Mathematical Problems of Computer Science 44, 22–32, 2015.

Computation Statistical Properties of Disordered Spin Systems from the First Principles of Classical Mechanics

Ashot S. Gevorkyan[1,2] and Vahe V. Sahakyan[1]

[1] Institute for Informatics and Automation Problems of NAS RA
[2] Institute of Chemical Physics of NAS of RA
e-mail: g_ashot@sci.am

Abstract

We study the classical $1D$ spin glasses in the framework of Heisenberg model. Based on the Hamilton equations we obtained the system of recurrence equations, which allows performing node-by-node calculations of a spin-chain. It is shown that the calculations from the first principles of classical mechanics lead to $\mathbb{NP}$ hard problem, that however, in the limit of the statistical equilibrium can be calculated by $\mathbb{P}$ algorithm. For the partition function of the ensemble a new representation is offered in the form of one-dimensional integral of spin-chains' energy distribution.

Keywords: Disordered system, Heisenberg spin glass, Ergodic ensemble, $\mathbb{NP}$ hard problem, $\mathbb{P}$ algorithm.

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., are well described mathematically by models of spin glasses [1]–[10]. Despite of numerous studies 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 and useful in terms of developing modern technology. We can mention a few important ones;

a) The simulation of spin glasses far from thermodynamic equilibrium. Obviously, in such cases, we cannot 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 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, moreover spin glasses, always are in metastable states, where parameters characterizing spin glass 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 spin-chains which are unstable from the point of view of 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 requires 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 is in the diverging equilibration at simulations by the Monte Carlo methods [15]. Recently in the statistical physics a rapid growth of the number of works has accurred which are using combinatorial optimization methods [16, 17, 18]. In particular, a number of disordered statistical systems have been mapped onto combinatorial problems for which fast combinatorial optimization algorithms are available [19, 20]. So, combinatorial methods and the corresponding algorithms are often used for 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 study by traditional techniques, for example, by Monte Carlo simulations [11]). However, the above-mentioned problems, for which we want to receive clear answers obviously require the development of principally new approaches.

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

And lastly, one of the important purposes of this work is argumentation of the possibility of reduction of the initial $\mathbb{NP}$-hard problem to the $\mathbb{P}$ problem, when the spin-chains' ensemble comes to the statistical equilibrium state.

2. Definition of Model

The disordered $1D$ spin system, in the nearest-neighboring model is written as ([21]):

$$H = -\sum_{i\in\mathcal{N}} J_{i,\,i+1} s_i s_{i+1}, \qquad s_i \in \mathbb{R}^3, \qquad ||s_i|| = ||s_{i+1}|| = 1, \tag{1}$$

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 spatial spins. The distribution of the coupling constants will be found below, in the result of numerical modeling.

Since the norm of vector $s_i = (x_i, y_i, z_i)$ is equal to the unit, then the projection, z_i can be represented in the following form:

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

Substituting (1) into the Hamilton equations (see, for example, ([22])) we can find:

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

where the following notations are made, $\ddot{\xi}_i = \partial^2\xi_i/\partial t^2$ and $\xi = (x, y)$, in addition "t" denotes the usual time. We will assume that near the nodes spins are localized and quasi-periodic movements commit, $\xi_i(t) = \xi_i^0 + \delta_i^{\xi}(t)$, where ξ_i^0 and $\delta_i(t)$ denote the position of the equilibrium and quasi-periodic function of the time, respectively. Below we will study the statistical properties of the system, which are formed on time scales $\tau >> \tau_0$, where τ_0 is a characteristic time of spins oscillation and obviously, in this case; $\langle\ddot{x}\rangle_{\tau_0} = \langle\ddot{y}\rangle_{\tau_0} \approx 0$.

Averaging equations (3) on the period τ_0 can be found:

$$\begin{aligned} J_{i-1,\,i}(x_{i-1} - x_i z_i^{-1} z_{i-1}) + J_{i,\,i+1}(x_{i+1} - x_i z_i^{-1} z_{i+1}) = 0, \\ J_{i-1,\,i}(y_{i-1} - y_i z_i^{-1} z_{i-1}) + J_{i,\,i+1}(y_{i+1} - y_i z_i^{-1} z_{i+1}) = 0, \end{aligned} \tag{4}$$

where for simplicity in equations the index "0" over of variables are omitted, i.e., $x_i^0 \to x_i$, $y_i^0 \to y_i$ and $z_i^0 \to z_i$. As it is easy to verify these equations define the condition at which the Hamiltonian (1) in the *i-th* node takes an extremal value.

