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MAGNETISM

Construction of Approximate Methods within the Ising Model of a Diluted Magnet Using Averaging over Interaction Fields

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Abstract—The method of averaging over interaction fields has been analyzed as applied to the problems of statistical physics. This method has been theoretically justified as applied to a spin cluster. Based on the general relations obtained, approximate solutions for the bond-diluted Ising model are found. These approximate solutions are compared with the exact solution for a one-dimensional chain of bond-diluted Ising spins.

Keywords: Ising model, interaction field, diluted magnet, Bethe lattice

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1. INTRODUCTION

It is known that the properties of diluted and disordered magnets differ from those of pure magnets [1–3, 10]. However, exact solutions to the models of diluted magnetic systems have not been obtained yet. Therefore, it is reasonable to construct approximate solutions for diluted magnets. Some of these solutions can be obtained using averaging over interaction fields.

Chandrasekhar was the first to study the properties of a system of many interacting particles using the function of distribution over interaction fields [4]. In that study, motion of a system of galaxies bound by gravitational interactions was under consideration. Later, this method was used to estimate the influence of magnetostatic interaction of small ferrimagnetic particles located in a nonmagnetic matrix [5]. In [6–8], the method of averaging over interaction fields was used to analyze the magnetic properties of pure and diluted magnets. The application of this method for solving the problems of statistical physics was based on the results of [9], where it was shown that the following expression is valid for the Ising model in the thermodynamic equilibrium state for any spin σ_0

$$\langle\sigma_0\rangle = \langle\tanh(Kh + h_{ex})\rangle,$$

where $K = J/kT$, $h_{ex} = H_{ex}/kT$, J is the exchange-interaction constant, H_{ex} is the external magnetic field, k is the Boltzmann constant, and T is temperature. In this case, interaction field h is a sum of all spins interacting with σ_0.

In this study, we formulate and verify the relations (formula (2)), which can underlie the method of averaging over exchange fields as applied to clusters of several spins. As an example, two versions of the approximate methods are constructed for this model by applying the relations obtained to the bond-diluted Ising model. These methods are verified for the one-dimensional bond-diluted Ising model, for which the exact solution was constructed [17]. In addition, we compare the magnetization values at zero temperature, obtained within these approximations, with the probability that a site of the bond-diluted Bethe lattice belongs to an infinite cluster.

2. AVERAGING OVER INTERACTION FIELDS

Let us consider a system of N interacting particles, each characterized by some parameter σ (taking into account that the method is applied to the Ising model, this parameter will be referred below to as spin). We denote the set of all these spins and the Hamiltonian of the system as Ω and $\mathcal{H}(\Omega)$, respectively. A specific form of the Hamiltonian is of little importance; however, we assume that, for each spin σ_i, there is a finite number of terms in the Hamiltonian that contain σ_i. Note that this number is also finite in the thermodynamic limit $N \to \infty$. Two spins (σ_i and σ_j) are referred to as interacting spins, if the Hamiltonian contains a term which nonadditively depends on σ_i and σ_j.

Let us consider a group in the system, which contains n spins. Below, this group will be referred to as a cluster. The set of spins entering the cluster is denoted as c. The set of spins, which do not enter the cluster and interact with at least one spin from the cluster, is denoted as r. The set of the rest spins is denoted as s. Obviously, Ω is a union of nonoverlapping sets c, r, and s.

