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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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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 advanced Sylvester conditions which allows one to step by step construct a huge number of stable spin chains in parallel. The distribution functions of different parameters of spin glass system are constructed from first principles by analyzing the calculation results of the 1D SSCs ensemble. It is shown that the behaviors of different distributions parameters are quite different even at weak external fields. The ensemble energy and constants of spin–spin interactions are being 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 the ensemble and parameters of its orderings are frustrated. We have also studied some critical properties of the ensemble such as catastrophes in the Clausius–Mossotti equation depending on the value of the external field. We have shown that the generalized complex-classical approach excludes these catastrophes, which allows 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 is suggested based on these investigations. Being opposite to the usual definition, it is a complex function and its derivatives are everywhere defined, including at critical points.

Исследованы статистические свойства ансамбля неупорядоченных 1D-пространственных спин-цепей (ПСЦ) конечной длины, помещенных во внешнее поле, с учетом релаксационных эффектов. Для решения этой проблемы впервые был использован короткодействующий комплексно-классический гамильтониан. Получена система рекуррентных уравнений на узлах решетки спин-цепи. На основе этих уравнений разработан эффективный математический алгоритм с учетом обобщенных условий Сильвестра, которые позволяют параллельно, шаг за шагом, построить огромное количество стабильных спиновых цепочек. Построены функции распределения различных параметров системы спинового стекла, исходя из первых принципов на основе анализа результатов расчетов 1D ПСЦ ансамбля. Показано, что поведение различных параметров распределений значительно различается даже при слабых внешних полях. Энергия ансамбля и константы спин-спиновых взаимодействий в пределе статистического равновесия в зависимости от внешнего поля меняются плавно, в то время как некоторые из них, такие как среднее значение поляризаций ансамбля и параметры упорядочения, фрустрируют. Изучены также некоторые критические свойства

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ансамбля, такие как катастрофы уравнения Клаузиуса–Моссотти, в зависимости от величины внешнего поля. Показано, что обобщенный комплексно-классический подход исключает эти катастрофы, что позволяет организовать непрерывные параллельные вычисления во всей области значений внешнего поля, включая критические точки. На основе этих исследований предлагается новое представление функций статистической суммы. Оно, в отличие от обычного определения, является комплексной функцией, и ее производные всюду определены, в том числе в критических точках.

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INTRODUCTION

A wide class of phenomena which raise important and difficult calculation problems in physics, chemistry, materials 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-glass models (see, for example, [1–10]). In the literature, two types of mean field models were developed. The first consists of true random-bond models, where the coupling between interacting spins is assumed to be independent random variables [11–13]. The solution of the model problems 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 superficial nature. It has been pointed out in works [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 started our investigation with the classical problem concerning the study of statistical properties of 1D spatial spin-chains (SSCs) ensemble in external fields [20]. Then we investigated the 3D spin-glass problem. We have suggested a new idea which is based on the 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 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 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 Heiseberg Hamiltonian, the meaning of which is similar to the idea of classical Newtonian mechanics generalization on complex-classical trajectories [23–27].

In Sec. 1 we formulate problems arising under the generalization of the Clausius–Mossotti equation on space-time scales of external fields. It is shown that the problem is mathematically equivalent to the studying of the 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. 2 the recurrent equations on the nodes of a 1D lattice are analyzed and solutions of the $(i+1)$th angular configuration are found depending on the spin–spin interaction constant $J_{i\,i+1}$, angular configurations of the 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 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. 3 the pseudo-code of parallel numerical experiments is adduced for simulation of a 1D SSCs ensemble with the length $25d_0$. Distributions of the complex energy, polarizations and spin–spin interaction constants of relaxing ensemble are investigated in detail.

In Sec. 4 the frustration phenomena of the mean value of ensemble polarization are investigated in detail depending on the external field energy parameter. The necessity of mean values additional averaging for the frustrating parameters of an ensemble is substantiated 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 the Conclusion, the obtained theoretical and computational results are analyzed in detail. Further development of the proposed approach is suggested.

