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A NEW PARALLEL ALGORITHM FOR SIMULATION OF SPIN GLASSES ON SCALES OF SPACE-TIME PERIODS OF EXTERNAL FIELDS WITH CONSIDERATION OF RELAXATION EFFECTS

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Новый параллельный алгоритм для моделирования спиновых стекол
на масштабах периодов пространства-времени внешних полей
с учетом релаксационных эффектов

Исследованы статистические свойства ансамбля неупорядоченных 1D-пространственных спин-цепочек (ПСЦ) с определенной длиной во внешнем поле с учетом релаксационных эффектов. Для решения этой проблемы впервые был использован короткодействующий комплексно-классический гамильтониан. Получена система рекуррентных уравнений в узлах решетки спин-цепочки. На основе этих уравнений разработан эффективный математический алгоритм, который с учетом расширенных условий Сильвестра позволяет параллельно шаг за шагом построить большое количество стабильных 1D ПСЦ. Функции распределения различных параметров спинового стекла построены из первых принципов комплексно-классической механики на основе анализа результатов расчета 1D ПСЦ ансамбля. Показано, что распределения разных параметров спинового стекла по-разному ведут себя в зависимости от внешнего поля. Так, распределения энергии и констант спин-спиновых взаимодействий меняются плавно, в то время как распределения поляризации по различным координатам, их средние значения и т. д. даже при небольших внешних полях являются хаотическими (фрустрируют). Исследованы также некоторые критические свойства ансамбля спин-цепочек, такие как возникновение катастроф в уравнении Клаузиуса–Моссотти в зависимости от величины внешнего поля. Показано, что обобщенный комплексно-классический подход исключает возможность возникновения этих катастроф, что позволяет организовать непрерывные параллельные вычисления на всем интервале значений внешнего поля, включая критические точки. На основе проведенных исследований предложен новый, более точный способ построения статистической суммы системы. Эта система в отличие от обычных представлений является комплексной функцией, и ее производные определены везде, включая критические точки.

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Gevorkyan A. S., Abajyan H. G. E5-2011-74
A New Parallel Algorithm for Simulation of Spin Glasses on Scales
of Space-Time Periods of External Fields with Consideration of Relaxation Effects

We have investigated the statistical properties of an ensemble of disordered 1D spatial spin chains (SSCs) of finite length, placed in an external field, with consideration of relaxation effects. The short-range interaction complex-classical Hamiltonian was first used for solving this problem. A system of recurrent equations is obtained on the nodes of the spin-chain lattice. An efficient mathematical algorithm is developed on the basis of these equations with consideration of the advanced Sylvester conditions which allows one step by step to construct a huge number of stable spin chains in parallel. The distribution functions of different parameters of spin-glass system are constructed from the first principles of the complex classical mechanics by analyzing the calculation results of the 1D SSCs ensemble. It is shown that the behavior of the parameter distributions is quite different depending on external fields. The energy ensembles and constants of spin–spin interactions are changed smoothly depending on the external field in the limit of statistical equilibrium, while some of them such as the mean value of polarizations of ensemble and parameters of its orderings are frustrated. We have also studied some critical properties of the ensemble of such catastrophes in the Clausius–Mossotti equation depending on value of the external field. We have shown that the generalized complex-classical approach excludes these catastrophes allowing one to organize continuous parallel computing on the whole region of values of the external field including critical points. A new representation of the partition function based on these investigations is suggested. As opposed to usual definition, this function is a complex one and its derivatives are everywhere defined, including critical points.

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1. INTRODUCTION

A wide class of phenomena which raise important and difficult calculation problems in physics, chemistry, material science, biology, nanoscience, evolution, organization dynamics, environmental and social structures, human logic systems, financial mathematics, etc., are mathematically well described in the framework of spin-glasses models (see, for example, [1–10]). In literature, two types of mean field models were developed. The first consists of true random-bond models, where the coupling between interacting spins are assumed to be independent random variables [11–13]. The solution of these models is obtained by n-replica trick [11, 13] and requires an invention of sophisticated schemes of replica-symmetry breaking [13, 14]. In the second type of models the bond-randomness is expressed in terms of some underlining hidden site-randomness and is thus of a superficial nature. It has been pointed out in [15–17], however, that this feature retains an important physical aspect of true spin glasses, viz. they are random with respect to the positions of magnetic impurities. Recently, it was shown [18, 19] that the critical properties in some type of dielectrics can be studied by the model of quantum 3D spin glass, on the scales of space-time of external standing electromagnetic fields. As a result, the superlattice of a dielectric constant is formed in the medium. In particular, it was proved that the initial 3D quantum problem can be reduced to two conditionally separable 1D problems on space-time scales of an external field, where one of the problems describes 1D spin glass with random environment.

We have started our investigation from the classical problem concerning the study of statistical properties of 1D spatial spin-chains (SSCs) ensemble in the external fields [20]. Then we have investigated 3D spin-glass problem. We have suggested a new idea which is based on 3D spin-system consideration as a set (ensemble) consisting of 1D spatial spin chains which randomly interact with each other (1D SSCs nonideal ensemble). In particular, we have argued that the model of 1D SSCs nonideal ensemble describes 3D spin glass [22] in the limit of the statistical equilibrium. New high performance parallel algorithms

are developed for both cases. However, as numerical simulation of spin-glass problem shows, critical phenomena can occur even for weak external fields, which makes the calculation of different thermodynamical potentials problematic near the mentioned critical points. The solution of this problem is found by taking into account the relaxation effects within the medium under the influence of external fields. In this paper we discuss in detail the statistical properties of classical 1D spin glasses which suggest that interactions between spins have short-range character and that the system has a possibility to relax under the influence of an external field. Mathematically we solve this problem in the framework of complex-classical Heisenberg Hamiltonian the meaning of which is similar to the idea of classical Newtonian mechanics generalization on complex-classical trajectories [23–27].

In Sec. 2, we formulate problems arising under the generalization of the Clausius–Mossotti equation on space-time's scales of external fields. It is shown that the problem is mathematically equivalent to that of studying statistical properties of a classical ensemble consisting of one-dimensional chains of spatial spins, where all interactions between spins are random and the system of spins is under the influence of external fields. We obtain the recurrent equations and Sylvester's conditions for the construction of stable spin chains of a given length. Definitions of the distribution parameters of the appropriate statistical system are adduced.