Now we select the terms in the Hamiltonian, which are related to the interaction of spins belonging to c and r:

$$\mathcal{H}(\Omega) = \mathcal{H}_c(c,r) + \mathcal{H}_s(r,s).$$

Hamiltonian $\mathcal{H}_c(c, r)$ contains only the terms which depend on the spins of cluster c and the terms describing the interaction between the cluster spins and the spins from set r. Hamiltonian $\mathcal{H}_s(r, s)$ contains the rest terms entering $\mathcal{H}(\Omega)$. Then, the partition function of the system can be written as

$$Z = \sum_r Z_c(r)Z_s(r), \quad (1)$$

where

$$Z_s(r) = \sum_s \exp\left(-\frac{1}{kT}\mathcal{H}_s(r,s)\right)$$

and

$$Z_c(r) = \sum_c \exp\left(-\frac{1}{kT}\mathcal{H}_c(c,r)\right).$$

Each term in (1) has the sense of (unnormalized) probability that the system of spins r is in a certain state. Normalized probability $W(r) = Z_c(r)Z_s(r)/Z$ is the distribution function for the sets of states of the spins interacting with the cluster.

Let $f(r)$ be a function of spins belonging to r, while $\varphi(c)$ is a function of cluster spins c. Then, the value of product $f\varphi$ averaged over the ensemble can be written as

$$\langle f\varphi\rangle = \frac{1}{Z}\sum_c f(r) \times\left(\sum_c \varphi(c)\exp\left(-\frac{1}{kT}\mathcal{H}_c(c,r)\right)\right)Z_s(r).$$

Having divided and multiplied each term in this sum by "cluster" statistical sum $Z_c(r)$, we obtain the following expression:

$$\langle f\varphi\rangle = \sum_r f(r)\langle\varphi\rangle_r W(r), \quad (2)$$

where

$$\langle\varphi\rangle_r = \frac{1}{Z_c(r)}\sum_c \varphi(c)\exp\left(-\frac{1}{kT}\mathcal{H}_c(c,r)\right). \quad (3)$$

Formula (2) can be interpreted as follows. Expression (3) can be considered as the "cluster mean" of the function $\varphi(c)$ calculated provided that the configuration of the spins interacting with the cluster is given and invariable. In this case, expression (2) can be considered as the averaging of the product $f(r)\langle\varphi\rangle_r$ over the distribution function $W(r)$. The method of averaging over interaction fields is based on the use of formula (2).

Let us consider the Ising model on some lattice. This lattice can be a periodic lattice with coordination number q; however, an arbitrary graph (obviously, containing no loops and parallel edges) can in principle be considered as a lattice. Let each lattice site contain an Ising "spin" with values of +1 and –1 and only spins located at the bound sites can interact. Then the Hamiltonian of the Ising model can be written as

$$\mathcal{H}(\Omega) = -J\sum_{(i,j)}\sigma_i\sigma_j - H_{ex}\sum_i\sigma_i. \quad (4)$$

Summation in the first and second sums is over all pairs of bound spins and over all sites, respectively.

Now we select a cluster on the lattice that contains only one spin σ_0. The cluster Hamiltonian is $\mathcal{H}_c(c, r) = -J\sigma_0\sum_{\sigma_i\in r}\sigma_i - \sigma_0\mathcal{H}_{ex}$, and formula (2), in which it is assumed that $f = 1$ and $\varphi = \sigma_0$, yields that

$$\langle\sigma_0\rangle = \sum_r \tanh\left(K\sum_{\sigma_i\in r}\sigma_i + h_{ex}\right)W(r), \quad (5)$$

which coincides with the result obtained in [9].

For a simple lattice, the average values of each spin are identical and equal to the M macroscopic magnetization of the system. In more complex cases, different spins may have different average values (5) (and the distribution functions $W(r)$).

Conditional probability (5) is a function of the sum of the spins belonging to r (i.e., the sum of the spins directly interacting with σ_0). This sum will be referred below to as an interaction field and denoted as h. The averaging in (5) is actually averaging over the distribution function of this interaction field

$$\langle\sigma_0\rangle = \int \tanh(Kh + h_{ex})W(h)dh, \quad (6)$$

where

$$W(h) = \sum_r \delta\left(h - \sum_{\sigma_i\in r}\sigma_i\right)W(r). \quad (7)$$

Here, δ is a delta function.

