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MAGNETIC SUSCEPTIBILITY OF A DILUTED ISING MAGNET

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For the Ising model with nonmagnetic dilution, we consider a method for constructing the "pseudochaotic" impurity distribution based on the condition that the position correlation of movable impurity atoms in neighboring sites vanishes. For the one-dimensional Ising model with nonmagnetic dilution, we find the exact solution and show that the pseudochaotic approximation method gives the exact value of the magnetic susceptibility for this model in a zero external field. We assume that the pseudochaotic impurity distribution is completely uncorrelated in the region of zero magnetization for any lattice. This assumption is based on calculating the correlation functions for the Ising model with nonmagnetic dilution on the Bethe lattice. We find the magnetic susceptibility for that model.

Keywords: Ising model, diluted magnet, Bethe lattice, magnetic susceptibility

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1. Introduction

In most cases, a good approximation for describing a diluted magnet is the assumption of a random distribution of nonmagnetic impurities among the lattice sites [1], [2]. Therefore, in theoretical papers devoted to studying diluted magnets, a random impurity distribution, as a rule, is introduced at the beginning.

Here, we propose a somewhat different approach to analyzing the properties of diluted magnets. Instead of initially assuming that impurities are randomly distributed in the lattice, we consider a magnet in which the magnetic atoms and impurity atoms can interchange and are in thermodynamic equilibrium. The energy of such system is determined not only by the orientation of the magnetic moments but also by the distribution of the impurity atoms among the lattice sites. In other words, the Hamiltonian of one or another model of a magnet with movable impurities comprises terms related to the exchange interaction of the magnetic atoms and terms related to the interatomic interaction in the crystal lattice, in which case the equilibrium distribution of the impurity atoms depends on the parameters characterizing these interactions. For each value of the temperature, external magnetic field, and concentration (fraction) of magnetic atoms in the system, we can then find the parameters of the interatomic interaction such that the equilibrium distribution of impurity atoms is as nearly as possible random. In [3], we applied this method to the Potters model with nonmagnetic dilution on the Bethe lattice.

Here, we realize this approach as follows. We consider the Ising model on a lattice with the coordination number q. We assume that some of the magnetic atoms are replaced with impurity atoms, which can

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move through the lattice sites and are in thermodynamic equilibrium. We first we choose an interatomic interaction potential for which, in our opinion, the equilibrium distribution of nonmagnetic impurities is nearly random; we say that such a distribution is pseudochaotic. To demonstrate the effectiveness of the pseudochaotic approximation, we consider the one-dimensional Ising model with a random distribution of immobile nonmagnetic impurities. For this model, we obtain the exact solution, which we compare with the solution found with the pseudochaotic approximation. Based on the results of this comparison, we assume that the pseudochaotic distribution with zero magnetization is equivalent to the totally uncorrelated positions of impurity atoms. Further considering the Ising model with nonmagnetic dilution on an arbitrary Bethe lattice, we find an expression for the magnetic susceptibility with zero magnetization, which we regard as an exact result for this model based on our assumption.

2. Pseudochaotic approximation

We formulate the Ising model with movable nonmagnetic impurities on an arbitrary crystal lattice. We consider a crystal lattice with the coordination number q, in whose sites both magnetic and nonmagnetic atoms can be placed (respectively atoms of the first and second types). Each magnetic atom is related to the Ising spin $s_i = \pm 1$ such that the energy of the exchange interaction of two magnetic atoms with the spins s_i and s_j is $-Js_is_j$ if the atoms are in neighboring lattice sites and is zero otherwise.