In Sec. 3, the recurrent equations on nodes of 1D lattice are analyzed and solutions of angular configuration of $(i+1)$th are found depending on spin–spin interaction constant $J_{i\,i+1}$, angular configurations of previous ith, $(i-1)$th spins and constant $J_{i-1\,i}$. The developed algorithm for simulation of stable spin chains is generalized by means of extension of recurrent equations and the Sylvester inequalities on a complex region taking into account relaxation effects occurring in the spin chain on both internal and external degrees of freedom.

In Sec. 4, the pseudocode of parallel numerical experiments is adduced for simulation of 1D SSCs ensemble with length of $25d_0$. Distributions of complex energy, polarizations and spin–spin interaction constants of relaxing ensemble are investigated in detail.

In Sec. 5, frustration phenomena of mean value of ensemble polarization are investigated in detail depending on external field energy parameter. The necessity of mean values additional averaging for the frustrating parameters of an ensemble is substantiates on fractal structures. The appropriate formulas are provided for the mean polarization and Edwards–Anderson-type orderings parameter of an ensemble. A new kind of complex partition function is formulated the different thermodynamic potentials of which have a regular behavior at critical points.

In section 6, the obtained theoretical and computational results are analyzed in detail. Further development of the proposed approach is suggested.

2. FORMULATION OF THE PROBLEM AND BASIC FORMULAS

It is well known that in isotropic mediums (as well as in the crystals with cubic symmetry) the dielectric constant ϵ_s is well described by the Clausius–Mossotti equation (see [28–31])

$$\frac{\epsilon_s - 1}{\epsilon_s + 2} = \frac{4\pi}{3} \sum_m N_m^0 \alpha_m^0, \tag{1}$$

where N_m^0 is the concentration of particles (electrons, atoms, ions, molecules or dipoles) with given m types of polarizabilities and α_m^0 are correspondingly coefficients of polarizabilities. From this equation follows that the static dielectric constant ϵ_s depends on the polarizability properties of the particles as well as on their topological order. The homogeneity and isotropy of the medium are disturbed in external fields. Nevertheless, there is every reason to expect that formula (1) will be applicable after a minor generalization.

Taking into account the influence of the external electromagnetic fields, the equation for dielectric constant formally may be written like that:

$$\epsilon_{st}(\mathbf{g}) = \frac{1 + 2\Lambda(\mathbf{g})}{1 - \Lambda(\mathbf{g})}, \quad \Lambda(\mathbf{g}) \simeq \frac{4\pi}{3} \left[\sum_m N_m^0 \alpha_m^0 + \varrho(\mathbf{g}) \right]. \tag{2}$$

In (2) the symbol $\epsilon_{st}(\mathbf{g})$ designates the dielectric constant depending on the external field parameters $\mathbf{g} = (\Omega, h_0)$, where Ω and h_0 designate the frequency and the amplitude of the external field, in addition, if the medium can be represented respectively as a model of disordered spin system (spin glass), then $\varrho(\mathbf{g})$ designates the coefficient of polarizability which is connected to orientational effects of spins in an external field. Following from the general considerations, we can represent the medium as an ensemble of 1D spatial spin chains (SSCs) of a certain length L_x (see Fig. 1). Note that the coefficient of polarizability $\varrho(\mathbf{g})$ is the mean value of the polarization of an ensemble in per spin, which is should be complex in general and equal to

$$\varrho(\mathbf{g}) = \frac{\bar{p}(\mathbf{g})}{N_x}, \quad \bar{p}(\mathbf{g}) = \int p(E; \mathbf{g})\, F(E; \mathbf{g})\, dE, \quad \operatorname{Re} E \leqslant 0, \tag{3}$$

where N_x denotes the number of spins in the chain, E — the complex energy of spin chain with length L_x and $F(E; \mathbf{g})$ — its distribution function defined on the ensemble (see definition (11)).

It is obvious that for some value of $\varrho(\mathbf{g})$ the expression for $\Lambda(\mathbf{g})$ goes to unit which means that in the equation of Clausius–Mossotti (2) a catastrophe occurs.

So, our aim will be the calculation of polarizibility coefficient $\varrho(\mathbf{g})$ with consideration of relaxation effects occurring in the system of spins under the

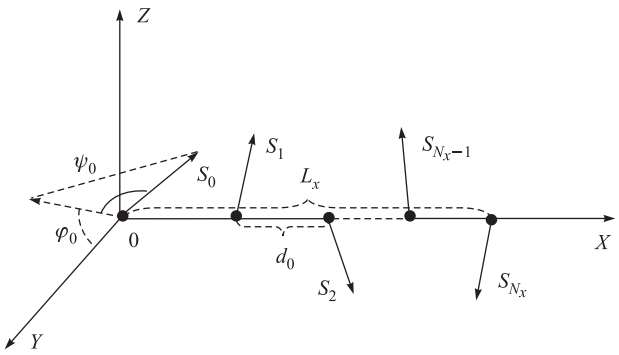

Fig. 1. A stable 1D spatial spin chain with random interactions and length $L_x = d_0 N_x$, where d_0 is the distance between nearest neighboring spins, N_x designates the number of spins in the chain. The spherical angles φ_0 and ψ_0 describe the spatial orientation of $\boldsymbol{S}_0$ spin, the pair of angles (φ_i, ψ_i) defines the spatial orientation of $\boldsymbol{S}_i$ spin

influence of external field. Note that in this case coefficient $\varrho(\mathbf{g})$ will have a complex value and correspondingly the problem of the catastrophe will be solved in natural way (for more details see Sec. 3).

We consider the classical ensemble of disordered 1D spatial spin chains (SSCs) with length L_x, where for simplicity it is supposed that the interactions between spin chains are absent. The specificity of this problem is such that statistical properties of the system interest us on very short time intervals δt at which the system cannot be thermally relaxed. Let us note that for a problem the following times correspondences take place $\tau \ll \delta t < \Omega^{-1} \ll \tau_T \ll 1$, where τ is the relaxation time of spin in the external field and τ_T is the time of thermal relaxation. In other words, we suppose that the spin-glass system is frozen and nonsusceptible to thermal evolution.

