Theoretical and Mathematical Physics, **202**(2): 265–271 (2020)

ISING MODEL WITH NONMAGNETIC DILUTION ON RECURSIVE LATTICES

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Using a method for composing self-consistent equations, we construct a class of approximate solutions of the Ising problem that are a generalization of the Bethe approximation. We show that some of the approximations in this class can be interpreted as exact solutions of the Ising model on recursive lattices. For these recursive lattices, we find exact values of the thresholds of percolation through sites and couplings and show that for the Ising model of a diluted magnet, our method leads to exact values for these thresholds.

Keywords: Ising model, crystal lattice, magnet with nonmagnetic dilution, recursive lattice

DOI: 10.1134/S0040577920020099

1. Introduction

We construct a class of self-consistent solutions that can serve as an approximate solution of the Ising model on different crystal lattices. The well-known Bethe approximation [1], [2] is a particular (and simplest) example of equations in this class. Therefore, our class of self-consistent solutions can be regarded as a generalization of the Bethe approximation. As is known [1], the Bethe approximation can be interpreted as a replacement of a real crystal lattice with a so-called Bethe lattice, which is an internal part of a Cayley tree. Similarly to this, the solutions of some of our proposed equations can be interpreted as exact solutions of the Ising problem on recursive lattices constructed in a special manner, as shown below. In addition, we extend our method to the Ising model with nonmagnetic dilution over sites and couplings [3]. We show that in the cases where our method gives an exact solution for a pure magnet on the recursive lattice, its generalization to the diluted magnet leads to the exact value of the percolation threshold for this lattice.

2. Recursive lattices and self-consistent equations

We consider a simple crystal lattice with the coordination number q, Ising spins $\sigma = \pm 1$ at its sites, and a nonzero exchange interaction only for neighboring spins. (Our method can be generalized to the case where the lattice is not simple, but this generalization is beyond the scope of this paper.) We seek the average magnetic moment (magnetization) of a lattice site in the form

$$M_1(h_1) = \tanh(Kh_1 + h_{\text{ex}}),$$

where $K = J/kT$ (J is the exchange integral, k is the Boltzmann constant, and T is the temperature), $h_{\text{ex}} = H_{\text{ex}}/kT$, H_{ex} is the external field, and h_1 has the meaning of an *effective exchange field* produced by neighboring spins.

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Translated from Teoreticheskaya i Matematicheskaya Fizika, Vol. 202, No. 2, pp. 304–311, February, 2020. Received May 22, 2019. Revised July 10, 2019. Accepted September 18, 2019.

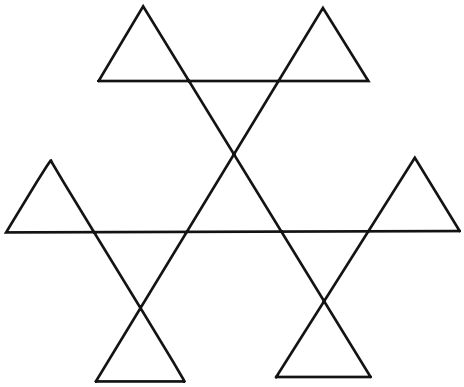

Fig. 1. Recursive lattice for $N = 3$ and $L = 1$.

On the lattice, we now consider a cluster consisting of two neighboring atoms, a dimer. Assuming that both dimer atoms are located in an effective exchange field h_2, we find the average magnetization of the dimer atom:

$$M_2(h_2) = \frac{\sinh(2Kh_2 + 2h_{\text{ex}})}{\cosh(2Kh_2 + 2h_{\text{ex}}) + e^{-2K}}.$$

Assuming that $h_2 = \frac{q-1}{q}h_1$ (based on each dimer atom having $q-1$ external neighbors), then the equality $M_1(h_1) = M_2(h_2)$ is a self-consistent equation whose solution is the Bethe approximation [4].

In the lattice, we select a closed chain of N sites of minimum possible length (which depends on the lattice form). Assuming that each atom in the chain is located in an effective field h_N, we find the atom magnetization of this cyclic cluster [5]:

$$M_N(h_N) = \frac{\lambda_1^N - \lambda_2^N}{\lambda_1^N + \lambda_2^N} \frac{e^K \sinh(Kh_N + h_{\text{ex}})}{\sqrt{e^{2K}\sinh^2(Kh_N + h_{\text{ex}}) + e^{-2K}}},$$

where

$$\lambda_{1,2} = e^K \cosh(Kh_N + h_{\text{ex}}) \pm \sqrt{e^{2K}\sinh^2(Kh_N + h_{\text{ex}}) + e^{-2K}}.$$

Setting $h_N = \frac{q-2}{q}h_1$, we can obtain the self-consistent equation

$$M_1(h_1) = M_N(h_N). \tag{1}$$

We now show that for even q, the obtained equation gives the exact solution of the Ising problem for the recursive lattice constructed as follows. We take N sites and couplings forming a closed N-gon. We construct L such nonintersecting N-gons at each vertex of this N-gon. Repeating this construction at each vertex of the new N-gons, we obtain a recursive lattice (Fig. 1), which is an infinite cactus (the Husimi cactus) [6]. The coordination number of such a lattice is always even and is equal to $q = 2L + 2$.

