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On Modeling of Statistical Properties of Classical 3D Spin Glasses

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The 3D spin glass is represented as an ensemble of disordered 1D spatial spin-chains (SSC) where interactions are random between spin-chains. It is proved that at 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 construct 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.

Key words and phrases: random 3D networks, 3D regular lattice, spin glass Hamiltonian, ergodic hypothesis, statistic distributions, parallel simulation.

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 mentioned investigations as a rule conduct at equilibrium's conditions of medium. This fact plays a key role both in 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 fields 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 glass system 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.

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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 the structure of this type compound can be well described by $3D$ random network [7]. As shown [17] compounds of this type can be represented as a disordered $3D$ system of similar rigid dipoles (hereinafter will be termed a $3D$ disordered spin system).

The Hamiltonian of 3D classical spin glass system reads:

$$H(\{\mathbf{r}\}) = -\sum_{\langle i\,j\rangle} J_{i\,j}\boldsymbol{S}_i\boldsymbol{S}_j, \quad \{\mathbf{r}\} \equiv \mathbf{r}_1, \mathbf{r}_2, ...$$

where indices i and j run over all nodes of 3D lattice, $\mathbf{r}_i$ correspondingly denotes the coordinates of i-th spin. For further investigation we will consider a spin glass layer of certain width L_x and infinite length (see Fig. 1). We will consider 3D compound in the framework of nearest-neighboring Hamiltonian model. Let us note that even for this relatively simplest model numerical simulations of spin glasses are extremely hard to solve NP problems.

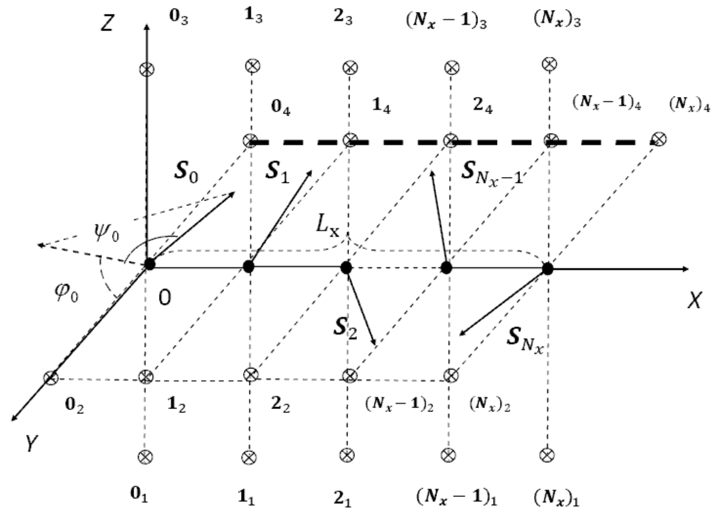

Figure 1. **1D SSC with the random environment. Recall that each spin-chain is surrounded by four spin-chains which are randomly interacted with it. By symbols $\otimes$ are designated spins from the random environment (four spin-chains of surrounding)**

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 $H_0^{(1)}(\{\mathbf{r}\};\, N_x) = -\sum\limits_{i=0}^{N_x-1} J_{i\,i+1}\boldsymbol{S}_i\boldsymbol{S}_{i+1}$, describes the disordered 1D *spatial spins chain* (SSC) while the second term $H_0^{(2)}(\{\mathbf{r}\};\, N_x) = -\sum\limits_{i=0}^{N_x-1}\sum\limits_{\sigma=1}^{4} J_{i\,i_\sigma}\boldsymbol{S}_i\boldsymbol{S}_{i_\sigma}$, 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, $\boldsymbol{S}_i$, $\boldsymbol{S}_{i+1}$ and $\boldsymbol{S}_{i_\sigma}$ are spins (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. 1). 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.

