

## SELF-CONSISTENT APPROXIMATION IN THE ISING MODEL OF PURE AND DILUTE MAGNETS USING A PAIR CORRELATION

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*We construct a self-consistent approximation for calculating the magnetization and Curie temperature in the Ising model on an arbitrary lattice based on using the magnetization and pair correlation of nearest neighbors. We find the Curie temperatures for simple lattices in this approximation and generalize the approximation to the case of lattices diluted in lattice sites or bonds, for which we find the approximate values of the percolation thresholds.*

**Keywords:** Ising model, dilute magnet, self-consistent approximation

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### 1. Introduction

As is known [1], [2], one of the classical approaches for solving the problem of many interacting particles is to construct self-consistent equations. For the Ising model, for example, the mean field approximation or the Bethe approximation is constructed using this method [1], [2]. The basic idea of this method is that some single quantity is calculated for different finite-size clusters of particles and the interaction with other particles not included in the cluster is taken into account in terms of an unknown parameter. The condition for the equality of this quantity for different clusters of particles (this is self-consistency) gives the equation for this parameter. Moreover, magnetization in the Ising model is taken as the quantity for which self-consistency is established. For example, a comparison of the magnetization in a cluster consisting of one spin and in a cluster consisting of a spin and its nearest neighbors is used in the Bethe approximation [1]. In [3]–[7], we constructed different variants of a generalization of this approach. In many cases (including for the Bethe method itself), the self-consistent approximation can be regarded as an exact solution for recursive lattices constructed in a certain way [3], [7]. Constructing self-consistent equations in this way is also possible for other models, for example, for the Potts model [4], [6].

It seems quite natural to try to extend the method of self-consistent equations by establishing self-consistency using not only magnetization but also some other quantity that is not expressed in terms of magnetization. Here, we attempt this by using the average product of adjacent spins as the additional quantity.

In [3], we constructed a class of self-consistent equations for the approximate solution of the Ising model of pure and dilute magnets. Some, although not all, equations for pure magnets in this class can be interpreted as exact solutions of the Ising problem on recursive lattices. In addition, we showed that in those cases where our method gives an exact solution on a recursive lattice for a pure magnet, its generalization

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to a dilute magnet leads to an exact value of the percolation threshold for this particular lattice. All self-consistent equations constructed in [3] were based on comparing the average magnetization calculated for clusters of various types and sizes.

Here, we investigate the possibility of constructing self-consistent equations (for both pure magnets and magnets diluted in sites or bonds) by comparing not only the magnetizations for different clusters but also the correlations of nearest neighbors. We show that the approximation constructed in this way gives values of the Curie temperature for simple lattices closer to the exact values than those obtained in [3] (if the recursive lattices constructed here are regarded as an approximation of real simple lattices). In addition, we extend our method to Ising magnets diluted in sites or bonds and obtain approximate values of the percolation thresholds.

## 2. Self-consistent equations for pure magnets

We consider a simple crystal lattice with a coordination number  $q$  with Ising spins  $\sigma = \pm 1$  located at the sites and a nonzero exchange interaction only for neighboring spins. Let  $J$  be the exchange integral,  $k$  be the Boltzmann constant, and  $T$  be the temperature. The temperature parameter is  $K = J/kT$ . We assume that the external field is zero and the temperature  $T < T_C$ , where  $T_C$  is the Curie temperature. Then there is a spontaneous magnetization  $M(K)$  in the lattice. We consider a cluster of two neighboring atoms (dimer) on this lattice. Then  $M(K)$  is the average magnetization of an atom of a dimer, and  $S(K)$  is the average product of its spins. The spontaneous magnetization  $M(K)$  vanishes for  $T > T_C$ .

