma}\cos\psi_{i_\sigma}\sin(\varphi_i-\varphi_{i_\sigma})\Big\}\cos\psi_i=0. \end{aligned}$$

In order to satisfy the conditions of local minimum (Silvester conditions) for H_0, it is necessary that the following inequalities be valid:

$$A_{\psi_i\psi_i}(\Theta_i^0) > 0, \quad A_{\psi_i\psi_i}(\Theta_i^0)A_{\varphi_i\varphi_i}(\Theta_i^0) - A^2_{\psi_i\varphi_i}(\Theta_i^0) > 0, \tag{5}$$

where $A_{\alpha_i\alpha_i} = \partial^2 H_0/\partial\alpha_i^2$ and $A_{\alpha_i\beta_i} = A_{\alpha_i\beta_i} = \partial^2 H_0/\partial\alpha_i\partial\beta_i$, in addition:

$$\begin{aligned} A_{\psi_i\psi_i}(\Theta_i^0) &= J_{i-1\,i}\Big\{\cos\psi_i^0\cos\psi_{i-1}\cos(\varphi_i^0-\varphi_{i-1})+\sin\psi_i^0\sin\psi_{i-1}\Big\}+ \\ &\quad + J_{i\,i+1}\Big\{\cos\psi_i^0\cos\psi_{i+1}\cos(\varphi_i^0-\varphi_{i+1})+\sin\psi_i^0\sin\psi_{i+1}\Big\}+ \\ &\quad + \sum_{\sigma=1}^{4} J_{i\,i_\sigma}\Big\{\cos\psi_i^0\cos\psi_{i_\sigma}\cos(\varphi_i^0-\varphi_{i_\sigma})+\sin\psi_i^0\sin\psi_{i_\sigma}\Big\}, \\ A_{\varphi_i\varphi_i}(\Theta_i^0) &= \Big\{J_{i-1\,i}\cos\psi_{i-1}\cos(\varphi_i^0-\varphi_{i-1})+J_{i\,i+1}\cos\psi_{i+1}\cos(\varphi_i^0-\varphi_{i+1})+ \\ &\quad + \sum_{\sigma=1}^{4} J_{i\,i_\sigma}\cos\psi_{i_\sigma}\cos(\varphi_i^0-\varphi_{i_\sigma})\Big\}\cos\psi_i^0, \quad A_{\psi_i\varphi_i}(\Theta_i^0)=0. \end{aligned}$$

Recall that $\Theta_i^0 = (\psi_i^0, \varphi_i^0)$ designates the angular configuration of the spin in the case that the condition of local minimum for H_0 is satisfied.

Thus, it is obvious that the classical 3D spin glass system (see Fig. 1, *b*) can be considered as a nonideal ensemble of 1D SSCs (see Fig. 2) and there are random interactions between spin chains.

Now we can construct distribution functions of different parameters of 1D SSCs nonideal 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 the real energy axis. The number of stable 1D SSC configurations with length 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 $M_{L_x}^{\text{full}} = \sum\limits_{j=1}^{n} M_{L_x}(\varepsilon_j)$. Accordingly, the energy distribution function can be defined by the expression

$$F_{L_x}(\varepsilon; d_0(T)) = M_{L_x}(\varepsilon)/M_{L_x}^{\text{full}}, \tag{6}$$

where the distribution function is normalized to unit:

$$\lim_{n\to\infty} \sum_{j=1}^{n} F_{L_x}(\varepsilon_j; d_0(T))\delta\varepsilon_j = \int\limits_{-\infty}^{0} F_{L_x}(\varepsilon; d_0(T))d\varepsilon = 1.$$

In a similar way we can also construct distribution functions for polarizations, spin–spin interaction constant, etc.

3. REDUCTION OF 3D SPIN GLASS PROBLEM TO 1D SSCS ENSEMBLE PROBLEM

Modeling of 3D spin glasses is a typical NP hard problem. This type of problems are hard-to-solve even on modern supercomputers if the number of spins in the system are more or less significant. In connection with the aforesaid, the significance of new mathematical approaches development is obvious and on this basis an effective parallel algorithm for numerical simulation of spin glasses can be elaborated.

Theorem: *The classical 3D spin glass problem at the limit of isotropy and homogeneity (ergodicity) of superspins distribution (sum of spins in chain) in 3D configuration space is equivalent to the problem of disordered 1D SSCs ensemble.*

It is obvious that the theorem will be proved if we can prove that in the case that the distribution of superspins in 3D configuration space is homogeneous and isotropic, the following two propositions take place:

a) In any random environment which consists of four arbitrary spin chains, it is always possible to find at least one physically admissible solution for spin chain (the direct problem),

b) It is possible to surround an arbitrary spin chain from the given environment with such environment which can make it physically admissible spin-chain solution (the reverse problem).