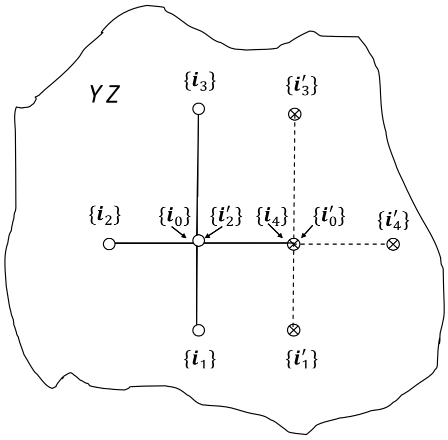

Figure 2. **The projection of spin-chains ensemble on the (Y, Z) plane. Spin-chains are designated by symbols $\bigcirc$ and $\bigotimes$ which correspondingly form the old and new environments**

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

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

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:

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

where $\Theta_i=(\psi_i,\varphi_i)$ defines the orientation of i-th spin (ψ_i,φ_i are correspondingly the polar and the azimuthal angles). In addition, $\mathbf{\Theta}=(\Theta_1,\Theta_2....\Theta_{N_x})$ describes the angular configuration of spin-chain consisting of N_x spins.

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

$$\sum_{\alpha=-1,\,\alpha\neq0}^{1} J_{i+\alpha\,i}\left[-\tan\psi_i\cos\psi_{i+\alpha}\cos(\varphi_i-\varphi_{i+\alpha})+\sin\psi_{i+\alpha}\right]+$$

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

$$\sum_{\alpha=-1,\,\alpha\neq 0}^{1} J_{i+\alpha\,i}\,\cos\psi_{i+\alpha}\sin(\varphi_i-\varphi_{i+\alpha})+\sum_{\sigma=1}^{4} J_{i\,i_\sigma}\cos\psi_{i_\sigma}\sin(\varphi_i-\varphi_{i_\sigma})=0. \qquad (4)$$

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

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

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:

$$A_{\psi_i\psi_i}(\Theta_i^0)=\sum_{\alpha=-1,\,\alpha\neq 0}^{1} J_{i+\alpha\,i}\Big\{\cos\psi_i^0\cos\psi_{i+\alpha}\cos(\varphi_i^0-\varphi_{i+\alpha})+\sin\psi_i^0\sin\psi_{i+\alpha}\Big\}+$$
$$+\sum_{\sigma=1}^{4} J_{i\,i_\sigma}\Big\{\cos\psi_i^0\cos\psi_{i_\sigma}\cos(\varphi_i^0-\varphi_{i_\sigma})+\sin\psi_i^0\sin\psi_{i_\sigma}\Big\},$$

$$A_{\varphi_i\varphi_i}(\Theta_i^0)=\sum_{\alpha=-1,\,\alpha\neq 0}^{1}\Big\{J_{i+\alpha\,i}\cos\psi_{i+\alpha}\cos(\varphi_i^0-\varphi_{i+\alpha})+$$
$$+\sum_{\sigma=1}^{4} J_{i\,i_\sigma}\cos\psi_{i_\sigma}\cos(\varphi_i^0-\varphi_{i_\sigma})\Big\}\cos\psi_i^0,$$

$$A_{\psi_i\varphi_i}(\Theta_i^0)=0.$$

Recall that $\Theta_i^0=(\psi_i^0,\varphi_i^0)$ designates the angular configuration for which conditions of local minimum are satisfied.

Thus, it is obvious that the classical 3D spin glass system can be considered as an nonideal ensemble of 1D SSCs (see Fig. 1) where interactions between spin-chains are random.

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 $0>\varepsilon_0>...>\varepsilon_n$, 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 $M_{L_x}^{full}=\sum_{j=1}^{n} M_{L_x}(\varepsilon_j)$. Accordingly, the energy distribution function can be defined by the expression:

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

where distribution function is normalized to unit:

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

By similar way we can construct also 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 told, the significance of new mathematical approaches development is obvious and on the basis of which an effective parallel algorithms for numerical simulation of spin glasses can be elaborated.

Theorem. *The classical 3D spin glass in the limit of isotropy and homogeneity (ergodicity) of superspins (sum of spins of chain) in statistical sense is equivalent to the problem of nonideal 1D SSCs ensemble.*

It is obvious that the theorem will be proved if we can prove that in case when 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), and
b) it is possible to surround an arbitrary spin-chain from the given environment with such new environment which can make it physically admissible spin-chain solution (the reverse problem).