Thus, the average magnetization of each specific spin in the Ising model on any lattice can be considered as the value of $\tanh(Kh + h_{ex})$ averaged over the distribution function of the "interaction fields" $W(h)$ calculated for this spin.

Let us now consider a cluster of two neighboring spins σ_1 and σ_2 (dimer). On the assumption that $f = 1$ and $\varphi = \frac{\sigma_1 + \sigma_2}{2}$ in (2), we obtain

$$\left\langle\frac{\sigma_1 + \sigma_2}{2}\right\rangle = \int \frac{\sinh(K(h_1 + h_2) + 2h_{ex})}{\cosh(K(h_1 + h_2) + 2h_{ex}) + e^{-2K}\cosh(K(h_1 - h_2))} \times W(h_1, h_2)dh_1dh_2, \quad (8)$$

where $h_{1,2}$ are the interaction fields (i.e., the sums of the spins from set r, which interact with spins σ_1 and σ_2, respectively). Distribution function $W(h_1, h_2)$ of these fields is determined similarly to (6). For a simple lattice, means (8) are identical for each dimer and equal to the macroscopic magnetization of the system per atom.

Let us now consider the Ising model on some simple lattice exhibiting nonmagnetic bond dilution. (The considerations presented below can also be extended (with small changes) to a site-diluted model.) We assume that the bond of the initial lattice is dangling with a probability of $1 - b$ (i.e., the term describing the interaction of the spins via this bond is excluded from Hamiltonian (4)). We assume that dangling bonds are randomly and without correlation distributed over the lattice sites. Having considered each individual ith magnetic atom in this lattice and applied equality (6), we obtain that the average value of its spin is

$$\langle\sigma_i\rangle = \int \tanh(Kh + h_{ex})W(h)dh,$$

where $W(h)$ is the "local" distribution function over the interaction fields at this specific atom. According to the self-averaging method [10], to calculate the macroscopic magnetization M of a diluted magnet, one should calculate the mean of all $\langle\sigma_i\rangle$ values in the system with sufficiently large N (more specifically, in the thermodynamic limit):

$$M = \overline{\langle\sigma_i\rangle} = \int \tanh(Kh + h_{ex})W(h,b)dh, \qquad (9)$$

where $W(h, b) = \overline{W(h)}$ is the "average" distribution function of the interaction fields. Formula (9) can also be generalized to an arbitrary cluster; however, one should take into account that bonds in the cluster may be dangling. Therefore, the "self-averaging" should be performed separately for each configuration of dangling bonds in the cluster, and the results obtained should be averaged over these configurations with weights equal to the probabilities of the corresponding configurations. For example, there are two configurations for a two-site cluster: one with a dangling interatomic bond and the other with a not dangling bond. The probabilities of these configurations are $1 - b$ and b, respectively.

Therefore,

$$M = \overline{\left\langle\frac{\sigma_1 + \sigma_2}{2}\right\rangle} = (1-b)\int\frac{1}{2}(\tanh(Kh_1 + h_{ex}) + \tanh(Kh_2 + h_{ex}))W_1(h_1,h_2,b)dh_1dh_2 + b\int\frac{\sinh(K(h_1+h_2)+2h_{ex})}{\cosh(K(h_1+h_2)+2h_{ex}) + e^{-2K}\cosh(K(h_1-h_2))}W_2(h_1,h_2)dh_1dh_2. \qquad (10)$$

The average distribution functions $W_1(h_1, h_2, b)$ and $W_2(h_1, h_2, b)$ can be obtained by averaging over the clusters with dangling and not dangling bonds, respectively.

3. APPROXIMATE METHODS

Obviously, the magnetization in the diluted Ising model can be calculated directly from formulas (9) or (10) only with the corresponding distribution functions of the interaction fields known. As follows from these formulas, determination of the distribution functions is actually equivalent to exact solution of the problem. However, formulas (9) and (10) (or formulas, which can be similarly obtained from (2) for clusters with a large number of atoms) can be used for constructing approximate methods of determination of the magnetization in the diluted Ising model. To this end, particular approximations for distribution functions W, W_1, and W_2 entering formulas (9) and (10) should be accepted. In this study, we consider two approximation versions and estimate their accuracy.

