Simulation of statistical parameters of 3D classical spin glasses at influence of external electromagnetic fields

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ABSTRACT

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 the 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 all they interact with each other randomly. For minimization of the Hamiltonian in an arbitrary node of the 1D lattice obtained recurrent equations and corresponding Sylvester's criterion, which allow to find energy local minimum. On the bases of these equations the high-performance parallel algorithm is developed which allows to calculate all statistical parameters of 3D spin glass, including distribution of a constant of spin-spin interac- tion, from the first principles of the classical mechanics.

Keywords

Neural networks, spin glass Hamiltonian, Birkhoff's ergodic hypothesis, statistic distributions, parallel simulation.

1. INTRODUCTION

Spin glasses and in general disordered spin systems as models often are used for study of different complex natural and social phenomena in 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, the economy (modelization of financial markets), etc. [1, 2, 3, 5, 6, 4, 7, 8, 9, 10, 11, 13].

There are different theoretical and numerical methods to study of 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 are 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 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, 18, 19], however, this feature retains an important physical aspect of true spin-glasses, viz. that they are random with respect to the positions of magnetic impurities.

The problem of simulation 3D spin glass is a typical NP hard problem. Nevertheless, the solution of problem becomes more difficult and even problematic when spin glasses are in states far from thermodynamic equilibrium. In this case standard methods based on Monte Carlo simulations, as a rule, are 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.

2. FORMULATION OF 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 a 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;

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

describes the disordered 1D chain of spatial spins (CSS) (below we will name the central spin-chain).

The second term:

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

describes a random environment of the central 1D CSS (see on Fig. 1) and the external field $\boldsymbol{h}_i$. Note that; $||\boldsymbol{h}_i|| = h_i = h_0 \cos(i2\pi/N_x)$ designates an external field

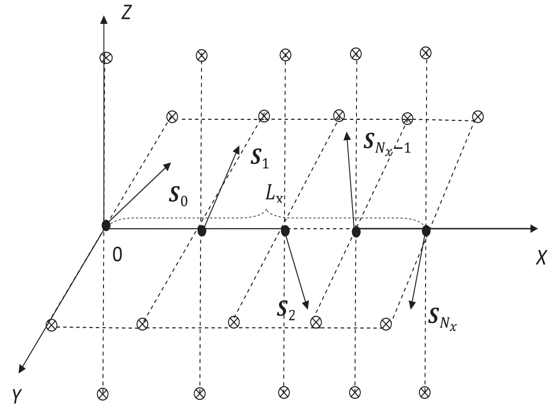

Figure 1: The 1D CSS with the random environment. The random environment consists of spins denoted by symbols ⊗.

which is propagated by direction of x-axis, h_0 its amplitude and N_x is the number of spins into standing wave formed by the external field. In (1) $J_{i\ i+1}$ and $J_{i\ i_\sigma}$ are random interaction constants between arbitrary i and $i + 1$ spins and between i and i_σ spins, correspondingly, $\boldsymbol{S}_i$, $\boldsymbol{S}_{i+1}$ and $\boldsymbol{S}_{i_\sigma}$ are spins (vectors) of the unit length $||\boldsymbol{S}_i|| = 1$, which in O(3) space are orientated randomly. The main aim of our study is the development of a theoretical approach and the relevant algorithm which will allow to exactly compute all statistical parameters of classical 3D spin glass, including the distribution of spin-spin interactions' constant, at the influence of external fields. Based on general physical considerations we need to construct such spins 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; $\boldsymbol{S}_i = (x_i,\ y_i,\ z_i)$, then we can find equations which define the condition of an extremum of Hamiltonian (1) in the node *i-th*:

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

Recall that the 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 equal to unit.

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

$$\boldsymbol{S}_{i+1} = -\frac{J_{i-1,i}\boldsymbol{S}_{i-1} + \boldsymbol{U}_i}{J_{i,i+1}} + \boldsymbol{S}_i\left\{\frac{(J_{i-1,i}\boldsymbol{S}_{i-1} + \boldsymbol{U}_i)\boldsymbol{S}_i}{J_{i,i+1}}\right.$$

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

where the constant of spin-spin coupling satisfies an inequality:

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

The energy of Hamiltonian in the *i-th* node will be minimal if the following inequalities would be satisfied:

$$A_{x_ix_i} > 0, \quad A_{x_ix_i}A_{y_iy_i} - A_{x_iy_i}^2 > 0, \tag{5}$$

where $A_{\eta_i\eta_i} = \partial^2 H/\partial{\eta_i}^2$ and $A_{x_iy_i} = \partial^2 H/(\partial x_i \partial y_i)$. Now we can calculate the second derivatives of Hamiltonian:

$$A_{\eta_i\eta_i} = \left(\eta_i^2 + z_i^2\right)\delta_i, \qquad A_{x_iy_i} = x_iy_i\delta_i, \tag{6}$$

