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Frustrations in a Diluted Ising Magnet on the Bethe Lattice

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Abstract—We consider the calculation of the entropy of an Ising ferromagnet with nonmagnetic impurities distributed at random over the lattice sites or bonds. The Ising magnet on the Bethe lattice is analyzed. On such a lattice, the situations with a random nonmagnetic dilution over the sites and bonds are indistinguishable. For calculating the entropy, the magnetization determined in the pseudo-chaotic approximation is used. In this approximation, we obtain the entropy as a function of the temperature, the concentration of magnetic atoms, and the external magnetic field. It is found that in zero external field, the system is frustrated in the sense that the ground-state entropy differs from zero. The value of this entropy is determined for concentrations magnetic atoms below as well as above the percolation threshold.

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1. INTRODUCTION

This study is devoted to the calculation of the free energy and entropy of a diluted Ising magnet on the Bethe lattice. The Bethe lattice is an infinite graph without closed routes, in which each node is connected with coordination number q by other nodes [1]. On such a lattice, the Ising model can be defined by placing the Ising "spin" that takes values of $+1$ or -1 in each node. Each pair of adjacent spins σ_i and σ_j is connected with Hamiltonian term $J_{ij}\sigma_i\sigma_j$ that simulates the exchange interaction, J_{ij} being preset constants. When all J_{ij} are identical and positive, it is possible to construct the exact solution for arbitrary q [1].

If we now replace some of the spins by nonmagnetic atoms distributed in the lattice at random without a correlation, we obtain the model of a magnet diluted over the sites; if, however, nonmagnetic impurities are located on lattice bonds and block the exchange interaction on the given bond, we obtain the model of the magnet diluted over the bonds [2, 3]. For the Bethe lattice, the models with dilution over sites and bonds are formally indistinguishable [4]. The exact solution for the Ising model with dilution can be obtained for $q = 2$ (1D chain) [5]; however, for an arbitrary q, the exact solution to the problem does not exist.

In our previous publications [4, 6, 7], we proposed an approach to analysis of the properties of diluted magnets with nonmagnetic impurities, which is based on the following considerations. Instead of assuming from the very outset that the impurities are distributed in the lattice at random, we consider a magnet in which magnetic atoms and impurity atoms can move and are in thermodynamic equilibrium. The energy of such a system is determined not only by the orientation of magnetic moments, but also by the distribution of impurity atoms over lattice sites. Therefore, the Hamiltonian of a certain model of a magnet with mobile impurities consists of the terms connected with the exchange interaction of magnetic atoms as well as the terms associated with the interatomic interaction in the crystal lattice; the equilibrium distribution of impurity atoms in this case depends on parameters characterizing both these interactions. Then it is possible to choose for each value of temperature, external magnetic field, and concentration (fraction) b of magnetic atoms in the system the values of the interatomic interaction parameters so that the equilibrium distribution of impurity atoms is as close as possible to the random distribution [4, 6, 7]. For the criterion of closeness of the impurity atom distribution to the random distribution, we can use, for example, the equality to zero of the correlation in the location of impurity atoms for two nearest sites, which forms the basis of the pseudo-chaotic approximation used in this study. In this approximation, we calculate the free energy and entropy of a diluted Ising magnet on the Bethe lattice and draw conclusions concerning possible frustrated states in this system.

2. FREE ENERGY AND ENTROPY OF A DILUTED ISING MAGNET

In accordance with the principles of statistical physics and thermodynamics, the total free energy of a thermodynamic system is given by [1, 8]

$$F = -kT\ln Z, \quad (1)$$

where k is the Boltzmann constant, T is the absolute temperature, and Z is the partition function of the system. Knowing the free energy as a function of temperature, we can express internal energy U and entropy S as [8]

$$U = -T^2\frac{\partial}{\partial T}\left(\frac{F}{T}\right), \quad S = -\frac{\partial F}{\partial T}. \quad (2)$$

The Ising model is a simple and frequency used model of a magnetic system [1]. In this model, a magnetic atom is represented by variable σ taking values of $+1$ and -1 (so-called Ising spin), which is localized in the position of this atoms (lattice site). For the Ising model on an arbitrary lattice, we have

$$Z = \sum_{\Omega}\exp\left(-\frac{1}{kT}\mathcal{H}(\Omega, H)\right). \quad (3)$$