Solving the system of equations (4) with respect to variables x_{i+1} and y_{i+1} may be found:

$$x_{i+1} = C_x/J_{i,\,i+1}, \qquad y_{i+1} = C_y/J_{i,\,i+1}, \tag{5}$$

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) the conditions of a local minimum can be set. It is obvious *i-th* spin is in stable equilibrium if the following inequalities are satisfied:

$$A_{x_i x_i}(s_i^0) > 0, \qquad A_{x_i x_i}(s_i^0) A_{y_i y_i}(s_i^0) - A_{x_i y_i}^2(s_i^0) > 0, \tag{6}$$

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 s_i^0 denotes *i-th* spin which is in a stable equilibrium.
Using (2), (4) and (6), the explicit forms of the second order derivatives can be calculated:

$$A_{\eta_i\eta_i} = (\eta_i^2 + z_i^2) z_i^{-3} \Delta_i, \quad A_{x_i y_i} = x_i y_i z_i^{-3} \Delta_i, \quad \Delta_i = (J_{i-1,\,i} z_{i-1} + J_{i+1,\,i} z_{i+1}), \tag{7}$$

and taking into account (6) and (7) the conditions of a local minimum energy may be found:

$$A_{x_i x_i} = (1 - y_i^2) z_i^{-3} \Delta_i > 0, \quad A_{x_i x_i} A_{y_i y_i} - A_{x_i y_i}^2 = z_i^{-4} \Delta_i^2 > 0. \tag{8}$$

Since, at the $z_i > 0$ both conditions in (8) are satisfied:

$$\Delta_i = (J_{i-1,\,i} z_{i-1} + J_{i+1,\,i} z_{i+1}) > 0. \tag{9}$$

Thus, in each node the solutions determining the orientation of the spin in the state of the local equilibrium can be found. If there is such coupling constants $J_{i,\,i+1}$, for which not only the conditions (8) or (9) are satisfied, but also the following inequality holds:

$$J_{i,\,i+1}^2 \geq C_x^2 + C_y^2 > 0. \tag{10}$$

3. The Statistical Ensemble of $1D$ Disordered Spin-Chains

It is easy to show, that the solutions of equations (5) satisfying inequalities (8) can be of two types:

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

Note that the solutions which are denoted with signs "+" and "−" are characterized as follows, if the previous solution is the *queen* "+", up to two different solutions may be found; $\boldsymbol{s}^{+}_{i+1}$ and $\boldsymbol{s}^{-}_{i+1}$, while after the *drone* "−" the solution is 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 branchings number depending on the height of $\widehat{FsT}_i$ can be calculated as follows:

$$M(n) = M(n-1)\lfloor(2\xi_n)\rfloor = \lfloor 2^{n\eta(n)}\rfloor, \quad \eta(n) = 1 + n^{-1}\sum_{k=1}^{n}\log_2(\xi_k) > 0, \tag{11}$$

where $M(n-1)$ number of branchings at the height $(n-1)$ and ξ_k denotes a random coefficient which belongs to the interval $[1/2, 1]$. For simplification in the expression (11) the subtree's number i is omitted. Since each $\widehat{FsT}_i$ consists of the set of nodes and the set of edges (the set of constants $\{J\} = [J_{1,2}, J_{2,3}, ...J_{n-1,n}]$), 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 [23, 24].