Mathematically, such a type of spin glass can be described by 1D Heisenberg spin-glass Hamiltonian [1–3]:

$$H(\{\mathbf{r}\}; N_x) = -\sum_{i=0}^{N_x-1} J_{i\,i+1} \boldsymbol{S}_i \boldsymbol{S}_{i+1} - \sum_{i=0}^{N_x-1} \boldsymbol{h}_i \boldsymbol{S}_i, \tag{4}$$

where $\{\mathbf{r}\} = \mathbf{r}_0, \mathbf{r}_1 \ldots$ designates the set of spins' coordinates ($\mathbf{r}_i$ is the coordinate of ith spin), $\boldsymbol{S}_i$ describes the ith spin which is the unit length vector and has a random orientation, $\boldsymbol{h}_i$ — the external field which is orientated along axis x:

$$h_i = h_0 \cos(k_x x_i), \quad x_i = i \cdot d_0, \quad k_x = 2\pi / L_x. \tag{5}$$

In addition, $J_{i\,i+1}$ characterizes the random interaction constant between i and $i+1$ spins in (4). $J_{i\,i+1}$ can have positive as well as negative values (see [1, 4]).

For further investigations, expression (4) is convenient to write in spherical coordinates (see Fig. 1):

$$H(\{\mathbf{r}\};N_x) = -\sum_{i=0}^{N_x-1}\Big\{J_{i\,i+1}[\cos\,\psi_{i+1}\cos\left(\varphi_i-\varphi_{i+1}\right)+\tan\,\psi_i\sin\,\psi_{i+1}]+ \\ +h_0\cos\left(2\pi i/N_x\right)\tan\,\psi_i\Big\}\cos\,\psi_i. \quad (6)$$

Equation (6) of stationary points of Hamiltonian will play a central role for the consecutive calculations of the problem:

$$\frac{\partial H}{\partial\psi_i}=0, \quad \frac{\partial H}{\partial\varphi_i}=0, \tag{7}$$

where $\Theta_i=(\psi_i,\varphi_i)$ are angles of ith spin in spherical coordinates (ψ_i is the polar and φ_i — the azimuthal angle).

Using expression (4) and equations (7), it is easy to find the following system of trigonometric equations:

$$\sum_{\nu=i-1;\nu\neq i}^{i+1} J_{\nu i}[\sin\,\psi_\nu-\tan\,\psi_i\cos\,\psi_\nu\cos\left(\varphi_i-\varphi_\nu\right)]+h_i=0, \\ \sum_{\nu=i-1;\nu\neq i}^{i+1} J_{\nu i}\,\cos\,\psi_\nu\sin\left(\varphi_i-\varphi_\nu\right)=0, \quad J_{\nu i}\equiv J_{i\nu}. \tag{8}$$

If the interaction constants between ith spin with its nearest neighboring spins, $J_{i-1\,i}$, $J_{i\,i+1}$, as well as the angles $(\psi_{i-1},\varphi_{i-1})$, (ψ_i,φ_i) are known, it is possible to explicitly calculate the pair of angles $(\psi_{i+1},\varphi_{i+1})$. Correspondingly, the ith spin will be in the ground state (in the state of minimum energy) if the following conditions are satisfied (Sylvester conditions) at the stationary point $\Theta_i^0=(\psi_i^0,\varphi_i^0)$:

$$A_{\psi_i\psi_i}(\Theta_i^0)>0, \quad A_{\psi_i\psi_i}(\Theta_i^0)\,A_{\varphi_i\varphi_i}(\Theta_i^0)-A^2_{\psi_i\varphi_i}(\Theta_i^0)>0, \tag{9}$$

where $A_{\alpha_i\alpha_i}(\Theta_i^0)=\partial^2H_0/\partial\alpha_i^2$, $A_{\alpha_i\beta_i}(\Theta_i^0)=A_{\beta_i\alpha_i}(\Theta_i^0)=\partial^2H_0/\partial\alpha_i\partial\beta_i$, in addition:

$$A_{\psi_i\psi_i}(\Theta_i^0)=\Big\{\sum_{\nu=i-1;\nu\neq i}^{i+1} J_{\nu i}[\cos\,\psi_\nu\cos\left(\varphi_\nu-\varphi_i^0\right)+\tan\,\psi_i^0\sin\,\psi_\nu] \\ +h_0\cos\left(2\pi i/N_x\right)\tan\,\psi_i^0\Big\}\cos\,\psi_i^0, \quad A_{\psi_i\,\varphi_i}(\Theta_i^0)=0,$$

$$A_{\varphi_i\,\varphi_i}(\Theta_i^0) = \sum_{\nu=i-1;\nu\neq i}^{i+1} J_{\nu i}\cos\,\psi_\nu\cos\left(\varphi_\nu - \varphi_i^0\right)\cos\,\psi_i^0. \tag{10}$$

With the help of equations (8) and conditions (9)–(10) we can calculate a huge number of stable 1D SSCs which will allow us to investigate the statistical properties of 1D SSCs ensemble. It is supposed that the average polarization (magnetization) of 1D SSCs ensemble (polarizability of 1D SSC) is equal to zero in the absence of an external field.

Now we can construct the distribution function of the energy of the 1D SCCs ensemble subject to an external influence. To this aim it is useful to divide the dimensionless real energy axis E into regions $0 > E_0 > \ldots > E_n$, where $n \gg 1$. The number of stable 1D SSC configurations with length L_x in the range of energy $[E-\delta E, E+\delta E]$, $\delta E \ll 1$, will be denoted by $M_{L_x}(E)$ while the number of all stable 1D SSC configurations by the symbol $M_{L_x}^{\text{full}} = \sum_{j=1}^{n} M_{L_x}(E_j)$. Accordingly, the energy distribution function of the ensemble may be defined by the expressions

$$F_{L_x}(E,\mathbf{g};d_0) = M_{L_x}(E,\mathbf{g})/M_{L_x}^{\text{full}}, \tag{11}$$

$$\lim_{n\to\infty}\sum_{j\,=1}^{n} F_{L_x}(E_j,\mathbf{g}\,;d_0)\,\delta E_j = \int_{-\infty}^{0} F_{L_x}(E,\mathbf{g};\,d_0)\,dE = 1,$$

where the second one expresses the normalization condition of the distribution function to unity.