Hamiltonian $\mathcal{H}(\Omega, H)$ of the system depends on external field H and on configuration Ω of Ising spins, and the summation in expression (3) is performed over all such configurations. For the model with the pair interaction, we have

$$\mathcal{H}(\Omega, H) = \sum_{(i,j)} J_{ij}\sigma_i\sigma_j - H\sum_i \sigma_i. \quad (4)$$

The first summation in this expression is performed over all ordered pairs of spins, while the second summation is carried out over all lattice spins, J_{ij} being the energy of the exchange interaction of the ith and jth spins. For the Hamiltonian of this type, the total magnetization of the system is

$$\sum_i M_i = -\frac{\partial F}{\partial H}, \quad (5)$$

where $M_i = \langle\sigma_i\rangle$ is the thermodynamic mean of the ith spin (i.e., local magnetization of the ith site). Let us calculate the free energy of the system using the arguments analogous to those in [1]. For a very strong external field (i.e., for $H \to \infty$), the largest contribution to sum (3) comes from the term in which all spins $\sigma_i = +1$. In this limit, we have

$$F = -\sum_{(ij)} J_{i,j} - HN. \quad (6)$$

Here, N is the number of lattice sites. Taking into account asymptotic equality (6), assuming that all $M_i \to 1$ for $H \to \infty$, and integrating relation (5), we obtain

$$F(H_0, T) = -\sum_{(i,j)} J_{ij} - H_0 N + \int_{H_0}^{\infty}\left(\sum_i M_i - H\right)dH. \quad (7)$$

Differentiating this expression with respect to T, we obtain, in accordance with relation (2), the entropy of the system:

$$S(H_0, T) = -\sum_i \int_{H_0}^{\infty}\frac{\partial M_i(H.T)}{\partial T}dH. \quad (8)$$

We assume that only the spins of the nearest sites are interacting, while the exchange interactions constants are $J_{ij} = J$ for the nearest neighbors and are equal to zero in all remaining cases. Then

$$\sum_{(ij)} J_{ij} = J\bar{q}\frac{N}{2},$$

where $\bar{q}$ is the coordination number averaged over the lattice. For a simple lattice with coordination number q, we obviously have $\bar{q} = q$ for a pure magnet. In the case of an uncorrelated nonmagnetic dilution over sites or bonds, $\bar{q} = qb$, where b is the concentration of magnetic atoms or bonds [4].

Dividing now expressions (7) and (8) by NkT and introducing specific (per magnetic atom) free energy $f = F/N$, entropy $s = S/N$, and magnetization

$$M = \frac{\sum_i M_i}{N}$$

we obtain

$$\frac{f(h_0, K)}{kT} = -\frac{1}{2}\bar{q}K - h_0 + \int_{h_0}^{\infty}(M(h) - 1)dh, \quad (9)$$

$$\frac{s(h_0, K)}{kT} = -\int_{h_0}^{\infty}\frac{\partial M(h)}{\partial T}dh. \quad (10)$$

Here, $K = J/kT$ and $h = H/kT$.

Expressions (9) and (10) imply that if average magnetization M as a function of temperature, magnetic field, and concentration of magnetic atoms or bonds is known, we can find the free energy and entropy.

3. BETHE LATTICE AND THE PSEUDO-CHAOTIC APPROXIMATION

It was shown in our previous publications [4, 6, 7] that the approximate value of the magnetization of a diluted Ising magnet on a lattice with coordination number q can be determined using expression

$$M = \tanh(Kq\mu + h), \quad (11)$$

where μ can be determined from the following equation:

$$\tanh(Kq\mu + h) = (1-b)\tanh(K(q-1)\mu + h) + b\frac{\sinh(2K(q-1)\mu + 2h)}{\cosh(2K(q-1)\mu + 2h) + e^{-2K}}. \quad (12)$$

It turns out [4] that approximation (11) for a pure magnet ($b = 1$) is the exact solution for the Ising model on the Bethe lattice, while for $b < 1$, it can be treated as the "pseudo-chaotic" approximation for the Ising model with a nonmagnetic dilution on the Bethe lattice [4]. The pseudo-chaotic approximation can be obtained from the solution of the problem with mobile nonmagnetic impurities by imposing the additional condition of zero correlation in the location of impurities in neighboring lattice sites [6]. The situations of dilution over sites and bonds on the Bethe lattice are indistinguishable; therefore, b can be treated as the concentration of magnetic atoms as well as the probability that the bond with neighboring sites is not ruptured.