We now consider a system consisting of only two spins coupled by the exchange interaction in the field  $h_2$  (in units  $kT$ ) and find the average magnetization  $m_2(h_2, K_2)$  of an atom in such an individual dimer and the average value  $s_2(h_2, K_2)$  of the product of its spins. For such a system,

$$-\frac{H(\sigma_1, \sigma_2)}{kT} = K_2 \sigma_1 \sigma_2 + h_2(\sigma_1 + \sigma_2),$$

where  $H(\sigma_1, \sigma_2)$  is the Hamiltonian. Calculating the partition function

$$Z_2 = \sum_{\sigma_1, \sigma_2} e^{-H(\sigma_1, \sigma_2)/kT},$$

we obtain

$$m_2(h_2, K_2) = \frac{1}{Z_2} \sum_{\sigma_1, \sigma_2} \left( \frac{\sigma_1 + \sigma_2}{2} \right) e^{-H(\sigma_1, \sigma_2)/kT},$$

$$s_2(h_2, K_2) = \frac{1}{Z_2} \sum_{\sigma_1, \sigma_2} \sigma_1 \sigma_2 e^{-H(\sigma_1, \sigma_2)/kT},$$

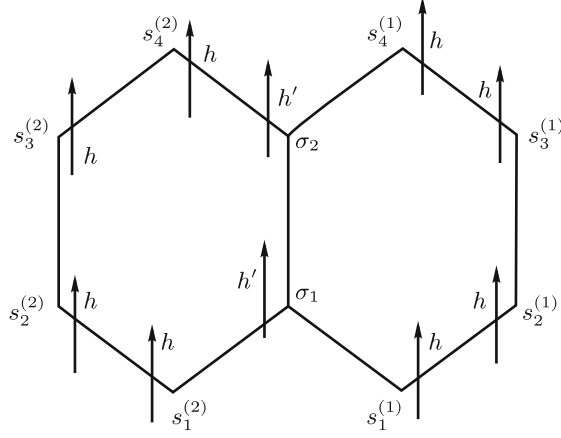
which gives

$$m_2(h_2, K_2) = \frac{\sinh(2h_2)}{\cosh(2h_2) + e^{-2K_2}}, \quad s_2(h_2, K_2) = \frac{\cosh(2h_2) - e^{-2K_2}}{\cosh(2h_2) + e^{-2K_2}}. \quad (1)$$

We assume that for any lattice, we can always choose the values of the parameters  $h_2$  and  $K_2$  such that we have the equalities

$$M(K) = m_2(h_2, K_2), \quad S(K) = s_2(h_2, K_2). \quad (2)$$

Of course, giving these exact values for any  $K$  is equivalent to exactly solving the Ising problem on this lattice. The essence of the method proposed here is to construct self-consistent equations such that by solving them, we can find the approximate values of  $h_2$  and  $K_2$  satisfying equalities (2).



**Fig. 1.** Spins  $\sigma_1$  and  $\sigma_2$  at the vertices of the common side  $L = 2$  of identical  $N$ -gons ( $N = 6$ ).

To construct the self-consistent equations, we consider a system of Ising spins located at the vertices  $L$  of identical nonintersecting  $N$ -gons with a common side (Fig. 1). We regard the spins  $\sigma_1$  and  $\sigma_2$  at the vertices of this common side as a dimer. We let  $s_i^{(j)}$ , where  $i = 1, \dots, N - 2$ ,  $j = 1, \dots, L$ , denote the spins located at the other vertices of the  $j$ th  $N$ -gon. Let the atoms of the dimer be in the field  $h'$  and the other atoms of the  $N$ -gons be in the field  $h$  (Fig. 1). In addition, we assume that there is an exchange interaction with the temperature parameter  $K$  between any adjacent spins of this structure. We then calculate the average magnetization of the dimer atom  $m_{N,L}(h, h')$  and the average value of the product of its spins  $s_{N,L}(h, h')$  as follows. We represent the partition function in the form of three terms corresponding to the dimer spin values  $(+1, +1)$ ,  $(-1, -1)$ , and  $(+1, -1)$ :

$$Z = e^{K+2h'} Z_N^L(+1, +1) + e^{K-2h'} Z_N^L(-1, -1) + 2e^{-K} Z_N^L(+1, -1),$$

where

$$Z_N(\sigma_1, \sigma_2) = \sum_{s_1, \dots, s_{N-2}} e^{K(\sigma_1 s_1 + s_1 s_2 + \dots + s_{N-2} \sigma_2) + h(s_1 + \dots + s_{N-2})}.$$

