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Construction of an approximate solution for a dilute magnet based on the solution for a pure magnet on the same lattice

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The paper proposes a method for approximate calculation of the magnetization of a dilute Ising magnet on a certain lattice, based on the use of an exact or approximate solution for a pure Ising magnet on the same lattice. Using the proposed method, it is possible to calculate the dependence of magnetization on temperature and concentration of non-magnetic impurities and the Curie temperature as a function of concentration for a diluted magnet. The proposed method is applied in the work to the solution in the mean field approximation, to the solution in the beta approximation, and to the exact solution on a square lattice.

Keywords: phase transitions, Ising model, dilute magnet.

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1. Introduction

Properties of dilute and unordered magnets differ from properties of pure magnets [1–5]. However, accurate solutions for models of dilute magnetic systems can be obtained only in rare cases [6]. That's why it makes sense to construct approximate solutions for dilute magnets. Some of these solutions can be constructed by way of averaging over interaction fields.

In our paper [7] we developed a common approach based on averaging over interaction fields as applied to spin clusters on a magnetic lattice. In the present paper, also on the basis of the method of averaging over interaction fields, we introduce a „function of relation of effective exchange interaction fields". This function is defined as a relation of values of exchange interaction fields at which the cluster average value of spin is equal to the ensemble average value. Thereat, we limit ourselves to clusters of one and two magnetic atoms only. A relationship between the relation function and spontaneous magnetization as a temperature function is established in the paper. The relationship makes it possible to calculate the relation function if an approximate or accurate solution for the Ising model is available. In this paper we assume that the relation function as a function of spontaneous magnetization in case of non-magnetic dilution is approximately the same as for a pure magnet. This conjecture is based on the fact that, as demonstrated in [6,8,9], a similar assumption for a Bethe lattice provides reasonable results. Therefore, the goal of the present paper is to study the outcome of the assumption of relation function's independence from non-magnetic dilution in a more general case.

2. Averaging over interaction fields, relation function for a pure and dilute magnet

Let us consider an Ising model on a certain lattice. Let each lattice site contain an Ising „spin", which takes on values $+1$ and -1, and let only the spins, located at adjacent sites, interact. Then the Ising model Hamiltonian can be written down as follows [10]:

$$\mathscr{H} = -J \sum_{(i,j)} \sigma_i \sigma_j - H_{ex} \sum_i \sigma_i, \tag{1}$$

where J is the exchange interaction energy, H_{ex} is the external field; summation in the first sum is performed for all pairs of adjacent spins, in the second one — for all sites.

Let us now select a certain spin σ_0 on the lattice. Let h be the sum of values of spins which directly interact with σ_0 (spins of the first coordination sphere). This sum will be called the „interaction field". Then, as shown in [7], the thermodynamic average $\langle\sigma_0\rangle$ is obtained by averaging of $\mathrm{th}\,(Kh)$ over the distribution function $W(h)$:

$$\langle\sigma_0\rangle = \sum_h W(h)\,\mathrm{th}\,(Kh), \tag{2}$$

where $K = \frac{J}{kT}$, k is the Boltzmann constant, T is temperature. In the general case, $\langle\sigma_0\rangle$ and $W(h)$ depend on the site where spin σ_0 is located. If an Ising model is assigned on a simple lattice with coordination number q, then all $\langle\sigma_0\rangle = M$, where M is the average magnetization per site, while function $W(h)$ does not depend on site number. In this case, since magnetization M takes on values from 0 to 1, for any distribution function $W(h)$ there is a

value of $h = \chi_1$ for which

$$M = \mathrm{th}\,(K\chi_1). \tag{3}$$

This value of χ_1 will be called the „effective field".