First we prove the direct problem.
By using the following notation:

$$\xi_{i+1} = \cos\psi_{i+1}, \quad \eta_{i+1} = \sin(\varphi_i - \varphi_{i+1}), \tag{7}$$

the system of equations (6) can be transformed as follows:

$$\begin{aligned} C_1 + J_{i\,i+1}\big[\sqrt{1-\xi_{i+1}^2} - \tan\psi_i\,\xi_{i+1}\sqrt{1-\eta_{i+1}^2}\big] = 0, \\ C_2 + J_{i\,i+1}\,\xi_{i+1}\,\eta_{i+1} = 0, \end{aligned} \tag{8}$$

where parameters C_1 and C_2 are defined by the expressions

$$\begin{aligned} C_1 = J_{i-1\,i}\big[\sin\psi_{i-1} - \tan\psi_i\cos\psi_{i-1}\cos(\varphi_i - \varphi_{i-1})\big] + \sum_{\sigma=1}^{4} J_{i\,i_\sigma} \times \\ \times \Big[\sin\psi_{i_\sigma} - \tan\psi_i\cos\psi_{i_\sigma}\cos(\varphi_i - \varphi_{i_\sigma})\Big], \\ C_2 = J_{i-1\,i}\cos\psi_{i-1}\sin(\varphi_i - \varphi_{i-1}) + \sum_{\sigma=1}^{4} J_{i\,i_\sigma}\cos\psi_{i_\sigma}\sin(\varphi_i - \varphi_{i_\sigma}). \end{aligned}$$

From the system (8) we can find the equation for the unknown variable η_{i+1}:

$$C_1\eta_{i+1} + C_2\sqrt{1-\eta_{i+1}^2}\tan\psi_i + \sqrt{J_{i\,i+1}^2\eta_{i+1}^2 - C_2^2} = 0. \tag{9}$$

We have transformed Eq. (9) to the equation of fourth order which is exactly solved further:

$$\xi_{i+1}^2 = \frac{C_2^2}{J_{i\,i+1}^2\eta_{i+1}^2}, \quad \eta_{i+1}^2 = \frac{A}{B}, \tag{10}$$

where

$$\begin{aligned} A = C_2^2\Big\{J_{i\,i+1}^2\cos^2\psi_i + C_3 + 2C_1^2\sin^2\psi_i\Big[1 \pm C_1^{-1}\sqrt{J_{i\,i+1}^2 - C_1^2 - C_2^2}\,\cot\psi_i\Big]\Big\}, \\ C_3 = -C_1^2 + C_2^2\sin^2\psi_i, \\ B = J_{i\,i+1}^4\cos^4\psi_i + 2C_3J_{i\,i+1}^2\cos^2\psi_i + (C_1^2 + C_2^2\sin^2\psi_i)^2. \end{aligned}$$

Note that from the condition of nonnegativity of the value under the root we can find the following nonequality:

$$J_{i\,i+1}^2 \geqslant C_1^2 + C_2^2. \tag{11}$$

In consideration of (7), we can write the following conditions:

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

As it follows from Eq. (10), if the solutions in previous two nodes $(i-1)$ and i are known, then the solutions $(\psi_{i+1}, \varphi_{i+1})$ in the node $(i+1)$ can be defined only by constant $J_{i\,i+1}$. In this connection, a natural question arises: are there solutions for spin chain in arbitrarily given environment?

Let us consider the Silvester conditions (5) which can be written in the form of the following inequalities:

$$J_{i\,i+1} \cos\psi_i^0 \cos\psi_{i+1} \cos\left(\varphi_i^0 - \varphi_{i+1}\right) > -a_1 - \sin\psi_i^0 \sin\psi_{i+1},$$

$$J_{i\,i+1} \cos\psi_{i+1} \cos\left(\varphi_i^0 - \varphi_{i+1}\right) \cos\psi_i^0 > -a_2, \qquad (12)$$

where constants a_1 and a_2 are defined by the expressions

$$a_1 = J_{i-1\,i}\Big[\cos\psi_i^0 \cos\psi_{i-1} \cos\left(\varphi_i^0 - \varphi_{i-1}\right) + \sin\psi_i^0 \sin\psi_{i-1}\Big] +$$

$$+ \sum_{\sigma=1}^{4} J_{i\,i_\sigma}\Big[\cos\psi_i^0 \cos\psi_{i_\sigma} \cos\left(\varphi_i^0 - \varphi_{i_\sigma}\right) + \sin\psi_i^0 \sin\psi_{i_\sigma}\Big],$$

$$a_2 = \Big\{J_{i-1\,i} \cos\psi_{i-1} \cos\left(\varphi_i^0 - \varphi_{i-1}\right) + \sum_{\sigma=1}^{4} J_{i\,i_\sigma} \cos\psi_{i_\sigma} \cos\left(\varphi_i^0 - \varphi_{i_\sigma}\right)\Big\} \cos\psi_i^0.$$

So, the problem leads to the answer to the following question: are inequalities (11) and (12) compatible or not. Taking into account solutions (10), it is easy to prove that conditions (12) are automatically compatible at large absolute values of $J_{i\,i+1}$. On the other hand, there is no any contradiction with condition (11). Thus, the direct problem or the proposition *a*) is proved.