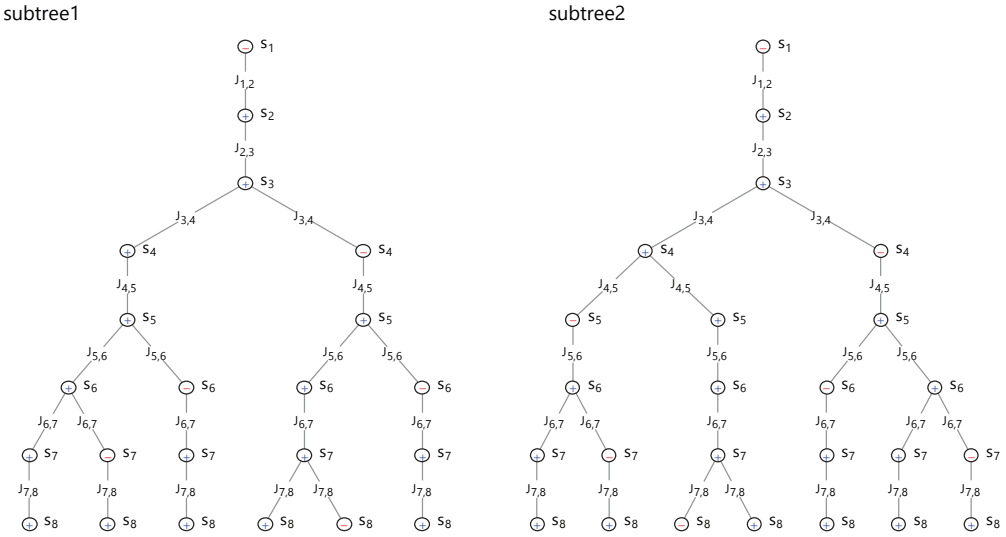

Fig. 1. Two different Fibonacci subtrees (graphs) each with the height 8. Both of graphs grow from the same initial data (*root*) in the result of two independent numerical experiments. The same symbols s_i and $J_{i,j}$ on different graphs can have completely different values.

Thus, for calculations of different physical parameters of the statistical ensemble, it is necessary to take into account the contribution of all independent graphs $\{G(n)\} = [G_1(n), ...G_i(n), ...]$.

With regard to the graph computation complexity, it is easy to prove that:

$$K_G(n) \propto M(n)K_s(n), \tag{12}$$

where $M(n) \propto 2^n$ is the value of branching on the step n, $K_s(n)$ denotes Kolmogorov's complexity of the string $g_j(n)$, while $K_G(n)$ denote the complexity of the graph $G_i(n) \subset \{G(n)\}_N$. The computational complexity of $\{G(n)\}_N$ obviously will be $K_{ens} \propto NM(n)K_s(n)$, where N is the total number of graphs in the ensemble.

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

$$E[f] = \bar{f} = \frac{\sum_{i=1}^{N} w_i \bar{f}_i}{\sum_{i=1}^{N} w_i}, \qquad w_i = N_i/\bar{N}, \tag{13}$$

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 random variable f in the $G_i(n)$, which is calculated similarly to formula (13).

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 (13) writing it as:*

$$E[f] = \bar{f} = \frac{1}{N} \sum_{j=1}^{N} \tilde{f}_j + O(N^{-1/3}), \tag{14}$$

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

Thus, the computation of statistical parameters of the disordered spin system by the formula (13) is algorithmically equivalent to solving of $\mathbb{NP}$ hard problem, while the simulation by the formula (14) is the $\mathbb{P}$ problem.

4. The Numerical Experiments

As a rule the problems of spin glasses are studied in the framework of the partition function representation by methods of Monte Carlo which, however, do not allow to answer 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, obviously, cannot be studied using Monte Carlo methods, because these methods are adapted only for calculating the *ground state*.

At first let us consider one set of initial data Ω_i^1 (roots) 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 (5), with consideration of inequality conditions (8), 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 log-normal distribution ([25]) a random constant $J_{i,\,i+1}$ and exactly to calculate the orientation of spin 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.

We calculated the characteristic distributions and parameters of the $1D$ spin glass, which is in the state of the statistical equilibrium using two algorithms which are based on formulas (13) and (14), respectively. For the simulation of the problem, first of all we need