Similarly to what is accepted in studying binary alloys [4], we assume that there are interatomic forces in the system with an interaction potential of the Lennard-Jones type rapidly decreasing over large distances [4]. Therefore, we assume that the action radios of these forces is restricted to the first coordination sphere; for brevity in what follows, we call them "Coulomb" forces, although, strictly speaking, they have a different nature. We let $-U_{\alpha\beta}$, $\alpha, \beta = 1, 2$ denote the potential of these forces. If we now associate each lattice site with the variable σ_i equal to s_i if a magnetic atom is in this site and zero if the atom is nonmagnetic, then the energy E_{ex} of the exchange interaction and the Coulomb energy E_{K} can be written as sums over all ordered pairs of neighboring sites:

$$\begin{split} E_{\rm ex} &= -\sum_{(i,j)} J\sigma_i \sigma_j, \\ E_{\rm K} &= -\sum_{(i,j)} \left\{ U_{11} \sigma_i^2 \sigma_j^2 + U_{22} (1 - \sigma_i^2) (1 - \sigma_j^2) + U_{12} [\sigma_i^2 (1 - \sigma_j^2) + \sigma_j^2 (1 - \sigma_i^2)] \right\}. \end{split}$$

The last expression up to an additive constant can be written as

$$E_{\rm K} = -\sum_{(i,j)} U\sigma_i^2 \sigma_j^2 - \sum_i f\sigma_i^2,$$

where $U = U_{11} + U_{22} - 2U_{12}$ and $f = q(U_{12} - U_{22})$. We call U the effective Coulomb interaction potential; the magnetic atoms attract each other if U > 0 and repel each other if U < 0.

Taking into account that the number of magnetic atoms on the lattice equals $\sum_i \sigma_i^2$, we write the grand partition function of the system as

$$Z = \sum_{\{\sigma\}} \exp\left\{\frac{1}{kT} \left(\sum_{(i,j)} (J\sigma_i \sigma_j + U\sigma_i^2 \sigma_j^2) + (f+\mu) \sum_i \sigma_i^2 + H_e \sum_i \sigma_i\right)\right\},\tag{1}$$

where μ is the chemical potential, H_e is the external magnetic field, k is the Boltzmann constant, and the sum is over all possible configurations $\{\sigma\}$.

We introduce the quantities $b = \langle \sigma_i^2 \rangle$ and $M = \langle \sigma_i \rangle / b$, where the angle brackets denote the ensemble average. Clearly, these quantities are independent of *i* because all lattice sites are equivalent (in the thermodynamic limit) and have a simple meaning: *b* is the probability for a magnetic atom to be at the given site (concentration), and *M* is the mean value of its spin. For such a model, we can define several types of correlation functions characterizing the relations between magnetic moments and relations between impurity atom positions. We introduce the positional correlation function (characterizing distribution of impurity atoms)

$$g_{ij}^b = \langle \sigma_i^2 \sigma_j^2 \rangle - b^2.$$

If impurities are distributed completely randomly and independently among the lattice sites, then $\langle \sigma_i^2 \sigma_j^2 \rangle = \langle \sigma_i^2 \rangle \langle \sigma_j^2 \rangle = b^2$ and $g_{ij}^b = 0$ for any *i* and *j*. If $g_{ij}^b = 0$ for any *i* and *j*, then we say that the impurity distribution is uncorrelated. Strictly speaking, uncorrelated impurities does not mean (although it does not exclude) that their distribution is completely random, because not only pairwise covariations but also triple, quadruple ones, and so on must equal zero for a completely random distribution.

For the Ising model with movable impurities, the positional correlation function depends on the effective Coulomb interaction potential U together with the temperature T and external field H_e . Instead of regarding U as a constant, we now find the value of U for each values of T and H_e such that the equality $g_{12}^b = 0$ holds, i.e., the impurity positions in two neighboring sites of the lattice are uncorrelated. We call the impurity distribution satisfying this condition the pseudochaotic distribution, and the calculations for this distribution the pseudochaotic approximation. As shown below, the condition $g_{12}^b = 0$ in some cases leads to the positional correlation function vanishing at any distance.