The simplest (and roughest) approximation implies replacement of the averaging over fields in (9) and (10) with the average values of these fields. In other words, the distribution functions in (9) and (10) can be written in the following form:

$$W(h,b) = \delta(h - h_a)$$

and

$$W_1(h_1,h_2,b) = W_2(h_1,h_2,b) = \delta(h_1 - h_{1a})\delta(h_2 - h_{2a}).$$

Concerning the average fields h_a, h_{1a}, and h_{2a}, we assume that $h_{1a} = h_{2a}$ and the field values are proportional to the numbers of external neighboring sites ($h_{1a}/h_a = (q-1)/q$). Having denoted this proportionality factor as x, we find from (9) and (10) that

$$M = \tanh(Kqx + h_{ex}), \qquad (11)$$

where x is determined from the equation

$$\tanh(Kqx + h_{ex}) = (1-b)\tanh(K(q-1)x + h_{ex}) + b\frac{\sinh(2K(q-1)x + 2h_{ex})}{\cosh(2K(q-1)x + 2h_{ex}) + e^{-2K}}. \qquad (12)$$

It turns out [11] that approximation (11) for a pure magnet ($b = 1$) is the exact solution for the Ising model on the Bethe lattice. At $b < 1$, this approximation can be considered as a "pseudorandom" approximation for the Ising model with nonmagnetic dilution on the Bethe lattice [12]. (The pseudorandom approximation is obtained by solving the problem with mobile non-

magnetic impurities under an additional condition of zero correlation in the arrangement of impurities in the neighboring lattice sites [13].)

Another approximation for the distribution functions entering (8) and (9) is as follows [18]. Each ith site of the bond-diluted lattice has k bound neighbors. This is a random number ranging from 0 to q and distributed according to the binomial law at random and uncorrelated arrangement of dangling bonds in the lattice. Therefore, the function $W(h, b)$ entering (9) can always be written as

$$W(h,b) = \sum_{k=0}^{q} C_q^k b^k (1-b)^{q-k} W^{(k)}(h,b).$$

Here, $W^{(k)}(h, b)$ is the conditional distribution function over the interaction fields, provided that a site has k bound neighboring sites, and C_q^k are binomial coefficients. Similarly, the functions $W_{1,2}(h_1, h_2, b)$ entering expression (10) can be written as

$$W_{1,2}(h_1,h_2,b) = \sum_{p=0}^{q-1}\sum_{l=0}^{q-1} C_{q-1}^p C_{q-1}^l b^{p+l} \times (1-b)^{2(q-1)-(p+l)} W_{1,2}^{(p,l)}(h_1,h_2,b).$$

Now we construct the following approximation. We replace the averaging over the conditional distribution functions $W^{(k)}$ and $W_{1,2}^{(p,l)}$ with the conditional means in the corresponding expressions. In other words, we take the conditional distribution functions in the form

$$W^{(k)}(h,b) = \delta(h - h_a^{(k)})$$

and

$$W_1^{(p,l)}(h_1,h_2,b) = W_2^{(p,l)}(h_1,h_2,b) = \delta(h_1 - h_{1a}^{(p)})\delta(h_2 - h_{2a}^{(l)}).$$

