Modeling of $1D$ spin glasses from first principles of classical mechanics

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Abstract. We study the classical $1D$ Heisenberg spin glasses assuming that spins are spatial. The system of recurrence equations is derived by minimization of the nearest-neighboring Hamiltonian in nodes of $1D$ lattice. We have proved that in each node of the lattice there is a probability that the solution of recurrence equations can bifurcate. This leads to the fact that, performing a consecutive node-by-node calculations on the *n-th* step instead of a single stable spin-chain we get a set of spin-chains which form Fibonacci subtree (graph). We have assessed the complexity of computation of one graph and have shown that it is $\propto 2^n K_s$, where n and K_s denote the subtree's height (the length of spin-chain) and the Kolmogorov's complexity of a string (the branch of subtree) respectively. It is shown that the statistical ensemble may be represented as a set of random graphs, where the computational complexity of each graph is $\mathbb{NP}$ hard. It is proved, that all strings of the ensemble have the same weights. The latter circumstance allows in the limit of statistical equilibrium with predetermined accuracy to reduce the $\mathbb{NP}$ hard problem to the $\mathbb{P}$ problem with complexity $\propto NK_s$, where N is the number of spin-chains in the ensemble. As it is shown by comparing statistical distributions of different parameters which are performed by using $\mathbb{NP}$ and $\mathbb{P}$ algorithms the coincidence of the corresponding curves is ideal. This allows to claim that it is possible to calculate all parameters and the corresponding distributions of the statistical ensemble from the first principles of classical mechanics without using any additional considerations. Finally, using formal similarity between of the ergodic dynamical system and the ensemble of spin-chains, it is proposed a new representation for the partition function in the form of one dimensional integral from the spin-chains' energy distribution.

1. Introduction

A wide class of phenomena in physics, chemistry, material science, biology, nanoscience, neural network, evolution, organization dynamics, hard-optimization, environmental and social structures, human logic systems, financial mathematics etc, mathematically are well described by models of spin glasses [1, 2, 3, 5, 6, 4, 7, 8, 9, 10]. Despite numerous studies nonetheless there are still a number of topical issues in the field of spin glasses and disordered systems as a whole, the solution of which is extremely important from the point of view of the development of modern technologies. We can mention important ones of them;

a) The simulation of spin glasses far from thermodynamic equilibrium. Obviously, in such cases, we can not enter the ambient temperature and, respectively, write and use a standard representation for partition function.

b) Even if it is assumed that spin glass is in the state of the thermodynamic equilibrium, and for it may be written in the standard form the partition function, in the frameworks of standard theoretical and numerical methods,it remains an open research question of metastable states. Recall that the Monte Carlo simulation methods allow us to study the spin systems only in the *ground state*, at the time when the real statistical system, all the more spin glasses, always are in the metastable states, i.e in the state where characterizing the spin glass parameters have some distributions.

c) At definition of the partition function, a priori is assumed that the total weight of nonphysical spin configurations in the configuration space is a zero that in a number of cases may be an incorrect assumption. Recall that under the nonphysical spin configurations, we mean such spin-chains, which are unstable based on the basic principles of classical mechanics.

d) The computational complexity of spin glasses often applies to the class of the $\mathbb{NP}$ hard problems. This circumstance to require the development of new efficient algorithms for a numerical simulation of spin glasses that one way or another leads to the problem of reduction of the $\mathbb{NP}$ to the $\mathbb{P}$ problem.

As it was shown in works [11, 12, 13, 14], the problem of spin glasses even in the state of the thermodynamic equilibrium often are $\mathbb{NP}$ hard problems, whose source of which is in the diverging equilibration at simulations by the Monte Carlo methods [15]. In the last time in the statistical physics occurs a rapid growth the number of works on methods of the combinatorial optimization [16, 17, 18]. In particular a number of disordered statistical systems have been mapped onto combinatorial problems, for which a fast combinatorial optimization algorithms are available [19, 20]. So, combinatorial methods and corresponding algorithms are often used for a simulation of spin glasses especially when studying the phenomena such as phase transitions where they have given valuable insights about questions that are hard to investigate by traditional techniques, for example by Monte Carlo simulations [11]). However, the above-mentioned problems, on which we want to receive clear answers, obviously require to development principally new approaches.

In this paper we will study the classical $1D$ spin glass problem suggesting that only the nearest neighboring spins interact. Recall despite the simplicity of the model, since in a known sense it's an exactly solvable model [21], as it will shown below, all the aforementioned problems in this model are present, if we try to solve the task from first principles of classical mechanics.

One of the important goals of this work is to prove, that in the limit of statistical equilibrium the initial $\mathbb{NP}$-hard problem with the prescribed accuracy can be reduced to the $\mathbb{P}$ problem, that in turn implies the creation of high-performance algorithm for simulation of the Heisenberg type spin glasses. In the work possibilities of generalization of the model for descriptions of more complex and realistic disordered systems of nature are also discussed.

2. Definition of model

The Hamiltonian of the $1D$ chain of disordered spatial spins, in the framework of the nearest-neighboring model may be written as:

$$H = -\sum_{i\in\mathcal{N}} J_{i,\,i+1}\boldsymbol{s}_i\boldsymbol{s}_{i+1}, \qquad \boldsymbol{s}_i \in \mathbb{R}^3, \qquad ||\boldsymbol{s}_i|| = ||\boldsymbol{s}_{i+1}|| = 1, \tag{1}$$

where $\mathcal{N} = \{1, ..., n\}$ is the set of nodes on $1D$ lattice, the couplings $J_{i,\,i+1}$ are independent random variables characterizing the power of interactions between the spins. The distribution of the coupling constants will be found below as a result of the numerical simulation.

Since the norm of vector $\boldsymbol{s}_i = (x_i, y_i, z_i)$ is equal to the unit, then the projection, z_i can be represented in the following form:

$$\boldsymbol{z}_i = q_i|z_i|, \qquad z_i = (1 - x_i^2 - y_i^2)^{1/2} > 0, \quad q_i = \mathrm{sign}(\boldsymbol{z}_i), \tag{2}$$

where q_i is a discrete variable which can take two possible values +1 and -1.

The local minimum of the Hamiltonian (1) in an arbitrary node i is defined by the equations of stationary point and by the Sylvester conditions. Hamiltonian takes an extreme value in the node *i-th*, if the vector equation is performed; $\partial H/\partial\boldsymbol{s}_i = (\partial H/\partial x_i; \partial H/\partial y_i) = 0$, that is equivalent to the following system of recurrence equations:

$$\begin{aligned} &J_{i-1,\,i}(x_{i-1} - x_i {z_i}^{-1} z_{i-1}) + J_{i,\,i+1}(x_{i+1} - x_i {z_i}^{-1} z_{i+1}) = 0,\\ &J_{i-1,\,i}(y_{i-1} - y_i {z_i}^{-1} z_{i-1}) + J_{i,\,i+1}(y_{i+1} - y_i {z_i}^{-1} z_{i+1}) = 0. \end{aligned} \tag{3}$$