Then

$$m_{N,L}(h, h') = \frac{e^{K+2h'} Z_N^L(+1, +1) - e^{K-2h'} Z_N^L(-1, -1)}{Z},$$

$$s_{N,L}(h, h') = \frac{e^{K+2h'} Z_N^L(+1, +1) + e^{K-2h'} Z_N^L(-1, -1) - 2e^{-K} Z_N^L(+1, -1)}{Z},$$

or

$$m_{N,L}(h, h') = \frac{e^{2h'} - e^{-2h'} X_N^L(h)}{e^{+2h'} + e^{-2h'} X_N^L(h) + 2e^{-2K} Y_N^L(h)}, \quad (3)$$

$$s_{N,L}(h, h') = \frac{e^{2h'} + e^{-2h'} X_N^L(h) - 2e^{-2K} Y_N^L(h)}{e^{2h'} + e^{-2h'} X_N^L(h) + 2e^{-2K} Y_N^L(h)}, \quad (4)$$

where  $X_N(h) = Z_N(-1, -1)/Z_N(+1, +1)$  and  $Y_N(h) = Z_N(+1, -1)/Z_N(+1, +1)$ .

Just as for a system of two spins, we assume that there exist values of the parameters  $h$  and  $h'$  such that for any lattice, we have the equalities

$$M(K) = m_{N,L}(h, h'), \quad S(K) = s_{N,L}(h, h'). \quad (5)$$

Equating the right-hand sides of the corresponding equalities in (2) and (5), we now obtain

$$m_2(h_2, K_2) = m_{N,L}(h, h'), \quad s_2(h_2, K_2) = s_{N,L}(h, h'). \quad (6)$$

System (6) is the self-consistency condition for the equations for the unknowns  $K_2$ ,  $h_2$ ,  $h$ , and  $h'$ . Of course, two equations are insufficient for determining four unknown parameters in the general case, and we must therefore supplement system (6) with two more conditions. Before we do this, we note that from system (6) with (1), (3), and (4) taken into account, we can easily obtain an equation that does not contain  $K_2$ :

$$X_N(h) = e^{-4(h_2-h')/L}. \quad (7)$$

As can be seen from (1) and (7), zero spontaneous magnetization corresponds to the values  $h_2 = 0$ ,  $h = h_0$ , and  $h' = h'_0$ , which are related by the condition

$$X_N(h_0) = e^{4h'_0/L}. \quad (8)$$

As can be seen from (4) with (8) taken into account, the value of  $S(K)$  (the correlation of neighboring spins for  $M(K) = 0$ ) is equal to

$$S(K) = \frac{X_N^{L/2}(h_0) - e^{-2K}Y_N^L(h_0)}{X_N^{L/2}(h_0) + e^{-2K}Y_N^L(h_0)}. \quad (9)$$

The zero solution is unstable in the region of the existence of spontaneous magnetization ( $T < T_C$ ), and the derivatives with respect to  $h_2$  of the left- and right-hand sides of (7) evaluated at  $h_2 = 0$  are equal to each other for  $T = T_C$  [2]. Therefore, for  $T = T_C$ ,

$$\left. \frac{\partial \log(X_N(h))}{\partial h} \right|_{h=h_0} = \frac{4(\beta - 1)}{\alpha L}, \quad (10)$$

where  $\alpha = \partial h / \partial h_2|_{h_2=0}$  and  $\beta = \partial h' / \partial h_2|_{h_2=0}$ .

We now return to the question of the additional conditions that must be imposed on the fields  $h_2$ ,  $h$ , and  $h'$  for a unique solution of system (6). These conditions can be obtained from various heuristic considerations. For example, comparing the constructions described above with a concrete lattice (as we do in what follows), we can regard the number  $N$  as the number of sites in the minimum closed path along the bonds of the lattice. For example,  $N = 3$  for hexagonal lattices,  $N = 4$  for square or simple cubic lattices, and so on. The value  $L$  is the number of different closed paths of length  $N$  that contain a dimer:  $L = 2$  for planar lattices and  $L \geq 3$  for volumetric lattices. We can regard the fields  $h_2$ ,  $h$ , and  $h'$  as effective exchange fields associated with interactions with spins not included in the structures described above. We assume that the fields  $h_2$ ,  $h$ , and  $h'$  are proportional to the number of lattice atoms that are adjacent to the dimer atoms and are not included in the  $N$ -gons, i.e.,  $h_2 = (q - 1)\mu$ ,  $h = (q - 2)\mu$ , and  $h' = (q - 1 - L)\mu$ , where  $q$  is the coordination number and  $\mu$  is some unknown parameter.