3. One-dimensional chain with dilution: Exact solution

We consider a one-dimensional Ising magnet (chain), where some magnetic atoms are replaced with nonmagnetic impurities such that the probability to find a magnetic atom at any site of the chain equals b and the probability to find an impurity at the same site equals 1 - b. With such a dilution, the chain is broken into segments of different lengths consisting of magnetic atoms with the segments separated by nonmagnetic impurities. The mean value of the Ising spin for one magnetic atom can be calculated as

$$M = \sum_{n=1}^{\infty} m_n p_n,\tag{2}$$

where m_n is the mean magnetization of the atom belonging to a segment of length n and p_n is the probability that an arbitrary magnetic atom belongs to such segment. Obviously, $p_n = nb^{n-1}(1-b)^2$. We calculate the magnetization m_n as follows. Let Z_n be the partition function for a segment of n Ising spins s_1, \ldots, s_n ,

$$Z_{n} = \sum_{\sigma_{1},...,\sigma_{n}} \exp\left(K \sum_{i=1}^{n-1} s_{i} s_{i+1} + h \sum_{i=1}^{n} s_{i}\right),$$

where K = J/kT and $h = H_e/kT$. In Z_n , we select the sum over the last spin s_n of a given segment:

$$Z_n = F_n(+1) + F_n(-1),$$

where

$$F_n(s_n) = \sum_{s_1,\dots,s_{n-1}} \exp\left(K\sum_{i=1}^{n-1} s_i s_{i+1} + h\sum_{i=1}^n s_i\right)$$

Then

$$m_n = \frac{1}{n} \frac{\partial}{\partial h} \log Z_n = \frac{1}{n} \frac{F_{n,h}(+1) + F_{n,h}(-1)}{F_n(+1) + F_n(-1)},$$
(3)

where $F_{n,h}(s)$ is the derivative of $F_n(s)$ with respect to h. For the functions $F_n(\pm 1)$ and their derivatives, we can construct the recurrence relations

$$F_{n+1}(s) = \sum_{s'=\pm 1} F_n(s') e^{Kss'+hs} = F_n(+1) e^{Ks+hs} + F_n(-1) e^{-Ks+hs},$$

$$F_{n+1,h}(s) = \left(F_{n,h}(+1) + sF_n(+1)\right) e^{Ks+hs} + \left(F_{n,h}(-1) + sF_n(-1)\right) e^{-Ks+hs},$$

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

Introducing the notation

$$x_n = \frac{F_n(-1)}{F_n(+1)}, \qquad y_n = \frac{F_{n,h}(+1)}{F_n(+1)}, \qquad z_n = \frac{F_{n,h}(-1)}{F_n(+1)},$$

we obtain the expression

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

and the recurrence relations

$$x_{n+1} = \frac{e^{-2K} + x_n}{1 + x_n e^{-2K}} e^{-2h}, \qquad y_{n+1} = \frac{y_n + z_n e^{-2K}}{1 + x_n e^{-2K}} + 1,$$

$$z_{n+1} = \frac{z_n + y_n e^{-2K}}{1 + x_n e^{-2K}} e^{-2h} - x_{n+1},$$

$$x_1 = e^{-2h}, \qquad y_1 = 1, \qquad z_1 = -e^{-2h}.$$

The magnetization M given by formula (2) can be represented by a power series in the concentration b of magnetic atoms,

$$M = m_1 + 2(m_2 - m_1)b + \sum_{k=2}^{\infty} ((k+1)m_{k+1} - 2km_k + (k-1)m_{k-1})b^k,$$

whence we can find the derivatives $\partial^k M / \partial b^k$ at b = 0. In particular,

$$\left. \frac{\partial M}{\partial b} \right|_{b=0} = 2(m_2 - m_1) = 2\left(\frac{\sinh(2h)}{\cosh(2h) + e^{-2K}} - \tanh h \right). \tag{4}$$

From relation (2), we obtain the magnetic susceptibility $\chi = \partial M / \partial h$:

$$\chi = \sum_{n=1}^{\infty} \chi_n p_n, \qquad \chi_n = \frac{1}{n} \frac{F_{n,hh}(+1) + F_{n,hh}(-1)}{F_n(+1) + F_n(-1)} - nm_n^2.$$
(5)