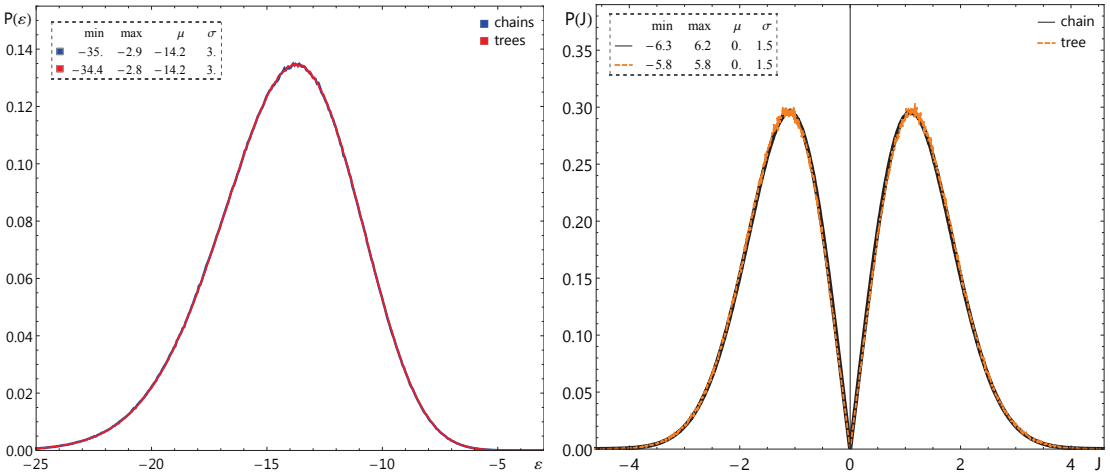

Fig. 2. The distributions of energies and spin-spin coupling constant. The beige curves denote the results of calculations using the algorithm with the complete enumeration of all branches of graphs (conditionally we will call $\mathbb{NP}$ algorithm), while black curves are constructed in the result of calculations by $\mathbb{P}$ algorithm.

to specify initial conditions 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; $\{\Omega_1^1 = (s_1^1, s_1^1; J_{1,2}^1)_1, ...\Omega_N^1 = (s_1^1, s_2^1; J_{1,2}^1)_N\} = \hat{\Omega}$.

The steps of simulation using the algorithm $\mathbb{NP}$ are as follows. 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 the set of classical trajectories that go out from one initial value (*root*). 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 which is based on the formula (14), 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 a *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 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 of the $5 \cdot 10^4$ strings of lengths 20. As it can be seen from Fig. 2, the distributions of various parameters of the statistical ensemble that have been calculated in the limit of statistical equilibrium using two $\mathbb{NP}$ and $\mathbb{P}$ algorithms coincide ideally.

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

5. Partition Function

Now we can return to the definition of the main object of statistical physics, i.e., the partition function. As known the multiparticle classical system in the state of the statistical equilibrium in the configuration space is described by the partition function of type:

$$Z(\beta) = \int ... \int \exp\{-\beta\,\mathcal{H}(\{\mathbf{r}\})\} \lceil \mathbf{r}_\infty ..., \lceil \mathbf{r}_\mathcal{N}, \qquad \beta = \infty/\|_\mathcal{B}\mathcal{T}, \quad \{\mathbf{r}\} = (\mathbf{r}_\infty, ..., \mathbf{r}_\mathcal{N}), \tag{15}$$

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]):

$$Z(\beta, \{J\}) = \prod_{i=1}^{n} \frac{sinh(a_i)}{a_i}, \qquad a_i = \beta J_{i,\,i+1}, \tag{16}$$

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, can be found by way of averaging over the distribution of the coupling constant. It is often assumed that the distribution is Gaussian:

$$W(J) = \frac{1}{\sigma_J\sqrt{2\pi}} \exp\Big\{-\frac{(J-J_0)^2}{2\sigma_J^2}\Big\}, \tag{17}$$

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

Averaging of the partition function (16) by the distribution (17) can find:

$$\bar{Z}(\beta) = \int_{-\infty}^{+\infty} Z(\beta, \{J\}) W(J) dJ = \frac{K(\beta)}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Big(\frac{\sinh(\sigma_J\beta x)}{\sigma_J\beta x}\Big)^n e^{-\frac{1}{2}(x-x_0)^2} dx, \tag{18}$$

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

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

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

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

$$F(\beta) = -\frac{1}{n\beta} \ln \bar{Z}(\beta). \tag{19}$$

Since the integration in representation (15) is carried out over the complete configuration space, then obviously we take into account also the contributions of physically unrealizable spin configurations. Recall that usually the measure of a set of such spin configurations is assumed to be equal to zero without any serious proof, that not only groundless, but in some cases may be wrong. Taking into account the fact that a set of strings describing the statistical ensemble in configuration space formally can be represented as a trajectory