Under the above conditions, Eq. (7) becomes an equation for  $\mu$ ,

$$X_N((q - 2)\mu) = e^{-4\mu}, \quad (11)$$

solving which we find the magnetization  $m(K)$  and the average product of adjacent spins  $s(K)$  by formulas (3) and (4). Of course, these quantities can no longer be regarded as an exact solution of the problem,

but as the calculations below show, the obtained approximation turns out to be quite accurate compared with other known approximations.

Therefore, in the considered approximation, we have

$$\begin{aligned} m(K) &= \frac{\sinh(2(q-1)\mu)}{\cosh(2(q-1)\mu) + (Y_N(h))^L e^{2(L\mu-K)}}, \\ s(K) &= \frac{\cosh(2(q-1)\mu) - (Y_N(h))^L e^{2(L\mu-K)}}{\cosh(2(q-1)\mu) + (Y_N(h))^L e^{2(L\mu-K)}}, \end{aligned} \quad (12)$$

where  $h = (q-2)\mu$  and the parameter  $\mu$  is determined from the solution of Eq. (11). Hence, to calculate the magnetization  $m(K)$  and the average product of adjacent spins  $s(K)$  by formulas (11) and (12), we must calculate the functions  $X_N(h) = Z_N(-1, -1)/Z_N(+1, +1)$  and  $Y_N(h) = Z_N(+1, -1)/Z_N(+1, +1)$ . Perhaps, general expressions for these functions can be found for an arbitrary  $N$ , but there is no special need for this: the length of the minimum closed path along the bonds is no more than six sites for realistic lattices. For example,  $N = 3$  for a triangular lattice, and direct calculation gives

$$X_3(h) = \frac{\cosh(2K-h)}{\cosh(2K+h)}, \quad Y_3(h) = \frac{\cosh(h)}{\cosh(2K+h)}.$$

For square and cubic lattices,  $N = 4$ , and we obtain

$$X_4(h) = \frac{\cosh(2K-2h) + e^{-2K}}{\cosh(2K+2h) + e^{-2K}}, \quad Y_4(h) = \frac{\cosh(2h) + (1 + e^{-4K})/2}{\cosh(2K+2h) + e^{-2K}}.$$

In the region of zero spontaneous magnetization ( $T \geq T_C$ ), we have  $h_0 = h'_0 = 0$ , and condition (8) is satisfied automatically. Because  $X_N(0) = 1$  (due to the symmetry of the Hamiltonian of the Ising model in a zero external field under a simultaneous reversal of the signs of all spins), from (9), we obtain

$$s(K) = \frac{1 - e^{-2K} Y_N^L(0)}{1 + e^{-2K} Y_N^L(0)}. \quad (13)$$

Ratio (10) becomes a condition from which we can determine the Curie temperature:

$$\left. \frac{\partial \log(X_N(h))}{\partial h} \right|_{h=0} = -\frac{4}{q-2}. \quad (14)$$

For a planar triangular lattice, we have  $N = 3$ ,  $L = 2$ , and  $q = 6$ . The correlation of neighboring spins in the region of the absence of spontaneous magnetization in accordance with (13) has the form

$$s(K) = \frac{\cosh(2K)^2 - e^{-2K}}{\cosh(2K)^2 + e^{-2K}}.$$

The critical temperature parameter  $K_c = J/kT_C$  can be found from (14) and is equal to  $K_c = (1/4) \log 3 \approx 0.275$ , which coincides with the exact value for the lattice [2]. The correlation of adjacent spins at the critical point is  $s(K_c) = (19 - 8\sqrt{3})/13 \approx 0.396$ .

Equation (11) reduces to the form  $e^{4K} = 2 \cosh(4\mu) + 1$ . Taking this and expressions (12) into account, we can represent  $m(K)$  and  $s(K)$  in the parametric forms

$$m(K) = \frac{1-x^5}{1+x^5+\varphi(x)}, \quad s(K) = \frac{1+x^5-\varphi(x)}{1+x^5+\varphi(x)}, \quad K = \frac{1}{4} \log \left( x + \frac{1}{x} + 1 \right),$$

where

$$\varphi(x) = \frac{2x^3 \sqrt{x^2 + x + 1}}{(1+x)^2}, \quad 0 < x \leq 1.$$

Calculations using these formulas shows that the correlation  $r(K) = s(K) - m^2(K)$  of neighboring spins is maximum at  $K = K_c$ , and its derivative with respect to  $K$  has a discontinuity at this point. The dependence  $r(K)$  also behaves similarly for other simple lattices, and the values of  $K_c$  and  $s(K_c)$  found for them in the same approximation are given in Table 1.