Now our aim is to prove the reverse problem or the proposition *b*) which consists in the following. We choose a spin chain from the environment (see Fig. 2), for example, $\{i_4\} \equiv (0_4, 1_4, \ldots, N_{x4})$. In this spin chain all angular configurations of spins $(\Theta_0^{(4)}, \ldots \Theta_{N_x}^{(4)})$ are known, but the constants that define spin–spin interactions in spin chain and interactions between spin chain and its environment still are not defined. We will prove that it is always possible to surround each spin chain by environment such that the selected spin chain will be the correct solution from the main physical laws point of view (see conditions (4), (5)). In the considered case $\{i_4\} \equiv \{i_0^{'}\}$, the spin chain is surrounded by four neighbors, one of which $\{i_0\} \equiv \{i_2^{'}\}$ is fully determined, while three spin chains $\{i_1^{'}\}, \{i_3^{'}\}$ and $\{i_4^{'}\}$ should be still specified (see Fig. 3). Recall that the mark «$'$» designates a new environment with three spin chains. However, for simplicity we will omit or more clearly make change them in the subsequent calculations

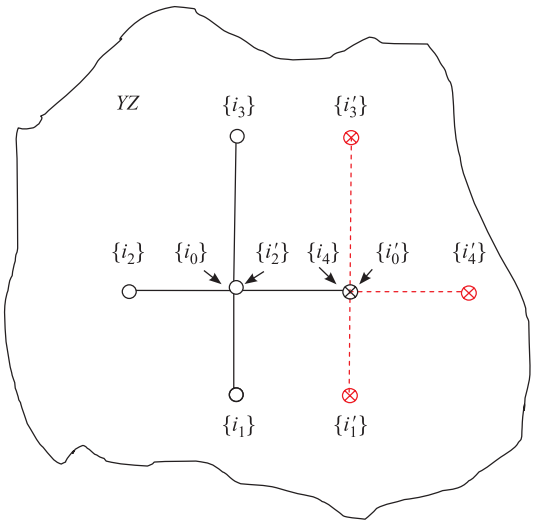

Fig. 3. The projection of spin-chains ensemble onto the (Y, Z) plane. Spin chains are designated by symbols ◯ and ⊗ which correspondingly form the old and new environments

$\big(\{i_0^{'}\},\{i_1^{'}\},\{i_2^{'}\},\{i_3^{'}\},\{i_4^{'}\}\big) \rightarrow \big(\{i_0\},\{i_1\},\{i_2\},\{i_3\},\{i_4\}\big)$. The proof of the proposition should be conducted as follows. We will suppose that the constants of spin–spin interactions in the considered chain and the corresponding parameters of two spin chains of environment are known. We will show that by special choosing of parameters of the third spin chain $\{i_3\}$, it is possible to ensure the condition of local minimum energy is satisfied in the considered spin chain.

Let us define the following denotations for constants:

$$\begin{aligned}
c_1 &= J_{i-1\,i}[-\sin\psi_i\cos\psi_{i-1}\cos(\varphi_i-\varphi_{i-1})+\cos\psi_i\sin\psi_{i-1}]+\\
&\quad + J_{i\,i_\sigma}[-\sin\psi_i\cos\psi_{i_\sigma}\cos(\varphi_i-\varphi_{i_\sigma})+\cos\psi_i\sin\psi_{i_\sigma}],\\
c_2 &= -\sin\psi_i\cos\psi_{i+1}\cos(\varphi_i-\varphi_{i+1})+\cos\psi_i\sin\psi_{i+1},\\
c_3 &= J_{i-1\,i}\cos\psi_{i-1}\sin(\varphi_i-\varphi_{i-1})+J_{i\,i_\sigma}\cos\psi_{i_\sigma}\sin(\varphi_i-\varphi_{i_\sigma}),\\
c_4 &= \cos\psi_{i+1}\sin(\varphi_i-\varphi_{i+1}),\quad \sigma=4.
\end{aligned} \tag{13}$$

Using (13), we can transform Eq. (4) to the following form:

$$c_1 + c_2 J_{i\,i+1} + \sum_{\sigma=1}^{3} J_{i\,i_\sigma}[-\sin\psi_i\cos\psi_{i_\sigma}\cos(\varphi_i-\varphi_{i_\sigma})+\cos\psi_i\sin\psi_{i_\sigma}] = 0,$$

$$c_3 + c_4 J_{i\,i+1} + \sum_{\sigma=1}^{3} J_{i\,i_\sigma}\cos\psi_{i_\sigma}\sin(\varphi_i-\varphi_{i_\sigma}) = 0,$$

which are equivalent to the following relations:

$$J_{i\,i+1} = -\frac{c_1}{c_2} - \frac{1}{c_2}\sum_{\sigma=1}^{3} J_{i\,i_\sigma}[-\sin\psi_i\cos\psi_{i_\sigma}\cos(\varphi_i-\varphi_{i_\sigma}) + \cos\psi_i\sin\psi_{i_\sigma}],$$
$$J_{i\,i+1} = -\frac{c_3}{c_4} - \frac{1}{c_4}\sum_{\sigma=1}^{3} J_{i\,i_\sigma}\cos\psi_{i_\sigma}\sin(\varphi_i-\varphi_{i_\sigma}). \tag{14}$$