Here, $F_{n,hh}(s)$ are the second derivatives of the function $F_n(s)$ with respect to h; recurrence relations can also be constructed for them. If the external field h = 0, then it follows from these recurrence relations that $F_n(-1) = F_n(+1)$, $F_{n,h}(-1) = -F_{n,h}(+1)$, and $F_{n,hh}(-1) = F_{n,hh}(+1)$ for any n. Introducing the notation $t_n = F_{n,hh}(+1)/F_n(+1)$ and $w_n = F_{n,h}(+1)/F_n(+1)$, we derive the relation for χ_n and recurrence relations for t_n and w_n :

$$\chi_n = \frac{t_n}{n}, \qquad t_{n+1} = 1 + t_n + 2w_n \tanh K, \qquad w_{n+1} = 1 + w_n \tanh K, \qquad t_1 = w_1 = 1.$$

It follows from the recurrence relation for w_n and the initial condition $w_1 = 1$ that

$$w_n = \sum_{i=0}^{n-1} (\tanh K)^i = \frac{1 - (\tanh K)^n}{1 - \tanh K}.$$

Using this result in the recurrence relation for t_n , we obtain

$$t_n = n \frac{1 + \tanh K}{1 - \tanh K} - \frac{2 \tanh K}{\left(1 - \tanh K\right)^2} \left(1 - \left(\tanh K\right)^n\right)$$

Substituting $\chi_n = t_n/n$ in (5) and summing the power series, we finally obtain

$$\chi = \frac{1 + b \tanh K}{1 - b \tanh K}.$$
(6)

4. One-dimensional chain with dilution: Pseudochaotic approximation

We now consider the one-dimensional Ising model with nonmagnetic impurities in the pseudochaotic approximation. We write partition function (1) for the one-dimensional chain consisting of N sites in the form

$$Z_N = \sum_{\{\sigma\}} \exp\bigg\{\sum_{i=1}^N (K\sigma_i\sigma_{i+1} + L\sigma_i^2\sigma_{i+1}^2 + r\sigma_i^2 + h\sigma_i)\bigg\},\tag{7}$$

where $r = \mu/kT$, L = U/kT, and we use the cyclic boundary condition $\sigma_1 = \sigma_{N+1}$. Calculating partition function (7) one way or another, we can find the chemical potential, the spontaneous magnetization, and the mean $\langle \sigma_i^2 \sigma_{i+1}^2 \rangle$ using the relations

$$bM = \frac{1}{N} \frac{\partial \log Z_N}{\partial h}, \qquad b = \frac{1}{N} \frac{\partial \log Z_N}{\partial r}, \qquad \langle \sigma_i^2 \sigma_{i+1}^2 \rangle = \frac{1}{N} \frac{\partial \log Z_N}{\partial L}.$$
(8)

Passing to the limit $N \to \infty$, we obtain a system from which we can obtain the magnetization and chemical potential as functions of the parameters K, L, b, and h. Eliminating the Coulomb interaction parameter L using the uncorrelation conditions for the positions of magnetic atoms in neighboring sites,

$$\langle \sigma_i^2 \sigma_{i+1}^2 \rangle - b^2 = 0$$

which is the main point of the pseudochaotic approximation, we now obtain [5]

$$M_{\rm a} = \tanh(2x - h), \qquad b = \frac{\tanh(2x - h) - \tanh x}{\frac{\sinh(2x)}{\cosh(2x) + e^{-2\kappa}} - \tanh x},\tag{9}$$

where x varies from $x_1 = h$ to $x_2 = (h + 2K)/2 + (1/2)\log(\sinh h + \sqrt{\sinh^2 h} + e^{-4K})$.

At h = 0, the magnetization $M_{\rm a}$ vanishes for any value of the concentration b, as does exact magnetization value (2). For b = 0 and for b = 1 (i.e., for the paramagnetic and for the chain without dilution), the magnetization $M_{\rm a}$ calculated using pseudochaotic approximation (9) coincides with exact magnetization value (2). The derivatives of the magnetization $M_{\rm a}$ with respect to the magnetic atom concentration b calculated using (9) with b = 0 and with b = 1 also coincide with the corresponding derivatives of the exact solution. In addition, it is easy to show that the susceptibility $\chi = \partial M_{\rm a}/\partial h$ calculated using (9) at h = 0 exactly coincides with susceptibility (6) found above for the exact solution. But there is still no complete match between the exact magnetization value and the approximate magnetization value calculated using pseudochaotic approximation (9) for all values of K, h, and b. Nevertheless, as our calculations show, the relative difference $(M_{\rm a} - M)/M$ does not exceed 10^{-5} to 10^{-4} in absolute value.