**Table 1**

Lattice	$(q, N, L)$	Exact value	Bethe approximation	Approximation [3]	$K_c$	$s(K_c)$
Square	(4, 4, 2)	0.441	0.347	0.370	0.402	0.473
Hexagonal	(3, 6, 2)	0.658	0.549	0.575	0.592	0.664
Triangular	(6, 3, 2)	0.275	0.203	0.219	0.275	0.396
Cubic	(6, 4, 4)	0.214	0.203	0.206	0.212	0.243
Tetrahedral	(4, 6, 3)	0.370	0.347	0.349	0.351	0.437

Values of  $K_c = J/kT_C$  in various approximations for simple lattices.

For comparison, we also give the values of  $K_c$  in the known Bethe approximation [2] and in the most accurate approximation in [3] in Table 1. It can be seen that in the approximation considered here, the value of  $K_c$  turns out to be closer to the exact values for all lattices and coincides with the exact value for a triangular lattice.

### 3. Magnets diluted in sites and bonds

For the Ising model with site or bond dilution, it is rarely possible to obtain an exact solution even in the cases where such a solution is obtainable for the model without dilution [5]. The method described above can be generalized to the case of dilute magnets as follows, for example. To calculate  $m(K)$  and  $s(K)$  when diluted in sites or bonds, we can average the right-hand sides of Eqs. (6) over dilution configurations  $\xi_i$  of each individual  $N$ -gon:

$$m(K) = \left\langle \frac{e^{2h'} - e^{-2h'} \prod_{i=1}^L X_N(h, \xi_i)}{e^{2h'} + e^{-2h'} \prod_{i=1}^L X_N(h, \xi_i) + 2e^{-2K} \prod_{i=1}^L Y_N(h, \xi_i)} \right\rangle_{W(\xi_1, \dots, \xi_L)}, \quad (15)$$

$$s(K) = \left\langle \frac{e^{2h'} + e^{-2h'} \prod_{i=1}^L X_N(h, \xi_i) - 2e^{-2K} \prod_{i=1}^L Y_N(h, \xi_i)}{e^{2h'} + e^{-2h'} \prod_{i=1}^L X_N(h, \xi_i) + 2e^{-2K} \prod_{i=1}^L Y_N(h, \xi_i)} \right\rangle_{W(\xi_1, \dots, \xi_L)}.$$

Here,  $X_N(h, \xi_i)$  and  $Y_N(h, \xi_i)$ , just as before, are the respective ratios

$$Z_N(-1, -1)/Z_N(+1, +1) \quad \text{and} \quad Z_N(+1, -1)/Z_N(+1, +1)$$

of the partition function, but calculated for the  $N$ -gon with the dilution configuration  $\xi_i$ . We now assume that the crystal fields  $h$  and  $h'$  are the same in all terms in the right-hand sides of relations (15) and, as in the case of a pure magnet, are proportional to the number of neighboring atoms in the lattice with the same coefficient of proportionality  $\mu$ . The value of this proportionality coefficient of course depends on the concentration of magnetic atoms or lattice bonds. To determine  $\mu$ , we use an analogue of Eq. (7) averaged over the configurations of all  $N$ -gons:

$$\left\langle \prod_{i=1}^L X_N(h, \xi_i) \right\rangle_{W(\xi_1, \dots, \xi_L)} = e^{-4L\mu}. \quad (16)$$

The probability  $W(\xi_1, \dots, \xi_L)$  is calculated as the product of the probabilities of the configurations for each  $N$ -gon separately:

$$W(\xi_1, \dots, \xi_L) = \prod_{i=1}^L P(\xi_i). \quad (17)$$

As in the case of a pure magnet, we can then find the equation for the critical temperature from the stability loss condition for the zero solution (with respect to  $\mu$ ) of Eq. (16). Hence, derivatives with respect to  $\mu$  of the right- and left-hand sides of (16) must be equal at  $\mu = 0$ :

$$\left\langle \sum_{i=1}^L \chi_N(\xi_i) \right\rangle_{W(\xi_1, \dots, \xi_L)} = \frac{2}{q-2}, \quad (18)$$

