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Approximate Accounting of Spin Correlations in the Ising Model

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 Received March 3, 2021; revised April 6, 2021; accepted April 10, 2021

Abstract—The expressions for average products of three neighboring spins in the Ising model have been found on lattices with coordination numbers 3 and 4 as functions of temperature and spontaneous magnetization. These expressions are used to compare the exact solution for the Ising model on a square lattice and the solutions found by approximate methods. A method of improving approximate methods is proposed for applying, in particular, to the Bethe approximation and to a change in the critical index of the temperature dependence of the spontaneous magnetization.

Keywords: Ising model, spin correlations, critical indices **DOI:** 10.1134/S1063783421080278

1. INTRODUCTION

Effective instruments of analyzing systems of many interacting particles, such as magnets, are simple lattice models, for example, the Ising model, the Potts model, or the Heisenberg model [1].

In spite of the fact that these models have been used in the statistical physics of phase transitions already for a long time, many problems related to them are topical up to now. In particular, in recent years, very many studies [5-9] were devoted to the Ising model (which is used not only in the magnetism theory [3, 4]). The detailed review [2] contains a quite voluminous bibliography which includes as the scientific works becoming classical and recent studies devoted to the Ising model and analogous models. It is a pity the efficiency of lattice models is restricted, as a rule, by the impossibility to obtain exact solutions in most of nontrivial cases. The known Onsager's solution for the twodimensional Ising model on a square lattice [1] in the absence of any external magnetic field is a rare exception to this rule. However, exact solutions are of importance for studies of phase transitions themselves and also the estimation of the accuracy of approximate solution methods. Exact solutions obtained, for example, for the Ising model can be used to estimate the efficiency of the algorithms of the numerical simulation of phase transitions in magnets [6, 7]. Thus, the obtainment of exact results for the Ising model or other lattice models is a quite topical problem.

There are, of course, also many approximate methods of solving the Ising model: the mean field method, the Bethe approximation, and their various generalizations [1-6, 10]. The solution obtained by these methods give different (as a rule, overestimated) estimations for the Curie temperature and have a number of common features which unite them and distinguish them from the exact Onsager's solution. Namely, critical indices of the solutions obtained by approximate methods which have so-called "classical" values, in particular, the critical index of the temperature dependence of the spontaneous magnetization near the Curie temperature is 1/2 [1], while it is 1/8 in the Onsager's solution [1]. One of the reasons of this difference is the circumstance that, in any real lattice with the coordination number q > 2, there are infinitely many various ways connecting any two lattice sites, but approximate methods use, as a rule, a finite (and small) number of such ways [9]. Thus, spin correlations in real lattices have a greater importance than it is taken into account in approximate methods. In this work, we found the exact expressions which relate some spin correlations in the Ising model for a lattice with coordination number q = 4 to the spontaneous magnetization for this lattice. Certain assumptions with respect to these correlations are shown to lead to various approximate methods of determining the magnetization; in this case, some of them can give a nonclassic critical index of the temperature dependence of spontaneous magnetization. Using the expressions relating the magnetization and correlations, we calculated the spin correlations for a square lattice (using the Onsager's solution), for the Bethe lattice (using the Bethe approximation) and also built correlations using the expressions for the magnetization found by some approximate methods.

The comparison of exact correlations with the approximate ones suggests a method of an artificial "correction" of approximate spin correlations which leads to a modification of an initial approximate solution. It turns out that the such-modified solutions have a nonclassic critical index of the temperature dependence of the spontaneous magnetization and the Curie temperature becomes significantly closer to the known exact values.

2. AVERAGING ON EXCHANGE FIELDS AND SPIN CORRELATIONS

Consider the Ising model on a lattice. Let us assume that each lattice site contains an "Ising" spin taking values +1 and -1 and only spins in the bound sites interact. Let Ω be a set of all these spins, $\mathcal{H}(\Omega)$ be Hamiltonian. Then,

$$\mathcal{H}(\Omega) = -J\sum_{(i,j)} \sigma_i \sigma_j - H_{\text{ex}} \sum_i \sigma_i.$$
(1)

The summation in the first sum is performed over all pairs of bound spins and in the second sum, over all sites; J is the exchange interaction energy, H_{ex} is the external field.