Solving the system of equations (3), with respect to the variables x_{i+1} and y_{i+1}, it can be found:

$$x_{i+1} = C_x/J_{i,\,i+1}, \qquad y_{i+1} = C_y/J_{i,\,i+1}, \tag{4}$$

where the following notations are made:

$$C_{x(y)} = \frac{A_{x(y)} - B_{y(x)}(C \pm \sqrt{D})}{1 + B_x^2 + B_y^2}, \quad A_\eta = \eta_i {z_i}^{-1} z_{i-1} - \eta_{i-1}, \qquad B_\eta = \eta_i {z_i}^{-1} q_{i+1},$$

$$D = (1 + B_x^2 + B_y^2 - A_x^2 - A_y^2 - C^2) > 0, \quad C = A_x B_y - A_y B_x, \qquad \eta = (x, y).$$

Now, for the Hamiltonian (1) we can obtain the conditions of the local minimum. It is obvious that *i-th* spin is in the stable equilibrium, if in the stationary point the following inequalities are satisfied:

$$A_{x_i x_i}(\boldsymbol{s}_i^0) > 0, \qquad A_{x_i x_i}(\boldsymbol{s}_i^0) A_{y_i y_i}(\boldsymbol{s}_i^0) - A_{x_i y_i}^2(\boldsymbol{s}_i^0) > 0, \tag{5}$$

where $A_{\eta_i \eta_i} = \partial^2 H / \partial \eta_i^2$ and $A_{x_i y_i} = \partial^2 H / \partial x_i \partial y_i$; in addition $\boldsymbol{s}_i^0$ denotes *i-th* spin which is in a stable equilibrium.

Using (2), (3) and (5), we can calculate the explicit forms of the second order derivatives:

$$A_{\eta_i \eta_i} = (\eta_i^2 + z_i^2) z_i^{-3} \Delta_i, \quad A_{x_i y_i} = x_i y_i z_i^{-3} \Delta_i, \quad \Delta_i = (J_{i-1,\,i} z_{i-1} + J_{i+1,\,i} z_{i+1}), \tag{6}$$

and taking into account (5) and (6) we find the conditions of the local minimum energy:

$$A_{x_i x_i} = (1 - y_i^2) z_i^{-3} \Delta_i > 0, \quad A_{x_i x_i} A_{y_i y_i} - A_{x_i y_i}^2 = z_i^{-4} \Delta_i^2 > 0. \tag{7}$$

Since, by definition (2) $z_i > 0$, then both of the conditions in (7) are satisfied:

$$\Delta_i = (J_{i-1,\,i} z_{i-1} + J_{i+1,\,i} z_{i+1}) > 0. \tag{8}$$

Thus in each node the solutions defining the orientation of the spin in the state of the local equilibrium can be found, if we find such coupling constants $J_{i,\,i+1}$, for which not only conditions (7) or (8) are satisfied, but also holds the inequality:

$$J_{i,\,i+1}^2 \geq C_x^2 + C_y^2 > 0. \tag{9}$$

As will be shown below, the additional condition (9) will play an important role at simulation.

Thus, we have obtained the system of recurrence equations (4) and corresponding Sylvester's conditions (7) on the basis of which we must to develop a parallel algorithm for calculations of the spin glass.

3. Geometric properties of disordered $1D$ spin-chain

Theorem. *If the set of spatial spins;* $\{\boldsymbol{s}\} = (\boldsymbol{s}_1, .., \boldsymbol{s}_n)$ *forms the stable* $1D$ *spin-chain (see conditions (7)) then they necessarily are coplanar in the sense, that at parallel moving to the origin all spins lie in the same plane.*

Proof. Let us consider the three consecutive spatial spins $\boldsymbol{s}_{i-1}, \boldsymbol{s}_i$ and $\boldsymbol{s}_{i+1}$ on the $1D$ lattice. If we join the origins of two consecutive spins $\boldsymbol{s}_{i-1}$ and $\boldsymbol{s}_i$, they will form a plane Λ_0. In this connection arises the question namely as subsequent spins are oriented relative to the plane Λ_0? Since these spins are in the positions of local minimums, we can use the system of equations (3) for defining bonds between projections of three nearest-neighboring spins. In particular from the first equation in (3) we can find the following expression for z_{i+1}:

$$z_{i+1} = \frac{J_{i-1,\,i}(x_{i-1} z_i - x_i z_{i-1}) + J_{i,\,i+1} x_{i+1} z_i}{J_{i,\,i+1} x_i}. \tag{10}$$

Substituting z_{i+1} into the second equation in (3) we can find the expression of bond between projections of two spins $\boldsymbol{s}_{i-1}$ and $\boldsymbol{s}_i$:

$$x_{i-1}y_i - x_i y_{i-1} = \frac{J_{i,\,i+1}}{J_{i-1,\,i}}(x_{i+1}y_i - x_i y_{i+1}). \tag{11}$$

The spin $\boldsymbol{s}_{i+1}$ is a parallel to the plane Λ_0, if the following equation is satisfied:

$$\begin{vmatrix} x_{i-1} & y_{i-1} & z_{i-1} \\ x_i & y_i & z_i \\ x_{i+1} & y_{i+1} & z_{i+1} \end{vmatrix} = 0. \tag{12}$$

We can write the equation (12) in the explicit form:

$$\det|\cdot| = x_{i-1}y_i z_{i+1} + x_{i+1}y_{i-1}z_{i+1} + x_i y_{i+1}z_{i-1} - x_{i+1}y_i z_{i-1} - x_i y_{i-1}z_{i+1} - x_{i-1}y_{i+1}z_i =$$

$$x_{i+1}\Big[-\frac{J_{i,\,i+1}}{J_{i-1,\,i}}(y_{i+1}z_i - y_i z_{i+1})\Big] + y_{i+1}\Big[\frac{J_{i,\,i+1}}{J_{i-1\,,i}}(x_{i+1}z_i - x_i z_{i+1})\Big] + z_{i+1}\Big[-\frac{J_{i,\,i+1}}{J_{i-1,\,i}}(x_{i+1}y_i - x_i y_{i+1})\Big],$$

Finally, using the expression (11) it is easy to show that:

$$\det|\cdot| = \frac{J_{i,i+1}}{J_{i-1,i}}\Big\{x_{i+1}(y_i z_{i+1} - z_i y_{i+1} - y_i z_{i+1} + z_i y_{i+1}) + x_i(y_{i+1}z_{i+1} - y_{i+1}z_{i+1})\Big\} = 0.$$

Thus the theorem is proved.

Note that, the specified geometric property allows simplifying the Hamiltonian (1). Let us consider the set of spins in the spherical coordinate system $(\alpha_i, \theta_i, \vartheta_i)$. In the new coordinates for the two consecutive spins we can write the following relation:

$$\boldsymbol{s}_i\boldsymbol{s}_{i+1} = ||\boldsymbol{s}_i|| \cdot ||\boldsymbol{s}_{i+1}|| = \cos(\alpha_i - \alpha_{i+1}), \tag{13}$$

where $(\alpha_i, \alpha_{i+1}) \in [-\pi, +\pi]$ are the angles of corresponding spins in planes parallel to plane Λ_0.