1. FORMULATION OF THE PROBLEM AND BASIC FORMULAS

It is well known that in isotropic media (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 the coefficients of polarizabilities, correspondingly. From this equation it 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 the dielectric constant formally may be written as

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

where $\eta = (x, y, z)$ designates the spatial coordinates.

In (2) the symbol $\epsilon_{\rm st}^{(\eta)}(\mathbf{g})$ designates the dielectric constant depending on the external field parameters $\mathbf{g} = (\Omega, h_0)$, where Ω and h_0 correspond to the frequency and amplitude of the external field; in addition, if the medium can be represented respectively as a model of disordered spin system (spin glass), then $\varrho_\eta(\mathbf{g})$ 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 certain length L_x (see Fig. 1). Note that the coefficient of polarizability $\varrho_\eta(\mathbf{g})$ is the mean value of polarization of an ensemble per spin, which should be complex in general and equal to

$$\varrho_\eta(\mathbf{g}) = \frac{\bar{p}_\eta(\mathbf{g})}{N_x}, \quad \bar{p}_\eta(\mathbf{g}) = \int p_\eta F_{L_x}(E, \mathbf{p}; \mathbf{g})\, dE\, d\mathbf{p}, \quad \operatorname{Re} E \leqslant 0, \quad \mathbf{p} = (p_x, p_y, p_z), \tag{3}$$

where N_x denotes the number of spins in the chain, E is the energy of a spin chain with the length L_x and $F_{L_x}(E, \mathbf{p}; \mathbf{g})$ is the distribution function of 1D spatial spin-chains ensemble (see definition (11).

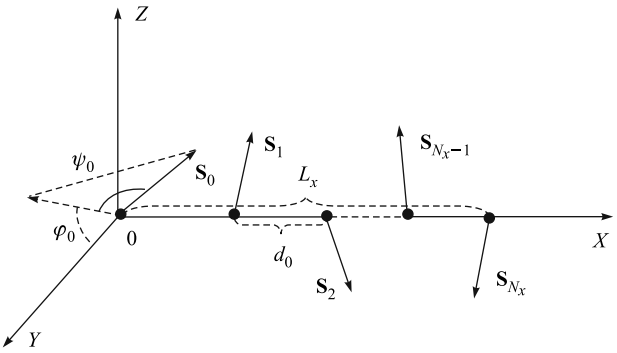

Fig. 1. A stable 1D spatial spin chain with random interactions and length $L_x = d_0 N_x$, where d_0 is the distance between nearest-neighboring spins. The spherical angles φ_0 and ψ_0 describe the spatial orientation of $\mathbf{S}_0$ spin, the pair of angles (φ_i, ψ_i) defines the spatial orientation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

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

Now, our aim is the calculation of the polarizibility coefficient $\varrho_\eta(\mathbf{g})$ with consideration of relaxation effects occurring in a system of spins under the influence of external field. Note that in this case the coefficient $\varrho_\eta(\mathbf{g})$ will have a complex value and, correspondingly, the problem of catastrophe will be solved in a natural way (for more details, see Sec. 2).

We consider a classical ensemble of disordered 1D spatial spin chains (SSC) with the length L_x, where for simplicity it is supposed that the interactions between spin chains are absent. The specificity of the 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 the problem the following time correspondences take place $\tau \ll \delta t < \Omega^{-1} \ll \tau_T \ll 1$, where τ is the time of spin relaxation in an external field and τ_T is the time of thermal relaxation. In other words, we suppose that the spin-glass system is frozen and insusceptible to thermal evolution.