Consider a spin σ_0 . Let $h = \sum_{i=1}^{q} \sigma_i$ be the sum of the values of the spins which immediately interact with σ_0 (spins of the first coordination sphere). We call this sum an "interaction field," and let f(h) be a function of this field. Then, as shown in [11], the thermodynamically average value of product $f(h)\sigma_0$ is

$$\langle f(h)\sigma_0 \rangle = \sum_h f(h) \tanh(Kh + h_{\rm ex})W(h),$$
 (2)

where K = J/kT, $h_{ex} = H_{ex}/kT$, and k is the Boltzmann constant, and the averaging is performed over the distribution function of interaction field W(h).

For the Ising model on a simple lattice with coordination number q, interaction field h can take only discrete values $h_i = q - 2i$, i = 0, ..., q. The average value of any lattice spin is the same and it is M (the average magnetization in the system). In the absence of an external field, we obtain from Eq. (2) at $f(h) = h^n$

$$\langle h^n \sigma_0 \rangle = \sum_i h_i^n \tanh(Kh_i)W(h_i).$$
 (3)

Let n = 2p be an even integral number. Then, we obtain from Eq. (3)

$$\left\langle h^{2p} \sigma_0 \right\rangle = \sum_{i=0}^{n(q)} X_i (q-2i)^{2p} \tanh(K(q-2i)),$$
 (4)

where $X_i = W(h_i) - W(-h_i)$ and $n(q) = \left[\frac{q-1}{2}\right]$ is the

integral part of $\frac{q-1}{2}$.

Averaging value h^{2p+1} over distribution functions $W(h_i)$, we obtain

$$\left\langle h^{2p+1} \right\rangle = \sum_{i=0}^{n(q)} X_i (q-2i)^{2p+1}.$$
 (5)

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Equations (4)–(5) allow us to determine some spin correlations in the Ising model on simple lattices with coordination numbers 3 and 4. Consider a lattice with q = 4. In this case, Eqs. (4)–(5) contain only terms containing X_0 and X_1 . At p = 0, Eq.(5) gives the average value of h equal to 4M:

$$4M = 4X_0 + 2X_1$$

and Eq. (4) gives, at p = 0, the average value of σ_0 equal to *M*:

$$M = X_0 \tanh(4K) + X_1 \tanh(2K),$$

from where

$$X_0 = \frac{2\tanh(2K) - 1}{2\tanh(2K) - \tanh(4K)}M$$

and

$$X_1 = \frac{2(1 - \tanh(2K))}{2\tanh(2K) - \tanh(4K)}M.$$
 (6)

Now, let p = 1 in Eq. (5). We raise interaction field $h = \sum_{i=1}^{4} \sigma_i$ to the third power and denote $S_3 = \langle \sigma_i \sigma_j \sigma_k \rangle$, where *i*, *j*, and *k* are different. (We assume that S_3 is independent of the specific choice *i*, *j*, and *k_i*, which is valid, in particular, for the isotropic Ising model on square or tetrahedral lattices.). Then, from Eq. (5), we obtain

$$S_3 = X_0 - \frac{1}{2}X_1 = \frac{(\tanh(4K) + 2\tanh(2K)) - 2}{2\tanh(2K) - \tanh(4K)}M.$$
 (7)

Quantity $S_3 - M^3$ (or S_3 itself) can be considered as a correlation measure of any three spins of the first coordination sphere. Equation (7) enables one to calculate the dependence of S_3 on temperature parameter K as the dependence of the spontaneous magnetization on this parameter is known. We know, in particular, the exact solution for the Ising model on a square lattice in the absence of external magnetic field obtained by L. Onsager and C.N.Yang [12, 13]:

$$M^8 = 1 - \frac{1}{\sinh^4(2K)}.$$
 (8)

Substituting *M* expressed from Eq. (8) into Eq. (7), we obtain the exact value $S_3(K)$ for a square lattice:

$$S_{3}(K) = \frac{(\tanh(4K) + 2\tanh(2K)) - 2}{2\tanh(2K) - \tanh(4K)} \times \left(1 - \frac{1}{\sinh^{4}(2K)}\right)^{1/8}.$$
(9)

If the expression for spontaneous magnetization M(K) found in the Bethe approximation for q = 4 is substituted into Eq. (7), the obtained expression for $S_3(K)$ can be considered as the exact one for the Bethe lattice [1], since the Bethe approximation can be interpreted as the exact solution for this lattice [1].