We place the Ising spins σ_i at the sites of this lattice and assume that neighboring spins interact with the energy $-J\sigma_1\sigma_2$ and, moreover, the entire system is located in an external field H_{ex}. We find the magnetization, the average value of each such spin. This can be done as follows. We consider a separate lattice site with the spin σ. This site is the common vertex of $L+1$ N-gons forming $L+1$ nonintersecting branches with the root point σ. Letting s_i denote the set of spins (except σ) of the ith branch, we represent the partition function of the system in the form

$$Z = \sum_{\sigma, s_1, \ldots, s_{L+1}} e^{\sigma h_{\text{ex}}} \Omega(\sigma, s_1) \cdots \Omega(\sigma, s_{L+1}),$$

where $\Omega(\sigma, s_i)$ is a factor depending only on σ and the set s_i of spins. We set $g(\sigma) = \sum_s \Omega(\sigma, s)$ (by symmetry, this quantity is the same for all branches, i.e., is independent of i). The partition function is then

$$Z = e^{h_{\text{ex}}} g^{L+1}(+1) + e^{-h_{\text{ex}}} g^{L+1}(-1),$$

and the average magnetization of the spin σ is

$$m_1 = \frac{e^{h_{\text{ex}}} g^{L+1}(+1) - e^{-h_{\text{ex}}} g^{L+1}(-1)}{e^{h_{\text{ex}}} g^{L+1}(+1) + e^{-h_{\text{ex}}} g^{L+1}(-1)} = \frac{e^{h_{\text{ex}}} - x^{L+1} e^{-h_{\text{ex}}}}{e^{h_{\text{ex}}} + x^{L+1} e^{-h_{\text{ex}}}},$$

where $x = g(-1)/g(+1)$. If we set $h_1 = \frac{-L+1}{2K} \log x$, then the expression for the magnetization m_1 becomes

$$m_1 = \tanh(Kh_1 + h_{\text{ex}}).$$

We now consider one of the N-gons of the recursive lattice. Each vertex of this N-gon is the root point of L nonintersecting branches such as considered above. We can therefore represent the partition function as

$$Z = (g(+1)x^{1/2})^{NL} \sum_{\sigma_i} \exp\left[K \sum \sigma_i \sigma_{i+1} + (Kh_N + h_{\text{ex}}) \sum \sigma_i\right],$$

where $h_N = -\frac{L}{2K} \log x$. Calculating this partition function, we find the average value $m_N = \left\langle \sum \sigma_i / N \right\rangle$:

$$m_N = \frac{\lambda_1^N - \lambda_2^N}{\lambda_1^N + \lambda_2^N} \frac{e^K \sinh(Kh_N + h_{\text{ex}})}{\sqrt{e^{2K} \sinh^2(Kh_N + h_{\text{ex}}) + e^{-2K}}}.$$

Equating m_1 to m_N and taking

$$h_N = \frac{L}{L+1} h_1 = \frac{q-2}{q} h_1$$

into account, we now obtain an equation that exactly coincides with self-consistent equation (1) given above. That is, similarly to how the Bethe approximation can be interpreted as the replacement of a crystal lattice with a Cayley tree with the same coordination number, the approximation based on Eq. (1) with even q can be interpreted as the replacement of the initial lattice with the recursive lattice described above with the corresponding value of L.

These two examples (the Bethe lattice and the recursive lattice consisting of N-gons) suggest the following generalization. We consider a recursive lattice constructed from the same clusters. For example, we can take a cubic cluster (sites that are the vertices of a cube with couplings along the edges of this cube) or a closed N-gon with one or several internal sites connected to all N vertices such as, for example, in [7], [8]. The recursive lattice is constructed from these clusters in the same way as the lattice consisting of N-gons, i.e., by adding L such clusters to each external vertex of the cluster, and so on. On one hand, each external site of any cluster in an infinite recursive lattice can then be regarded as the root point for the same $L+1$ branches; on the other hand, it can be regarded as the root point for L such branches if this site is assumed to be in the cluster composition. Therefore, if Ising spins are placed at the sites of this recursive lattice, then the average magnetization of an external site can be calculated using the formula