Using (13) Hamiltonian (1) can be written in the form:

$$H = -P(\theta, \vartheta)\sum_{i=1}^{n} J_{i,i+1}\cos(\alpha_i - \alpha_{i+1}), \tag{14}$$

where, as it follows from the proof of the proposition, $\theta = \theta_1 = ... = \theta_n \in (-\pi, +\pi]$ and $\vartheta = \vartheta_1 = ... = \vartheta_n \in [0, \pi]$. In addition, the pair of angles (θ, ϑ) defines the orientation of a plane Λ_0 in $3D$ space. It is natural to propose that $P(\theta, \vartheta)$ is the homogeneous distribution function from angles, which is normalized on unit $\int\int P(\theta, \vartheta)d\theta d\vartheta = 1$. For finding the extreme value of the Hamiltonian (14) in nodes, let us consider the first derivative by the angle α_i:

$$\frac{dH}{d\alpha_i} = P(\theta, \vartheta)[J_{i-1,\,i}\sin(\alpha_{i-1} - \alpha_i) - J_{i,\,i+1}\sin(\alpha_i - \alpha_{i+1})]. \tag{15}$$

It is obvious that derivatives of Hamiltonian (14) by angles θ and ϑ are identically equal to zero. Now by equating the expression (15) to zero and solving it, we will get two possible solutions for a stationary point:

$$\alpha_{i+1} = \alpha_i - \arcsin\Big[\frac{J_{i-1,\,i}}{J_{i,\,i+1}}\sin(\alpha_{i-1} - \alpha_i)\Big], \tag{16}$$

$$\alpha_{i+1} = \alpha_i + \pi + \arcsin\Big[\frac{J_{i-1,\,i}}{J_{i,\,i+1}}\sin(\alpha_{i-1} - \alpha_i)\Big].$$

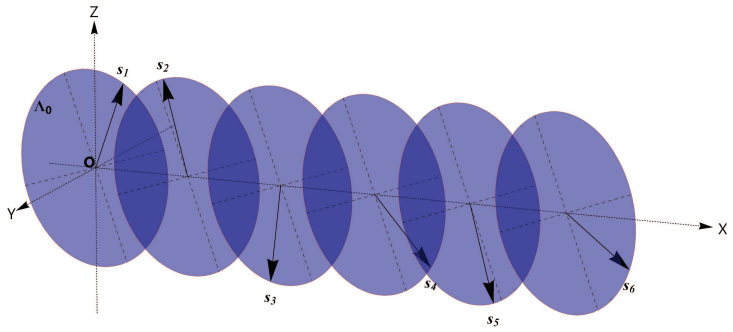

Figure 1. The disordered $1D$ spin chain where spins lie in planes parallel to the plane Λ_0.

The condition on existence of these solutions in the region of real numbers is equivalent to the following inequality:

$$-1 \leq \frac{J_{i-1,\,i}\sin(\alpha_{i-1}-\alpha_i)}{J_{i,\,i+1}} \leq 1, \quad or \quad |J_{i,\,i+1}| \geq |J_{i-1,\,i}\sin(\alpha_{i-1}-\alpha_i)|. \tag{17}$$

Using two equations from (17) and substituting i instead of $i-1$ we can find the value of $J_{i-1,i}\sin(\alpha_{i-1}-\alpha_i)$, and for both solutions result will be same:

$$J_{i-1,\,i}\sin(\alpha_{i-1}-\alpha_i) = J_{i-1,\,i}\frac{J_{i-2,\,i-1}\sin(\alpha_{i-2}-\alpha_{i-1})}{J_{i-1,\,i}} = J_{i-2,\,i-1}\sin(\alpha_{i-2}-\alpha_{i-1}).$$

It is clear that by continuing this process we will get:

$$J_{i-1,\,i}\sin(\alpha_{i-1}-\alpha_i) = J_{1,2}\sin(\alpha_1-\alpha_2). \tag{18}$$

Using (18) we can transform condition (17) to

$$|J_{i,\,i+1}| \geq |J_{1,2}\sin(\alpha_1-\alpha_2)|. \tag{19}$$

Let us note that the angles, α_1, α_2 and also the coupling constant, $J_{1,2}$ in condition (18) as an initial conditions of problem are specified. Finally we can write the condition of the local minimum energy in the arbitrary *i-th* node:

$$\frac{\partial^2 H}{\partial \alpha_i^2} = P(\theta,\vartheta)[J_{i-1,\,i}\cos(\alpha_{i-1}-\alpha_i) - J_{i,\,i+1}\cos(\alpha_i-\alpha_{i+1})] > 0. \tag{20}$$

4. The statistical ensemble of $1D$ disordered spin-chains

As it is easy to verify the solutions of equations (4) satisfying the inequalities (7) can be of two types:

a. If $J_{i-1,\,i}\boldsymbol{s}_{i-1}\cdot\boldsymbol{s}_i \leq 0$ and $|J_{i,\,i+1}| > |J_{i-1,\,i}|$, then there is only one solution, which we denote by; $\boldsymbol{s}_{i+1}^{+}$ (*queen*), and respectively,

b. If $J_{i-1,\,i}\boldsymbol{s}_{i-1}\cdot\boldsymbol{s}_i > 0$ and $|J_{i,\,i+1}| \geq |J_{0,1}|\cdot|\boldsymbol{s}_0\times\boldsymbol{s}_1|$, then $\boldsymbol{s}_{i+1}^{+}$ is the solution, in addition there is another solution; $\boldsymbol{s}_{i+1}^{-}$ (*drone*) under the condition that, $|J_{i,\,i+1}| < |J_{i-1,\,i}|$.

It is important to note that the solutions which are denoted with signs "+" and "−" are characterized as follows, if the previous solution is the *queen* "+" it is possible to find up two different solutions $\boldsymbol{s}_{i+1}^{+}$ and $\boldsymbol{s}_{i+1}^{-}$, while after the *drone* "−" the solution only one $\boldsymbol{s}_{i+1}^{+}$. Taking into account this we can construct solutions graphically in the form of separate *Fibonacci subtrees* ($\widehat{FsT}_i$) (see Fig. 2).

The mathematical expectation of the branching's number depending on the height of $\widehat{FsT}_i$ can be calculated by the following formula:

$$M(n) = M(n-1)\lfloor (2\xi_n)\rfloor = \lfloor 2^{n\eta(n)}\rfloor, \quad \eta(n) = 1 + n^{-1}\sum_{k=1}^{n}\log_2(\xi_k) > 0, \qquad (21)$$

where $M(n-1)$ the number of the branching at the height $(n-1)$ and ξ_k denotes a random coefficient which belongs to the interval $[1/2, 1]$. Recall that for simplification of the formula (21) designating the subtree's number i is omitted. Since, an each $\widehat{FsT}_i$ consists of the set of nodes and the set of edges (the set of constants $\{J\} = [J_{1,2}, J_{2,3}, ...J_{n-1,n}]$ therefore it can be represented as a graph $G_i(n) \cong \{g_j(n), j \in M\}$, where $g_j(n)$ denotes a random string by length n which is characterized by Kolmogorov's complexity [22, 23].

Note that each Fibonacci subtree (graph) depending on its height n can be represented itself as a random process. To compare them it is necessary to formulate the appropriate criteria.

