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NEW ALGORITHM FOR SIMULATION OF 3D CLASSICAL SPIN GLASSES UNDER THE INFLUENCE OF EXTERNAL ELECTROMAGNETIC FIELDS

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We study statistical properties of 3D classical spin glass under the influence of external fields. It is proved that in the framework of the nearest-neighboring model, 3D spin-glass problem at performing of Birkhoff's ergodic hypothesis regarding to orientations of spins in 3D space, can be reduced to the problem of disordered 1D spatial spin-chains (SSC) ensemble, where each spin chain interacts with a random environment. The 1D SSC is defined as a periodic 1D lattice, where spins in nodes are randomly oriented in 3D space, in addition, they all interact with each other randomly. For minimization of the Hamiltonian in an arbitrary node of 1D lattice the recurrent equations and corresponding Sylvester's criterion are obtained, which allow one to find energy local minimum. On the basis of these equations, the high-performance parallel algorithm is developed, which allows one to calculate all statistical parameters of 3D spin glass, including distribution of a constant of spin–spin interaction, from the first principles of the classical mechanics.

Изучаются статистические свойства 3D классического спинового стекла, находящегося под воздействием внешних полей. Доказано, что в рамках модели ближайших соседей задача 3D спинового стекла, при выполнении эргодической гипотезы Биркгофа относительно ориентации спинов в 3D-пространстве, может быть сведена к проблеме ансамбля неупорядоченных 1D пространственных спин-цепочек (ПСЦ), где каждая спиновая цепочка взаимодействует со случайным окружением. 1D ПСЦ определяется как периодическая 1D-решетка, где спины в узлах в 3D-пространстве ориентированы случайным образом, кроме того, все они взаимодействуют друг с другом случайным образом. Для минимизации гамильтониана в произвольном узле 1D-решетки получены рекуррентные уравнения и соответствующие критерии Сильвестра, которые позволяют найти локальный минимум энергии. На основе этих уравнений развит высокопроизводительный параллельный алгоритм, который позволяет рассчитать все статистические параметры 3D спинового стекла, в том числе распределение константы спин-спинового взаимодействия, исходя из первых принципов классической механики.

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INTRODUCTION

Spin glasses and in general disordered spin systems as models are often used for study of different complex natural and social phenomena in the fields as diverse as physics, chemistry, theoretical computer science (combinatorial optimization, traveling salesman, material science), biology (Hopfield model), population genetics (hierarchical coalescence), nanoscience, evolution, organization dynamics, human logic systems, economy (modeling of financial markets), etc. [1–11, 13].

There are different theoretical and numerical methods to study spin glasses and disordered spin systems in general. In all these approaches, the main object of investigation is a partition function in its standard Gibbs' representation. One of the important directions of investigation of partition function is the mean-field method. They, as a rule, are divided into two types. The first consists of the true random-bond models, where the coupling between interacting spins is taken to be independent random variables [12, 14, 15]. The solution of these models is obtained by n-replica trick [12, 15] and has required the invention of sophisticated schemes of replica-symmetry breaking [15, 16]. In the models of the second type, the bond-randomness is expressed in terms of some underlining hidden site-randomness and, thus, has superficial nature. It has been pointed out in works [17–19], however, that this feature retains an important physical aspect of true spin glasses, viz., they are random with respect to the positions of magnetic impurities.

The problem of 3D spin-glass simulation is a typical NP hard problem. Nevertheless, solution of the problem becomes more difficult and even problematic when spin glasses are in states far from thermodynamic equilibrium. In this case, standard methods based on the Monte Carlo simulations are, as a rule, not suitable for using.

In this paper, we study statistical properties of spin glasses at conditions when the time of an influence of external fields is much less of the characteristic relaxation times of a medium, but much more of the response time of individual spins. The last means that we have a typical example when medium is in the nonequilibrium state, which is impossible to study using a standard representation of partition function, defined in the framework of Gibbs' hypothesis. In conjunction with this, the importance of development of new approaches and corresponding parallel algorithms for solving problems of 3D spin glasses in external field is obvious.