The direct Problem. Using the following notation:

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

equations system (6) can be transformed to the following form:

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

where parameters C_1 and C_2 are defined by expressions:

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

$$C_2 = J_{i-1\,i}\cos\psi_{i-1}\sin(\varphi_i - \varphi_{i-1}) + \sum_{\sigma=1}^{4} J_{i\,i_\sigma}\cos\psi_{i_\sigma}\sin(\varphi_i - \varphi_{i_\sigma}).$$

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 the equation (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

$$A = C_2^2\Big\{J_{i\,i+1}^2\cos^2\psi_i + C_3 + 2C_1^2\sin^2\psi_i\Big[1 \pm C_1^{-1}\sqrt{J_{i\,i+1}^2 - C_1^2 - C_2^2}\,\cot\psi_i\Big]\Big\},$$

$$C_3 = -C_1^2 + C_2^2\sin^2\psi_i, \quad B = J_{i\,i+1}^4\cos^4\psi_i + 2C_3J_{i\,i+1}^2\cos^2\psi_i + (C_1^2 + C_2^2\sin^2\psi_i)^2,$$

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 following conditions: $0 \leqslant \xi_{i+1}^2 \leqslant 1$, $0 \leqslant \eta_{i+1}^2 \leqslant 1$. As it follows from equations (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 Silvester conditions (5) which can be written in the form of the following inequalities:

$$\begin{gathered} J_{i\,i+1}\cos\psi_i^0\cos\psi_{i+1}\cos(\varphi_i^0-\varphi_{i+1}) > -a_1 - \sin\psi_i^0\sin\psi_{i+1}, \\ J_{i\,i+1}\cos\psi_{i+1}\cos(\varphi_i^0-\varphi_{i+1})\cos\psi_i^0 > -a_2, \end{gathered} \tag{12}$$

where constants a_1 and a_2 are defined by expressions:

$$a_1 = J_{i-1\,i}\Big[\cos\psi_i^0\cos\psi_{i-1}\cos(\varphi_i^0-\varphi_{i-1}) + \sin\psi_i^0\sin\psi_{i-1}\Big] + \\ + \sum_{\sigma=1}^{4} J_{i\,i_\sigma}\Big[\cos\psi_i^0\cos\psi_{i_\sigma}\cos(\varphi_i^0-\varphi_{i_\sigma}) + \sin\psi_i^0\sin\psi_{i_\sigma}\Big],$$

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

So, the problem leads to the answer of the following question - are inequality (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 of the following. We choose a spin-chain from the environment (see Fig. 1), for example $\{i_4\} \equiv (0_4, 1_4, ..., N_{x4})$. In this spin-chain all angular configurations of spins $(\Theta_0^{(4)}, ...\Theta_{N_x}^{(4)})$ 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 such environment 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 $\{i_4\} \equiv \{i_0^{'}\}$ 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. 1). 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 $\big(\{i_0^{'}\}, \{i_1^{'}\}, \{i_2^{'}\}, \{i_3^{'}\}, \{i_4^{'}\}\big) \to \big(\{i_0\}, \{i_1\}\{i_2\}, \{i_3\}, \{i_4\}\big)$. The proof of the proposition should be conducted as follows. We will suppose that the constants of spin-spin interactions in considered chain and 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:

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

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

Using (13) we can transform equations (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:

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

After excluding $J_{i\,i+1}$ from (14) we find the following equation:

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

$$
\left. -\frac{J_{i\,i_\sigma}}{c_4}\cos\psi_{i_\sigma}\sin(\varphi_i-\varphi_{i_\sigma})\right\} - c_5 = 0, \qquad c_5 = \frac{c_1}{c_2}-\frac{c_3}{c_4}. \tag{15}
$$

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 equation (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: $x=\cos\psi_{i_3}$, in (16) we find the equation:

$$
D + \frac{J_{i\,i_3}}{c_2}[-x\sin\psi_i\cos(\varphi_i-\varphi_{i_3})+\sqrt{1-x^2}\,\cos\psi_i] - x\frac{J_{i\,i_3}}{c_4}\sin(\varphi_i-\varphi_{i_3}) = 0, \tag{17}
$$

From (17) the following square equation can be found :

$$
K_0x^2 + 2K_1x + K_2 = 0, \tag{18}
$$

where the following designations are made:

$$K_0 = \cos^2\psi_i + \Big(\sin\psi_i \cos(\varphi_i - \varphi_{i_3}) + \frac{c_2}{c_4}\sin(\varphi_i - \varphi_{i_3})\Big)^2,$$