Definition. *Two graphs with the same height; $G_1(n)$ and $G_2(n)$ are equivalent with a given accuracy $\epsilon \ll 1$, if the following conditions take place:*

1) *The difference of Shannon's entropy of the two Fibonacci subtrees (graphs) satisfies:*

$$|S^1(n) - S^2(n)| \le \epsilon, \qquad S^{1(2)}(n) = -\sum_{i=1}^{n} M_i^{1(2)} \ln M_i^{1(2)}, \qquad (22)$$

where $S^1(n)$ and $S^2(n)$ denote the Shannon's entropies of graphs $G_1(n)$ and $G_2(n)$, in addition M_i^1 and M_i^2 are the branching numbers of corresponding graphs on the i-th height,

2) *the difference of average polarizations of two graphs in per one spin satisfies:*

$$\Big\|\frac{1}{n}\sum_{i=1}^{n}\Big(\boldsymbol{s}_i^{(1)} - \boldsymbol{s}_i^{(2)}\Big)\Big\| \le \epsilon, \qquad (23)$$

where $\boldsymbol{s}_i^{(1,2)} = \sum_{G_{1,2}(i)} \boldsymbol{s}_i$ denotes the total value of spins on the corresponding graph at the i-th height,

3) *the difference of the average energies of two graphs in per one spin satisfies:*

$$\frac{1}{n}\sum_{i=1}^{n}\Big|\frac{1}{m_1}\sum_{j=1}^{m_1} J^{(1)}_{i,\,i+1;(j)}\boldsymbol{s}_{i;(j)}\boldsymbol{s}_{i+1;(j)} - \frac{1}{m_2}\sum_{j=1}^{m_2} J^{(2)}_{i,\,i+1;(j)}\boldsymbol{s}_{i;(j)}\boldsymbol{s}_{i+1;(j)}\Big| \le \epsilon, \qquad (24)$$

with $m_1 = M_n^1$ and $m_2 = M_n^2$. Note that, the small parameter ϵ is chosen with consideration of simulation accuracy. In the case when at least one condition from (22)-(24) is violated, we will consider that $G_1(n)$ and $G_2(n)$ are inequivalent or independent.

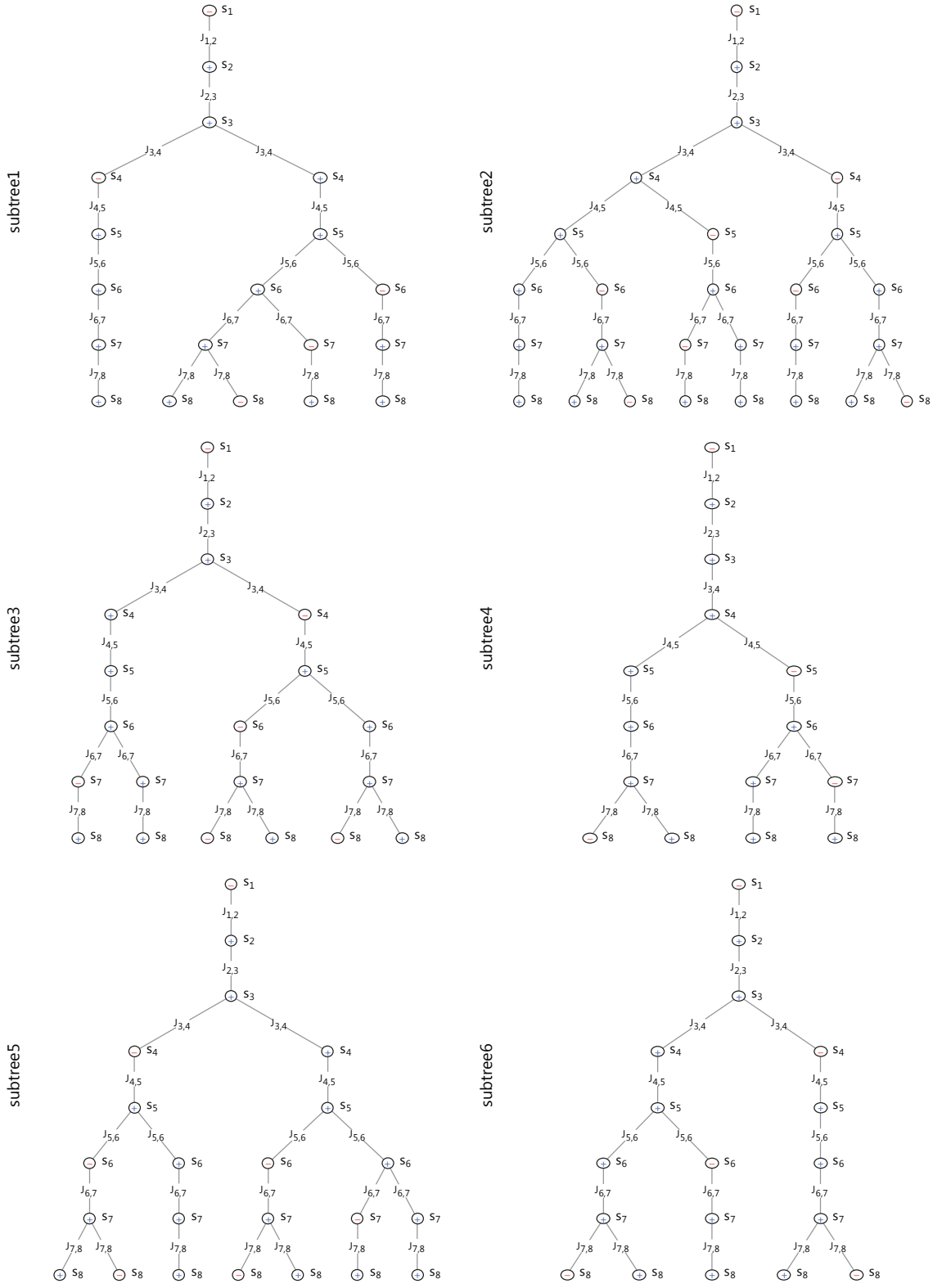

Figure 2. The six different Fibonacci subtrees (graphs) an each of which with the height 8. All these graphs are growing from the same initial data (*root*) in result of the six independent numerical experiments. The same symbols s_i and $J_{i,j}$ on different graphs can have completely different values.

Thus for calculations of different physical parameters of the statistical ensemble, it is necessary to take into account the contribution of all independent graphs (set of graphs) $\{G(n)\} = [G_1(n), ...G_i(n), ...]$. It is easy to verify that the system of equations (4) which satisfies conditions (7)-(8) in each node can have up to two solutions, which means that the number of solutions on the step n due to branching will be of order $M(n) \propto 2^n$. In other words the calculation problem of statistics even of a single graph algorithmically is a NP hard problem, since the number of solutions grows exponentially at increasing of spins number. The estimation of computational complexity of statistics for an one graph gives:

$$K_t(n) \propto M(n)K_s(n), \tag{25}$$

where $K_s(n)$ denotes the Kolmogorov complexity of the string $g_j(n)$, while $K_t(n)$ denote the complexity of the graph $G_i(n) \subset \{G(n)\}_N$. The computational complexity of the $\{G(n)\}_N$ obviously will be $K_{ens} \propto NM(n)K_s(n)$, where n is the height of graphs and N the total number of graphs of the ensemble.

The mathematical expectation of random variable f characterizing the ensemble $\{G(n)\}_N$ can be calculated by the formula:

$$E[f] = \bar{f} = \frac{\sum_{i=1}^{N} w_i \bar{f}_i}{\sum_{i=1}^{N} w_i}, \qquad w_i = N_i/\bar{N}, \tag{26}$$

where N_i and $\bar{N}$ denote the number of strings of the graph $G_i(n)$ and the total number of strings in the ensemble respectively, in addition $\bar{f}_i = \sum_{G_i(n)} f$ denotes the expectation of a random variable f on the $G_i(n)$, which is calculated similarly to formula (26).