After excluding $J_{i\,i+1}$ from (3) we find the following equation:

$$\sum_{\sigma=1}^{3}\left\{\frac{J_{i\,i_\sigma}}{c_2}[-\sin\psi_i\cos\psi_{i_\sigma}\cos(\varphi_i-\varphi_{i_\sigma}) + \cos\psi_i\sin\psi_{i_\sigma}] - \right.$$
$$\left. - \frac{J_{i\,i_\sigma}}{c_4}\cos\psi_{i_\sigma}\sin(\varphi_i-\varphi_{i_\sigma})\right\} - c_5 = 0, \quad c_5 = \frac{c_1}{c_2} - \frac{c_3}{c_4}. \tag{15}$$

Having made the following designation:

$$D = \sum_{\sigma=1}^{2}\left\{\frac{J_{i\,i_\sigma}}{c_2}[-\sin\psi_i\cos\psi_{i_\sigma}\cos(\varphi_i-\varphi_{i_\sigma}) + \cos\psi_i\sin\psi_{i_\sigma}] - \right.$$
$$\left. - \frac{J_{i\,i_\sigma}}{c_4}\cos\psi_{i_\sigma}\sin(\varphi_i-\varphi_{i_\sigma})\right\} - c_5,$$

we can transform Eq. (15) to the following form:

$$D + \frac{J_{i\,i_3}}{c_2}[-\sin\psi_i\cos\psi_{i_3}\cos(\varphi_i-\varphi_{i_3}) + \cos\psi_i\sin\psi_{i_3}] -$$
$$- \frac{J_{i\,i_3}}{c_4}\cos\psi_{i_3}\sin(\varphi_i-\varphi_{i_3}) = 0. \tag{16}$$

Now substituting

$$x = \cos\psi_{i_3} \tag{17}$$

into (16), we find the equation

$$D + \frac{J_{i\,i_3}}{c_2}[-x\sin\psi_i\cos(\varphi_i-\varphi_{i_3}) + \sqrt{1-x^2}\,\cos\psi_i] -$$
$$- x\frac{J_{i\,i_3}}{c_4}\sin(\varphi_i-\varphi_{i_3}) = 0. \tag{18}$$

From (18) the following square equation can be found:

$$K_0x^2 + 2K_1x + K_2 = 0, \tag{19}$$

where the following designations are made:

$$K_0 = \cos^2\psi_i + \left(\sin\psi_i\cos\left(\varphi_i - \varphi_{i_3}\right) + \frac{c_2}{c_4}\sin\left(\varphi_i - \varphi_{i_3}\right)\right)^2,$$
$$K_1 = -\frac{Dc_2}{J_{i\,i_3}}\left(\sin\psi_i\cos\left(\varphi_i - \varphi_{i_3}\right) + \frac{c_2}{c_4}\sin\left(\varphi_i - \varphi_{i_3}\right)\right),$$
$$K_2 = \left(\frac{Dc_2}{J_{i\,i_3}}\right)^2 - \cos^2\psi_i.$$

The discriminant of the square equation (19) has the form

$$D_x = \left(\sin\psi_i\cos\left(\varphi_i - \varphi_{i_3}\right) + \frac{c_2}{c_4}\sin\left(\varphi_i - \varphi_{i_3}\right)\right)^2\cos^2\psi_i + \\ + \left\{\cos^2\psi_i - \left(\frac{Dc_2}{J_{i\,i_3}}\right)^2\right\}\cos^2\psi_i \geqslant 0, \quad (20)$$

which on some set of $J_{i\,i_3}$ can be positive; i.e., the ith spin in spin chain $\{i_4\}$ will satisfy the local minimum conditions.