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

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

where $\mathbf{S}_i$ describes the ith spin which is a unit length vector and has a random orientation, $\mathbf{h}_i$ is the external field which is orientated along the 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, (4) is convenient to write in spherical coordinates (see Fig. 1):

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

Equations (6) for the stationary points of the Hamiltonian will play a central role in 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 the angles of the ith spin in the 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:

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

If the interaction constants between the 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 $A_{\alpha_i\alpha_i}(\Theta_i^0) = \partial^2 H_0/\partial\alpha_i^2$, $A_{\alpha_i\beta_i}(\Theta_i^0) = A_{\beta_i\alpha_i}(\Theta_i^0) = \partial^2 H_0/\partial\alpha_i\partial\beta_i$, in addition:

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

$$\left. + \; h_0 \cos(2\pi i/N_x)\tan\psi_i^0 \right\} \cos\psi_i^0, \quad A_{\psi_i\varphi_i}(\Theta_i^0) = 0,$$

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

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 the 1D SSCs ensemble. It is supposed that the average polarization (magnetization) of the 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 the external influence. To this aim it is useful to divide the dimensionless real energy axis E into the regions $0 > E_0 > \ldots > E_n$ and the polarization axis $\mathbf{p}$ into the regions $(0 > p_{0;x} > \ldots > p_{n;x})$, $(0 > p_{0;y} > \ldots > p_{n;y})$ and $0 > p_{0;z} > \ldots > p_{n;z}$, where $n \gg 1$. The number of stable 1D SSC configurations with the length L_x within the energy range $[E - \delta E, E + \delta E]$, $\delta E \ll 1$, and polarizations range $[p_x - \delta p_x, p_x + \delta p_x]$, $[p_y - \delta p_y, p_y + \delta p_y]$ and $[p_z - \delta p_z, p_z + \delta p_z]$ will be denoted by $M_{L_x}(E, \mathbf{p}; \mathbf{g})$, while the number of all stable 1D SSC configurations by the symbol $M_{L_x}^{\text{full}} = \sum\limits_{i,j,l,k=1}^{n} M_{L_x}(E_i, p_{j;x}, p_{l;y}, p_{k;z})$. Accordingly, the energy distribution function for the ensemble may be defined by the expressions:

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

$$\lim_{n\to\infty} \sum_{i,\,j,\,l,\,k=1}^{n} F_{L_x}(E_i, p_{j;x}, p_{l;y}, p_{k;z})\delta\varepsilon_i \delta p_{j;x}\delta p_{l;y}\delta p_{k;z} = \int\limits_{-\infty}^{0} dE \int F_{L_x}(E, \mathbf{p}; \mathbf{g}) d\mathbf{p} = 1, \tag{11}$$

where the second one expresses the normalization condition of the distribution function to unity. Recall that the energy E and polarization $\mathbf{p}$ in general can be complex quantities and accordingly integrations on these values must be understood as multidimensional integrations.

2. SIMULATION ALGORITHM

2.1. Spin Glass without Consideration of Relaxation Effects of the 1D SSCs Ensemble. Using the following notation:

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

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

$$\begin{gathered} C_1 + J_{ii+1}\left[\sqrt{1-\xi_{i+1}^2} - \tan\psi_i \xi_{i+1}\sqrt{1-\eta_{i+1}^2}\right] = 0, \\ C_2 + J_{ii+1}\xi_{i+1}\eta_{i+1} = 0, \end{gathered} \tag{13}$$

where parameters C_1 and C_2 are defined by the expressions

$$C_1 = J_{i-1i}[\sin\psi_{i-1} - \tan\psi_i \cos\psi_{i-1}\cos(\varphi_i - \varphi_{i-1})] + h_0 \cos(2\pi i/N_x)\cos\psi_i,$$
$$C_2 = J_{i-1i}\cos\psi_{i-1}\sin(\varphi_i - \varphi_{i-1}).$$

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

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

We can transform equation (14) to the following equation of 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

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

The discriminant of equation (15) is equal to

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

From the condition of nonnegativity 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 a new condition to be satisfied by the interaction constant between two successive spins:

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

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

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

where

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

Finally, in consideration of (12) for calculating the 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 a correct and effective simulation algorithm (see also [20]).

2.2. Spin Glass with Consideration of Relaxation Effects in the 1D SSCs Ensemble. As was shown by the 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 there arise such values of polarization which lead to catastrophe in equation (2). In order to solve this issue, it is necessary to consider 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 to solve the above-mentioned problem. Note that the idea of complex Hamiltonian is often used for solution of classical and semiclassical problems near zero scattering angles [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 the spin system.