1. FORMULATION OF THE PROBLEM

The 3D spin-glass system (the width of the layer is defined by the length of spin chain, which includes N_x spins) in the framework of the nearest-neighboring model can be represented by Hamiltonian:

$$H(N_x) = H^{(1)}(N_x) + H^{(2)}(N_x), \tag{1}$$

where the first term

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

describes the disordered 1D spatial spin chains (SSC) (below we will name the central spin chain). The second term

$$H^{(2)}(N_x) = -\sum_{i=1}^{N_x} \mathbf{U}_i \mathbf{S}_i, \quad \mathbf{U}_i = \sum_{i_\sigma=1}^{4} J_{ii_\sigma} \mathbf{S}_{i_\sigma} + \mathbf{h}_i$$

describes a random environment of the central 1D SSC (see Fig. 1) and the external field $\mathbf{h}_i$. Note, that $||\mathbf{h}_i|| = h_i = h_0 \cos(i2\pi/N_x)$ designates an external field, which is propagated by direction of x-axis, h_0 is its amplitude and N_x is the number of spins in standing wave formed by external field. In (1), J_{ii+1} and J_{ii_σ} are random interaction constants between arbitrary i and $i+1$ spins and between i and i_σ spins, correspondingly, $\mathbf{S}_i, \mathbf{S}_{i+1}$ and $\mathbf{S}_{i_\sigma}$ are spins (vectors) of the unit length $||\mathbf{S}_i|| = 1$, which in $\mathrm{O}(3)$ space are orientated randomly. Ambient vectors, for fixed σ and $i = 1, 2, \ldots, N_x$ are spin chains in state of energy local minimum, thus, they have their own inter-spin interaction constants $J^{\sigma}_{i,i+1}$. The main aim of our study is development of a theoretical approach and the relevant algorithm, which will allow one to compute exactly all statistical parameters of classical 3D spin glass, including the distribution of spin–spin interactions' constant, at influence of external fields. Based on general physical considerations, we need to construct such spin configurations, where each spin in chain will be in a state of a local energy minimum that obviously will provide a quasistability of a spin chain. Given that each spin is represented by three projections, $\mathbf{S}_i = (x_i, y_i, z_i)$, then we can find equations, which define the condition of an extremum of Hamiltonian (1) in the ith node:

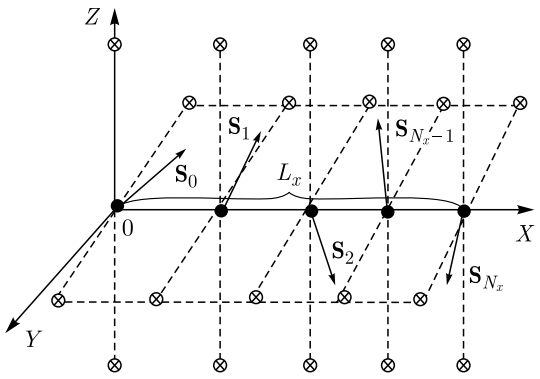

Fig. 1. The 1D SSC with the random environment. The random environment consists of spins denoted by ⊗ symbols

$$\frac{\partial H}{\partial x_i} = 0, \quad \frac{\partial H}{\partial y_i} = 0. \tag{2}$$

Recall that equation $\partial H/\partial z_i = 0$ is not considered, since it is linearly dependent on the previous two equations due to the fact that the length of a spin is a constant and equals to unit.