Let us define:

$$y = \cos\left(\varphi_i - \varphi_{i_3}\right). \quad (21)$$

Substituting (21) into (16), we will find that

$$D + \frac{J_{i\,i_3}}{c_2}[-y\,\sin\psi_i\cos\psi_{i_3} + \cos\psi_i\sin\psi_{i_3}] - \frac{J_{i\,i_3}}{c_4}\cos\psi_{i_3}\sqrt{1-y^2} = 0,$$

After squaring we will have the following equation:

$$M_0 y^2 + 2M_1 y + M_2 = 0, \quad (22)$$

where the following designations are made:

$$M_0 = \left(\left(\frac{c_2}{c_4}\right)^2 + \sin^2\psi_i\right)\cos^2\psi_{i_3},$$
$$M_1 = -\sin\psi_i\cos\psi_{i_3}\left(\cos\psi_i\sin\psi_{i_3} + \frac{Dc_2}{J_{i\,i_3}}\right),$$
$$M_2 = \left(\cos\psi_i\sin\psi_i + \frac{Dc_2}{J_{i\,i_3}}\right)^2 - \left(\frac{c_2}{c_4}\right)^2\cos^2\psi_{i_3}.$$

The discriminant of the square equation (22) has the form

$$D_y = \left(\frac{c_2}{c_4}\right)^2\cos^2\psi_i + \sin^2\psi_i\cos^2\psi_{i_3} - \left(\frac{Dc_2}{J_{i\,i_3}} + \cos\psi_i\sin\psi_{i_3}\right)^2 \geqslant 0. \quad (23)$$

Obviously, there are some set of constants $J_{i\,i_3}$ on which $D_y \geqslant 0$. However, it is more important to find the region of the interaction constant $J_{i\,i_3}$ values for which both determinants D_x and D_y are positive.

In particular, as the analysis of the following condition shows:

$$-\left|\frac{Dc_2}{\cos\psi_i}\right| \geqslant J_{i\,i_3} \geqslant \left|\frac{Dc_2}{\cos\psi_i}\right|, \tag{24}$$

discriminant D_x is always nonnegative. On the other hand,

$$\sin\psi_{i_3} \cong -\frac{Dc_2}{J_{i\,i_3}\cos\psi_i}, \tag{25}$$

which will assure that the D_y discriminant is always nonnegative. A simple analysis of the conditions (24) and (25) shows that they are compatible. In other words, the set of constants $J_{i\,i_3}$ which satisfies the energy local minimum condition is not empty and therefore the proposition *b*) is proved.

So, we have proved the validity of *a*) and *b*) propositions. It is obvious that at the simulation of 1D SSC problem we can in this way fill up 3D space by 1D SSC, which is equivalent to obtaining 3D spin glass. When the number of 1D SSCs is so much that the directions of spins in 3D space are distributed isotropically and homogeneous, the statistical properties of both problems (3D spin glass and 1D SSCs nonideal ensemble) will be obviously identical.

The theorem is proved.

4. RESULTS OF PARALLEL SIMULATIONS

One important consequence of the theorem is that for the numerical simulation of the problem we can use the algorithm for solving the direct problem. Obviously, a large number of independent computations of 1D SSC, which can be carried out in parallel, in statistical sense make it equivalent to the problem of 3D spin glass. This approach considerably reduces the amount of needed computations and helps us effortlessly simulate statistical parameters of 3D spin glasses of large size.

The strategy of simulation consists of the following steps (see Fig. 4). At first, the angular configurations of four spin chains are randomly generated which form random environment of the spin chain that we plan to construct later. On a following step, a set of random constants $J_{i\,i_\sigma}$ are generated, which characterizes the interactions between the random environment and the spin chain. The interaction constants are generated by Log-normal distribution. The angular configurations of the random environment are generated in the same way as it is described in [18]. Now that the environment and its influence on disordered

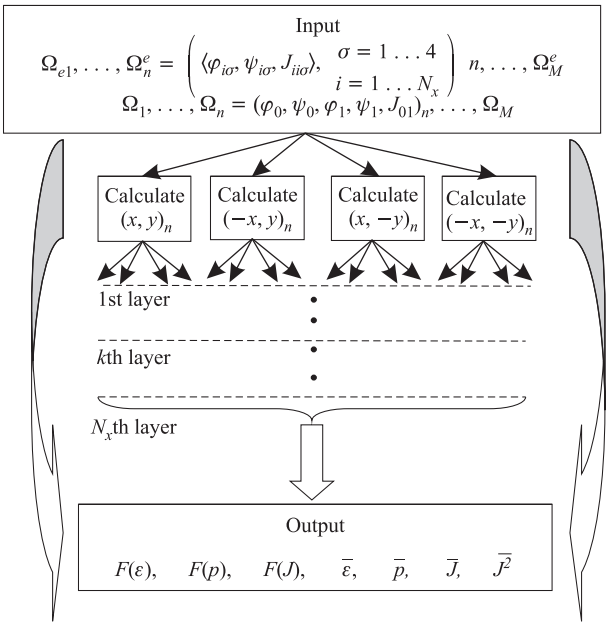

Fig. 4. The algorithm of parallel simulation of statistical parameters of disordered 1D SSCs nonideal ensemble. The symbol Ω_n^e describes the input of environment, M is a number of simulation or overall number of spin chains in the nonideal ensemble, N_x is a number of spins in chain

1D SSC are defined, we can go over to the computation of a spin chain which must satisfy the condition of local energy minimum. Note that the scheme of further computation of nonideal ensemble of 1D SSCs (see Fig. 2) is identical to the scheme of the computation of an ideal ensemble of disordered 1D SSCs (see [18]). Note that all calculations of 1D SSCs nonideal ensemble are done for spin chains with $10^3\, d_0$ length which require huge computational resources.