3. SIMULATION ALGORITHM

3.1. Spin Glass without Consideration of Relaxation Effects

Using the following notation:

$$\xi_{i+1} = \cos\,\psi_{i+1}, \quad \eta_{i+1} = \sin\left(\varphi_i - \varphi_{i+1}\right), \tag{12}$$

equations system (8) can be transformed to the following form:

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

$$C_2 + J_{i\,i+1}\,\xi_{i+1}\,\eta_{i+1} = 0, \tag{13}$$

where parameters C_1 and C_2 are defined by the expressions

$$C_1 = J_{i-1\,i}\left[\sin\,\psi_{i-1} - \tan\,\psi_i\cos\,\psi_{i-1}\cos\left(\varphi_i\,-\,\varphi_{i-1}\right)\right]+ \\ + h_0\cos\left(2\pi i/N_x\right)\cos\,\psi_i,$$

$$C_2 = J_{i-1\,i}\cos\,\psi_{i-1}\sin\left(\varphi_i - \varphi_{i-1}\right).$$

From system (13) we can find the equation for the unknown variable η_{i+1}:

$$C_1\eta_{i+1} + C_2\sqrt{1-\eta_{i+1}^2}\tan\,\psi_i + \sqrt{J_{i\,i+1}^2\eta_{i+1}^2 - C_2^2} = 0. \tag{14}$$

We can transform equation (14) to the following equation of the fourth order:

$$(A^{\,2} + 4C_1^2C_2^2\sin\,\psi_i)\eta_{i+1}^4 - 2(AC_2^2 + 2C_1C_2^2\sin^2\psi_i)\eta_{i+1}^2 + C_2^4 = 0, \tag{15}$$

where

$$A = J_{i\,i+1}^2\cos^2\psi_i - C_1^2 + C_2^2\sin^2\psi_i. \tag{16}$$

The discriminant of equation (15) equals

$$D = C_2^4(A + 2C_1\sin^2\psi_i)^2 - C_2^4(A^{\,2} + 4C_1^2C_2^2\sin^2\psi_i) = \\ = 4C_2^4C_1^2\sin^2\psi_i(A + C_1^2\sin^2\psi_i - C_2^2).$$

From the condition of non-negativity of the discriminant $D \geqslant 0$ we get

$$A + C_1^2\sin^2\psi_i - C_2^2 \geqslant 0. \tag{17}$$

Substituting the value of A from (16) into (17), we can find the new condition to be satisfied by the interaction constant between two successive spins:

$$J_{i\,i+1}^2 \geqslant C_1^2 + C_2^2. \tag{18}$$

Now we can write the following expressions for unknown variables ξ_{i+1} and η_{i+1}:

$$\xi_{i+1}^2 = \frac{C_2^2}{J_{i\,i+1}^2\eta_{i+1}^2}, \quad \eta_{i+1}^2 = C_2^2\frac{A}{B}, \tag{19}$$

where

$$A = J_{i\,i+1}^2\cos^2\psi_i + C_3 + 2C_1\sin^2\psi_i\big[C_1 \pm \sqrt{J_{i\,i+1}^2 - C_1^2 - C_2^2}\,\cot\psi_i\big], \\ B = J_{i\,i+1}^4\cos^4\psi_i + 2C_3J_{i\,i+1}^2\cos^2\psi_i + (C_1^2 + C_2^2\sin^2\psi_i)^2, \\ C_3 = -C_1^2 + C_2^2\,\sin^2\psi_i.$$

Finally, in consideration of (12) for calculating angles $(\varphi_{i+1}, \psi_{i+1})$ we find:

$$0 \leqslant \xi_{i+1}^2 \leqslant 1, \quad 0 \leqslant \eta_{i+1}^2 \leqslant 1. \tag{20}$$

These conditions are very important for elaborating correct and effective simulation algorithm (see also [20]).

3.2. Spin Glass with Consideration of Relaxation Effects

As was shown by numerical simulation, the algorithm described in the previous Section, allows very fast and correct parallel simulation of the spin-glass problem [20]. In particular, we have shown that even for weak external fields such values of polarization which lead to the catastrophe in Eq. (2) are arized. For solution of this issue, we need consideration of occurring relaxation effects in 1D SSCs ensemble under the influence of an external field. Mathematically the consideration of a complex Hamiltonian can be one of the effective ways for solution of the mentioned problem. Note that the idea of complex Hamiltonian is often used for solutions of the classical and semiclassical problems near zero angles of scattering [21]. In the specified cases the divergence problems are successfully solved by using the so-called complex-classical trajectories. We consider that spin chains, as a matter of fact, are classical trajectories where the analogue of time is the sequence of nodes. It is obvious, that in a complex-classical trajectory (spin chain) it is possible to take into account the relaxation effects in spins system.

We, thus, propose that the Hamiltonian (4) is a complex function where the constants $J_{i\,i+1}$ and the angles between spins have complex values. One might expect that such a Hamiltonian will describe the relaxation of spins inside the chain (excitation of external degrees of freedom) and correspondingly the excitation of internal degrees of freedom in the result of which the absolute values of spins can be changed. Mathematically such a kind of extension of the problem is equivalent to the analytic continuation of the classical solution in the complex region. In other words, we must extend equations (19) and inequalities (9), (18), by considering them as a complex.

The system of recurrent equations which will allow one to calculate spin chains with consideration of relaxation effects can be written in the following form:

$$\begin{aligned}
\mathrm{Re}\{\,\tilde{\xi}_{i+1}^{2} - \tilde{C}_2^{2}\,\tilde{J}_{i\,i+1}^{-\,2}\,\tilde{\eta}_{i+1}^{-\,2}\,\} &= 0,\\
\mathrm{Im}\,\{\,\tilde{\xi}_{i+1}^{2} - \tilde{C}_2^{2}\,\tilde{J}_{i\,i+1}^{-\,2}\,\tilde{\eta}_{i+1}^{-\,2}\,\} &= 0,\\
\mathrm{Re}\,\{\,\tilde{\eta}_{i+1}^{2} - \tilde{C}_2^{2}\,\tilde{A}\,\tilde{B}^{-1}\,\} &= 0,\\
\mathrm{Im}\,\{\,\tilde{\eta}_{i+1}^{2} - \tilde{C}_2^{2}\,\tilde{A}\,\tilde{B}^{-1}\,\} &= 0,\\
\mathrm{Im}\,\{\,\tilde{A}_{\,\tilde{\psi}_{i+1}\,\tilde{\psi}_{i+1}}\,(\tilde{\Theta}_{i+1})\,\} &= 0,\\
\mathrm{Im}\,\{\,\tilde{A}_{\,\tilde{\varphi}_{i+1}\,\tilde{\varphi}_{i+1}}\,(\tilde{\Theta}_{i+1})\,\} &= 0,\\
\mathrm{Im}\,\{\,\tilde{J}_{i\,i+1}^{2} - \tilde{C}_1^{2} - \tilde{C}_2^{2}\,\} &= 0.
\end{aligned} \tag{21}$$

The tildas over the symbols designate the analytic extension of the functions in complex region: $\tilde{\sigma} = \sigma^{\,r} + i\sigma^{\,I}$, where $\sigma^{\,r}$ and $\sigma^{\,I}$ are the real and the imaginary parts of the function, correspondingly. Note that the first four equations in (21) are found from the complex extension of equations (19) by separating the real and

imaginary parts. The next three equations are found from the zeroing condition of imaginary parts of the Sylvester conditions (9) and the inequality (18).