On the other hand, Eq. (7) itself can be considered as a base for an approximate estimation of spontaneous magnetization M(K). If we completely neglect the ternary spin correlation and assume that $S_3 = M^3$, we obtain the approximate expression for M(K)

$$M^{2} = \frac{(\tanh(4K) + 2\tanh(2K)) - 2}{2\tanh(2K) - \tanh(4K)}.$$
 (10)

As is easy to show that it is precisely the expression for M(K) that is obtained when using the approximate binominal distribution function on the interaction fields [14].

From Eq. (4) at p = 1, we can determine, by analogy, the quantity $S_{03} = \langle \sigma_i \sigma_j \sigma_0 \rangle$ that is the average value of the products of the central spin and two various spins from the first coordination sphere. For a tetrahedral lattice, S_{03} is independent of the choice of *i* and *j*; for a plane square lattice, we determine S_{03} as a result of additional averaging over the versions of choosing two spins from the first coordination sphere. Then

$$S_{03} = X_0 \tanh(4K)$$

= $\frac{(2 \tanh(2K) - 1) \tanh(4K)}{2 \tanh(2K) - \tanh(4K)} M.$ (11)

This expression, as well as Eq. (7), can be used for finding the exact solution S_{03} and also for an approximate estimating M(K), neglecting the corresponding ternary correlation, i.e., equating S_{03} to M^3 . If p = 2 is substituted to Eq. (4), we can find $S_5 = \langle \sigma_0 \sigma_1 \sigma_2 \sigma_3 \sigma_4 \rangle$ that is the ensemble average value of the product of central spin σ_0 and all four its nearest neighbors

$$S_{5} = X_{4} \tanh(4K) - X_{2} \tanh(2K)$$
(12)
=
$$\frac{4 \tanh(2K) \tanh(4K) - (\tanh(4K) + 2 \tanh(2K))}{2 \tanh(2K) - \tanh(4K)} M.$$

By analogy with Eqs. (7) and (11), Eq. (12) can be used to find the exact average S_5 , if the expression for the spontaneous magnetization as a function of temperature parameter *K* is known. In addition, by analogy with the previous cases, we can approximately assume that $S_5 = M^5$ and obtain

$$M^{4} = \frac{4\tanh(2K)\tanh(4K) - (\tanh(4K) + 2\tanh(2K))}{2\tanh(2K) - \tanh(4K)}.$$
(13)

In approximation (13), spontaneous magnetization M becomes zero at $K = K_c$, where, as it is easy to show $\tanh(2K_c) = 2 - \sqrt{2}$ and $K_c \approx 0.336$. This value of K_c is slightly closer to the exact values for the tetrahedral (0.370) and square (0.441) lattices than the values obtained from approximations $S_3 = M^3$ (0.324) and $S_{03} = M^3$ (0.275). A more interesting feature of approximation (13) is that, as seen from Eq. (13), $M \sim (K - K_c)^{1/4}$ near K_c ; i.e., the critical index of the temperature dependence of the spontaneous magnetization is 1/4, which differs from the classical value 1/2.

Similar calculations can be also performed for lattices with coordination number q = 3, obtaining the expressions for the average values of spin products via temperature and spontaneous magnetization:

$$S_3 = \frac{3(\tanh(K) + \tanh(3K)) - 4}{3\tanh(K) - \tanh(3K)}M,$$

$$S_{03} = \frac{4\tanh(3K)\tanh(K) - \tanh(K) - \tanh(3K)}{3\tanh(K) - \tanh(3K)}M.$$

3. MODIFICATION OF THE APPROXIMATE METHODS ON SPIN CORRELATIONS

The mean values (7) and (11) calculated in Section 2 can be used, in particular, to estimate the efficiency of

the approximate methods of solving the Ising model. We introduce functions R(M) and $R_0(M)$ as follows:

$$R_0(M) = \frac{S_{03} - M^3}{M}$$
 and $R(M) = \frac{S_3 - M^3}{M}$.