$$m_1 = \tanh(Kh_1 + h_{\text{ex}}),$$

where $h_1 = \frac{-L+1}{2K} \log x$, $x = g(-1)/g(+1)$, and $g(\pm 1)$ are the factors of the partition function related to the spins of one of the $L+1$ branches. On the other hand, if the magnetization m_N of this site is calculated

as that of the site belonging to the cluster, then it can be expressed as the function of $h_N = -\frac{L}{2K}\log x$. Consequently, solving the equation $m_1 = m_N$ for x, we obtain the exact solution of the Ising problem for the recursive lattice. But we can regard the equation $m_1 = m_N$ as Eq. (1), i.e., as a self-consistent equation in which h_1 and h_N are effective exchange fields. These fields are related by $h_N = \frac{q-q'}{q}h_1$, where q' is the number of couplings of the external atom of the cluster to other atoms of this cluster and $q = q'(L+1)$ is the coordination number. We can consider the self-consistent equation $m_1 = m_N$ for any $q > q'$, but if the condition $q = q'(L+1)$ is not satisfied, then the solution of this equation cannot be interpreted as an exact solution of the Ising model for the recursive lattice.

3. Nonmagnetic dilution in the recursive lattice

We can formulate the percolation problem for the recursive lattices composed of N-gons and described above. We assume that each lattice site is randomly and independently of other sites "cut" with the probability $1 - b$ (i.e., all couplings leaving this site are removed) and it remains unchanged with the probability b. Uncut lattice sites belong to clusters with different dimensions. For small b, each such cluster contains a finite number of sites, and for rather large b, a cluster containing an infinitely large number of sites exists. The minimum b for which an infinite cluster exists is the threshold b_s of percolation through the sites. If each separate branch is cut with the probability $1-b$, then the minimum b for which an infinite cluster exists is the threshold b_b of percolation through the couplings.

We find the thresholds of percolation through the sites and couplings for recursive lattices constructed by the method described above. Let x be the probability that the branch of a cluster with an uncut initial vertex is finite. We can obtain the equation for x using the following simple reasoning. The branch is finite in four mutually exclusive cases:

1. Sites that are adjacent to the initial vertex are cut off: the probability of this is $(1-b)^2$.

2. All sites of the N-gon are present, but all branches leaving them are finite: the probability of this is $b^{N-1}x^{(N-1)L}$.

3. One of the vertices of the N-gon is absent, and the branches leaving the other vertices are finite: the probability of this is $(N-1)(1-b)b^{N-2}x^{(N-2)L}$.

4. Two vertices of the N-gon are absent, and the branches leaving the vertices connected to the initial vertex are finite: the probability of this is $(1-b)^2\sum_{k=1}^{N-3}(k+1)b^k x^{kL}$.

Summing these probabilities, we obtain the equation

$$x = (1-b)^2 + (1-b)^2\sum_{k=1}^{N-3}(k+1)b^k x^{kL} + (N-1)(1-b)b^{N-2}x^{(N-2)L} + b^{N-1}x^{(N-1)L}.$$

For any b, this equation has the solution $x = 1$. We let $F(x)$ denote the right-hand side of this equation. Because $F(0) = (1-b)^2 > 0$, the equation $x = F(x)$ has a nontrivial solution in the interval $(0,1)$ under the condition $F'(1) \geq 1$. Consequently, the percolation threshold b_s must satisfy the equation $F'(1) = 1$, i.e.,

$$(1-b_\mathrm{s})^2\sum_{k=1}^{N-3}k(k+1)b_\mathrm{s}^k + (N-1)(N-2)(1-b)b_\mathrm{s}^{N-2} + (N-1)b_\mathrm{s}^{N-1} = \frac{1}{L},$$

which transforms into

$$(N-3)b_{\rm s}^{N-1} - 2\sum_{i=1}^{N-2} b_{\rm s}^{i} + \frac{1}{L} = 0. \tag{2}$$

By analogy, we obtain

$$(N-1)b_{\rm b}^{N} - 2\sum_{i=1}^{N-1} b_{\rm b}^{i} + \frac{1}{L} = 0 \tag{3}$$

for the threshold of percolation through couplings.