5. Correlations in a chain with movable nonmagnetic impurities

To study the difference between the pseudochaotic approximation and the exact solution in more detail, we consider the correlation of magnetic atom positions not only at neighboring sites but at any two sites of the one-dimensional chain. This correlation can be calculated from partition function (7) both for an arbitrary value of L and in particular for L corresponding to the pseudochaotic distribution. We find the correlations in the chain of Ising spins with movable nonmagnetic impurities for an arbitrary value of L. For this, we can use the following method [4]. We consider the transfer matrix \mathbf{V} ,

$$\mathbf{V} = \begin{pmatrix} 1 & e^{(r+h)/2} & e^{(r-h)/2} \\ e^{(r+h)/2} & e^{K+L+r+h} & e^{-K+L+r} \\ e^{(r-h)/2} & e^{-K+L+r} & e^{K+L+r-h} \end{pmatrix}.$$
 (10)

If λ_1 , λ_2 , and λ_3 are the eigenvalues of matrix (10), then partition function (7) equals $Z_N = \lambda_1^N + \lambda_2^N + \lambda_3^N$. Let λ_1 be the maximum eigenvalue of **V**. In the thermodynamic limit $N \to \infty$, we then have

$$bM_{\rm m} = \frac{\partial \log \lambda_1}{\partial h}, \qquad b = \frac{\partial \log \lambda_1}{\partial r}.$$
 (11)

The eigenvalues of matrix (10) can be found from the characteristic equation

$$\lambda^3 + A\lambda^2 + B\lambda + C = 0, \tag{12}$$

where

$$\begin{split} A &= -\left(1 + 2e^{(1+\gamma)K+r}\cosh h\right),\\ B &= 2\left(e^{2(\gamma K+r)}\sinh(2K) + (e^{(1+\gamma)K} - 1)e^{r}\cosh h\right),\\ C &= -4e^{\gamma K+2r}\left(e^{\gamma K}\cosh K - 1\right)\sinh K, \qquad \gamma = \frac{L}{K} = \frac{U}{J} \end{split}$$

Solving Eq. (12) either numerically or using the Cardano formulas and calculating λ_1 , we can by virtue of relation (11) define the dependence of the magnetization $M_{\rm m}$ on b and h for any value of γ , in particular, for a value that corresponds to the pseudochaotic distribution of impurities; in this case $M_{\rm m} = M_{\rm a}$.

We define the correlation functions for the Ising model with movable impurities. As noted above, we call the covariation $g_{ij}^b = \langle \sigma_i^2 \sigma_j^2 \rangle - b^2$ of the quantities σ_i^2 and σ_j^2 (their means equal the magnetic atom concentration b), which we regard as a function of the distance between these sites, the positional correlation function. We call the covariation $g_{ij}^{mb} = \langle \sigma_i \sigma_j \rangle - b^2 M^2$ of the quantities σ_i and σ_j themselves the magnetic-positional correlation function because it characterizes the relation between positions and magnetic moments of atoms. We consider the calculation of these correlation functions for a linear chain:

$$\langle \sigma_i^2 \sigma_j^2 \rangle = \frac{1}{Z_N} \sum_{\{\sigma\}} V(\sigma_1, \sigma_2) \cdots V(\sigma_{i-1}, \sigma_i) \sigma_i^2 V(\sigma_i, \sigma_{i+1}) \cdots V(\sigma_{j-1}, \sigma_j) \sigma_j^2 V(\sigma_j, \sigma_{j+1}) \cdots V(\sigma_N, \sigma_1), \quad (13)$$

where

$$V(\sigma_i, \sigma_{i+1}) = \exp\left\{K\sigma_i\sigma_{i+1} + L\sigma_i^2\sigma_{i+1}^2 + r\frac{\sigma_i^2 + \sigma_{i+1}^2}{2} + h\frac{\sigma_i + \sigma_{i+1}}{2}\right\}$$

is the transfer matrix element.