From the point of view of statistics, it is important to investigate the ensemble in the state of the statistical equilibrium. This as a rule is realized at $N >> 1$ and when the average value of random variable f almost surely converges to the expected value [24]:

$$\Pr\Big(\lim_{N\to\infty} \bar{f}_N = \bar{f}\Big) = 1,$$

where $f_1, f_2, ...$ are infinite sequence of Lebesgue integrable random variables with the expected values $E[f_1] = E[f_2] = ... = \bar{f}$.

Lemma. *If statistical weights of all independent graphs $G_i(n) \subset \{G(n)\}_N$ are approximately the same it can be shown that the statistical weights of all strings $g_j(n) \subset \{G(n)\}_N$ are equal exactly. In this case we can use the law of large numbers and simplify the expression (26) writing it as:*

$$E[f] = \bar{f} = \frac{1}{N}\sum_{j=1}^{N} \tilde{f}_j + O(N^{-1/3}), \tag{27}$$

where $\tilde{f}_j = \sum_{g_j} f$ denotes the expectation of the random variable f on a randomly selected string $g_j(n) \subset G_i(n)$.

Note that the asymptotic convergence to the limit value in the expression (27) occurs with accuracy $\propto N^{-1/3}$ due to the fact that the spins are three-dimensional.

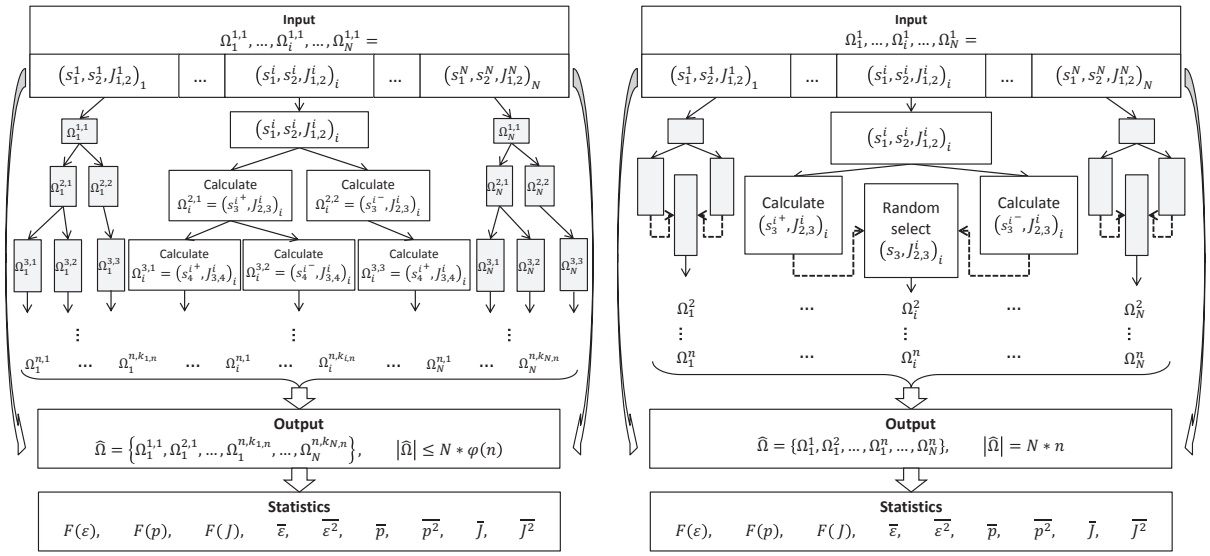

Figure 3. In the figure the left scheme describes $\mathbb{NP}$ algorithm while the right one describes $\mathbb{P}$ algorithm which allows implementing calculations of the problem in a polynomial time.

Thus, the computation of statistical parameters of the disordered spin system by the formula (26) is algorithmically equivalent to solving of $\mathbb{NP}$ hard problem (the left scheme in Fig. 3). In the case when the ensemble is in the state of statistical equilibrium then the numerical simulation can be realized by the formula (27) and respectively by the algorithm $\mathbb{P}$ (the right scheme in Fig. 3) having the polynomial complexity.

5. The numerical experiments

As it has been said, usually the problems of spin glasses are studied in the framework of the partition function representation by using Monte Carlo simulation methods which however does not allow to answer on many important questions of the statistical ensemble. In particular an important problem is the fact that the spin glass in the state of a statistical equilibrium generally speaking is in a metastable state and has some distribution near the *ground state*. The system in this state is obviously impossible to study by Monte Carlo methods, since these methods are adapted for calculations only the *ground state*. To take into account the influence and contribution of this distribution on different properties and values of parameters of a spin glass, it is necessary to implement numerical simulation from the first principles of classical mechanics.

Hypothesis. *If the Heisenberg* $1D$ *spin glass is in the state of the statistical equilibrium, then the computational* $\mathbb{NP}$ *hard problem with the prescribed accuracy* ϵ *can be reduced to the* $\mathbb{P}$ *problem.*

As it is shown above at study of $1D$ spin glass we face with the problem of numerical simulation of the set $\{G(n)\}_N$ which is a $\mathbb{NP}$ hard problem, since the number of branches in each subtree depending on its height is growing exponentially. It should be noted

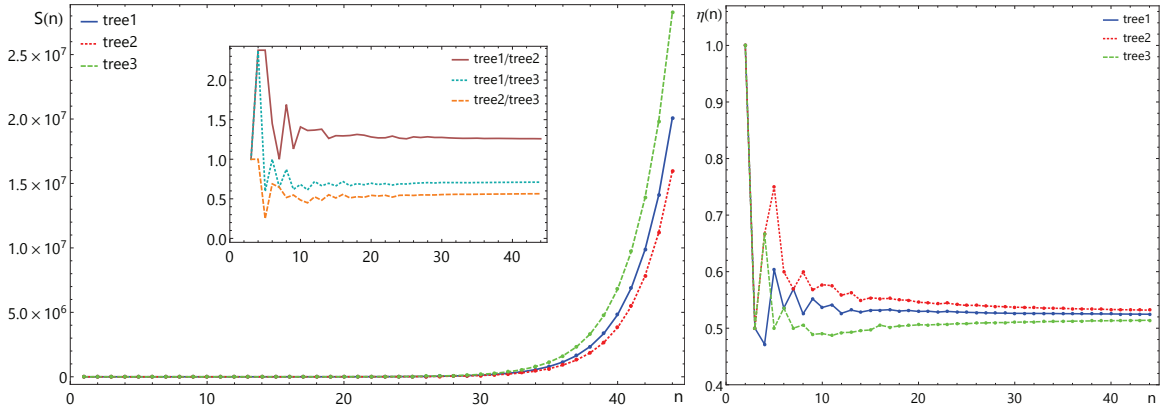

Figure 4. In the left figure are shown the entropies of graphs (subtrees) depending on their height (the red, blue, and green lines), while in the small frame are shown curves of relations of corresponding entropies. In the right figure are shown curves of the branching factor $\eta(n)$ depending of the graph height.