These functions (which we call "correlants" in the text) can be considered as a correlation measure of the values of a spin in a lattice and its two neighbors ($R_0(M)$ or three spins neighboring to one site (R(M)). For a square lattice (q = 4), these function are, according to Eqs. (7) and (11),

$$R_{0}(M) = \frac{(2 \tanh(2K) - 1) \tanh(4K)}{2 \tanh(2K) - \tanh(4K)} - M^{2}$$

$$= 1 - \left(\frac{1 - x}{x}\right)^{2} - M^{2}$$
(14)

and

$$R(M) = \frac{(\tanh(4K) + 2\tanh(2K)) - 2}{2\tanh(2K) - \tanh(4K)} - M^{2}$$

= $1 - \frac{1}{x} \left(\frac{1 - x}{x}\right)^{2} - M^{2}$, (15)

where $x = \tanh(2K)$. Relationships (14) and (15) allow one to find $R_0(M)$ and R(M) if the spontaneous magnetization is known as a function of temperature M = M(x) (more correctly, inverse function x = x(M)). However, the same relationships can be used in the "inverse direction": if for some reasons the expressions for correlants $R_0(M)$ or R(M) as functions of spontaneous magnetization M are found, the spontaneous magnetization can be found from Eqs. (14) and (15) as a function of temperature.

For the exact solution of the Ising model on a square lattice (8), we have

$$M^{8} = 1 - \frac{1}{\sinh^{4} 2K} = 1 - \left(\frac{1 - x^{2}}{x^{2}}\right)^{2},$$
 (16)

from where $x = 1/\sqrt{1 + \sqrt{1 - M^8}}$.

Using this solution, we find, from Eqs. (14) and (15), the exact values of correlants R(M) and R(M) for a square lattice in the absence of external field.

Let there be some approximate solution for the Ising model on a square lattice that determines an approximate value of the spontaneous magnetization as a function of temperature parameter x. Representing this solution as inverse function $x = \chi(M^2)$ and using it in Eqs. (14) and (15), we can obtain approximate values of spin correlants $\tilde{R}_0(M)$ and $\tilde{R}(M)$ corresponding to this solution. (We assume that x is a function of M^2 , since, in the absence of magnetic field, the Hamiltonian of the Ising model is symmetric with respect to the simultaneous change in the signs of all spins. Thus, when this circumstance is taken into account in an approximate solution, two values of the spontaneous magnetization +M and -M correspond to each value of parameter x; i.e., x is an even function of M.) As was said in Introduction, the correlation effect is usually underestimated in the approximate methods; thus, we expect that values $\tilde{R}_0(M)$ and $\tilde{R}(M)$ will be smaller than the exact values calculated by Eq. (16). In particular, the values of these functions at M = 0 must be smaller than the corresponding exact values. As seen from Eqs. (14) and (15), $R_0(0)$ and R(0)are monotonically increasing functions of x. Thus, the lower $R_0(0)$ and R(0), the smaller is the critical value of temperature parameter K_c ; i.e., the estimation of the Curie temperature $T_c = 1/K_c$ in the approximate solutions is overestimated one precisely due to an underestimation of spin correlations.

The value of function $x = \chi(M^2)$ at M = 0 determines the critical value of temperature parameter $x = \tanh(2K)$, i.e., the Curie temperature, and the critical index of the temperature dependence of the spontaneous magnetization is determined by the function expansion in powers of M^2 : if the first nonzero term of such an expansion is of an order of M^{2n} , the critical index is 1/2n.

Consider, as an example, the Bethe approximation [1] and its generalization on a class of recursive lattices [15]. As shown in [14], the Bethe approximation can be considered as a sort of the renormalization-group transformation from a unit lattice site with a coordination number to a dimer on the same lattice; i.e., we consider a cluster consisting of one atom existing in

crystal field h_1 . The average magnetization of this atom is

$$n_{\rm l}(h_{\rm l}) = \tanh(Kh_{\rm l}). \tag{17}$$

In addition, we consider a cluster consisting of two neighboring atoms (dimer) existing in crystal field h_2 .

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The average magnetization of an atom of this cluster is

$$m_2(h_2) = \frac{\sinh(2Kh_2)}{\cosh(2Kh_2) + e^{-2K}}.$$
 (18)

In the Bethe approximation, the spontaneous magnetization is found by equalizing the right sides of Eqs. (21) and (22)

$$M = m_1(h_1) = m_2(h_2)$$
(19)

at additional condition $\frac{h_2}{h_1} = \frac{q-1}{1}$ [14]. Such a "renor-

malization-group" interpretation of the Bethe approximation suggests the natural generalization [15]: in parallel to the dimer, we can consider a more complex cluster on a lattice; for example, a cyclic cluster consisting of N atoms existing in crystal field h_N . The value of N can be taken to be equal to the number of sites contained in the shortest closed way on this lattice: for example, N = 4 for a square lattice, N = 6 for a hexagonal lattice, and so on.