Theorem. *The Hamiltonian (1) is a solution of Eqs. (2) and it has an extremum in the ith node, if the spin in the $(i+1)$th node has the form*

$$\mathbf{S}_{i+1} = -\frac{J_{i-1,i}\mathbf{S}_{i-1} + \mathbf{U}_i}{J_{i,i+1}} + \\ + \mathbf{S}_i \left\{ \frac{(J_{i-1,i}\mathbf{S}_{i-1} + \mathbf{U}_i)\mathbf{S}_i}{J_{i,i+1}} \pm \frac{\sqrt{J^2_{i,i+1} - ||\mathbf{S}_i \times (J_{i-1,i}\mathbf{S}_{i-1} + \mathbf{U}_i)||^2}}{J_{i,i+1}} \right\}, \tag{3}$$

where the constant of spin–spin coupling satisfies the inequality

$$J_{i,i+1}^2 \geqslant ||\mathbf{S}_i \times (J_{i-1,i}\mathbf{S}_{i-1} + \mathbf{U}_i)||^2 = A_i^2. \tag{4}$$

The energy of Hamiltonian in the ith node will be minimal, if the following inequalities are satisfied:

$$A_{x_i x_i} > 0, \quad A_{x_i x_i} A_{y_i y_i} - A_{x_i y_i}^2 > 0, \tag{5}$$

where $A_{\eta_i \eta_i} = \partial^2 H / \partial \eta_i^2$ and $A_{x_i y_i} = \partial^2 H / (\partial x_i \partial y_i)$.

Now, we can calculate the second derivatives of Hamiltonian:

$$A_{\eta_i \eta_i} = \left(\eta_i^2 + z_i^2\right)\delta_i, \quad A_{x_i y_i} = x_i y_i \delta_i, \tag{6}$$

where $\delta_i = \left(z_{i-1}J_{i-1,i} + z_{i+1}J_{i,i+1} + u_i^z\right) z_i^{-3}$, and u_i^z is the projection of vector $\mathbf{U}_i$ on z-axis. Using (6), explicit forms of inequalities (5) can be easily found:

$$A_{x_i x_i} = \left(x_i^2 + z_i^2\right)\delta_i \geqslant 0, \quad A_{x_i x_i} A_{y_i y_i} - A_{x_i y_i}^2 = z_i^2 \delta_i^2 \geqslant 0. \tag{7}$$

As can be seen, the second inequality of (7) is always satisfied. Finally, taking into account (4), the conditions of local minimum of Hamiltonian (1) in the ith node can be written in the form

$$\delta_i \geqslant 0, \quad |J_{i,i+1}| \geqslant A_i. \tag{8}$$

In our previous work [20], it was shown that the unperturbed by external fields 3D spin glass at condition when in the reciprocal lattice regarding of directions of spins is implemented conditions for using of Birkhoff's ergodic hypothesis, the initial problem can be reduced to the problem of a nonideal ensemble of 1D SSC. Recall that, when we say that the ensemble is nonideal, we mean that 1D spin chain interacts with its random environment consisting of four disordered 1D spin chains. As analysis shows, at switching of weak external fields, the possibility of the reduction of 3D spin-glass problem to that of nonideal ensemble of 1D spin chains remains valid. In a nonideal ensemble, each classical spin chain is characterized by two parameters — energy and magnetization. The last means that many important properties of statistical ensemble can be studied in the space of an energy ε and magnetization $\mathbf{p}$, equivalently constructing the distribution function for an energy and magnetization of nonideal ensemble.

Thus, the main problem is concluded in a solution of direct problem, namely, the numerical simulation of the nonideal ensemble of disordered 1D SSC.

Now, we have to construct the distribution function of an energy and magnetization of the nonideal ensemble. In this connection, it is useful to divide axis of an energy ε and magnetization $\mathbf{p}$ into small regions $0 > \varepsilon_0 > \ldots > \varepsilon_n$, $(0 > p_{0;x} > \ldots > p_{n;x})$, $(0 > p_{0;y} > \ldots > p_{n;yx})$, and $(0 > p_{0;z} > \ldots > p_{n;z})$, where $n \gg 1$. The number of stable 1D SSC configurations with the length L_x in the range of energy $[\varepsilon - \delta\varepsilon, \varepsilon + \delta\varepsilon]$, where $|\delta\varepsilon| \ll 1$, and polarization range $[p_x - \delta p_x, p_x + \delta p_x]$, $|\delta p_x| \ll 1$, $[p_y - \delta p_y, p_y + \delta p_y]$, $|\delta p_y| \ll 1$ and $[p_z - \delta p_z, p_z + \delta p_z]$, $|\delta p_z| \ll 1$, will be denoted by $M_{L_x}(\varepsilon)$, while the number of all stable 1D SSC configurations — correspondingly, by symbol $M_{L_x}^{\text{full}} = \sum\limits_{i,j=1}^{n} M_{L_x}(\varepsilon_i, \mathbf{p}_j)$. Accordingly, the multidimensional distribution function of nonideal ensemble 1D SSC may be defined by the following formula:

$$F_{L_x}(\varepsilon, \mathbf{p}; g) = \frac{M_{L_x}(\varepsilon, \mathbf{p}; g)}{M_{L_x}^{\text{full}}}, \tag{9}$$

where the distribution function is normalized to unit

$$\lim_{n\to\infty}\sum_{i,j=1}^{n} F_{L_x}(\varepsilon_i,\mathbf{p}_j;g)\,\delta\varepsilon_j\,\delta\mathbf{p}_j=\int d^3\mathbf{p}\int\limits_{-\infty}^{0} F_{L_x}(\varepsilon,\mathbf{p};g)\,d\varepsilon=1, \tag{10}$$

where $\delta\mathbf{p}_j=\delta p_{j;x}\delta p_{j;y}\delta p_{j;z}$, and g denotes a set of external field's parameters.

2. SIMULATION ALGORITHM

The strategy of numerical simulation for one spin chain is the following. At first, we randomly generate initial spin configuration, which consists of four pairs of ambient vectors and interaction constants ($\mathbf{S}_{1_\sigma}$, $\mathbf{S}_{2_\sigma}$ and $J^{\sigma}_{1,2}$, $\sigma=1,\ldots,4$), one pair of SSC spin vectors and interaction constant ($\mathbf{S}_1$, $\mathbf{S}_2$ and $J_{1,2}$). Recall that previously the interaction constants in the case of unperturbed by external fields 3D spin glass [20] are generated by log-normal