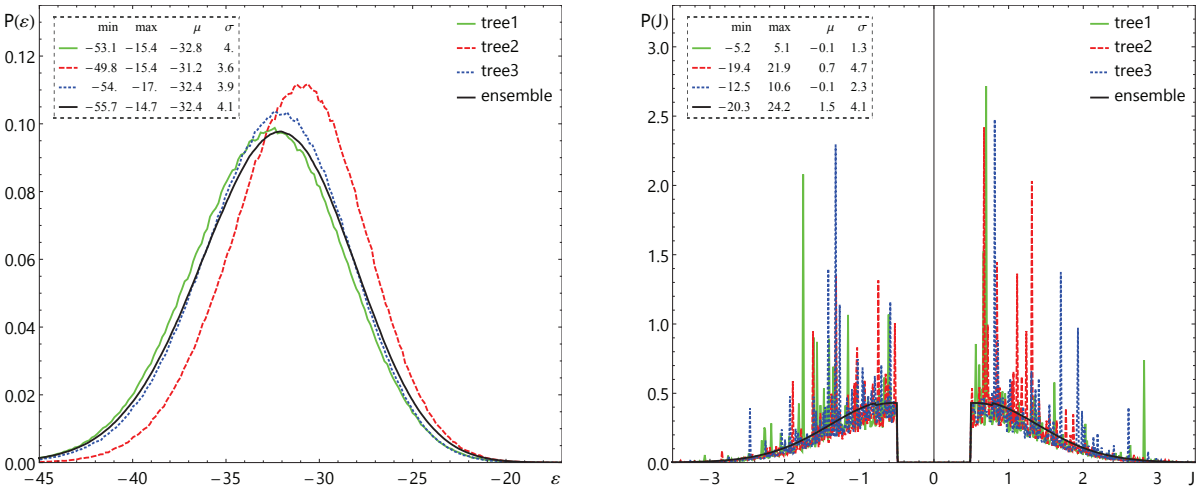

Figure 5. On the left picture are shown the distributions of strings' energies of the length 45 in the three different graphs (red, green and blue lines) which *grow* from the same *root* and correspondingly the black curve, which shows the energy distribution in statistically equilibrium ensemble $\{G(n)\}_N$, where all graphs from one *root* are *growing*. In addition, in tables adduced the important parameters that characterize the corresponding distributions; the maximal and minimal values, the average value of parameter $\mu = \int xP(x)dx$ and the dispersion σ. Note that the simulation has been conducted by $\mathbb{NP}$ algorithm (see the left scheme on Fig. 3).

that at performing of numerical simulations with a same initial data in each time t we find a new set of graphs $\{G(n)\}_N^t$ (see Fig. 2), nevertheless we expect that in the limit of statistical equilibrium all these sets must be identical in terms of statistical properties and this is the assumption of the hypothesis. It is obvious, if we prove that all strings in the statistical ensemble, $\{G(n)\}_N$, have the equal weight then this allows to use the law of big numbers and to reduce $\mathbb{NP}$ hard problem to $\mathbb{P}$ problem with the prescribed accuracy.

For the comprehensive study of graphs properties and their contributions to the statistics of the ensemble, we will consider two possible cases; when graphs are growing from one single *root* and respectively when they are growing from different *roots*.

At first let us consider one set of initial data Ω_i^1 (root) which includes orientations of the first two spins of the chain and the coupling constant between them which are generated randomly from the corresponding homogeneous distributions. Using the system of recurrence equations (4), with consideration of inequality conditions (7), we perform successive calculations of spin-chain. Recall that this system of equations connects three consecutive spins, so that knowing the configuration of two previous spins, we can generate from lognormal distribution [25] a random constant $J_{i,\,i+1}$ and exactly to calculate a spin orientation in the subsequent node. Conducting the consecutive node-by-node calculations on the *n-th* step, we generate a random graph $G_i(n) \subset \{G(n)\}_N$ at internal nodes of which the spins are in local minima of energies. With regard to spins in the external nodes, then it is supposed that they are in local minima of energies on the basis of other considerations.

Performing the simulation using the $\mathbb{NP}$ algorithm shows that all three graphs which *grow* from one *root* are independent by criteria (22)-(24). In particular the numerical simulations show that depending on height of the graph, the Shannon's entropy *grows* an exponential, in all cases starting with $n \simeq 15$ (see the left picture on Fig. 4). The ratios of entropies as follows from the Fig. 4, for the $n > 15$ they take values $\propto O(1)$ that means in the ensemble $\{G(n)\}_N$ the weights of separate graphs are approximately equal. The weight of individual branches in the statistical ensemble obviously will be the inverse of weights of graphs to which they belong. In other words all branches in the ensemble have the same weight. Note that the same picture is observed when graphs *grow* from different *roots*. In this case all graphs are also independent and the parameter of branching, at increasing of string length as in the previous case converges to the value $\eta(n) = 0.55$ (see the right picture on Fig. 4). When the length of string $n < 15$ then in the behaviour of entropy an oscillating character is observed (see Fig. 4), that is characteristic of the discrete systems and manifests itself in the form of *size effects*. We carried calculations of distributions of different parameters on the example of three graphs and also of the ensemble of graphs which *grow* from the same *root*. As the calculations show, the energies distributions for three graphs and the ensemble, $\{G(n)\}_N$ by criterion of Kullback-Leibler distance are close enough [26], while the distributions of the coupling constants are sufficiently far by the same criterion (see Fig. 5).

So, we have shown that there are necessary and sufficient conditions for performing of the **lemma**.

Now we can prove the **hypothesis** on the example of numerical experiments. We calculated the characteristic distributions and parameters of the $1D$ spin glass, which is in the state of the statistical equilibrium by two $\mathbb{NP}$ and $\mathbb{P}$ algorithms. It is obvious that the comparison of the simulation results of the relevant distributions will allow us to prove or disprove the **hypothesis**.

For the simulation of the problem, first of all we need to specify initial conditions

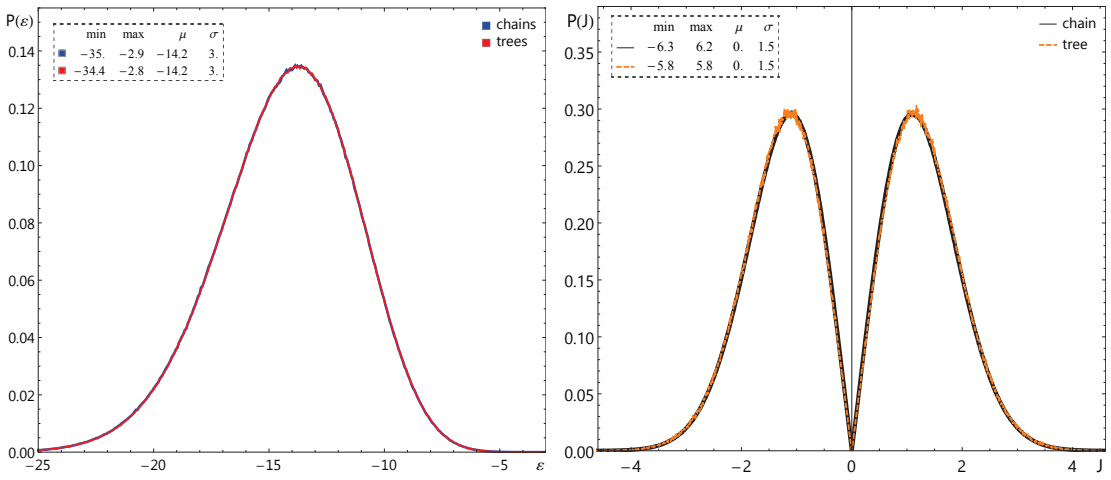

Figure 6. The distributions of energies and spin-spin coupling constant. The distributions of energies and spin-spin coupling constant. The black curves denote the results of calculations using $\mathbb{P}$ algorithm, while beige curves are constructed in result of calculations by $\mathbb{NP}$ algorithm.