We introduce the matrix $\mathbf{S} = \text{diag}(0, 1, 1)$ and write equality (13) in the form

$$\langle \sigma_i^2 \sigma_j^2 \rangle = \frac{1}{Z_N} \operatorname{Tr} \{ \mathbf{V}^{i-1} \mathbf{S} \mathbf{V}^{j-i} \mathbf{V}^{N-j+1} \}.$$
(14)

To calculate the trace in the right-hand side of (14), we consider the orthogonal matrix **P** transforming the symmetric transfer matrix **V** to the diagonal form: $\mathbf{P}^{-1}\mathbf{VP} = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$. We can then write (14) as

$$\langle \sigma_i^2 \sigma_j^2 \rangle = \frac{1}{Z_N} \operatorname{Tr} \Big\{ \operatorname{diag}(\lambda_1^{i-1}, \lambda_2^{i-1}, \lambda_3^{i-1}) \cdot \widetilde{\mathbf{S}} \times \\ \times \operatorname{diag}(\lambda_1^{j-1}, \lambda_2^{j-1}, \lambda_3^{j-1}) \cdot \widetilde{\mathbf{S}} \cdot \operatorname{diag}(\lambda_1^{N-j+1}, \lambda_2^{N-j+1}, \lambda_3^{N-j+1}) \Big\},$$
(15)

where $\widetilde{\mathbf{S}} = \mathbf{P}^{-1}\mathbf{SP}$. Taking $Z_N = \lambda_1^N + \lambda_2^N + \lambda_3^N$ into account and passing to the limit $N \to \infty$, we obtain

$$\langle \sigma_i^2 \sigma_j^2 \rangle = \frac{1}{\lambda_1^{j-1}} \operatorname{Tr} \Big\{ \operatorname{diag}(\lambda_1^{i-1}, \lambda_2^{i-1}, \lambda_3^{i-1}) \cdot \widetilde{\mathbf{S}} \cdot \operatorname{diag}(\lambda_1^{j-1}, \lambda_2^{j-1}, \lambda_3^{j-1}) \cdot \widetilde{\mathbf{S}} \cdot \operatorname{diag}(1, 0, 0) \Big\}$$

Expressing correlation function (13) in terms of the elements of the matrix $\tilde{\mathbf{S}}$, we obtain

$$\langle \sigma_i^2 \sigma_j^2 \rangle = \tilde{s}_{11}^2 + \tilde{s}_{12} \tilde{s}_{21} \left(\frac{\lambda_2}{\lambda_1}\right)^{j-i} + \tilde{s}_{13} \tilde{s}_{31} \left(\frac{\lambda_3}{\lambda_1}\right)^{j-i}.$$
(16)

Similarly calculating the mean $\langle \sigma_i^2 \rangle$, we can show that it equals \tilde{s}_{11} . Therefore, the positional correlation function is the sum of two decreasing geometric progressions:

$$g_{ij}^b = \langle \sigma_i^2 \sigma_j^2 \rangle - b^2 = \alpha x_1^{j-i} + \beta x_2^{j-i}, \qquad (17)$$

where $\alpha = \tilde{s}_{12}\tilde{s}_{21}$, $\beta = \tilde{s}_{13}\tilde{s}_{31}$, $x_1 = \lambda_2/\lambda_1$, $x_2 = \lambda_3/\lambda_1$. To calculate the magnetic-positional correlation function, we use the matrix $\mathbf{S}_1 = \text{diag}(0, 1, -1)$ instead of the matrix \mathbf{S} , which results in an equation for g_{ij}^{mb} analogous to Eq. (17):

$$g_{ij}^{\mathrm{mb}} = \alpha_1 x_1^{j-i} + \beta_1 x_2^{j-i}.$$
(18)

At h = 0 (in this case, the magnetization $M_{\rm m}$ also vanishes because spontaneous magnetization does not arise in a one-dimensional chain at a zero temperature), it turns out that one of the coefficients α or β in formula (17) vanishes (which one depends on the enumeration of roots λ_2 and λ_3 of the characteristic equation), i.e., the positional correlation function in this case has the form of decreasing geometric progression. Magnetic-positional correlation function (18) also becomes a geometric progression at h = 0. But if the ratio of the progression equals x_1 in (17), then it equals x_2 in (18), and vice versa. If $h \neq 0$, then all four coefficients α , β , α_1 , and β_1 in expressions (17) and (18) are nonzero.