We thus propose that Hamiltonian (4) is a complex function where the constants J_{ii+1} and angles between spins have complex values. One might expect that such a Hamiltonian will describe the relaxation of the spins inside the chain (excitation of external degrees of freedom) and, correspondingly, the excitation of internal degrees of freedom due to which the absolute values of spins can be changed. Mathematically, such 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) and (18) by considering them as 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:

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

The tildas over the symbols designate the analytic extension of the functions in the complex region: $\tilde{\sigma} = \sigma^r + i\sigma^i$, where σ^r and σ^i are the real and 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 Sylvester conditions (9) and inequality (18).

The condition of local minimum energy for spins requires 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)):

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

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.

Simulation of (21) with consideration of conditions (22), (23) can be realized under 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)):

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

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

3. NUMERICAL EXPERIMENTS

In this section we discuss the case when relaxation occurs by the above-mentioned two degrees of freedom.

We assume that the ensemble consists of M spin chains, each of them of length $25d_0$. 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 first and second spins of each chain in the ensemble and interaction constants between those spins) are generated as complex values $\{\Omega_1, \Omega_2, \ldots, \Omega_n = (\tilde{\Theta}_0, \tilde{\Theta}_1, \tilde{J}_{01})_n, \ldots, \Omega_M\}$. 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 at the following node if the conditions (22) are satisfied. If conditions (22) are not satisfied, a new constant J_{i_1+1} is randomly generated and, correspondingly, new solutions are found and constraints (22) are being checked. It is important to note that starting from the spin-chain second node the spin–spin interaction constants J_{ii+1} are generated taking into account inequality (23). This cycle is being repeated at each node until the solutions do satisfy the conditions for the local energy minimum. The process of computation is continued up to the N_xth node. The algorithm works until the simulation of all M parallel problems ends.

At first we conducted numerical simulation for the definition of different statistical parameters of an ensemble which consists of $3 \cdot 10^3$ spin chains with the length $25d_0$ 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 the energy are, correspondingly, equal to $E_0^{(r)} = -1.0549$ and $E_0^{(i)} = 0.00014$. The small value of the imaginary part of the 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

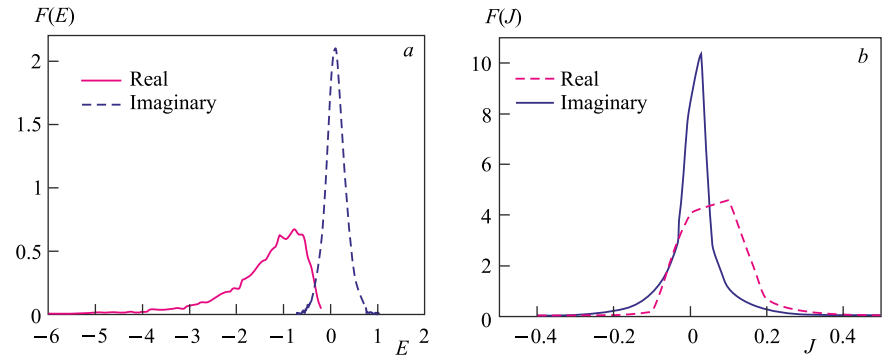

Fig. 2. *a*) The distribution of the energy (for the real and imaginary parts, correspondingly) of an ensemble, which consists of 1D SSCs, each of them being of length $L_x = 25d_0$. *b*) The distribution of constants of spin–spin interactions (for the real and imaginary parts, correspondingly). These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