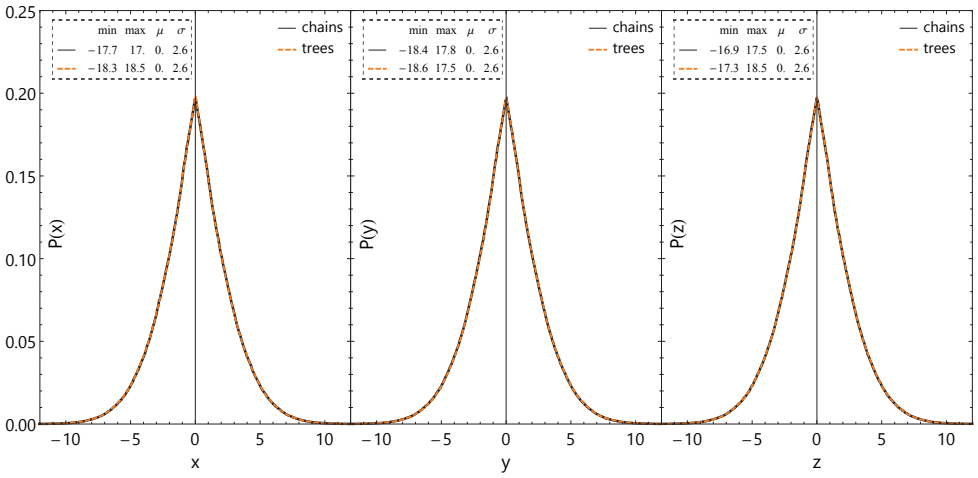

Figure 7. The distributions of polarizations in the ensemble of spin-chains by axes, which are calculated using $\mathbb{NP}$ (beige curves) and $\mathbb{P}$ (black curves) algorithms.

in the form of a large number of independent configurations (roots), i.e. the large set of the first two spins and coupling constants between them; $\{\Omega_1^1 = (\boldsymbol{s}_1^1, \boldsymbol{s}_1^1; J_{1,2}^1)_1, ...\Omega_N^1 = (\boldsymbol{s}_1^1, \boldsymbol{s}_2^1; J_{1,2}^1)_N\} = \hat{\Omega}$ (see the two scheme on Fig. 3).

The steps of simulation using the algorithm $\mathbb{NP}$ are as follows (the left scheme on Fig. 3). Using the initial data, $\hat{\Omega}$ we perform parallel calculations of all graphs $G_i(n)$ of the ensemble $G_i(n) \subset \{G(n)\}_N$. Note that each of these graphs in terms of classical mechanics, represents itself the set of classical trajectories that go out from one initial value (*root*). Recall that this is due to the fact that spins are in states of local minimum energy in all nodes of each graph with the exception of the set of nodes coinciding with the origin and ends of a graph. The database which is obtained in the result of simulation using $\mathbb{NP}$ algorithm allows to construct distributions of the main parameters

of the statistically equilibrium ensemble.

The simulation by $\mathbb{P}$ algorithm (the right scheme on Fig. 3), is performed in a similar way but with the difference that in this case instead of the set of graphs $\{G(n)\}_N$ we *grow* the set of strings $\{g(n)\}_N$. In this case from each graph we choose only one string as the *representative*. Note, that the string (branch) $g_j(n) \subset \{G(n)\}_N$ we grow by way of randomly selecting only one solution in each node. In the result of parallel simulation of the set of strings, we get the database which allows to construct the distributions of main parameters of the statistical equilibrium ensemble $\{G(n)\}_N$ with the asymptotic accuracy $O(N^{-1/3})$.

We compared the results of numerical simulations on the example of the statistical ensemble, $\{G(20)\}_{5\cdot 10^4}$ consisting from $5 \cdot 10^4$ graphs by heights 20 with the ensemble $\{g(20)\}_{5\cdot 10^4}$ which consists from the $5 \cdot 10^4$ strings of lengths 20. As can be seen from Fig. 6 and Fig. 7, in the limit of statistical equilibrium, the distributions of various parameters of the statistical ensemble that have calculated using of two $\mathbb{NP}$ and $\mathbb{P}$ algorithms coincide ideal.

Thus we have shown on the example of $1D$ Heisenberg spin glass, that the $\mathbb{NP}$ hard problem with given accuracy may be reduced to the $\mathbb{P}$ problem and respectively the **hypothesis** is proved.

6. Partition function

Now it is important to return to the definition of the main object of statistical physics, i.e. to the partition function. It is well known that the multiparticle classical system in the state of statistical equilibrium in the configuration space is described by the partition function of type:

$$Z(\beta) = \int ... \int \exp\{-\beta\, \mathcal{H}(\{\mathbf{r}\})\} d\mathbf{r}_1 ..., d\mathbf{r}_N, \qquad \beta = 1/k_B T, \quad \{\mathbf{r}\} = (\mathbf{r}_1, ..., \mathbf{r}_N), \tag{28}$$

where $\mathcal{H}(\{\mathbf{r}\})$ is the Hamiltonian of the system in the configuration space, k_B and T are the Boltzmann constant and temperature of the system respectively.

For the considered model the partition function is calculated exactly and has the following form [21]:

$$Z(\beta, \{J\}) = \prod_{i=1}^{n} \frac{sinh(a_i)}{a_i}, \qquad a_i = \beta J_{i,\,i+1}, \tag{29}$$

where the coupling constant $J_{i,\,i+1} \in \{J\} = (J_{1,\,2}, J_{2,\,3}, ...J_{n-1,\,n})$ is the random variable.

The average value of the partition function for the ensemble may be found after averaging over the distribution of the coupling constant. It is often assumed that this distribution is Gaussian:

$$W(J) = \frac{1}{\sigma_J \sqrt{2\pi}} \exp\Big\{-\frac{(J - J_0)^2}{2\sigma_J^2}\Big\}, \tag{30}$$

where σ_J is the variance and J_0 is the average value of coupling constant.

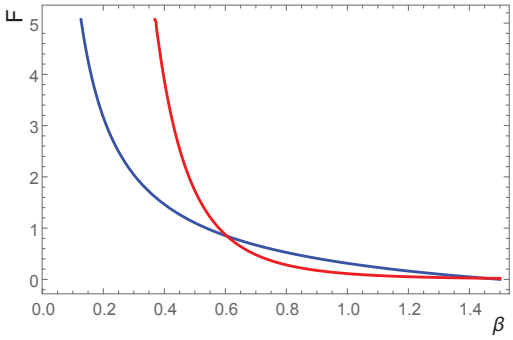

Figure 8. The free energy of the ensemble which is calculated by two methods. The red curve is obtained at using of the expression (33), while the blue curve is obtained in the result of calculation by the expression (32). Note that parameters of ε_0 and σ_ε are found by the way of simulation of problem from first principles, whereas parameters J_0 and σ_J chosen on the basis of the best approximation to the red curve.