We now consider the pseudochaotic approximation. We choose the quantity L such that the correlation function g_{12}^b equals zero for given values of the external field h, the temperature parameter K, and the magnetic atom concentration b. According to the above, such a choice of L at h = 0 leads to all values of the positional correlation function g_{ij}^b vanishing, i.e., the impurity distribution in this case is uncorrelated at any distance. If $h \neq 0$, then only the function g_{12}^b vanishing no longer results in all g_{ij}^b vanishing, but we still can consider that the impurity distribution is more chaotic than at $g_{12}^b \neq 0$.

Therefore, we have the following result for the one-dimensional chain with nonmagnetic dilution. At $M_{\rm m} = 0$, the distribution of the nonmagnetic impurities in the pseudochaotic approximation becomes uncorrelated at any interatomic distance, and the magnetic susceptibility at h = 0 calculated using the

pseudochaotic approximation simultaneously coincides with the exact value. We now assume that a similar situation holds not only for the one-dimensional chain with dilution but also for an arbitrary crystal lattice, i.e., we assume that for the Ising model with nonmagnetic dilution on any crystal lattice in the region of values of the parameters K, b, and h such that M = 0, the impurity distribution in the pseudochaotic approximation is uncorrelated at any distance. In addition, we assume that the magnetic susceptibility calculated on the boundary of the region M = 0 in this approximation coincides with the exact value of the magnetic susceptibility for the Ising model with fixed immobile impurities. As shown below, there are reasons to suppose that this assumption holds for the Ising model with nonmagnetic dilution on an arbitrary Bethe lattice.

6. Bethe lattice with dilution

The Bethe lattice can be constructed as follows [4]. The central site is connected to q other sites. Each of them is in turn connected to q-1 new sites. Performing this procedure n times, we obtain the so-called Cayley tree. The Bethe lattice is the inside part (which is far from the boundary points) of this graph as $n \to \infty$. We first consider the solution for the Ising model on the Bethe lattice with movable impurities, which are in thermodynamic equilibrium with the matrix. Partition function (1) on the Bethe Lattice can be calculated by the method based on constructing recurrence relations [4]. Applying this method yields the result [5]

$$M_{\rm m} = \tanh \frac{qx - h}{q - 1}, \qquad b = \frac{2y \cosh x + \cosh(2x) + e^{-2K}}{2y^2 e^{(1 + \gamma)K} + 4y \cosh x + \cosh(2x) + e^{-2K}},$$

$$\mu = -kT \log \left(2y^q e^{q(1 + \gamma)K} \left(\frac{p}{1 - p}\right)^{q - 1} (1 - M_{\rm m}^2)^{(q - 1)/2}\right),$$
(19)

where

$$y = \frac{1}{2} (1 - e^{-2K}) \frac{\sinh((qx - h)/(q - 1))}{\sinh((x - h)/(q - 1))} - \cosh x.$$
⁽²⁰⁾

These relations represent the parametric relations $M_{\rm m} = M_{\rm m}(x, h)$, b = b(x, h, K), and $\mu = \mu(x, h, K)$, and the parameter x varies in the interval from h to the value of x^* such that y vanishes. A detailed analysis of these expressions for different values of γ was presented in [5], where it was shown that a nonzero solution for $M_{\rm m}$ at h = 0 (i.e., spontaneous magnetization) exists only for $b > b_{\rm c}(K)$, where the threshold concentration $b_{\rm c}(K)$ also depends on the parameter γ [5].