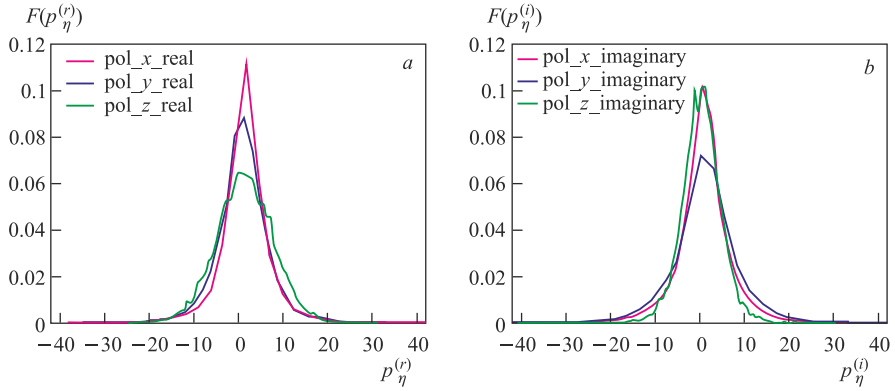

Fig. 3. *a*) Distributions of the real part of polarizations on the coordinates x, y, z. *b*) Distributions of the imaginary part of polarizations on the coordinates x, y, z

spin-spin interaction constants from first principles of classical mechanics. As calculations show, the distributions of the real and imaginary parts are not normal (Fig. 2, *b*). They satisfy the Lévy alpha-stable distribution class [33].

For the spin glass problem an important issue is the calculation of the spins magnetization (throughout the text also called polarization). As was numerically shown, the distributions of both real and imaginary parts of polarizations are symmetric in weak external fields γ (defined by the expression $\gamma = h_0/|E_0^{(r)}| = 2 \cdot 10^{-3}$), which means that the system is ergodic (see Figs.3, *a, b*). Recall that for the 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 the imaginary part of polarization, correspondingly: $(\bar{p}_x^{(i)} = 0.29102, \bar{p}_y^{(i)} = -0.39594, \bar{p}_z^{(i)} = 0.067269)$.

Such values of polarizations are possible if the absolute values are greater than the number 25 on all coordinates (Fig. 3, *a*). Recall that in the absence of external field the spin mag-

nitudes are equal to unity and, correspondingly, the maximal absolute value of the 1D SSC 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.

4. 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 very important parameter.

We have investigated the behavior of the ensemble polarization average value depending on the external field. Using definition (3), we have calculated the 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 the parameter γ. This frustration does not disappear at grid convergence of computation region, see Figs. 4, *a, b, c* (real part) and, correspondingly, Figs. 4, *d, e, f* (imaginary part). Moreover, at each separation the self-similarity of structure is conserved, which testifies to 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 the value $\gamma = 0.003$ the dimensionality $D_x^{(r)} \approx 1.2095$. Similar calculations can be done for $D_y^{(r)}$, $D_z^{(r)}$, etc. At increasing γ, all of them tend to unity.

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

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

where n stands for the number of points at which the average value of polarization $\bar{p}_\eta^{(o)}(\gamma_i)$ (averaged over the ensemble of 1D SSCs, see equation (3)) has an extremal value, in addition $\gamma_i \in [\gamma - \delta\gamma, \gamma + \delta\gamma], \delta\gamma \ll 1$, and the angle brackets $\langle\, . \,\rangle$ denote fractal averaging, i.e., the arithmetic mean. As it follows from Figs. 5, *a, b*, the mean value of polarization $\langle \bar{p}_\eta^{(o)}(\gamma) \rangle$ has a set of phase transitions of 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 the external influence. As is seen from the visualization of commutated evidence (Figs. 6, *a–f*), a similar pattern follows for the ordering parameters. The mean values of the square of polarizations on the ensemble are strongly frustrated and depend on the external field (Figs. 6, *a–f*):

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

where E and $\mathbf{p}$ correspondingly denote energy and polarization of 1D SSC, which have complex values, in addition $dE = dE^{(r)} dE^{(i)}$ and $d\mathbf{p} = dp_x^{(r)} dp_y^{(r)} dp_z^{(r)} dp_x^{(i)} dp_y^{(i)} dp_z^{(i)}$.