where  $\chi_N(\xi_i) = -(1/2)(\partial X_N(\xi_i)/\partial h)|_{h=0}$  and we take into account that all  $X_N(\xi_i) = 1$  for  $\mu = 0$ . Using (18), we obtain

$$\sum_{\xi} \chi_N(\xi) P(\xi) = \frac{2}{q-2}. \quad (19)$$

With dilution in sites, we can define a configuration  $\xi$  by assigning a variable  $\epsilon_j$  to each of  $N-2$  sites of an  $N$ -gon (except the sites forming a dimer), where  $\epsilon_j$  is equal to one if there is a magnetic atom at the site  $j$  and zero if there is a nonmagnetic impurity at the site  $j$ . With dilution in bonds, we define a similar variable for each of the  $N-1$  bonds of the  $N$ -gon. We can then calculate the probabilities  $P(\xi)$  in (19) by assuming that each magnetic atom is present in the  $N$ -gon with the probability  $b_s$  and is absent with the probability  $1 - b_s$  independently of the others. Similarly, for bond dilution, each bond is present with the probability  $b_b$  and absent with the probability  $1 - b_b$ . Substituting the calculated probabilities  $P(\xi)$  in (19), we obtain the equation for the critical temperature parameter  $K_c$  as a function of the concentration of sites or bonds.

As is known [8], spontaneous magnetization disappears in the dilute Ising model in a concentration of magnetic atoms (or bonds) equal to the percolation threshold of the corresponding lattice. Therefore, as  $K_c \rightarrow \infty$ , solution (19) for the concentration gives an approximate value of this percolation threshold. As  $K_c \rightarrow \infty$ , the value of  $\chi_N(\xi)$  tends to  $n(\xi)$ , the number of polygon sites that can be reached from the dimer atom via unbroken bonds. Therefore, from (19), we obtain the equation for the percolation threshold:

$$\sum_{\xi} n(\xi) P(\xi) = \frac{2}{q-2}. \quad (20)$$

From (19), we obtain

$$\tanh(2K_c) = \frac{1}{2b_s}$$

for a planar triangular lattice with dilution in sites and

$$b_b^2 \tanh(2K_c) + 2b_b(1 - b_b) \tanh(K_c) = \frac{1}{2}$$

with dilution in bonds. The percolation thresholds  $b_s^c$  and  $b_b^c$  for sites and bonds for this lattice turn out to be  $b_s^c = 0.5$  and  $b_b^c = 1 - 1/\sqrt{2} \approx 0.293$ . The approximate value of the percolation threshold in terms of the sites in this case coincides with the exact value [8].

In Table 2, we present the exact values of the percolation thresholds along the sites and bonds (first and second columns) and the value of the critical concentration in the Bethe approximation [8] (third column; the problems of percolation through sites and bonds do not differ in this approximation). We also give the

best approximate values of the percolation thresholds obtained in [3] (fourth and fifth columns) and the values found using Eq. (20) (sixth and seventh columns). It can be seen that Eq. (20) gives values closer to the exact values of the percolation thresholds for both sites and bonds in all cases.

**Table 2**

Lattice	Exact value of $b_s^c$	Exact value of $b_b^c$	Bethe approximation	$b_s^c$ [3]	$b_b^c$ [3]	$b_s^c$	$b_b^c$
Square	0.590	0.500	0.333	0.427	0.368	0.500	0.403
Hexagonal	0.700	0.653	0.500	0.558	0.532	0.581	0.546
Triangular	0.500	0.347	0.200	0.333	0.227	0.500	0.293
Cubic	0.310	0.250	0.200	0.219	0.205	0.250	0.214
Tetrahedral	0.430	0.390	0.333	0.343	0.337	0.350	0.340

Values of percolation thresholds for sites and bonds in various approximations for simple lattices.

#### 4. Conclusion

We have shown that using the average product of neighboring spins together with the magnetization for self-consistency allows constructing an approximate solution of the Ising model for both pure and dilute magnetic materials. It turns out that the values of the critical temperature parameter calculated in this approximation agree better with the known exact values than the values obtained in [3] (see Table 1). For the percolation thresholds of lattices diluted at sites and bonds, this approximation also gives more accurate values than in [3] (see Table 2).

**Conflicts of interest.** The authors declare no conflicts of interest.

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