We assume that the average values of the fields $h_a^{(k)}$, $h_{1a}^{(p)}$, and $h_{2a}^{(l)}$ are proportional to the k, p, and l values, respectively, with the same proportionality factor (denoted as y). Then, we find from (9) and (10) that

$$M = \sum_{k=0}^{q} C_q^k b^k (1-b)^{q-k} \tanh(Kky + h_{ex}), \qquad (13)$$

where y is determined from the equation

$$\sum_{k=0}^{q} C_q^k b^k (1-b)^{q-k} \tanh(Kky + h_{ex}) = (1-b)\sum_{p=0}^{q-1} C_{q-1}^p b^p (1-b)^{q-1-p} \tanh(Kpy + h_{ex}) + b\sum_{p=0}^{q-1}\sum_{l=0}^{q-1} C_{q-1}^p C_{q-1}^l b^{p+l} (1-b)^{2(q-1)-(p+l)} \times \frac{\sinh(K(p+l)y + 2h_{ex})}{\cosh(K(p+l)y + 2h_{ex}) + e^{-2K}\cosh(K(p-l)y)}. \qquad (14)$$

Approximation (13) will be referred below to as binomial. Now we consider the main properties of binomial approximation (13). First, it should be noted that, for a pure magnet ($b = 1$), approximation (13) coincides with (11); thus, it is the exact solution for the Ising model on the Bethe lattice. There is another similarity between approximations (13) and (11): if one finds the critical value of parameter $K = K_c$ for approximation (11), at which the nonzero root of (12) for $h_{ex} = 0$ disappears, the following expression can be obtained [11, 12]:

$$K_c = \frac{1}{2}\ln\frac{b + b_c}{b - b_c}, \quad b_c = \frac{1}{q-1}. \qquad (15)$$

It can easily be shown using (14) that the critical value of parameter K_c and percolation threshold b_c determined within the binomial approximation are the same as in (15). However, approximations (11) and (13) do not coincide in the general case. To compare the degrees of accuracy of these approximations, one should compare them with the exact solution. The exact solution for the site- or bond-diluted Ising model can be constructed for a one-dimensional chain [14]. It is known [15] that a one-dimensional chain is a kind of "pathological" lattice form: it cannot undergo a phase transition and does not exhibit spontaneous magnetization at nonzero temperature, and an infinite cluster of magnetic atoms is broken upon nonmagnetic dilution at any nonzero impurity concentration. In other words, when considering a one-dimensional chain with nonmagnetic impurities, we are always in the concentration range below the percolation threshold and at temperatures above the Curie temperature. Nevertheless, the exact solution can be obtained and, correspondingly, compared with the results of the approximate methods.

Let us consider a one-dimensional bond-diluted Ising magnet (chain). At bond dilution, the chain is broken into segments of magnetic atoms with different lengths separated by dangling bonds. The average value of the Ising spin per magnetic atom can be calculated as

$$M = \sum_{n=1}^{\infty} m_n p_n, \qquad (16)$$

where m_n is the average magnetization of an atom from a segment with length n and p_n is the probability that a randomly chosen magnetic atom belongs to this segment. Obviously, $p_n = nb^{n-1}(1-b)^2$, and magnetization

m_n can be calculated as follows. Let Z_n be a partition function for a segment of n Ising spins $\sigma_1, ..., \sigma_n$:

$$Z_n = \sum_{\sigma_1,\ldots,\sigma_n} \exp\left(K\sum_{i=1}^{n-1}\sigma_i\sigma_{i+1} + h_{ex}\sum_{i=1}^{n}\sigma_i \right) = F_n(+1) + F_n(-1),$$

where

$$F_n(\sigma_n) = \sum_{\sigma_1,\ldots,\sigma_{n-1}} \exp\left(K\sum_{i=1}^{n-1}\sigma_i\sigma_{i+1} + h_{ex}\sum_{i=1}^{n}\sigma_i \right).$$