The condition of local minimum energy for spins asks to satisfy the following inequalities:

$$\mathrm{Re}\left\{\tilde{A}_{\tilde{\psi}_i\,\tilde{\psi}_i}(\tilde{\Theta}_i^0)\right\} > 0, \quad \mathrm{Re}\left\{\tilde{A}_{\tilde{\varphi}_i\,\tilde{\varphi}_i}(\tilde{\Theta}_i^0)\right\} > 0, \tag{22}$$

and the additional condition (see also condition (18)):

$$\mathrm{Re}\big\{\tilde{J}_{i\,i+1}^2 - \tilde{C}_1^2 - \tilde{C}_2^2\big\} \geqslant 0. \tag{23}$$

The system (21) with the constraints conditions of inequalities (22) and (23) allows one to conduct computation and construct stable spin chains with consideration of relaxation effects which occur as a result of energy exchange between spins inside the chain and excitation of their internal degrees of freedom.

The simulation (21) with consideration of conditions (22)–(23) can be realized in various scenarios. In particular, if we assume that relaxation occurs only between the spins in chains without excitation of internal degrees of freedom, then a new additional condition arises (see also (20)):

$$\big|\,\tilde{\xi}_{i+1}^2\big| \leqslant 1, \quad \big|\,\tilde{\eta}_{i+1}^2\big| \leqslant 1. \tag{24}$$

The conditions (24) are equivalent to the assumption that the interaction constants $J_{i\,i+1}$ are only complex. When the relaxation goes on two degrees of freedom, then the conditions (24) are not satisfied.

4. NUMERICAL EXPERIMENTS

In this Section we discuss the case when the relaxation occurs by the abovementioned two degrees of freedom.

We assume that the ensemble consists of M spin chains each of them of $25d_0$ length. For the realization of simulation, we use a parallel algorithm the scheme of which is represented in [20, 32].

Briefly random M sets of initial parameters (the angular configurations of the first and the second spins of each chain in the ensemble and the interaction constants between those spins) are generated as complex values $\big\{\,\Omega_1,\,\Omega_2,\ldots,\Omega_n = (\tilde{\Theta}_0, \tilde{\Theta}_1, \tilde{J}_{01})_n, \ldots, \Omega_M\big\}$. The MAPLE tool for symbolic calculations of system (21) allows the separation of the real and imaginary parts of the complex equations. When the solutions of the recurrence equations are found, the conditions of stability of the spins at each node are being checked. The process of simulation proceeds on the following node if the conditions (22) are satisfied. If conditionts (22) are not satisfied, a new constant J_{i_1+1} is being randomly generated and correspondingly new solutions are being found, and the constraints (22)

being checked. It is important to note that starting from the spin-chain second node the spin–spin interaction constants $J_{i\,i+1}$ are generated taking into account the inequality (23). This cycle is being repeated on each node until the solutions do satisfy the conditions for the energy local minimum. The process of computation is continued up to N_xth node. The algorithm works until the simulation of all M parallel problems ends.

At first, we have conducted numerical simulation for the definition of different statistical parameters of an ensemble which consists of $3 \cdot 10^3$ spin chains of $25d_0$ length in the absence of external fields (the case of unperturbed Hamiltonian). The simulations showed that the distribution of the real part of the energy has a global maximum in the negative region while its imaginary part is symmetrically distributed around zero (Fig. 2, *a*). The mean values of the real and imaginary parts of energy are correspondingly equal to $E_0^{(r)} = -1.0549$ and $E_0^{(I)} = 0.00014$. The small value of the imaginary part of energy is understandable. There should not be relaxation in the absence of the external field in the ensemble and, respectively, the imaginary part of the energy must be zero. An important result is the calculation of spin–spin interaction constants from the first principles of classical mechanics. As calculations show, the distributions of the real and imaginary parts are not normal (Fig. 2, *b*). They satisfy Lévy alpha-stable distribution class [33].

For the spin-glass problem, an important issue is the calculation of the spins magnetization (in the text often called polarization). As was numerically shown, the distributions of both the real and imaginary parts of polarizations are symmetric in weak external fields γ (defined by the expression $\gamma = h_0/|E_0^{(r)}| = 2 \cdot 10^{-3}$),

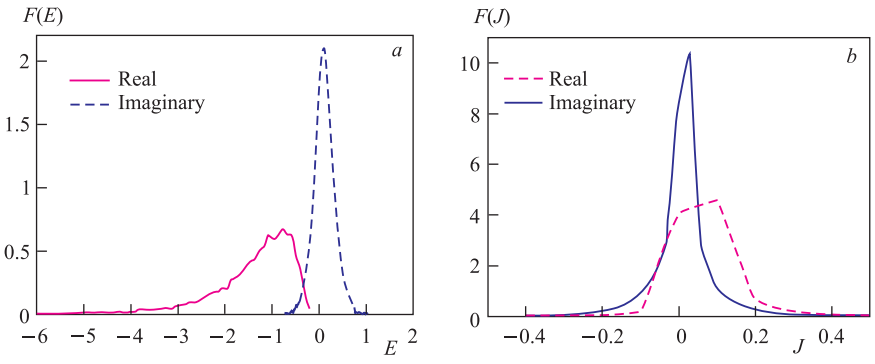

Fig. 2. *a*) The distribution of the energy (for the real and imaginary parts, correspondingly) of an ensemble which consists of 1D SSCs each of them of length $L_x = 25\,d_0$. *b*) The distribution of constants of spin–spin interactions (for the real and imaginary parts, correspondingly). These distributions essentially differ from the Gauss–Edwards–Anderson distribution and they correspond to the Lévy alpha-stable distributions class