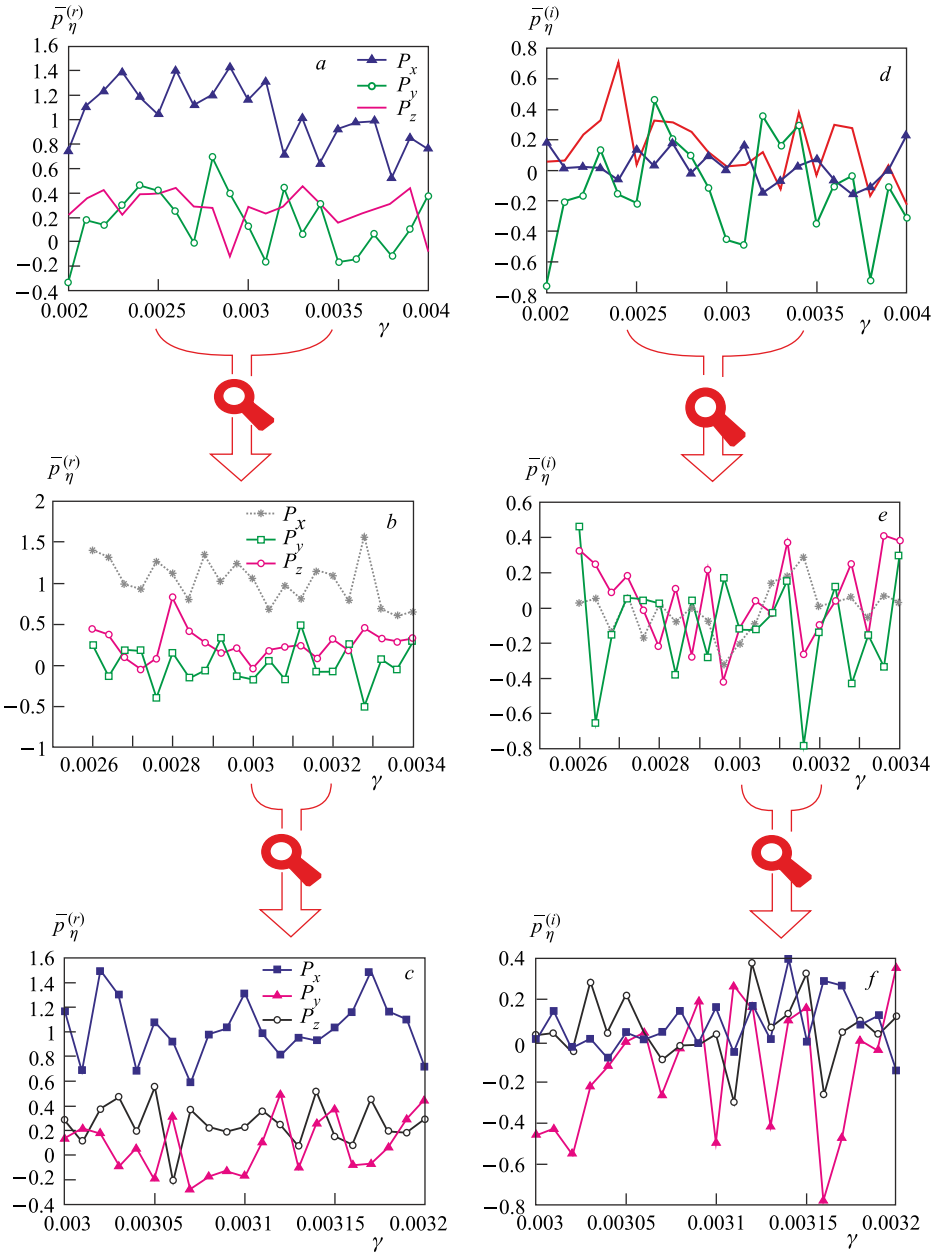

Fig. 4. *a, b, c*) Self-similar curves of the real part of polarization. *d, e, f*) Self-similar curves of the imaginary part of polarization. The x, y, z mean values of both the real and imaginary parts of the polarization are strongly frustrated on all coordinates depending on the external field

The expression $\overline{[p_\eta^{(o)}(\gamma_i)]^2}$ should be averaged on fractal structures like (26):