As the simulations show, for the ensemble which consists of 10^5 spin chains, the dimensional effects practically disappear (see Figs. 5, *a, b* and 6) and the energy distribution $F(\varepsilon)$ has one global maximum and is precisely approximated by Gaussian distribution (see Fig. 5, *a*).

Mean values of polarizations on coordinates are not very small, especially when it comes to coordinate x (thickness of spin glass layer): $p_x = -0.13508$, $p_y = 0.036586$, $p_z = -0.059995$ and correspondingly the average energy of 3D SSC is equal to $\bar{\varepsilon} = -990.88$, where $\bar{p} = \int\limits_{-\infty}^{+\infty} F(p) p dp$, $p = (p_x, p_y, p_z)$, $\bar{\varepsilon} =$

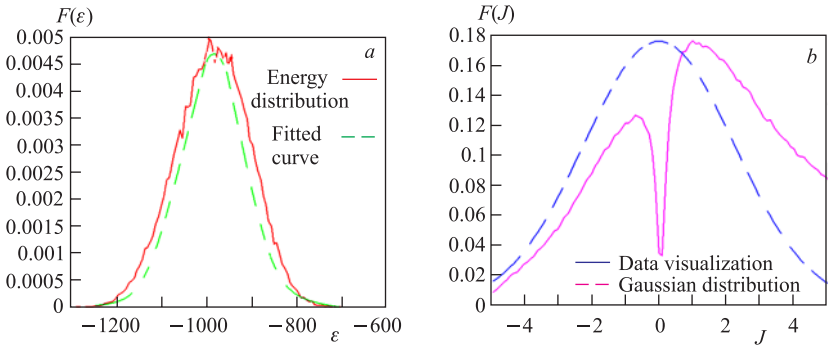

Fig. 5. *a*) The energy distribution of 1D nonideal ensemble of SSCs with 10^3 length. The red line shows a numerical data visualization, while the green one illustrates its fitting by Gaussian function. *b*) The visualization of numerical data of spin–spin interaction constants (pink line) and Gaussian distribution (blue line). The analysis of the numerical data proves that the green curve is not analytic function and by the character is the Lévy skew α-stable distribution function

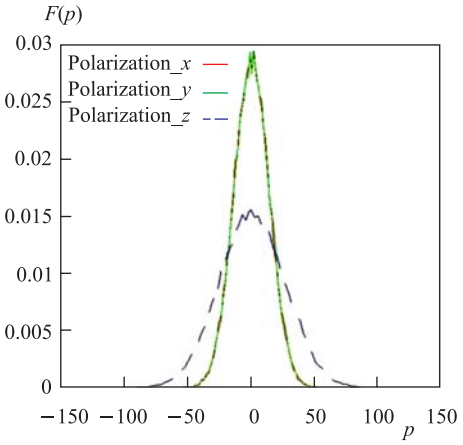

Fig. 6. The polarization distributions on different coordinates after 10^5 simulations

$\int_{-\infty}^{0} F(\varepsilon)\varepsilon d\varepsilon$ and F is the distribution function. As our numerical investigations have shown using the example of systems where the thickness of the spin glass layer is not so large $\propto 25d_0{-}100d_0$, for a full self-averaging of superspin it is necessary to make $\propto N_x^2$ simulations. In other words, the system can be fully ergodic in the considered case if we continue the numerical simulations of the spin chains up to $\propto 10^6$ times.

It is analytically proved and also the parallel simulation results show that the spin–spin interaction constant cannot be described by Gauss–Edwards–Anderson distribution (see Fig. 5, *b*). It essentially differs from the normal Gaussian distribution model and can be approximated precisely by Lévy skew alpha-stable distribution function. Let us recall that Lévy skew alpha-stable distribution is a continuous probability and a limit of certain random process $X(\alpha, \beta, \gamma, \delta; k)$, where the parameters correspondingly describe an index of stability or characteristic exponent $\alpha \in (0; 2]$, a skewness parameter $\beta \in [-1; 1]$, a scale parameter $\gamma > 0$, a location parameter $\delta \in \mathbf{R}$ and an integer k which shows the certain parametrization (see [19, 20]). Let us note that the mean of distribution and its variance are infinite. However, taking into account that spin–spin interaction constant has limited value in real physical systems, it is possible to calculate distribution mean and its variance. In particular, if $J \in [-5, +5]$, then $\overline{J} = 0.89717$ and $\overline{J^2} = 5.3382$.

In the work we also present polarization distributions on different coordinates (see Fig. 6). The polarization distributions are obviously very symmetric by coordinates in the considered case (see Fig. 6).