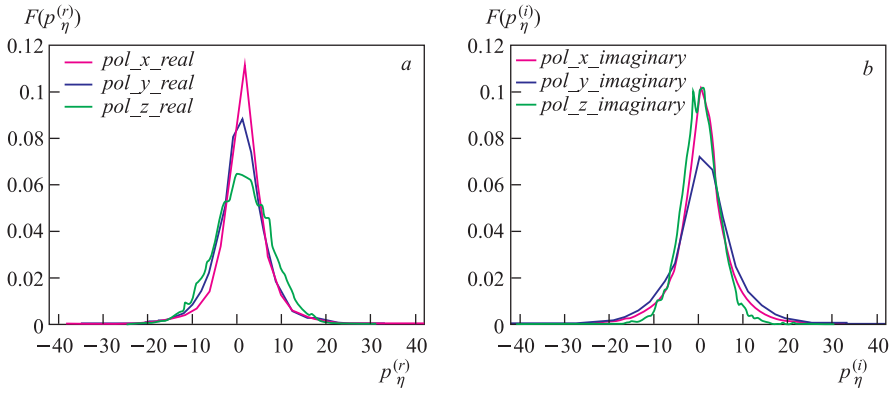

Fig. 3. *a*) Distributions of the real part of polarizations on x, y, z coordinates. *b*) Distributions of imaginary part of polarizations on x, y, z coordinates

which means that the system is ergodic (see Fig. 3, *a, b*). Recall that for considered case we have the following results for the mean values of 1D SSCs polarizations $(\bar{p}_x^{(r)} = 0.14921, \bar{p}_y^{(r)} = -0.45993, \bar{p}_z^{(r)} = 1.0893)$ and for imaginary part of the polarization, correspondingly $(\bar{p}_x^{(I)} = 0.29102,\ \bar{p}_y^{(I)} = -0.39594, \bar{p}_z^{(I)} = 0.067269)$.

Such polarizations are possible if the absolute values of 1D SSC polarization are more than 25 on all coordinates (Fig. 3, *a*). Recall that in the absence of external field the spin magnitudes are equal to unity and, correspondingly, the maximal absolute value of 1D SSD polarization is less than 25. The latter means that both the internal and external degrees of freedom of the spin system are excited under relaxation in the external field.

5. STATISTICAL PROPERTIES OF 1D SSCs ENSEMBLE IN EXTERNAL FIELD

The most interesting and important questions about statistical systems concern their critical behaviors in external fields. In this sense, the behavior of spin-chains ensemble magnetization (the mean value of polarizability) in the external field is a very important parameter.

We have investigated the behavior of the ensemble polarization average value depending on an external field. Using definition (3) we have calculated mean values of polarizations $\bar{p}_\eta^{(o)}(\gamma)$ on all coordinates $(\eta = x, y, z)$, where the index $(o = r, i)$ designates the real and imaginary parts.

The numerical simulation has shown that the mean values of both the real and imaginary parts of the polarizations are strongly frustrated [35] depending on parameter γ. This frustration does not disappear at grid convergence of computation region, see Fig. 4, *a, b, c* (real part) and correspondingly Fig. 4, *d, e, f* (imaginary part). Moreover, at each separation the self-similarity of structure is conserved which testifies about its fractal character. The dimensionality of fractal structure is calculated by the following simple formula:

$$D_{\eta}^{(o)}(\gamma) \; = \; \ln(n)/\ln(N), \tag{25}$$

where n is the number of partitions of the structure size, and N is the number of placing of the initial structure. At a value $\gamma = 0.003$ a dimensionality $D_x^{(r)} \approx 1.2095$. Similar calculations for $D_y^{(r)}$, $D_z^{(r)}$ etc., can be performed. At increasing γ all of them tend to unity.

Taking into account the above-mentioned results, the average value of the polarization (magnetization) is

$$< \bar{p}_{\eta}^{(o)}(\gamma) > \simeq \frac{1}{n} \sum_{i=1}^{n} \bar{p}_{\eta}^{(o)}(\gamma_i), \tag{26}$$

where n stands for the number of points on which the average value of polarization $\bar{p}_{\eta}^{(o)}(\gamma_i)$ (averaged over the ensemble of 1D SSCs) has an extremal value, where $\gamma_i \in [\gamma - \delta\gamma, \gamma + \delta\gamma], \delta\gamma \ll 1$; in addition, the angle brackets $\langle . \rangle$ denote fractal averaging, i.e., the arithmetic mean. As follows from Fig. 5, *a, b*, the mean value of polarization $\langle \bar{p}_{\eta}^{(o)}(\gamma) \rangle$ has a set of phase transitions of the first order depending on γ after averaging on fractals.

Now we can define the Edwards–Anderson-type ordering parameter which characterizes the process of orderings in the system depending on an external influence. As seen from the visualization of commutated evidence (Fig. 6, *a–f*), a similar pattern follows for the ordering parameters. The mean values of the square of polarizations on the ensemble

$$\overline{[p_{\eta}^{(o)}(\gamma_i)]^2} = \int [p^{(o)}(E; \mathbf{g}, N_x)]^2 F(E; \mathbf{g})\, dE, \quad \operatorname{Re} E \leqslant 0$$

are strongly frustrated and depend on the external field (Fig. 6, *a–f*). The expression $\overline{[p_{\eta}^{(o)}(\gamma_i)]^2}$ should be averaged on fractal structures like (26):

$$g_{\eta}^{(o)}(\gamma) \simeq \frac{1}{n} \sum_{i=1}^{n} \overline{[p_{\eta}^{(o)}(\gamma_i)]^2}. \tag{27}$$

As calculations are shown, an ordering occurs in the system depending on the increase of γ (Fig. 7, *a, b*).