Let us now take a cluster of two neighboring spins σ_1 and σ_2 (dimer). It was shown in [7] that the thermodynamic average $\langle\frac{\sigma_1+\sigma_2}{2}\rangle$ is equal to

$$\left\langle\frac{\sigma_1+\sigma_2}{2}\right\rangle = \sum_{h_1,h_2} W(h_1,h_2) \times \frac{\mathrm{sh}\big(K(h_1+h_2)\big)}{\mathrm{ch}\big(K(h_1+h_2)\big)+\mathrm{ch}\big(K(h_1-h_2)\big)\exp(-2K)}, \tag{4}$$

where h_1 and h_2 are interaction fields related to σ_1 and σ_2, $W(h_1,h_2)$ is their joint distribution function. Similarly to a one-atom cluster, it follows from the normalization condition for $W(h_1,h_2)$ that there is such a value of $h_1 = h_2 = \chi_2$ at which

$$M = \frac{\mathrm{sh}(2K\chi_2)}{\mathrm{ch}(2K\chi_2)+x}, \tag{5}$$

where $x = \exp(-2K)$, and χ_2 is the effective field of the dimer.

Many approximate methods in the theory of magnetism can be treated as the introduction of additional correlations between effective fields χ_1, χ_2 and magnetization M. For instance, by assuming $\chi_1 = qM$, we obtain a known mean field approximation [11], while correlation $\chi_2 = (q-1)M$ leads to a generalization of mean field approximation discussed in [8]. By complementing equalities (3) and (5) with correlation $\chi_2 = \frac{(q-1)}{q}\chi_1$, we obtain a Bethe approximation [10,11]. Let us consider in more detail a common correlation that can be represented as $\chi_2 = y(M)\chi_1$. Function $y(M)$ will be called the relation function. If an accurate or approximate value of spontaneous magnetization as temperature function $M = M(x)$ is known, then (3) and (5) can be used to find χ_1, χ_2 and relation function $y(M)$. Conversely, if function $y(M)$ is known from some considerations, then (3) and (5) can be used to find dependence $M = M(x)$ which corresponds to this function. A low-temperature decomposition of the statistical sum [10] can be used to show that for simple lattices with coordination number $q\,\chi_1 \to q$ and $\chi_2 \to q-1$ at $x \to 0$, i.e. $y(M)$ tends to $\frac{q-1}{q}$ within the low temperatures.

Let us now consider an Ising model with non-magnetic dilution. The most interesting [4] case is the so-called „frozen-in" dilution: when some of sites randomly and without correlation are filled with nonmagnetic impurities, so that any lattice site can contain a magnetic atom with probability b or an impurity with probability $1-b$. (Similarly, dilution for bonds can be considered: a bond between neighboring spins exists with probability b or is broken with probability $1-b$ [12].) The main difference of systems with frozen-in impurities from pure magnets is in the disruption of the lattice translation symmetry — the thermodynamic average values, for instance, $\langle\sigma_0\rangle$ in the general case are not equal for different system spins. Here we can opt for averaging over different configurations of impurities, or, according to the self-averaging idea [4] — over different spins in one and the same configuration. Then, „self-averaged" magnetization of a magnetic atom for dilution both for sites and bonds is represented as [7]:

$$M = \mathrm{th}\,(K\tilde{\chi}_1). \tag{6}$$

Here $\tilde{\chi}_1$ is the effective exchange field dependent on b. Similarly, for a dimer

$$M = (1-b)\mathrm{th}\,(K\tilde{\chi}_2) + b\,\frac{\mathrm{sh}(2K\tilde{\chi}_2)}{\mathrm{ch}(2K\tilde{\chi}_2)+x}. \tag{7}$$

Finding of the accurate form of function $\tilde{\chi}_1(x,b)$ (or $\tilde{\chi}_2(x,b)$) for dilution for sites or for bonds is equivalent to an accurate solution of the problem of magnetization of a dilute Ising magnet. Let us consider this method of an approximate solution of this problem. We will assume that the relation of effective exchange fields $\tilde{\chi}_2/\tilde{\chi}_1$, expressed as a function of M, does not depend on b. That is, it is assumed that $\tilde{\chi}_2 = y(M)\tilde{\chi}_1$, where $y(M)$ is the relation function determined above for a pure magnet. As demonstrated below, this conjecture for a Bethe lattice is equivalent to consideration of impurities on this lattice in a pseudo-chaotic approximation [8,9].