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

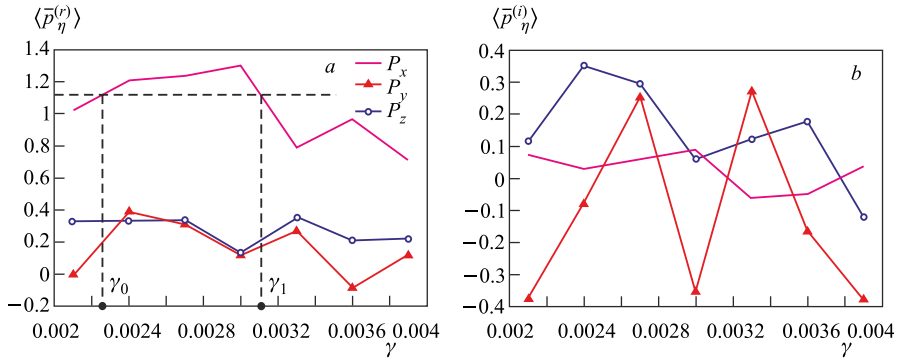

Fig. 5. *a*) Curves of the real part of polarizations on different coordinates (x, y, z) after averaging on the spin-chains ensemble and fractal structures. The usual Clausius–Mossotti equation (2) (without consideration of relaxation effects) has a catastrophe (plot *a*) for two values of external field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

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

It is important to note that in the system critical phenomena may occur connected with catastrophes in the Clausius–Mossotti equation (2) (Fig. 5, *a*) when the real part of denominator in the equation tends to one. 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 $\varrho_\eta(\gamma) \propto 0.025{-}0.05$ and the contribution coming from relaxation effects is not considered in equation (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 equation (2) (see Fig. 5, *b*). As is seen from Figs. 4 and 6, the above-mentioned parameters are frustrated in other directions, also where the external field is 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 a 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 $H(\{\mathbf{r}\})$ describes Hamiltonian of spins system in the direct lattice, 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 representation (28) configurations of spin chains which are not physically realizable do obviously contribute. Moreover, the weight of these configurations is not known in general and 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 the energy and polarization $(E, \mathbf{p})$ of superspin in the form