Then,

$$m_n = \frac{1}{n}\frac{\partial}{\partial h_{ex}}\ln Z_n = \frac{1}{n}\frac{F_{n,h}(+1) + F_{n,h}(-1)}{F_n(+1) + F_n(-1)},$$

where $F_{n,h}(\sigma)$ is the derivative of $F_n(\sigma)$ with respect to h_{ex}. The following recurrence relations can be obtained for parameters $F_n(\pm 1)$ and their derivatives:

$$F_{n+1}(\sigma) = \sum_{\sigma'=\pm 1} F_n(\sigma')e^{K\sigma\sigma'+h_{ex}\sigma} = F_n(+1)e^{K\sigma+h_{ex}\sigma} + F_n(-1)e^{-K\sigma+h_{ex}\sigma},$$

$$F_{n+1,h}(\sigma) = (F_{n,h}(+1) + \sigma F_n(+1))e^{K\sigma+h_{ex}\sigma} + (F_{n,h}(-1) + sF_n(-1))e^{-K\sigma+h_{ex}\sigma},$$

$$F_1(+1) = F_{1,h}(+1) = e^{h_{ex}}, \quad F_1(-1) = e^{-h_{ex}}, \quad F_{1,h}(-1) = -e^{-h_{ex}}.$$

Having introduced the designations

$$x_n = F_n(-1)/F_n(+1), \quad y_n = F(n,h)(+1)/F_n(+1), \quad z_n = F(n,h)(-1)/F_n(+1),$$

we arrive at

$$m_n = \frac{1}{n}\frac{y_n + z_n}{1 + x_n},$$

$$x_{n+1} = \frac{e^{-2K} + x_n}{1 + x_n e^{-2K}}e^{-2h_{ex}}, \quad y_{n+1} = \frac{y_n + z_n e^{-2K}}{1 + x_n e^{-2K}} + 1, \quad z_{n+1} = \frac{z_n + y_n e^{-2K}}{1 + x_n e^{-2K}}e^{-2h_{ex}} - x_{n+1}, \quad (17)$$

$$x_1 = e^{-2h_{ex}}, \quad y_1 = 1, \quad z_1 = -e^{-2h_{ex}}.$$

Now we compare solution (16) with approximations (11) and (13). Assuming that $q = 2$ in (11) and (13), we obtain

$$M_1 = \tanh(2x + h_{ex}), \quad (18)$$

$$M_2 = (1-b)^2\tanh(h_{ex}) + 2b(1-b)\tanh(y + h_{ex}) + b^2\tanh(2y + h_{ex}), \quad (19)$$

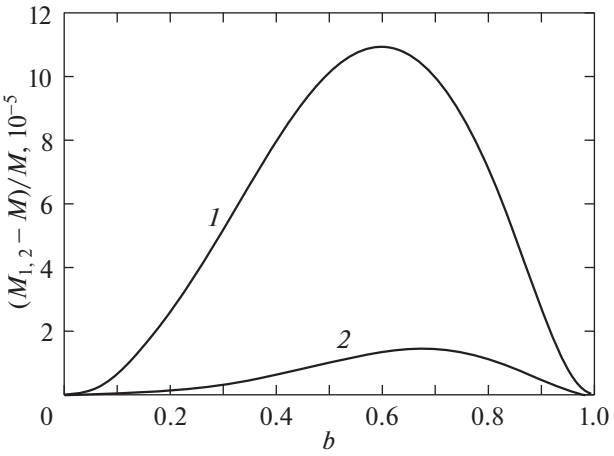

Fig. 1. Relative differences (*1*) $(M_1 - M)/M$ and (*2*) $(M_2 - M)/M$ between the approximate and exact solutions for a one-dimensional bond-diluted chain of Ising spins. The concentration of non-dangling bonds b is on the abscissa axis.

where x and y can be found from the equations

$$\tanh(2x + h_{ex}) = (1-b)\tanh(x + h_{ex}) + b\frac{\sinh(2x + 2h_{ex})}{\cosh(2x + 2h_{ex}) + e^{-2K}}$$

and

$$(1-b)\tanh(y + h_{ex}) + b\tanh(2y + h_{ex}) = (1-b)^2\frac{\sinh(2h_{ex})}{\cosh(2h_{ex}) + e^{-2K}} + 2b(1-b)\frac{\sinh(y + 2h_{ex})}{\cosh(y + 2h_{ex}) + e^{-2K}\cosh(y)} + b^2\frac{\sinh(2y + 2h_{ex})}{\cosh(2y + 2h_{ex}) + e^{-2K}}.$$