One of the advantages of the developed algorithm is that we are able to take into account the branching solutions at the successive constructing of the spin chain (see Fig. 7). As calculations show, the number of branching solutions ν for spin chains of length $10^3\, d_0$ is not more than 25. At the simulation process only those spin chains are considered for which Silvester conditions are satisfied on each node. If on some node the conditions are not satisfied, we try to regenerate $J_{i\,i+1}$ in order to obtain a new solution. However, if the solution is not found after a large quantity of simulations, it means that the weight of these solutions are all

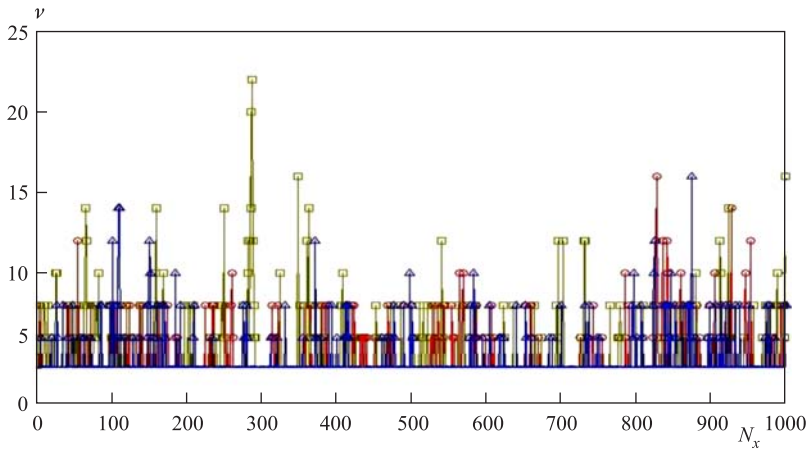

Fig. 7. The number of branching of solutions ν shown along with the spin-chain length depending on different initial conditions which are indicated by way of various colors

extremely small and further simulations of these spin chains are unpractical. Thus, when the ensemble consists of a large number of spin chains, the self-averaging of superspin (sum vector of spin chain) in 3D space occurs with high accuracy. It is important to note that the summation procedure on the number of spins in chain or on the number of spin chains in ensemble is similar to the procedure of averaging by the natural parameter or «timing» in the dynamical system. The latter means that at defined space scales of spin glasses it is possible to introduce the concept of ergodicity for both separate spin chains and ensemble as a whole.

5. PARTITION FUNCTION

The main object of investigation of statistical mechanics, information science, probability theory, etc., is the partition function which is defined for classical many-particle case in configuration space as follows [21]:

$$Z(\beta) = \int \exp\big[-\beta H(\{\mathbf{r}\})\big] d\mathbf{r}_1 d\mathbf{r}_2 \ldots, \quad \beta = \frac{1}{k_B T}, \tag{26}$$

where k_B is the Boltzmann constant and T is the thermodynamic temperature. Obviously, when the number of spins or spin chains in the system are large, we can consider the integral (26) as a functional integral. In any case the number of integration in the expression (26) as a rule is very large for many tasks and the main problem lies in the correct calculation of this integral. However, in the representation of (26) configurations of spin chains that are not physically realizable obviously make a contribution. Moreover, the weight of these configurations is not known in general scenario and it is unclear how to define it. With this in mind and also taking into account the ergodicity of the spin glass in the above-mentioned sense, we can define the partition function as

$$Z_*(\beta; N_x) = \int\limits_{-\infty}^{0} \exp\big[\beta\varepsilon\big] F(\varepsilon; N_x) d\varepsilon, \tag{27}$$

where $F(\varepsilon; N_x)$ is the energy distribution function in nonideal ensemble of 1D SSCs with certain length N_x (see also definition (6)). Note that the partition function will be defined more precisely and comprehensively if the distribution function $F(\varepsilon; N_x)$ is replaced by the new distribution function $F(\varepsilon; \mathbf{p}; N_x)$, where $\mathbf{p}$ is spin-chain three-climensional vector of polarization and the integration in (27) is performed on space $(\varepsilon; \mathbf{p})$.

Now we can define the Helmholtz free energy for ensemble of 1D SSCs in two different ways. Using standard definition for Helmholtz free energy, we can write

$$Q(\beta; N_x) = -\frac{1}{N_x \beta} \ln\big[Z(\beta; N_x)\big], \quad Q_*(\beta; N_x) = -\frac{1}{N_x \beta} \ln\big[Z_*(\beta; N_x)\big]. \tag{28}$$