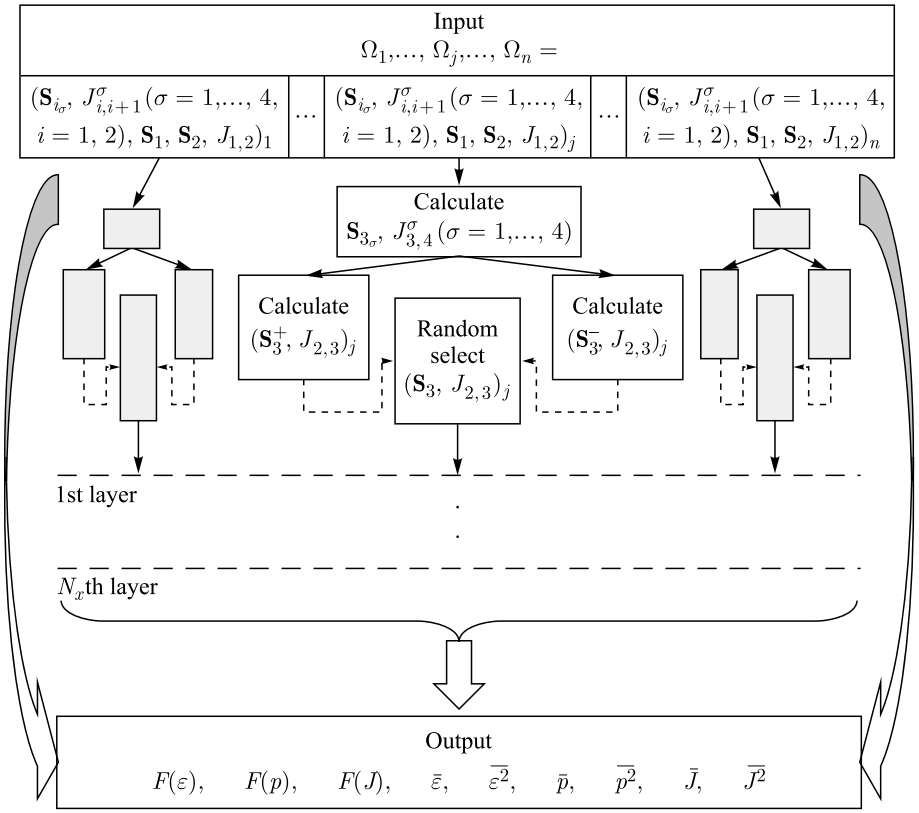

Fig. 2. The algorithm of parallel simulation of statistical parameters of a nonideal ensemble of disordered 1D SSC

distribution, while for the case when 3D spin glass is under the influence of external fields, spin–spin interaction constants are generated by normal distribution. Now, when the initial configuration is defined, we can go over to the computation of spin chain under the influence of external fields, which must satisfy conditions of local energy minimum (8). At first, ambient spin-chains next node is computed as 1D SSC using (3) and taking into consideration that $U_i = 0$ and $h_0 = 0$, which also should satisfy condition (8). Now, when we have environment vectors, central spin's next node can be calculated. Note, that in calculation of each node (for both ambient spin chains and central spin chain), two solutions are found (see the scheme in Fig. 2, they are designated by symbols $+$ and $-$), however, at continuation of simulation of the spin chain we leave in each node only one solution, which is being randomly selected. This algorithm is being executed in parallel in order to compute desired amount of different spin chains. Finally, in the last stage of simulation with the help of formulas (9) and (10), we calculate distributions of corresponding parameters, which characterize statistical properties of 3D spin glass under the influence of external fields.

3. NUMERICAL EXPERIMENTS

Note, that calculations of 3D spin glass or, more correctly, a nonideal ensemble of 1D SSC, are done for spin chains having the length 100. This approach considerably reduces the amount of needed computations and gives us a possibility to solve a conceptually NP hard problem, such as, in particular, 3D spin-glass problem, and to construct all statistical parameters, which describe 3D spin glass. It is analytically proved and by parallel simulation is shown, that the distribution of a spin–spin interaction constant cannot be described by the normal Gaussian distribution model (the Gauss–Edwards–Anderson distribution) (see Fig. 3).

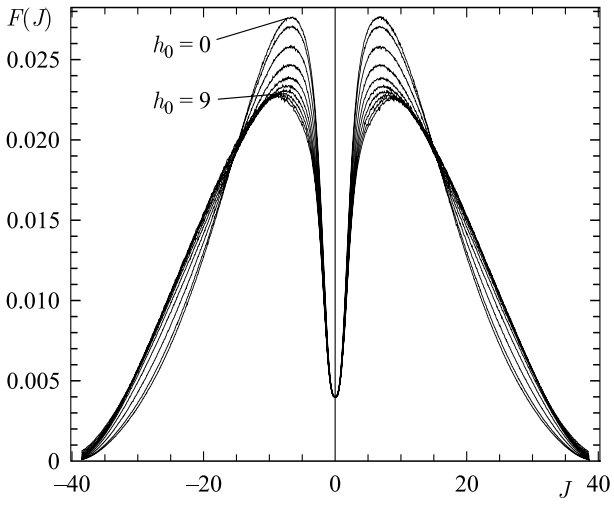

Fig. 3. Distribution of spin–spin interaction constant in a nonideal ensemble consisting of 1D spin chains with the length 100, depending on an external field