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

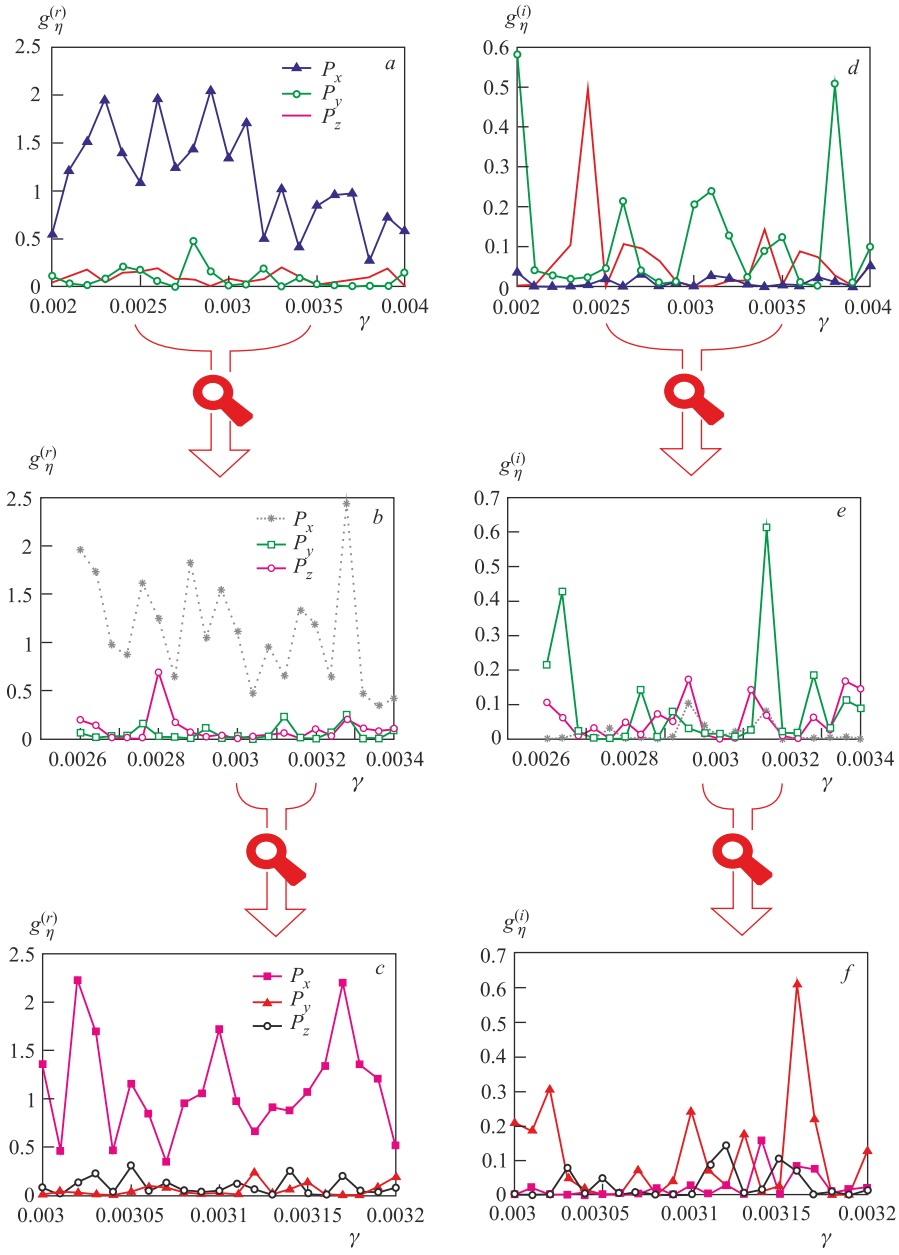

Fig. 6. Self-similar curves of the Edwards–Anderson ordering parameter on different coordinates. The curves (*a, b, c*) correspond to the real part of the ordering parameter, while the curves (*d, e, f*) correspond to its imaginary part. The (x, y, z) mean values of both the real and imaginary parts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

where $H(E, \mathbf{p})$ describes Hamiltonian of spins system in a space $(E, \mathbf{p})$, in addition $\langle \ldots \rangle$, correspondingly, designate the averaging by fractal structures like definition (26).

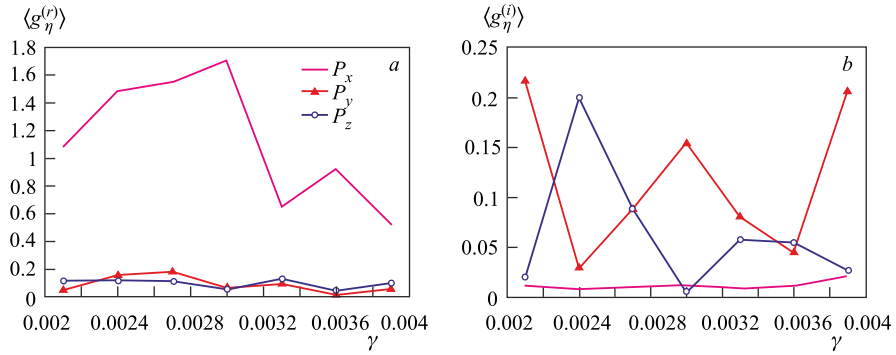

Fig. 7. *a*) Curves of the real part of ordering parameters on different coordinates (x, y, z) after averaging on the spin-chains ensemble and on the fractal structures. As is obvious, at increasing of γ parameter (energy of the external field) the system goes to ordering. *b*) Properties of the imaginary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

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

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 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 us to find a system of recurrent equations (7) or (8) based on the fact that stable spin chains are essentially classical trajectories, where the role of time in the context of this problem is the sequence of nodes. These equations together with 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 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 build up a reliable numerical algorithm for solving the spin glass problem taking into account relaxation effects. The developed approach allows us to generalize the Clausius–Mossotti equation and makes it suitable for qualitative and quantitative study of the dielectric constant's 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 at the critical points.

Finally, we note that the developed approach allows us to 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 were used before for the simulation of this class of problems.

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