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

Discriminant of the square equation (18) has the form:

$$D_x = \Big(\sin\psi_i \cos(\varphi_i - \varphi_{i_3}) + \frac{c_2}{c_4}\sin(\varphi_i - \varphi_{i_3})\Big)^2 \cos^2\psi_i + \\ + \left\{\cos^2\psi_i - \left(\frac{Dc_2}{J_{i\,i_3}}\right)^2\right\}\cos^2\psi_i \geqslant 0, \quad (19)$$

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

Let us define:

$$y = \cos(\varphi_i - \varphi_{i_3}), \quad (20)$$

Substituting (20) in (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:

$$M_0 y^2 + 2M_1 y + M_2 = 0, \quad (21)$$

where the following designations are made:

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

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

The discriminant of the square equation (21) has the form:

$$D_y = \Big(\frac{c_2}{c_4}\Big)^2\cos^2\psi_i + \sin^2\psi_i\cos^2\psi_{i_3} - \Big(\frac{Dc_2}{J_{i\,i_3}} + \cos\psi_i\sin\psi_{i_3}\Big)^2 \geqslant 0. \quad (22)$$

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:

$$-\Big|\frac{Dc_2}{\cos\psi_i}\Big| \geqslant J_{i\,i_3} \geqslant \Big|\frac{Dc_2}{\cos\psi_i}\Big|, \quad (23)$$

discriminant D_x is always nonnegative. From the other side:

$$\sin\psi_{i_3} \cong -\frac{Dc_2}{J_{i\,i_3}\cos\psi_i}, \quad (24)$$

which will assure that D_y discriminant is always nonnegative. A simple analysis of conditions (23) and (24) 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 by this way fill up 3D space by 1D SSC which is equivalent to obtaining 3D spin glass. In case 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 identic.

The theorem is proved.

4. 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 and 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. 3).

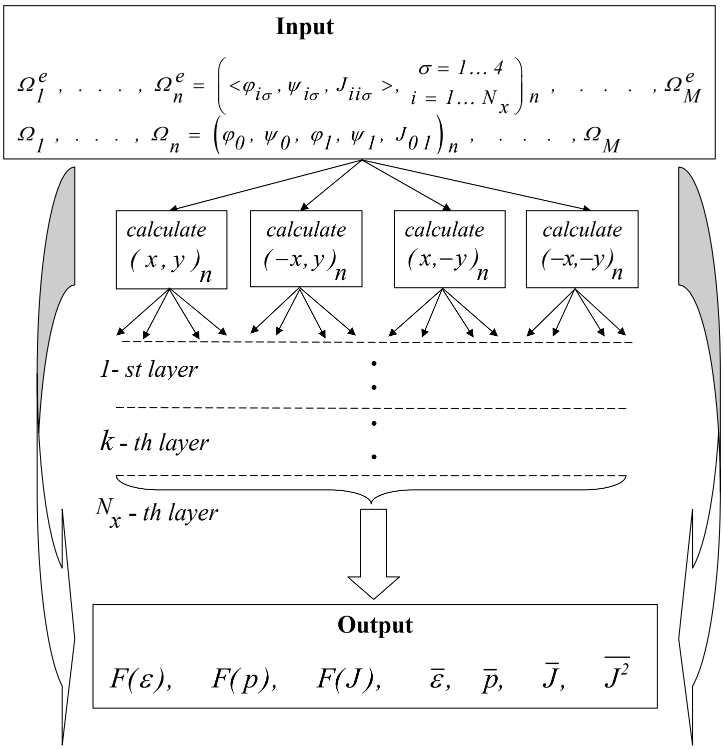

Figure 3. **The algorithm of parallel simulation of statistical parameters of disordered $1D$ SSCs nonideal ensemble. The symbol Ω_n^e describes the input of environment, M is a number of simulation or overall number of spin-chains in the nonideal ensemble, N_x is a number of spins in chain**

At first, the angular configurations of four spin-chains are randomly generated which form random environment of the spin-chain which 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 the same way as it is described in [18]. Now when the environment and its influence on disordered 1D SSC are defined, we can go over to the computation of spin-chain which must satisfy the condition of local energy minimum. Note that all calculations of 1D SSCs nonideal ensemble are done for spin-chains with 10^3 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 and the energy distribution $F(\varepsilon)$ has one global maximum which is precisely approximated by Gaussian distribution (see Fig. 4).