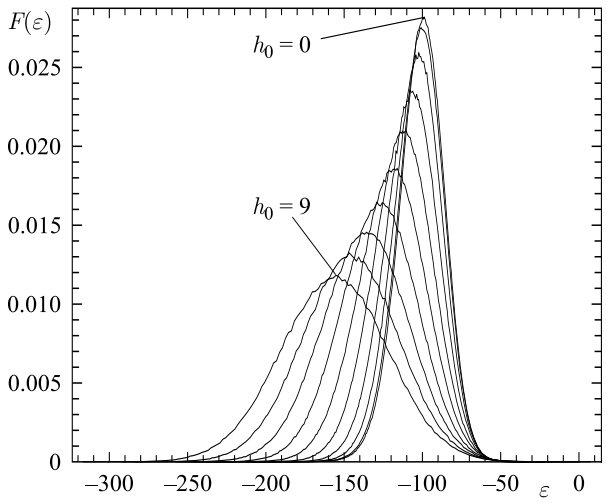

Fig. 4. The energy distributions in a nonideal ensemble depending on amplitude of an external field

As analysis shows, the curve of distribution is a nonanalytical function and probably it can be approximated precisely by the Lévy skew α-stable distribution function. As shown by calculations, at the increasing of the number of spin chains the ergodicity in a known sense comes already at $\propto N_x^2$. As we can see from Fig. 3, the distribution of a spin–spin interaction constant depends on an amplitude of the external field, however, its characteristic structure does not change. In the work, the energy distributions in a nonideal ensemble depending on an external field are also presented (see Fig. 4). As calculations show, for a nonideal ensemble consisting of 10000 spin chains, the dimensional effects practically disappear and the energy distributions $F(\varepsilon; g)$ have one global maximum (see Fig. 4). The maximum of distribution function at increasing of amplitude of an external field moves in area of lower negative values of energy. As to the magnetization distributions, as computation shows, at influence on media with the weak external field the distribution of magnetization in all coordinates frustrates. After procedure of averaging of magnetization by fractal structures [21], we find average values of magnetization on corresponding coordinates, depending on amplitude of an external field. As we can see at inclusion of an external field, a spin glass in all directions is magnetized, however, magnetization steadily goes up in direction of propagation of an external field, with increasing of amplitude of an external field (see Fig. 5).

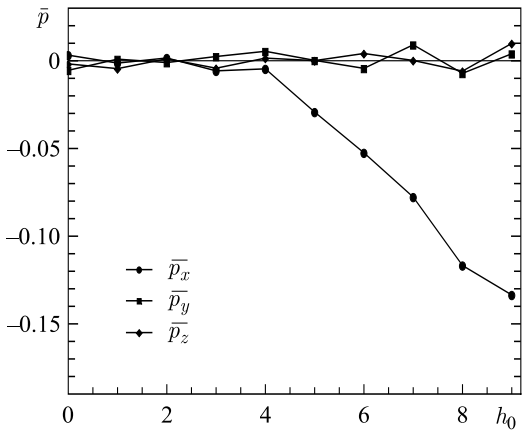

Fig. 5. The average value of polarization on corresponding coordinates depending on an external field

CONCLUSION

Using the proof about equivalence of models of 3D spin glass and nonideal ensemble 1D SSC, we have developed a new parallel algorithm for simulation of statistical properties of 3D spin glasses under the influence of external fields. The central idea based on numerical simulation is a method of construction of stable spin chains node by node with consideration of external random (random environment) and regular (external fields) influences. For realization of this idea we have used a model of the nearest-neighboring Hamiltonian of Heisenberg. The developed algorithm allows one on the basis of first principles of classical mechanics to calculate all statistical parameters of 3D spin glasses including the distribution of spin–spin interaction constant under external fields. An important peculiarity of the developed method is the possibility of exact simulation of 3D spin glasses including the situations when system is far from thermodynamic equilibrium, and we cannot use the well-known representations for the partition function, which are based on Gibbs's hypothesis. Let us note that the last is very important for investigation of properties of disordered spin systems on nanoscales of space-time, development of which is closely connected to development of modern technologies and in general of nanoscience. Finally, let us note that the program for numerical simulations of 3D spin glasses is created using the GPU technologies, which achieves high performance parallel calculations for the aforementioned problems.

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