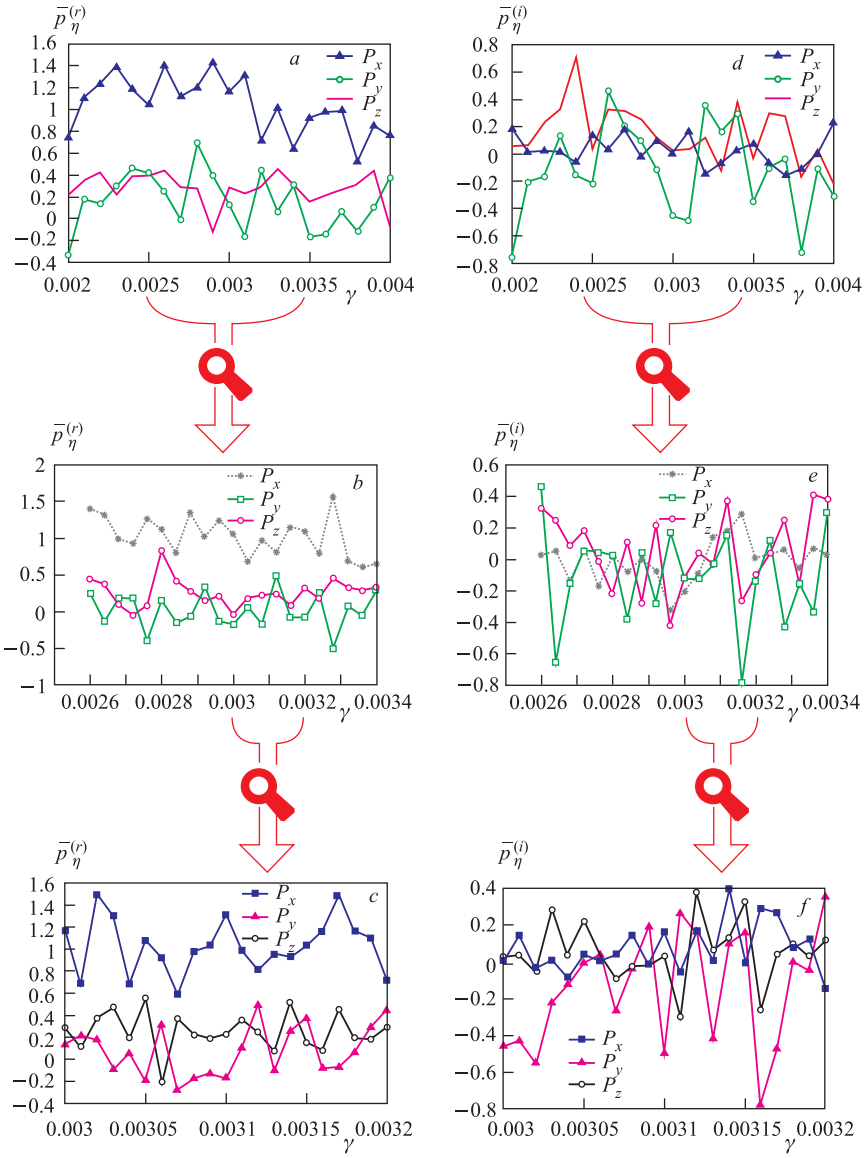

Fig. 4. *a, b, c*) Self-similar curves of the real part of polarization are shown. *d, e, f*) Self-similar curves of the imaginary part of polarization are correspondingly shown. The x, y, z mean values of both the real and imaginary parts of the polarization are strongly frustrated on all coordinates depending on the external field

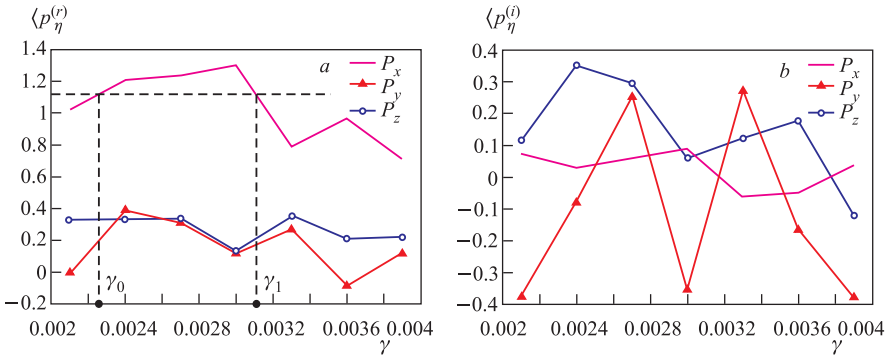

Fig. 5. *a*) Curves of the real part of polarizations are shown on different coordinates (x, y, z) after averaging on spin-chains ensemble and on fractal structures. The usual equation of Clausius–Mossotti (2) (without consideration of relaxation effects) for two values of external field (γ_0, γ_1) has catastrophes (plot (*a*)). *b*) Curves of the imaginary part of polarizations are shown after the full averaging by spin-chains ensemble and fractal structures

It is important to note that in the system critical phenomena may occur connected with catastrophes in the equation of Clausius–Mossotti (2) (Fig. 5, *a*), when the real part of denominator in the equation tends to zero. The analysis of a large class of spin glasses shows that catastrophes occur, when the real part of polarizability coefficient connected with orientational effects, varies between $\varrho(\gamma) \propto 0.025 \div 0.05$, and the contribution coming from relaxation effects is not being considered in Eq. (2).

These problems are solved by consideration of relaxation effects which lead to formation of the imaginary part in the polarizability coefficient which fully eliminates the divergence in Eq. (2) (see Fig. 5, *b*). As can be seen from Fig. 4 and 6 the above-mentioned parameters are frustrated in other directions also in which the external field are applied.

Finally, we return to the definition of the main object of statistical physics, which is the partition function. As is well known, the partition function of classical many particle system is defined in the configuration space as follows [36]:

$$Z(\beta) = \int \exp\left\{-\beta H(\{\mathbf{r}\})\right\} d\mathbf{r}_1 d\mathbf{r}_2 \ldots, \quad \beta = \frac{1}{k_B T}, \tag{28}$$

where k_B is the Boltzmann constant and T is the thermodynamic temperature. If the number of spins or spin chains in the system is large, the quantity (28) is a functional integral. Anyway, the number of integrals in expression (28) is very large, as a rule, and the main problem lies in their correct calculation. However, in the representation (28) configurations of spin chains which are not