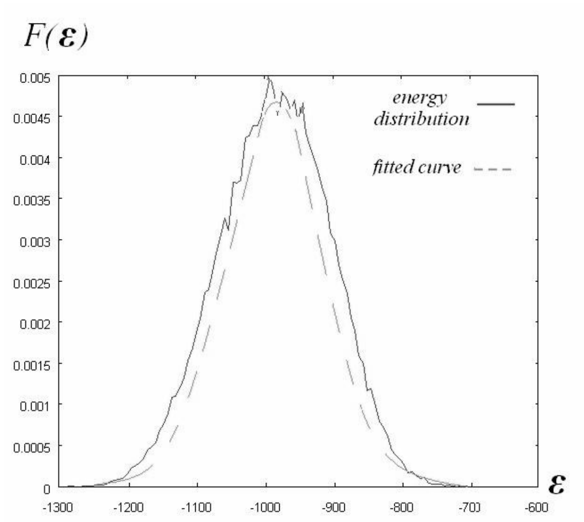

Figure 4. **The energy distribution of $1D$ nonideal ensemble of SSCs with 10^3 length is shown. The numerical data visualization and its fitted curve (by Gaussian function) are illustrated on the figure**

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

$$\bar{p} = \int\limits_{-\infty}^{+\infty} F(p)p dp, \quad p = (p_x, p_y, p_z), \quad \bar{\varepsilon} = \int\limits_{-\infty}^{0} F(\varepsilon)\varepsilon d\varepsilon$$

and F is the distribution function. As our numerical investigations have shown on the example of systems where thickness of spin glass layer is not so large $\propto 25 \div 100$, 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 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). It essentially differs from the normal Gaussian distribution model and can be approximated precisely by Lévy skew alpha-stable distribution function [19, 20]).

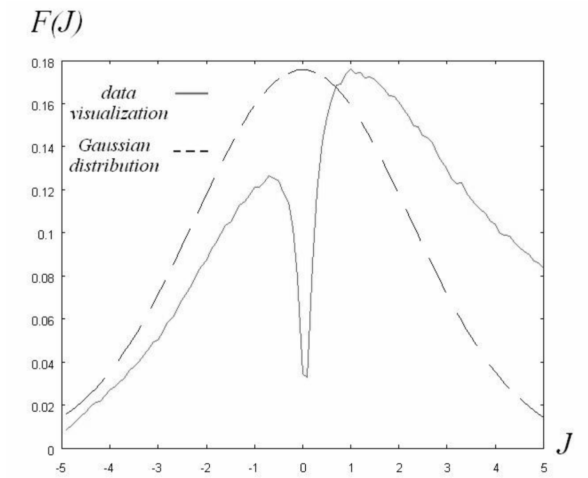

Figure 5. **The visualization of numerical data of spin-spin interaction constants and Gaussian distribution are shown. The analysis of the numerical data proves, that interaction distribution is not analytic function and by the character is the Lév's skew α-stabile distribution function**

5. 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 by 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) also can 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 step by step construct spin-chain of the specified length with taking into account the random surroundings. It is proved that at 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 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 large number of parallel simulations of the auxiliary problem in order to construct all statistical parameters of 3D spin glass at 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 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 principals of the classical mechanics is very important result of this work. As analysis show, 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 [21], by 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 figures 4 and 5.

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

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О моделировании статистических свойств классических 3D спин-стёкол

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Исследуются статистические свойства классического 3D спин-стекольного слоя определённой 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 Биргофа 3D спин-стекло может быть генерировано вспомогательным гамильтонианом неупорядоченной 1D ПСЦ со случайным окружением. Неупорядоченный 1D ПСЦ определяется на регулярной решётке, где в каждом узле решётки помещается один случайно ориентированный спин. Также предполагается, что каждый спин случайно взаимодействует с шестью ближайшими соседними спинами (два спина на решётке и четыре в окружении). В узлах решётки спин цепочки получены рекурентные трансцендентные уравнения. Эти уравнения совместно с условиями Сильвестра позволяют шаг за шагом построить спин-цепочку в основном состояни энергии, где все спины находятся в минимальной энергии классического гамильтониана. На основе этих уравнений разработан оригинальный высокопроизводительный параллельный алгоритм для моделирования 3D спинового стекла.

Ключевые слова: 3D случайная сеть, 3D регулярная решетка, гамильтониан спинового стекла, эргодическая гипотеза, статистические распределения, параллельное моделирование.