The positional correlation of two neighboring sites can be calculated using the formula

$$g_{12}^{b} = \frac{\cosh(2x) + e^{-2K}}{2y^{2}e^{(1+\gamma)K} + 4y\cosh x + \cosh(2x) + e^{-2K}} - b^{2}.$$
(21)

Similarly,

$$g_{12}^{\mathrm{mb}} = \frac{\cosh(2x) - e^{-2K}}{2y^2 e^{(1+\gamma)K} + 4y \cosh x + \cosh(2x) + e^{-2K}} - M_{\mathrm{m}}^2 b^2.$$
(22)

In addition, the functions g_{13}^b and g_{13}^{mb} were found in [5].

We assume that in the case of an arbitrary q, like for a one-dimensional chain, the positional and magnetic-positional correlation functions are sums of two decreasing geometric progressions:

$$g_{ij}^{b} = \langle \sigma_{i}^{2} \sigma_{j}^{2} \rangle - b^{2} = \alpha x_{1}^{j-i} + \beta x_{2}^{j-i}, \qquad g_{ij}^{\mathrm{m}b} = \langle \sigma_{i} \sigma_{j} \rangle - M_{\mathrm{m}}^{2} b^{2} = \alpha_{1} x_{1}^{j-i} + \beta_{1} x_{2}^{j-i}.$$
(23)

The coefficients α , β , α_1 , and β_1 and the ratios of the progressions x_1 and x_2 can be found by equating functions (23) to the correlation functions g_{12} and g_{13} . The calculation shows [5] that at h = 0 and for

 $0 < b < b_{c}(K)$ (the spontaneous magnetization $M_{\rm m} = 0$ in this region), the coefficients α and β_1 (or β and α_1) vanish, i.e., the positional and magnetic-positional correlation functions have the form of decreasing geometric progressions but with different ratios. In this case, in the region of existence of spontaneous magnetization (for h = 0, $b_{c}(K) < b < 1$, and $K > K_{c}(1)$), all four coefficients α , β , α_1 , and β_1 are nonzero in the general case.

We now pass to the pseudochaotic approximation, i.e., we chose the parameter γ such that the function g_{12}^b vanishes. We let γ_0 denote this value of γ (depending on b, K, and h). The parameter γ_0 is defined by the relation

$$e^{(1+\gamma_0)K} = \frac{1}{2y^2} \left(\frac{\cosh(2x) + e^{-2K}}{b^2} - (4y\cosh x + \cosh(2x) + e^{-2K}) \right), \tag{24}$$

where

$$b = \frac{\cosh(2x) + e^{-2K}}{2y\cosh x + \cosh(2x) + e^{-2K}}.$$
(25)

This implies that spontaneous magnetization can exist in the system only for $b > b_c(K) = 1/((q-1) \tanh K)$, i.e., the Curie temperature vanishes at $b = b_c = 1/(q-1)$.

The magnetization has the form

$$M_{\rm a} = \tanh \frac{qx - h}{q - 1}, \qquad b = \frac{\tanh((qx - h)/(q - 1)) - \tanh x}{\sinh(2x)/(\cosh(2x) + e^{-2K}) - \tanh x},\tag{26}$$

and x varies from $x_1 = h$ to a value x_2 such that b = 1. If $M_a = 0$, i.e., h = 0 and $K < K_c(b)$, then the condition $g_{12}^b = 0$ automatically leads to all the functions g_{ij}^b vanishing. This result supports the above proposed assumption. In this case, the value of the parameter γ_0 does not depend on b and equals

$$\tilde{\gamma}_0 = \frac{1}{K} \log \frac{2}{1 + e^{-2K}} - 1.$$
(27)

Because $g_{11}^{mb} = b$ and the magnetic-positional function is a decreasing geometric progression in this case, we obtain $g_{ij}^{mb} = b(b \tanh K)^{|j-i|}$. Differentiating the quantity M_a defined in (26) with respect to h, we find the magnetic susceptibility at $M_a = 0$, i.e., for h = 0 and $K < K_c(b)$,

$$\chi = b_{\rm c} \frac{1 + b \tanh K}{b_{\rm c} - b \tanh K}, \quad {\rm where} \ b_{\rm c} = \frac{1}{q - 1}.$$

According to the above assumption, we obtain the exact value of the magnetic susceptibility for the Ising model with immobile impurities on the Bethe lattice in the region M = 0.

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

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