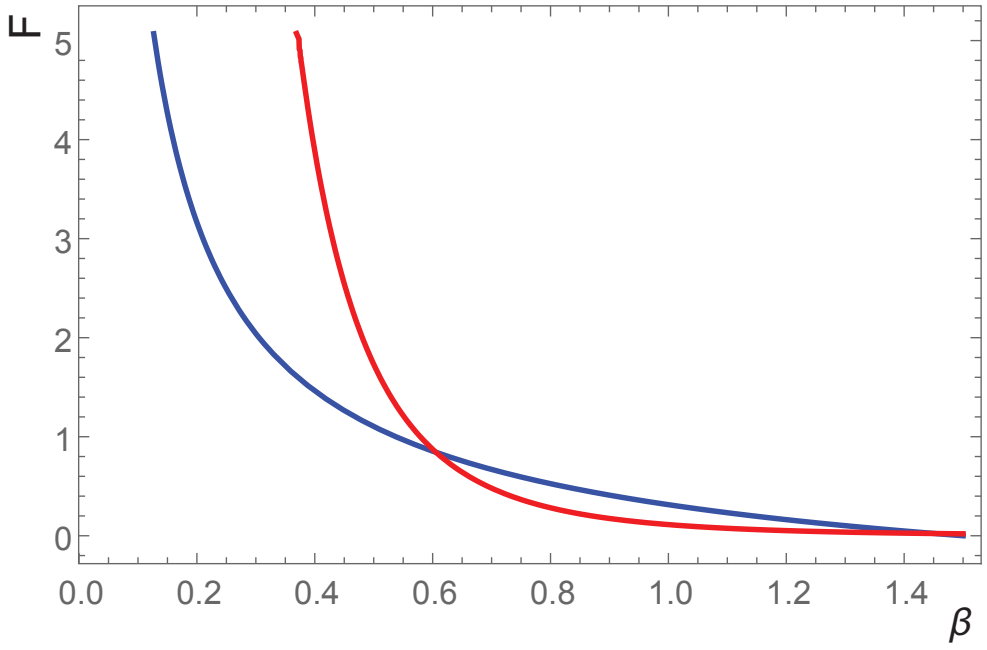

Fig. 3. The free energy of the ensemble. The red curve is obtained at using of the expression (20), while the blue curve is obtained in the result of calculation by the expression (19). Note that parameters of ε_0 and σ_ε are found by the way of simulation of problem from the first principles, whereas parameters J_0 and σ_J are chosen for reasons of the best approximation to red curve.

of dynamical system, in the limit of ergodicity of system (see [26, 27]), for the partition function the following representation may be written:

$$Z_\star(\beta) = \int_{-n\varepsilon_0}^{-n/\beta} \bar{P}(\varepsilon)d\varepsilon, \qquad \bar{P}(\varepsilon) = c^{-1}P(\varepsilon), \quad c = \int_{-n\varepsilon_0}^{0} P(\varepsilon)d\varepsilon, \tag{20}$$

where $\varepsilon < 0$ and $\varepsilon_0 = \mu < 0$ (see Fig. 2) denote the energy of $1D$ spin-chain and its average energy, respectively, $\bar{P}(\varepsilon)$ is the normalized energy distribution. If the energy distribution (see Fig. 2) to approximate by Gaussian function (see expression (17)), then using the representation (20), for the free energy attributable to a single spin we obtain the following analytical expression:

$$F_\star(\beta) = -\frac{1}{n\beta}\ln\Big\{\frac{1}{2}\Big[1 - erf\Big(\frac{\varepsilon_0 + n/\beta}{\sqrt{2}\sigma_\varepsilon}\Big)\Big]\Big\}, \tag{21}$$

where σ_ε 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 these curves diverge sharply already at finite temperatures (see Fig. 3). As we can see, near the temperature $\beta \simeq 0.3$, the ensemble of spin-chains exhibits a critical behavior, since the free energy tends to infinity (the red curve) that is characteristic to the phase transitions of the first order. The latter obviously is connected with the fact that in the expression (21), only the physically realizable spin configurations are taken into account.