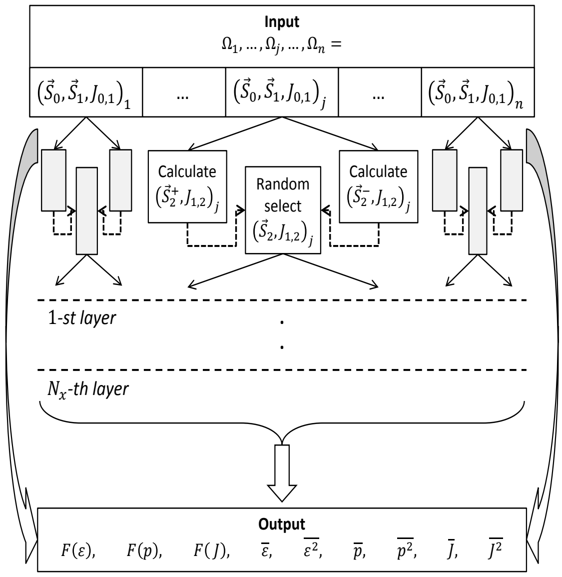

Figure 2: The algorithm of parallel simulation of statistical parameters of a non-ideal ensemble of disordered $1D$ CSS.

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 $\boldsymbol{U}_i$ on z-axis. Using (6) the explicit forms of inequalities can be easily found (5):

$$A_{x_ix_i} = \left(x_i^2 + z_i^2\right)\delta_i \geq 0,$$
$$A_{x_ix_i}A_{y_iy_i} - A_{x_iy_i}^2 = z_i^2\delta_i^2 \geq 0. \tag{7}$$

As can be seen the second inequality of (7) is always satisfied.

Finally, taking into account (4) the conditions of local minimum of the Hamiltonian (1) in the i-th node can be written in the form:

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

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 non-ideal ensemble of 1D CSS. Recall that when we say that the ensemble is non-ideal, we mean that the 1D spin-chain interacts with its random environment consisting of four disordered 1D spin-chains. As shows analysis at switching of weak external fields, the possibility of the reduction of 3D spin glass problem to the problem of non-ideal ensemble of 1D spin-chains remains valid. In a non-ideal 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 $\boldsymbol{p}$, that equivalently constructing the dis- tribution function for an energy and magnetization of non-ideal ensemble.

Thus, the main problem is concluded in a solution of direct problem, namely the numerical simulation of the non-ideal ensemble of disordered 1D CSS. Now we have constructed the distribution function of an energy and magnetization of the non-ideal ensemble. In this connection it is useful to divide axis of an energy, ε and magnetization, $\boldsymbol{p}$ 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 $n >> 1$. The number of

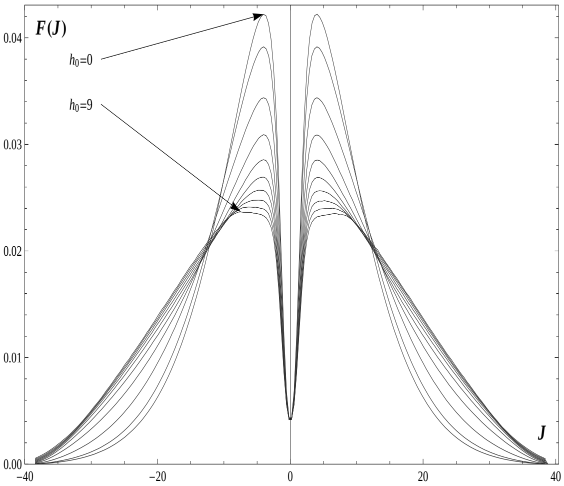

Figure 3: Distribution of spin-spin interaction constant in a non-ideal ensemble consisting of $1D$ spin-chains with the length 100, depending on an external field.

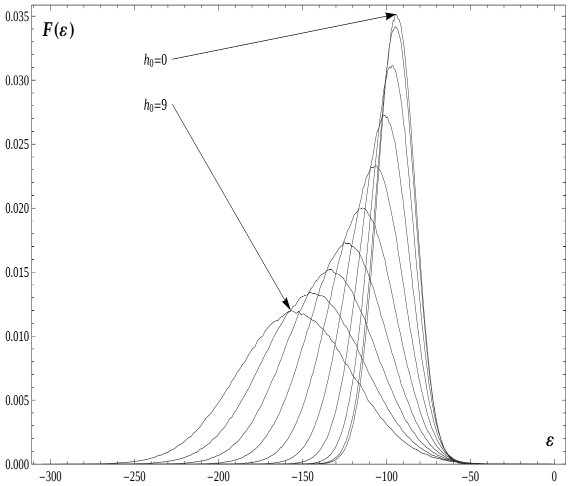

Figure 4: The energy distributions in a non-ideal ensemble depending on amplitude of an external field.