The average magnetization of an atom of this cluster is

$$m_N(h_N) = \frac{\lambda_1^N - \lambda_2^N}{\lambda_1^N + \lambda_2^N} \frac{e^K \sinh(Kh_N)}{\sqrt{e^{2K} \sinh^2(Kh_N) + e^{-2K}}},$$
 (20)

where $\lambda_{1,2} = e^K \cosh(Kh_N) \pm \sqrt{e^{2K} \sinh^2(Kh_N) + e^{-2K}}$. Now, equalizing the right sides of Eqs. (17) and (20) at additional condition $\frac{h_N}{h_1} = \frac{q-2}{q}$ and the right sides of Eqs. (18) and (20) $\frac{h_N}{h_2} = \frac{q-2}{q-1}$, we obtain, by analogy with Eq. (19), two approximations which improve the Bethe approximation and which will be called "cluster approximations 1 - N and 2 - N." (In [15], it was shown that, at some values of q, these approximations can be understood as the exact solution for recursive lattice constructed specially.) It is easy to show that both the Bethe approximation and its cluster improvements have the critical index of the temperature dependence of the spontaneous magnetization 1/2.

Figure 1 shows the plots of (curve *1*) correlant $R_0(M)$ and its approximate values $\tilde{R}_0(M)$ in (curve 2) the Bethe approximation, and cluster approximations 1 - N and 2 - N (curves 3 and 4, respectively) calculated for q = 4. It is seen that, for all the approximations, the values of the correlants at any *M* is lower than the exact values found by Eq. (16) (curves *1*),



Fig. 1. Correlant $R_0(M)$ as a function of spontaneous magnetization *M* for a square lattice. Curve *1* is the exact value; curve *2* is the Bethe approximation; curves *3* and *4* are cluster approximations 1 - N and 2 - N, respectively.

which confirms the above assumption. Correlant R(M) and its approximate values $\tilde{R}(M)$ behave similarly.

The behavior of these functions suggests a possibility of improving the approximate methods of calculating the spontaneous magnetization by a modification of the corresponding correlants. Namely, taking some approximate solution $x = \chi(M^2)$, we calculate, for example, correlant $\tilde{R}_0(M)$ (14) for it and then multiply it by the "modifying polynomial" $P(M^2)$ which is only dependent on even powers of M and whose maximum power is 2n

$$P(M^{2}) = A_{0} + A_{1}M^{2} + A_{1}M^{4} + \dots + A_{n}M^{2n}.$$
 (21)

This correlant will be called "modified" correlant. Now we substitute the modifying correlant to the left part of Eq. (14) and solve the obtained equation with respect M. This solution is exactly the modified spontaneous magnetization as a function of temperature: i.e., the modified spontaneous magnetization as a function of temperature parameter $x = \tanh(2K)$ is found, according to Eq. (14), from condition

$$F_0(x) = P(M^2)F_0(\chi(M^2)) - (P(M^2) - 1)M^2, \quad (22)$$

where

$$F_0(x) = 1 - \left(\frac{1-x}{x}\right)^2$$
.

The solution found by this method will be, of course, dependent on the maximum power and the coefficients of modifying polynomial (21). Thus, the final calculation of the modifying magnetization is dependent on the method which is used for determination of coefficients of Eq. (21).

One of such methods is as follows. The right side of Eq. (22) is expanded into a series in powers of $\mu = M^2$:

$$F_0(x) = a_0 + a_1 \mu + a_2 \mu^2 \dots$$
(23)

The terms of this expansion are dependent on the coefficients of modifying polynomial (21) and the initial approximate solution $\chi(M^2)$. Assume that the critical index of the temperature dependence of the spontaneous magnetization is 1/2, i.e., $\chi'(0) \neq 0$. If we will demand that coefficient a_1 in expansion (23) vanishes, then, in the modified solution, the critical index of the temperature dependence of the spontaneous magnetization becomes equal to 1/4. The simultaneous vanishing of coefficients a_1 and a_2 gives the modified solution with the critical index 1/6, and so on. Coefficient a_0 determines the value of x at which M becomes equal to zero, i.e., the Curie temperature of the modified solution. The simplest version of this method is that, in which only constant A_0 remains in polynomial (21). Then, we have in expansion (23)

$$a_0 = A_0 F_0(\chi(0))$$
 and $a_1 = 1 - A_0(1 - F_0'(\chi(0))\chi'(0))$.