That is, the proposed approximation to analysis of a dilute magnet consists in the following. Let there be an accurate or approximate value of magnetization of a pure magnet as a temperature function $M = \mu(x)$ (or an inverse function $x = \nu(M)$). This can be, for instance, a solution in a mean field approximation [10] or in a Bethe approximation [11] (which can be interpreted as an accurate solution on a Bethe lattice [10]) or an accurate Onsager solution on a square lattice [10]. Using this solution, we obtain an expression for relation function $y(M)$ from correlations (3) and (5):

$$y(M) = \frac{\ln\big(\nu M + \sqrt{(\nu M)^2 + (1-M^2)}\big) - \ln(1-M)}{\ln(1+M) - \ln(1-M)}. \tag{8}$$

Using this expression, we obtain the following from (6) and (7):

$$x(M,b) = \frac{\nu(M) - \gamma F_1(M)}{1 - \gamma F_2(M)}, \tag{9}$$

where $\gamma = \frac{1-b}{1+b}$ — measure of the „dilution" magnet,

$$F_1(M) = 2\,\frac{R-\nu}{R+1}\left(\frac{\nu M}{1-M} + \frac{1}{R+\nu M}\right) + \nu,$$

$$F_2(M) = \frac{1-R+2\nu}{R+1}, \tag{10}$$

here $R = \sqrt{(\nu M)^2 + (1-M^2)}$. For this, in order to find a concentration dependence of Curie temperature $T_c(b)$

or $K_c(b) = J/kT_c(b)$ we will go to limit $M \to 0$ in (9) and (10). Let us denote $x_c(b) = \exp(-2K_c(b))$, we obtain

$$x_c(b) = \frac{x_c(1) - \gamma}{1 - \gamma x_c(1)} \text{or} \operatorname{th} K_c(b) = \frac{1}{b} \operatorname{th} K_c(1). \qquad (11)$$

It follows from formula (11) that Curie temperature becomes zero at $b = \operatorname{th} K_c(1)$. It means that quantity $b_c = \operatorname{th} K_c(1)$ can be considered an estimate of the percolation threshold value in the given approximation [12]. For an Ising model with dilution, the value of spontaneous magnetization $M_0(b)$ at $T = 0$ is the probability that a given magnetic atom pertains to an infinite cluster [12]. This value can be obtained from (9)–(10) in the limit $T \to 0$. $M_0(b)$ satisfies the equation

$$\nu(M_0) = \gamma F_1(M_0). \qquad (12)$$

It should be noted that the above-mentioned method can be used not only for one- and two-atom clusters, but also for two clusters of a random size. Having determined the corresponding relation function for a pure magnet and assuming its independence from b, we obtain a more common form of the approximation given in the present paper. In such a common form there will be a difference in dilution for sites and for bonds, but in this paper we will consider only the simplest method implementation where this difference is absent.

3. Mean field theory, Bethe approximation and Onsager solution

Let us now apply the above-mentioned method to an Ising model on a square lattice. Selection of this lattice is due to the fact that an accurate Onsager solution exists for this lattice [10], in addition to approximate solutions. Let us first consider the approximate solutions. In a mean field approximation [11], spontaneous magnetization for this lattice is determined by expression $M = \operatorname{th}(4KM)$, from where

$$\nu(M) = \left(\frac{1 - M}{1 + M}\right)^{\frac{1}{4M}}. \qquad (13)$$

By substituting this function into (8), we obtain a relation function $y_a(M)$ in the mean field approximation. The plot of this function is shown in Fig. 1 (curve *1*). It is easy to show that $M \to 1$ $y_a(M) \to 3/4$, while $\nu(M) \to 0$. K_c in the mean field approximation is equal to 1/4, then $x_c(1) = \exp(-1/2) \approx 0.607$.