stable $1D$ CSS configurations with the length of L_x in the range of energy $[\varepsilon-\delta\varepsilon,\varepsilon+\delta\varepsilon]$, where $|\delta\varepsilon|<<1$ and polarizations range $[p_x-\delta p_x, p_x+\delta p_x]$, $|\delta p_x|<<1$, $[p_y-\delta p_y, p_y+\delta p_y]$, $|\delta p_y|<<1$ and $[p_z-\delta p_z, p_z+\delta p_z]$, $|\delta p_z|<<1$ will be denoted by $M_{L_x}(\varepsilon)$ while the number of all stable $1D$ CSS configurations - correspondingly by symbol $M_{L_x}^{full}=\sum_{i,j=1}^{n} M_{L_x}(\varepsilon_i,\boldsymbol{p}_j)$. Accordingly, the multidimensional distribution function of non-ideal ensemble $1D$ SSC may be defined by the following formulas:

$$F_{L_x}(\varepsilon,\boldsymbol{p};g)=M_{L_x}(\varepsilon,\boldsymbol{p};g)/M_{L_x}^{full}, \tag{9}$$

where the distribution function is normalized to unit:

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

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

3. SIMULATION ALGORITHM

The strategy of numerical simulation consists of the following steps. At first, we randomly sets configurations of four disordered 1D CSS without checking of spin-chains under formulas (8). Note that these four spin-chains form random environment in which we should construct central spin-chains (see Fig 1). On the second step a set of random constants of spin-spin interaction is generated, that characterizes the interactions between the random environment and the considered 1D CSS. Recall that the interaction constants as well as in a case of unperturbed by external fields 3D spin-glass [20], are generated by Log-normal distribution. Now when the random environment and its influence on disordered 1D SSC are defined, we can go over to the computation of spin-chain under the influence of external fields which must satisfy the conditions of local energy minimum (8). The central spin-chain consistently, node by node is being computed. Note that in each node two solutions are found (see the scheme on Fig 2, they are designated by symbols + and −), however, at continuation of simulation of the spin-chain we in each node leave only one solution which is randomly being selected. Finally in the last stage of simulation with the help of formulas (9)-(10) we calculate distributions of corresponding parameters which characterize the statistical properties of the 3D spin glass under the influence of external fields.

4. NUMERICAL EXPERIMENTS

Note, that calculations of 3D spin glass or more correctly a non-ideal ensemble of 1D CSS 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 as in particular is 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 normal Gaussian distribution model (Gauss-Edwards-Anderson distribution) (see Fig. 3). As shows an analysis, the curve of distribution is a non-analytical function and probably it can be approximated precisely by Lévy skew alpha-stable distribution function. As shown by calculations, at the increasing of the number of spin-chains 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 are also presented the energy distributions in a non-ideal ensemble depending on an external field (see Fig. 4). As calculations show, for a non-ideal 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 function of distribution, at increasing of amplitude of an external field moves in area of lower negative values of energy. As to the magnetization distributions, as shows computation at influence on media with the weak external field the distribution of magnetization in all coordinates frustrates. After the procedure of averaging of magnetization by fractal structures [21], we find the average values of magnetization on the corresponding coordinates, depending on the amplitude of an external field. As we can see at inclusion of an external field a spin glass on all directions is magnetized, however, magnetization steadily goes up on direction of propaga-

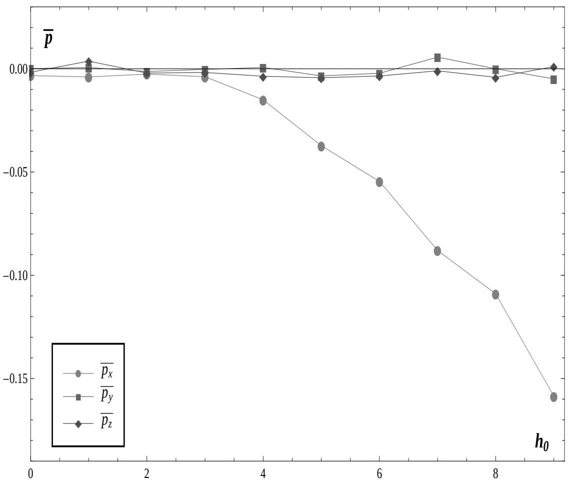

Figure 5: The average value of polarization on corresponding coordinates depending on an external field.

tion of an external field, with increasing the amplitude of an external field (see Fig. 5).

5. CONCLUSION

Using the proof about the equivalence of models of 3D spin glass and non-ideal ensemble 1D SSC we have developed a new parallel algorithm for simulation of statistical properties of 3D spin glasses under an influence of external fields. The central idea which lays in a based of 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 nearest-neighboring Hamiltonian of Heisenberg. The developed algorithm allows on a basis of first principles of classical mechanics to calculate all statistical parameters of 3D spin glasses including the distribution of constant of spin-spin interaction under external fields. An important peculiarity of the developed method is the possibility of an exact simulation of 3D spin glasses including situations when system is far from thermodynamic equilibrium and we cannot use 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 properties of disordered spin systems on a nano-scales of space-time, the development of which is closely connected with the development of modern technologies and in general of nanoscience.
Finally let us note that the programm for numerical simulations of 3D spin glasses is created using GPU technologies which achieves high performance parallel calculations for aforementioned problems.

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