6. Conclusion

We studied $1D$ spin glass in the framework of Heisenberg's nearest-neighboring Hamiltonian from the first principles of the classical mechanics. It was shown that in the framework of the considered approach, even this simple task, which in a sense, is exactly solvable, corresponds to the category of $\mathbb{NP}$-hard (see the estimation of complexity (11)). It was proved that in the limit of the statistical equilibrium the computational $\mathbb{NP}$-hard problem, with a given accuracy to the $\mathbb{P}$ problem is reduced. The developed method as opposed to standard approach allows to calculate the statistical distributions of all parameters of the ensemble, including the distribution of coupling constant (see Fig. 2).

In the paper, a new representation was suggested for the partition function in the form of one dimensional integral from the spin-chains' energy distribution (see the expression (20)). We have compared the Helmholtz's free energies which were calculated by using the usual (19) and new (21) representations. As it is shown (see Fig. 3), the corresponding curves are significantly different already at finite temperatures, moreover, near the value $\beta \sim 0.3$ the ensemble of spin-chains demonstrates a critical property, that usually occurs at first-order phase transitions. This is obviously due to the fact that in the formula (21), only such spin configurations are presented which satisfy the basic principles of classical mechanics (see expressions (4)-(9).

Thus, the main advantages of the developed approach are that we have received clear answers to all the raised questions on the example of study $1D$ spin glass from the first principles of the classical mechanics without using any additional assumptions.

The ideas lying in the base of the developed approach are enough universal and allow the generalization of model for a multidimensional case and at presence of external fields ([28]).

Lastly, note that the new formulation of the problem of spin glasses and disordered systems in general might become very useful for investigation of the more global problem: namely, the problem of reduction of $\mathbb{NP}$ hard to the $\mathbb{P}$ problem.

References

[1] K. Binder and A. Young, "Spin glasses, Experimental facts, theoretical concepts and open questions", *Rev. Mod. Phys.*, vol. 58, pp. 801-976, 1986.

[2] M. Mézard, G. Parisi and M. Virasoro, "Spin Glass Theory and Beyond (World Scientific)", Singapore 1987.

[3] A. Young, *Spin Glasses and Random Fields*, World Scientific, Singapore, 1998.

[4] R. Fisch and A. Harris, "Spin-glass model in continuous dimensionality", *Phys. Rev. Lett.*, vol. 47, page 620, 1981.

[5] C. Ancona-Torres, D. Silevitch, G. Aeppli and T. Rosenbaum, "Quantum and classical glass transitions in LiHoxY1-xF4", *Phys. Rev. Lett.*, vol. 101, no. 5, 057201, 2008.

[6] A. Bovier, *Statistical Mechanics of Disordered Systems, A Mathematical Perspective*, Cambridge Series in Statistical and Probabilistic Mathematics, 2006.

[7] Y. Tu, J. Tersoff and G. Grinstein, "Properties of a Continuous-Random-Network model for amorphous systems", *Phys. Rev. Let.*, vol. 81 ,page 2490, 1998.

[8] K. Chary and G. Govil, "NMR in biological systems, from molecules to human", Springer, vol. 6, page 511, 2008.

[9] E. Baake, M. Baake and H. Wagner, "Ising quantum chain is a equivalent to a model of biological evolution", *Phys. Rev. Let.*, vol. 78, page 559, 1997.