Now, equating, according to the abovementioned, a_1 to zero, we obtain

$$A_0 = 1/(1 - F_0'(\chi(0))\chi'(0)), \qquad (24)$$

i.e. the relationship between $x = \tanh(2K)$ and spontaneous magnetization M for the modified solution is determined by condition

$$1 - \left(\frac{1-x}{x}\right)^2 = A_0 \left(1 - \left(\frac{1-\chi(M^2)}{\chi(M^2)}\right)^2\right) - (A_0 - 1)M^2, (25)$$

where, according to Eq. (24),

$$A_0 = \frac{\chi^3(0)}{\chi^3(0) - 2(1 - \chi(0))\chi'(0)}.$$
 (26)

The critical temperature parameter K_c is found from condition $tanh(2K_c) = (1 + \sqrt{1 - a_0})^{-1}$.

From Eqs. (17)–(18), for the Bethe approximation at q = 4, it is easy to calculate that $\chi(0) = 3/5$ and $\chi'(0) = 2/25$. Using these values, we found modified value $K_c \approx 0.420$, which is closer to the exact value 0.441 obtained from Eq. (21) than the value 0.347 obtained by nonmodified Bethe method. Figure 2 shows the spontaneous magnetization as a function of K found in the Bethe approximation (curve 2) and in the Bethe approximation modified by correlant $R_0(M)$, according to Eqs. (25)–(26). Curve *I* in Fig. 2 shows the exact value of M(K) calculated by Eq. (16).

In equations (25)-(26), a approximation simpler than the Bethe approximation can be used as the ini-



Fig. 2. Spontaneous magnetization *M* as a function of temperature parameter K = J/kT for the Ising model on a square lattice. Curve *I* is the exact value; curve *2* is the Bethe approximation. Curve *4* is the mean field approximation. Curves *3* and *5* are the modified Bethe approximation and the mean field approximation, respectively.

tial one, namely, the mean field approximation [1]. For this approximation at q = 4, we have

$$\chi(M^2) = \tanh\left(\frac{1}{2M}\operatorname{arctanh}(M)\right).$$
(27)

Thus,

$$\chi(0) = \frac{e-1}{e+1}, \quad \chi'(0) = \frac{2e}{3(e+1)^2}$$

and

$$\tanh(2K_c) = (1 + 2/\sqrt{2e^2 + 1})^{-1}$$

The numerical value of K_c is ~0.440. Figure 2 shows the plots of the spontaneous magnetization as a function of K in the mean field approximation (curve 4) and the modified mean field (curve 5).

By analogy, cluster approximations 1 - N and 2 - N can be modified by correlant $R_0(M)$ and also all the approximations can be modified by correlant R(M).

4. CONCLUSIONS

Thus, in this work, the following results have been obtained. Using the method of averaging over exchange fields [11], it is shown that, for the Ising model on lattices with coordination numbers 3 and 4, the mean values of the products of three neighboring spins in the absence of magnetic field are proportional to the spontaneous magnetization; we calculated the coefficients of this proportionality depending only on temperature. For a square lattice, these expressions allow one to find the exact values of the spin means, using the known exact Onsager's solution.

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The obtained expressions can be also used to construct approximate values of spin means (or relevant mean correlants $R_0(M)$ and R(M)) if the values found by the approximate methods are used for the temperature dependence of the spontaneous magnetization. The Bethe approximation and some its generalizations are shown to give underestimated values of spin correlants as compares to the exact values (Fig. 1).

We proposed the method of modifying the approximate methods of solving the Ising model based on the artificial correction of approximate correlants. It is shown that, as applied to the Bethe approximation and the mean field approximation, such a modification gives more correct value of the critical temperature and changes the critical index of the temperature dependence of the spontaneous magnetization from 1/2 to 1/4.

CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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Translated by Yu. Ryzhkov