Let us now apply this solution to the analysis of a dilute magnet in compliance with the above-mentioned approach. From (11) $b_c = \operatorname{th}(1/4) \approx 0.245$. This value does not agree well with the accurate values of percolation thresholds for sites and for bonds either for a square or for a tetrahedral lattice [12]. However, a percolation transition and a percolation threshold are completely absent for a dilute magnet in the conventional mean field approximation [12]. Using (13) and (12), let us now plot the function $M_0(b)$ — it is shown in Fig. 2 (curve *1*).

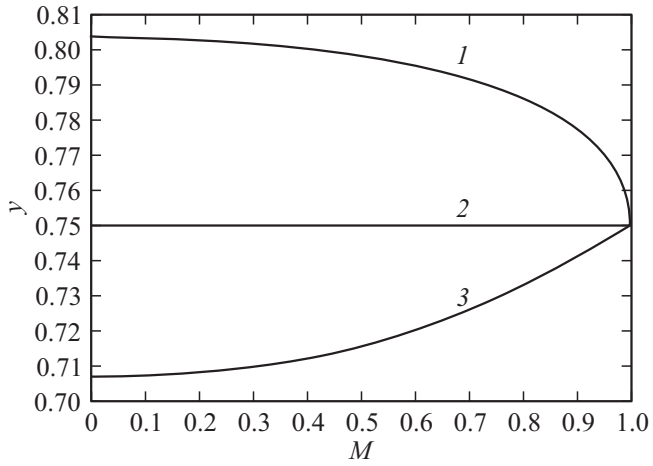

Figure 1. Effective field relation functions in different approximations depending on spontaneous magnetization for a square lattice. Curve *1* shows a mean field approximation, curve *2* shows a Bethe approximation and curve *3* shows an accurate solution.

Spontaneous magnetization on a lattice with coordination number q in a Bethe approximation [10] is equal to $M = (1-p^q)/(1+p^q)$, where p is the root of equation $p = (x + p^{q-1})/(1 + xp^{q-1})$. It can be easily shown that at $q = 4$

$$\nu(M) = \frac{\sqrt[4]{1 - M^2}}{\sqrt{1 + M} + \sqrt{1 - M}}. \qquad (14)$$

Substituting this expression into (8), we will obtain a relation function in this approximation $y_b(M) = 3/4$, that is, it does not depend on M. As already mentioned, the assertion that the relation function of the effective fields included in (3) and (5) is equal to $(q-1)/q$ can be considered a definition of Bethe approximation [8,9]. It can be seen from (14) that spontaneous magnetization in a Bethe approximation disappears at $x_c(1) = 1/2$ or $K_c = (1/2)\ln 2$. Let us now use a Bethe approximation in expressions (9)–(12). We obtain $\operatorname{th} K_c(b) = 1/(3b)$ or $b_c = 1/3$. The plot of function $M_0(b)$ in a Bethe approximation is shown in Fig. 2, curve *2*.

The authors of [8] considered a Bethe approximation for a dilute magnet in a „pseudo-chaotic“ approximation. The essence of this approximation is that mobile impurities are considered instead of frozen-in impurities on a Bethe lattice, with an additional condition of a zero correlation in the location of impurities in neighboring sites. It turns out that all the results obtained from (9)–(12) when using a Bethe approximation match those obtained in a pseudo-chaotic approximation for a Bethe lattice [8,9]. This makes it possible to assume that the suggested approach to analysis of a dilute magnet, based on the assumption that the relation function does not depend on b, can be in the general case