Figure 1 shows the relative differences $(M_1 - M)/M$ (curve *1*) and $(M_2 - M)/M$ (curve *2*) in dependence of b calculated at $K = 0.5$ and $h_{ex} = 0.1$. One can see that, in this case, binomial approximation (13) yields the more accurate result compared to pseudorandom approximation (11). Our calculations show that, at other values of parameters K and h_{ex}, the binomial approximation is also more accurate than the pseudorandom approximation for the one-dimensional diluted Ising model.

Unfortunately, the exact solution for the diluted Ising model cannot be constructed even for the Bethe lattice with $q > 2$. However, for the diluted Bethe lattice, the probability $P_0(b)$ that a random lattice site belongs to an infinite cluster can be found in a relatively simple way [16]:

$$P_0(b) = 1 - Z^q,$$

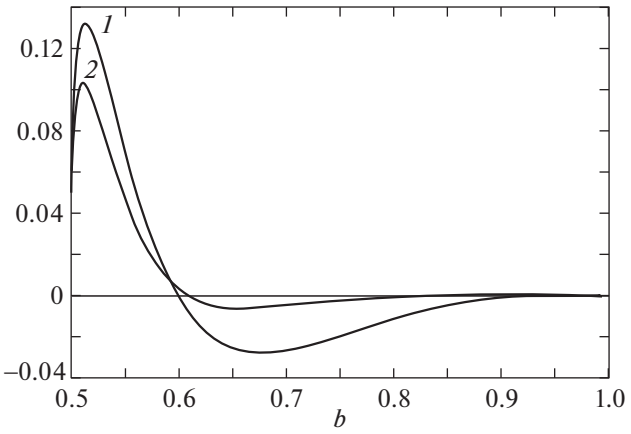

Fig. 2. Differences between the spontaneous magnetization at zero temperature and function $P_0(b)$ for (*1*) pseudorandom and (*2*) binomial approximations. The concentration of non-dangling bonds b is on the abscissa axis.

where Z is a root of the equation $\sum_{i=0}^{q-2} Z^i = 1/b$.

It is known [16] that the average spontaneous magnetization in the diluted Ising model at $T \to 0$ ($K \to \infty$) should be equal to $P_0(b)$. Since approximations (11) and (13) at $b = 1$ are the exact solutions for the Ising model on the Bethe lattice, at $b < 1$ they can be considered as approximate solutions for the diluted Ising model for this lattice. Therefore, it is reasonable to compare the probability $P_0(b)$ with the spontaneous magnetization in approximations (11) and (13) at $K \to \infty$.

Figure 2 shows the differences between the magnetization calculated at $T \to 0$ and the probability $P_0(b)$ for pseudorandom approximation (10) (curve *1*) and binomial approximation (13) (curve *2*) for the Bethe lattice with $q = 3$ in dependence of b. It can be seen that the difference for the binomial approximation is smaller than that for the pseudorandom approximation.

4. CONCLUSIONS

We can conclude the following. The method of averaging over interaction fields based on relation (2) was formulated and substantiated in the general form. It was shown that this method can be applied to diluted magnets in combination with the self-averaging method [10]. The described general algorithm was used for one- and two-site clusters (formulas (9) and (10), respectively).

Pseudorandom (11) and binomial (13) approximations for the bond-diluted Ising model were constructed using averaging over interaction fields. The accuracy of these approximations was estimated by comparing with the exact solution for the one-dimensional bond-diluted Ising model. In addition, the magnetizations at zero temperature obtained within these approximations were compared with $P_0(b)$ for the Bethe lattice at $q = 3$. These comparisons showed that binomial approximation (13) is more accurate than approximation (11).

CONFLICT OF INTEREST

The authors declare that they have no conflict of interest.

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