After averaging of the expression for the partition function (29) by the distribution (30), it is easy to find:

$$\bar{Z}(\beta) = \int_{-\infty}^{+\infty} Z(\beta, \{J\}) W(J) dJ = \frac{K(\beta)}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Big(\frac{\sinh(\sigma_J \beta x)}{\sigma_J \beta x} \Big)^n \exp\Big\{ -\frac{1}{2}(x - x_0)^2 \Big\} dx, \quad (31)$$

where $x = J/\sigma_J$ and $x_0 = J_0/\sigma_J$, in addition $K(\beta)$ denotes the normalization factor of the partition function:

$$K^{-1}(\beta) = \frac{1}{2\bar{J}} \int_{-\bar{J}}^{\bar{J}} \Big(\frac{\sinh(J\beta)}{J\beta} \Big)^n dJ = \frac{1}{\bar{y}} \int_0^{\bar{y}} \Big(\frac{\sinh(y)}{y} \Big)^n dy, \qquad J \in [\bar{J}, -\bar{J}],$$

with $\bar{J} > 0$ and $\bar{y} = \bar{J}\beta$. Recall that the coefficient $K(\beta)$ is constructed in such way that the Helmholtz free energy in the limit $\beta \to \infty$ converges to zero.

The Helmholtz free energy per one spin in chain is calculated by the following formula:

$$F(\beta) = -\frac{1}{n\beta} \ln \bar{Z}(\beta). \quad (32)$$

Since integration in the representation (28) is carried out by the full configuration space, then obviously we take into consideration also contributions of spin configurations, which are physically unrealizable. Let us note that usually, the measure of set of such spin configurations is assumed to be equal to zero without any serious proof, that not only groundlessly but in a number of cases may be incorrect. Taking into account the fact that a set of strings describing the statistical ensemble in configuration space formally can be represented as a trajectory of dynamical system, in the limit of ergodicity of system (see [27, 28]), for the partition function the following representation may be written:

$$Z_\star(\beta) = \int_{-\infty}^{-n/\beta} \bar{P}(\varepsilon) d\varepsilon, \qquad \bar{P}(\varepsilon) = c^{-1} P(\varepsilon), \quad c = \int_{-\infty}^{0} P(\varepsilon) d\varepsilon, \quad (33)$$

where $\varepsilon < 0$ denotes the energy of $1D$ spin-chain, while $\bar{P}(\varepsilon)$ the normalized energy distribution of the ensemble. If the energy distribution (see Fig. 6) to approximate by the Gaussian function (see (30)) then using the representation (33), for the free energy attributable to a single spin is found the following analytical expression:

$$F_\star(\beta) = -\frac{1}{n\beta}\ln\Big\{\frac{1}{2}\Big[1 - erf\Big(\frac{\varepsilon_0 + n/\beta}{\sqrt{2}\sigma_\varepsilon}\Big)\Big]\Big\}, \tag{34}$$

where $\varepsilon_0 = \mu < 0$ (see Fig. 6) denotes the average energy of spin-chain in the ensemble and σ_ε respectively denotes the variance of spin-chains energy distribution. Comparing Helmholtz's free energies $F(\beta)$ and $F_\star(\beta)$ for the ensemble $\{g(20)\}_{5\cdot 10^5}$ shows that already at finite temperatures these curves diverge sharply (see Fig. 8). Furthermore, near the temperature $\beta \simeq 0.3$, the ensemble of spin-chains exhibits a critical behavior, since the free energy tends to infinity that is characteristic at phase transitions of first order. The latter obviously connected with taking into account of contribution non-physical configurations in the representation (28) and in formulas (29) and (30) respectively.

7. Conclusion

We have studied $1D$ spin glass in the framework of Heisenberg's nearest-neighboring Hamiltonian. Using the Hamiltonian (1) we obtained the system of recurrent algebraic equations (3) which together with conditions of energy minimum in nodes (5) allow to implement node-by-node calculations and to construct stable spin-chains. It is proved, that in the considered model the system of spins form only such spin-chains where into in each spin-chain all spins lie in one plane, while the planes of two arbitrary spin-chains, relative to each other can have an any angle. Another important property of equations system (3) consists in the probability of branching of solution in each node of $1D$ lattice. This leads to the fact that in result of consecutive calculations, from the one initial condition (*root*) on the *n-th* step, we get a set of solutions (stable spin-chains or Kolmogorov's strings $g_i(n)$) that form the *Fibonacci subtree* (random graphs $G_j(n) \supseteq g_i(n)$).

Thus when we say on the statistical ensemble we mean the set of random graphs $\{G(n)\}_N$, where N denotes number of graphs in the ensemble and correspondingly the problem is consists in that to calculate all parameters and corresponding distributions characterizing the ensemble.

It is shown that the computational complexity of an arbitrary graph $G_j(n)$ is the $\mathbb{NP}$ hard of the order $2^n K_s(n)$, while complexity of the ensemble, with increasing number of elements is increases linearly, $\{G(n)\}_N$ is the $\sim 2^n N K_s(n)$. The properties of random graphs depending on their height are studied in detail (see Fig.s 4-5) by using $\mathbb{NP}$ algorithm (see the left scheme on Fig. 3) and conditions at which the ensemble $\{G(n)\}_N$ is in the state of the statistical equilibrium are formulated. We analyzed and proposed the hypothesis that the $1D$ spin glass in the limit of statistical equilibrium may be simulated by using $\mathbb{P}$ algorithm (see the right scheme on Fig. 3). Let us note, that all

theoretical results and predictions have been confirmed with high accuracy in numerical experiments that have been performed using $\mathbb{NP}$ and $\mathbb{P}$ algorithms (see Fig.s 5-7). It is noteworthy that the simulation by the algorithm $\mathbb{P}$ not only ensures high precision but also allows to find distributions of all parameters of the ensemble, including the distribution of a constant spin-spin coupling (see Fig. 5).

In the work has been suggested a new representation for the partition function in the form of one dimensional integral from the spin-chain's energy distribution (see the expression (33)). We have compared the Helmholtz's free energies which were calculated by using the usual (32) and new (34) representations. As it is shown (see Fig. 8), already at finite temperatures the corresponding curves significantly different, moreover near $\beta \sim 0.3$ the ensemble of spin-chains demonstrates critical property, that usually occurs at first order phase transitions. This is obviously due the fact that in the formula (31), only such spin configurations are counted which satisfy to the basic principles of classical mechanics (see expressions (3) and (5)).

Thus, the main advantages of developed approach are that we have received clear answers, to all raised questions on the example of study $1D$ spin glass from the first principles of the classical mechanics without using any additional assumptions. In addition we showed that in the limit of statistical equilibrium (at ergodicity of the statistical system), the initial $\mathbb{NP}$ hard problem is reduced to the $\mathbb{P}$ problem that allows the simulation of spin glasses radically simplify.

The ideas lying in the base of developed approach enough are universal and allow the generalization of model for a multidimensional case and at presence of external fields [29].

Finally, a new formulation of the problem of spin glasses and disordered systems in general can be very useful for study of a global problem, i.e the problem of reduction $\mathbb{NP}$ to the $\mathbb{P}$.

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