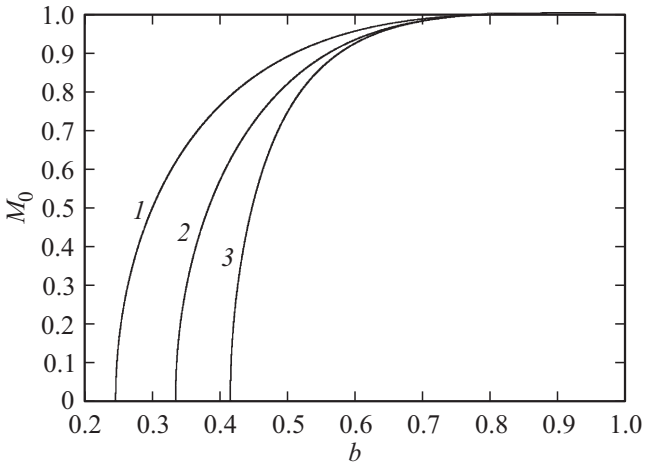

Figure 2. Spontaneous magnetization $M_0(b)$ as a function of magnetic atom concentration b on a square lattice. The plots were constructed based on a mean field approximation (curve *1*), based on a Bethe approximation (curve *2*) and based on an accurate solution (curve *3*).

physically interpreted as a certain variant of a pseudo-chaotic approximation.

It is to be recalled that the suggested approach to analysis of a dilute magnet is based on the use of an approximate or accurate solution for a pure magnet on the corresponding lattice. As is well-known [10], an accurate expression for spontaneous magnetization as a function of temperature can be found for an Ising model on a square lattice

$$M^8 = 1 - \frac{1}{\mathrm{sh}^4(2K)}. \qquad (15)$$

Hence

$$v(M) = \sqrt[4]{1-M^2}\,\frac{\sqrt[4]{(1+M^2)(1+M^4)}}{1+\sqrt{1+\sqrt{1-M^8}}}. \qquad (16)$$

It follows from these expressions that spontaneous magnetization disappears at $x_c(1) = \sqrt{2}-1$ or $K_c = (1/2)\ln(\sqrt{2}+1)$. The relation function $y_e(M)$, which corresponds to solution (16) is shown in Fig. 1, curve *3*. It can be shown that $y_e(M) \to 3/4$ at $M \to 1$.

Let us now use an accurate solution (16) as the basis for analysis of a dilute magnet. From (9)–(12) we obtain $b_c = \sqrt{2}-1 \approx 0.414$. Fig. 2 (curve *3*) shows the plot of function $M_0(b)$ calculated as per (12) for solution (16).

4. Conclusion

In the present paper we have constructed a universal relation function for an Ising model without non-magnetic dilution $y(M, x)$, which relates the effective fields of single-atom and two-atom clusters. This function depends on spontaneous magnetization M and temperature parameter $x = \exp(-2K)$. It means that the relation between M and x, obtained from an accurate or an approximate solution, determines the relation function $y(M)$ or $y(x)$.

Assuming that function $y(M)$ for a magnet with non-magnetic dilution has the same form as for a pure one, we have obtained the following main results.

1. The adopted conjecture results in a form of a concentration dependence of the critical temperature parameter $K_c(b) = J/kT_c(b)$, where $T_c(b)$ is the Curie temperature. This form is expressed by a simple correlation $b\,\mathrm{th}\,K_c(b) = \mathrm{th}\,K_c(1)$.

2. Based on any solution for a pure Ising magnet, we obtain the existence of a percolation transition at concentration $b_c = \mathrm{th}\,K_c(1)$. In particular, based on a mean field approximation, we obtain $b_c = \mathrm{th}\,(1/q)$ for a lattice with coordination number q.

3. The concentration dependence of spontaneous magnetization at zero temperature (which for an Ising model can be understood as a probability of appurtenance of a given magnetic atom to an infinite cluster) is determined by expression (12).

4. Universality of the relation function for pure and dilute Ising magnets on a Bethe lattice is equivalent to the consideration of nonmagnetic impurities in a pseudo-chaotic approximation [8,9]. We made an assumption that such universality in the general case is equivalent to certain additional conditions for correlation in the location of impurities in a model with mobile impurities.

Conflict of interest

The authors declare that they have no conflict of interest.

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