We now consider the Ising model with nonmagnetic dilution on a lattice. We take a closed chain composed of N sites in the lattice. In the case of the dilution over sites and couplings, we can divide the chain into some number of linear fragments. Calculating the average magnetization per atom for each such fragment and then the average magnetization per site for the chain, we obtain the latter as a function of K, h_N, and b. We let m_i denote the average magnetization per atom for the unclosed remainder of the chain (containing $i \le N$ magnetic atoms) and $m_N^{\rm c}$ denote the average magnetization per atom for a closed chain composed of N magnetic atoms (obviously, $M_N(K) = m_N^{\rm c}$ for a pure magnet). Then in the case of dilution over the sites, we have

$$M_N(K,b) = \sum_{l=1}^{N-1} b^l (1-b)^{N-l} \sum_{\{l,N\}} \left(\frac{1}{N} \sum_k i_k m_{i_k} \right) + b^N m_N^{\rm c}. \tag{4}$$

In this expression, the sums are constructed as follows. The external sum is taken over the number of magnetic atoms in the chain. The sum over $\{l, N\}$ is taken over all possible arrangements of l magnetic atoms at N sites of the closed chain. For each such arrangement, these l atoms form fragments containing $i_1, i_2, \ldots$ atoms, and the internal sum is taken over these fragments. By analogy, in the case of the dilution over couplings, we have

$$M_N(K,b) = (1-b)^N m_1 + \sum_{l=1}^{N-1} b^l (1-b)^{N-l} \sum_{\{l,N\}} \left(\frac{1}{N} \sum_k i_k m_{i_k} \right) + b^N m_N^{\rm c}. \tag{5}$$

We consider a lattice site. Replacing the action of atoms located at neighboring sites with the action of the crystal field h_1, we find the average magnetization per site

$$M_1(K,b) = b \tanh(Kh_1) \tag{6}$$

for the dilution over the sites and

$$M_1(K,b) = \tanh(Kh_1) \tag{7}$$

for the dilution over the couplings. We also consider the cluster composed of two neighboring sites located in the crystal field h_2. The average magnetization per cluster site has the form

$$M_2(K,b) = 2b(1-b)\tanh(Kh_2) + b^2 \frac{\sinh(2Kh_2)}{\cosh(2Kh_2) + e^{-2K}} \tag{8}$$

in the case of dilution over sites and the form

$$M_2(K,b) = (1-b)\tanh(Kh_2) + b \frac{\sinh(2Kh_2)}{\cosh(2Kh_2) + e^{-2K}} \tag{9}$$

in the case of dilution over the couplings.

We note that if the right-hand sides of equalities (6) and (8) (or (7) and (9)) are equated, then under the additional condition $h_2 = \frac{q-1}{q} h_1$, we obtain the solution of the model for the diluted Ising magnet on the Bethe lattice with a pseudochaotic impurity distribution [9], [10].

We now construct self-consistent equations by equating the right-hand sides of (4) and (6) for the dilution over sites and of (5) and (7) for the dilution over couplings under the condition $h_N = \frac{q-2}{q} h_1$. Solving these equations, we obtain the dependences of the magnetization on the concentration and temperature in different approximations. It turns out that all these equations have nonzero solutions for h_N under the condition $K > K_c$; in this case, K_c is determined by equating the derivatives of the right-hand sides of the corresponding equalities with respect to h_N at $h_N = 0$. Passing to the limit $K_c \to \infty$, we now obtain the equations for the percolation thresholds b_s and b_b. It turns out that

$$(N-3) b_s^{N-1} - 2 \sum_{i=1}^{N-2} b_s^i + \frac{2}{q-2} = 0 \tag{10}$$

and

$$(N-1) b_b^{N} - 2 \sum_{i=1}^{N-1} b_b^i + \frac{2}{q-2} = 0. \tag{11}$$

Clearly, these equations with $q = 2L + 2$ coincide with Eqs. (2) and (3).

We recall that we obtained Eqs. (2) and (3) for the percolation thresholds of the considered recursive lattice irrespective of the magnetic models that can be constructed on these lattices, i.e., their solutions are "geometric" property of these lattices. And Eqs. (10) and (11) are equations for the concentrations b_s and b_b at which the Curie temperature (and the spontaneous magnetization at zero temperature) in the considered approximation becomes zero in the Ising model with nonmagnetic dilution on the recursive lattice. It is known [11] that these quantities must vanish at concentrations of nonmagnetic atoms that are equal to the percolation thresholds. This implies that the coincidence between (2) and (10) (and also between (3) and (11)) means that the Curie temperature vanishes precisely at the percolation thresholds in the considered approximation. This does not mean that the self-consistent equations obtained by equating the right-hand ides of (4) and (6) (or of (5) and (7)) give an exact solution of the Ising model with the corresponding dilution (over the sites and couplings) for arbitrary temperatures and concentrations. Nevertheless, if we take into account that the self-consistent equations give exact solutions on the recursive lattice for pure magnets, then the coincidence between (2) and (3) and between (10) and (11) shows that our approximation coincides with the exact solution rather well not only for small impurity concentrations but also near the percolation thresholds.

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

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