[10] A. S. Gevorkyan and H. G. Abajyan, "A new parallel algorithm for simulation of spin glasses on scales of space-time periods of external fields with consideration of relaxation effects", *Phys. of Particles and Nuclei Letters*, vol. 9, no. 6-7, page 530, 2012.
[11] F. Liers, M. Palassini, A. K. Hartmann and M. Jünger,"Ground state of the Bethe lattice spin glass and running time of an exact optimization algorithm",*Phys. Rev. B*, **68**, 094406, 2003.
[12] J. C. Angles, D'Auriac, M. Preissmann and A. Sebo Leibniz-Imag, "Optimal cuts in graphs and statistical mechanics", *Mathl. Comput. Modeling*, **26**, no. S-10, page 11, 1997.
[13] C. Papadimitriou, *Computational Complexity*, (1st ed.). Addison-Wesley. Section 2.7: *Nondeterministic machines*, 1993.
[14] H. R. Lewis and C. Papadimitriou, *Elements of the Theory of Computation*, (1st ed.). Prentice-Hall. Section 4.6: *Nondeterministic Turing Machines*, 1981.
[15] N. Metropolis, A. Rosenbluth, M. Rosenbluth, A. Teller and E. Teller, "Equation of State Calculations by Fast Computing Machines", *J. Chem. Phys.*, vol. 21, no. 6, page 1087, 1953.
[16] B. Hayes, "Can't get no satisfaction", *Am. Scientist*, vol. 85, page 108, 1997.
[17] R. Monasson et all, Diameter of the world wide web, Nature, London, **400**, 133, 1999.
[18] Special issue of Theor. Comput. Sci. **265**, edited by O. Dubois, R. Monasson, B. Selman, and R. Zecchina, 2001.
[19] M. J. Alava, P. M. Duxbury, C. F. Moukarzel and H. Rieger, *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. Lebowitz, Academic Press, New York, **18**, 2001.
[20] A. K. Hartmann and H. Rieger, *Optimization Algorithms in Physics*, While-VCH, Berlin, 2001.
[21] C. J. Thompson, "Phase Transitions and Critical Phenomena", *Academic Press*, vol. 1, pp. 177-226, 1972.
[22] H. Goldstein, *Classical Mechanics*, Reading, MA: Addison-Wesley, 2nd ed., 1980.
[23] A. N. Kolmogorov, "Logical basis for information theory and probability theory", *IEEE Transactions on Information Theory*, vol. 14, no. 5, pp. 662–664, 1968.
[24] M. Li and P. Vitányi, *An introduction to Kolmogorov Complexity and its Applications*, New York, Springer-Verlag, 1997.
[25] S. Y. Park and A. K. Bera, "Maximum entropy autoregressive conditional heteroskedasticity model", *Journal of Econometrics*, Elsevier, vol. 50, no. 2, pp. 219–230, 2009.
[26] G. D. Birkhoff, "What is the ergodic theorem?", *The American Mathematical Monthly*, vol. 49, no. 4, pp. 222–226, 1942.
[27] V. I. Arnol'd and A. Avez, *Ergodic Problems of Classical Mechanics*, New York, W.A. Benjamin, 1968.
[28] E. A. Ayryan, A. S. Gevorkyan and V. V. Sahakyan, "New algorithm for simulation of 3D classical spin glasses under the influence of external electromagnetic fields", *Physics of Particles and Nuclei Letters*, vol. 2, no. 3, pp. 380–384, 2015.

Submitted 15.07.2015, accepted 27.11.2015

Չկարգավորված սպինային համակարգերի վիճակագրական հատկությունների հաշվարկը ելնելով դասական մեխանիկայի հիմնարար սկզբունքներից

Ա. Գևորգյան և Վ. Սահակյան

Ամփոփում

Մենք հետազոտել ենք դասական 1D սպինային ապակիները Հայզենբերգի մոդելի շրջանակներում: Հիմնվելով Համիլտոնի հավասարումների վրա դուրս է բերված ռեկուրենտ հավասարումների համակարգ, որը թույլ էտալիս իրականացնել սպինային շղթաների հաշվարկը հանգույց առ հանգույց: Ցույց է տրված, որը դասական մեխանիկայի հիմնարար սկզբունքների հիման վրա հաշվարկները բերում են NP բարդ խնդրի, որը սակայն վիճակագրական հավասարակշռության սահմանում տրված ժշտությամբ հաշվվում է P ալգորիթմի միջոցով: Անսամբլի վիճակագրական գումարի համար առաջարկված է մեկչափանի ինտեգրալային ներկայացում սպինային շղթաների էներգիայի բաշխման ֆունկցիայից:

Вычисление статистические свойства неупорядоченных спиновых систем из первых принципов классической механики

А. Геворкян и В. Саакян

Аннотация

Мы исследовали классические спиновые стекла в рамках 1D модели Гейзенберга. Основываясь на уравнениях Гамильтона, выведена система рекуррентных уравнений, которая позволяет осуществлять вычисление спиновой цепочки узел за узелом. Показано, что проведенные на основе основных принципов классической механики расчеты сводятся к NP трудной задаче, которая, тем не менее, в пределе статистического равновесия с заданной точностью вычисляется P алгоритмом. Для статистической суммы ансамбля предложено одномерное интегральное представление от распределения энергии спиновой цепочки.