Note that the dependence on N_x of the expressions in (28) arises due to the finite layer width. In particular, using the expression of partition function (26), we can find the average value of free energy coming on one spin in the chain (see also [22]):

$$Q(\beta; N_x) = -\frac{1}{N_x \beta} \left\langle \sum_{i=0}^{N_x - 1} \ln \left[\frac{\sinh x_i}{x_i} \right] \right\rangle, \quad x_i = J_{i\, i+1} \beta, \tag{29}$$

where $\langle \ldots \rangle$ designates averaging by 1D SSCs ensemble. Now the main problem is the investigation of behavior of free energy subject to the parameter β. Correspondingly, we can define two forms of free energy derivatives:

$$q(\beta; N_x) = \frac{\partial Q(\beta; N_x)}{\partial \beta} = \frac{1}{N_x \beta^2} \left\langle \sum_{i=0}^{N_x - 1} \left\{ 1 + \ln \left[\frac{\sinh x_i}{x_i} \right] - x_i \coth x_i \right\} \right\rangle,$$

$$q_*(\beta; N_x) = \frac{\partial Q_*(\beta; N_x)}{\partial \beta} = \frac{1}{N_x \beta} \left\{ \frac{1}{\beta} \ln Z_*(\beta; N_x) - \frac{Z_{*;\,\beta}(\beta; N_x)}{Z_*(\beta; N_x)} \right\}, \tag{30}$$

where $Z_{*;\,\beta}(\beta; N_x) = \partial Z_*(\beta; N_x)/\partial \beta$.

6. CONCLUSION

A new parallel algorithm is developed for the simulation of the classical 3D spin glasses. It is shown that 3D spin glasses can be investigated with the help of an auxiliary Heisenberg Hamiltonian (1). The system of recurrent transcendental equations (3) and Silvester conditions (4) are obtained by using this Hamiltonian. Let us note that exactly similar equations of stationary points (3) can also be obtained if the full 3D Hamiltonian (see the first unnumbered formula) is used in the framework of short-range interaction model. That allows us to construct step by step a spin chain of the specified length with taking into account the random surroundings. It is proved that in the limit of Birkhoff's ergodic hypothesis performance, 3D spin glass can be generated by Hamiltonian of disordered 1D SSC with random environment. We have proved that it is always possible to construct a spin chain in any given random environment which will be in ground-state energy (direct problem). We have also proved the inverse problem, namely, every spin chain of the random environment can be surrounded by an environment so that it will be the solution in the ground state. In the work, all the necessary numerical data were obtained by way of a large number of parallel simulations of the auxiliary problem in order to construct all the statistical parameters of 3D spin glass in the limit of ergodicity of 1D SSCs nonideal ensemble. As numerical simulations show, the distributions of all statistical parameters become stable after $\propto N_x^2$ independent calculations which are realized in parallel. The idea of 1D

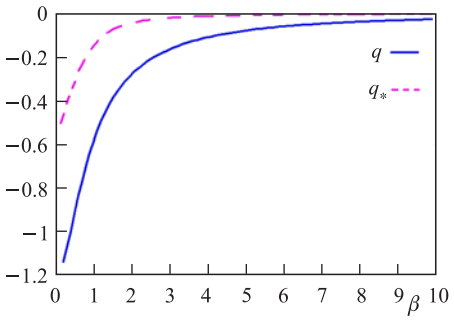

Fig. 8. Two derivatives of Helmholtz's free energy shown depending on reverse temperature β, which have been calculated by formulas (30) after 10^6 simulations. The figure shows that at low temperatures the curves approach each other which is rather natural, resulting from the decrease of the system's entropy

spin chains parallel simulations, based on this simple and clear logic, greatly simplifies the calculations of 3D spin glasses which are still considered as a subset of difficult simulation problems. Let us note that computation of spin–spin interactions distribution function from the first principles of the classical mechanics is a very important result of this work. Analysis shows that the distribution is not an analytic function. It is from the class of Lévy functions which does not have variance $\overline{J^2}$ and mean value $\bar{J}$.

Despite the absence of calculations by other methods, it is obvious that the developed scheme of calculations should differ from other algorithms, including the algorithms which are based on Monte Carlo simulation method [23], in the accuracy and efficiency. We were once again convinced in the accuracy and efficiency of the algorithm after analyzing the results of different numerical experiments by modeling the statistical parameters of 3D spin-glass system which are presented in Figs. 5, *a, b* and 6.

In the work a new way of partition function construction (configuration integral) is proposed in the form of one-dimensional integral of the energy distribution, which unlike the usual definitions does not include physically unrealizable spin chains configurations (see the difference of free energy derivatives on Fig. 8). It is obvious that the new definition of partition function is more correct and in addition it is very simple for computation.

Finally, the developed method can be generalized for the cases of external fields which will allow us to investigate a large number of dynamical problems including critical properties of 3D classical spin glasses.

Acknowledgements. The work is partially supported by RFBR grants 10-01-00467-a, 11-01-0027-a.

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Received on June 23, 2011.

Редактор *Е. И. Кравченко*

Подписано в печать 13.07.2011.
Формат 60 × 90/16. Бумага офсетная. Печать офсетная.
Усл. печ. л. 1,43. Уч.-изд. л. 1,93. Тираж 270 экз. Заказ № 57372.

Издательский отдел Объединенного института ядерных исследований
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