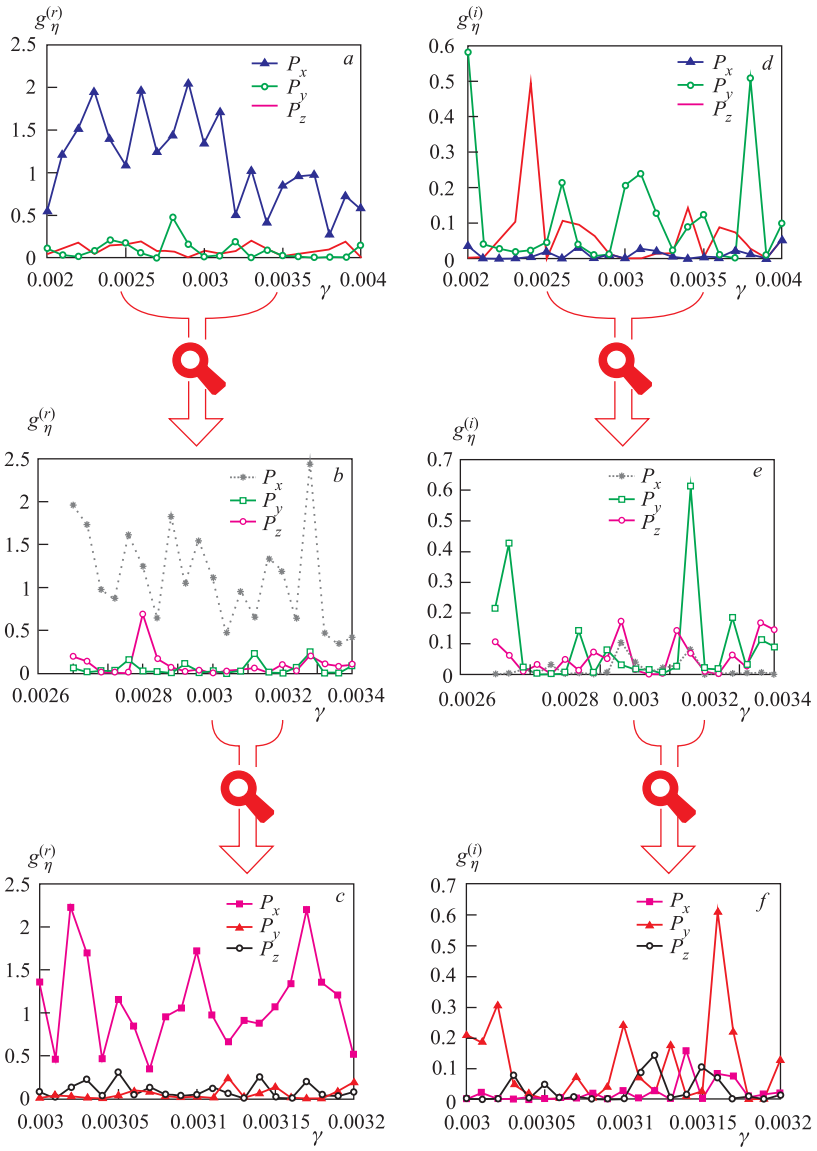

Fig. 6. Self-similar curves of the Edwards–Anderson ordering parameter on different coordinates. Curves (a, b, c) correspond to the real part of the ordering parameter while curves (d, e, f) correspond to its imaginary part. The (x, y, z) mean values of both the real and imaginary parts of polarization are strongly frustrated on all coordinates and depend on the external field

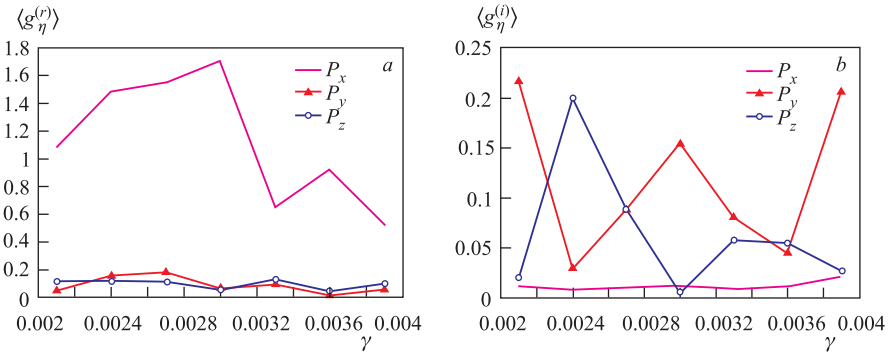

Fig. 7. *a*) Curves of the real part of ordering parameters on different coordinates (x, y, z) after averaging on spin-chains ensemble and on fractal structures are shown. As is visible at incising of γ parameter (energy external field) system going to ordering. *b*) Properties of the imaginary part of ordering parameter are shown

physically realizable do obviously contribute. Moreover, the weight of these configurations is not known and, in general, it is unclear how to define it. With this in mind and also taking into account the ergodicity of the spin glass in the above-mentioned sense, we can define the partition function in the space of an energy and polarization $(E, \mathbf{p})$ of superspin, in the form:

$$Z_*(\beta; N_x) = \left\langle \int \exp\left\{\beta H(E, \mathbf{p})\right\} F(E, \mathbf{p}; \mathbf{g}, N_x)\, dE\, d\mathbf{p} \right\rangle, \quad \operatorname{Re} E \leqslant 0, \quad (29)$$

where $F(E, \mathbf{p}; \mathbf{g}, N_x)$ is the distribution function of an ensemble, where $\mathbf{p}$ denotes the polarization of 1D SSC which is complex, $d\mathbf{p} = dp_x^{(r)} dp_y^{(r)} dp_z^{(r)} dp_x^{(i)} dp_y^{(i)} dp_z^{(i)}$. In addition $H(E, \mathbf{p})$ designates Hamiltonian in the new space $(E, \mathbf{p})$ and $\langle \ldots \rangle$ correspondingly designates the averaging by fractal structures as defined in (26).

Thus, according to the new definition, the partition function is a complex function and its derivatives have regular behaviors, respectively, at the critical points.

6. CONCLUSION

In order to solve the problem of critical phenomena in spin glasses under external fields, we first examined the possibility of its description in the framework of the complex Hamiltonian. We have studied a short-range interaction model of the spin glass which consists of 1D SSCs. We use the condition of stationarity point of the Hamiltonian on the nodes which allows one to find the

system of recurrent equations (7) or (8) based on the fact that stable spin chains essentially are classical trajectories, where the role of time in the context of this problem is the sequence of nodes. These equations together with the Sylvester conditions (9) allow step-by-step construction of stable spin chains as classical trajectories. The generalization of classical trajectories on the complex classical trajectories leads to a system of equations (21) which satisfy inequalities (22)–(23). The solutions of equations (22)–(23) for both the angles and spin–spin coupling constants are complex since all parameters of the problem are complex. As a result, it helps to avoid the catastrophe in equation (2) and to build up a reliable numerical algorithm for solving the spin-glass problem taking into account the relaxation effects. The developed approach allows us to generalize the equation of Clausius–Mossotti and makes it suitable for qualitative and quantitative study of the dielectric constant behavior of medium including the cases where critical phenomena occur in the medium.

Also it is important to note that the presented approach allows us to construct a new more correct partition function (29), which is a complex function and its derivatives do not diverge in the critical points.

Finally, we note that the developed approach allows us efficiently run the parallel algorithm for the numerical simulation of the considered problem on small (about 20–24) multiprocessor systems. It is a good result since large supercomputers for the simulation of this class of problems have been useed.

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