In expressions (11) and (12), we introduce the following notation:

$$z = Kq\mu + h, \quad w = K(q-1)\mu + h, \quad \eta = e^{-2K},$$
$$\beta = \frac{q-1}{q}, \quad x = h/q.$$

Then expressions (11) and (12) take form

$$M = \tanh(z),$$
$$M = (1-b)\tanh(w) + b\frac{\sinh(2w)}{\cosh(2w) + \eta}, \quad (13)$$
$$w = \beta z + x$$

or $M = \partial\psi/\partial w$, where

$$\psi(w) = (1-b)\ln(\cosh(w)) + \frac{b}{2}\ln(\cosh(2w) + \eta).$$

Equations (13) can be written in the form of a single equation in magnetization M:

$$M = (1-b)\frac{(1+M)^\beta - \xi(1-M)^\beta}{(1+M)^\beta + \xi(1-M)^\beta} + b\frac{(1+M)^{2\beta} - \xi^2(1-M)^{2\beta}}{(1+M)^{2\beta} + \xi^2(1-M)^{2\beta} + 2\xi\eta(1-M^2)^\beta}, \quad (14)$$

where $\xi = e^{-2x}$.

In deriving Eqs. (13) or (14), we have assumed that the mean value of spin (local magnetization) is the same for all inner lattice sites and is equal to M in the thermodynamic limit. In other words, magnetic sublattices are not formed in the system. This means that either the ferromagnetic exchange interaction exists in the system (i.e., $K > 0$), or $K < 0$, but external field H is large enough to prevent the formation of sublattices at any temperature.

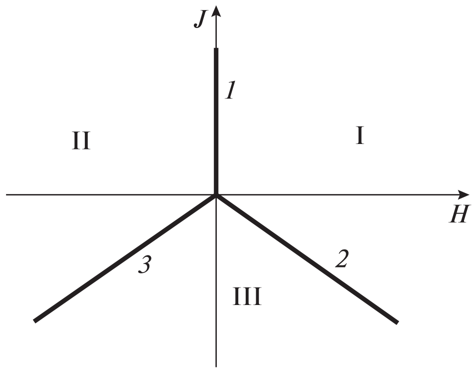

Fig. 1. Diagram of states of a diluted Ising magnet on the Bethe lattice.

To specify the domain of applicability of Eq. (14), we consider the phase diagram of the ground state ($T = 0$) of a diluted Ising magnet on the Bethe lattice with coordination number q (Fig. 1).

Passing to the limit $T \to 0$ in expression (14), we find that $M \to 1$ for $H > 0$ and $J > -H/q$ (domain I in Fig. 1) and $M \to 1$ for $H < 0$ and $J > H/q$ (domain II in Fig. 1). Therefore, in domains I and II, the ground state of the system is ferromagnetic. The boundary of these domains (line *1* in Fig. 1) is the zone in which ferromagnetic phase transitions occur. Analysis of Eqs. (13) shows [4] that for $T \to 1$ and $b < b_c = 1/(q-1)$, $M = 0$ in line *1*. For $b > b_c$, i.e., for the concentration of magnetic atoms, which exceeds the percolation threshold of the Bethe lattice, the system acquires spontaneous magnetization M_0, which can be determined from equation

$$M_0 = (1-b)\frac{(1+M_0)^\beta - (1-M_0)^\beta}{(1+M_0)^\beta + (1-M_0)^\beta} + b\frac{(1+M_0)^{2\beta} - (1-M_0)^{2\beta}}{(1+M_0)^{2\beta} + (1-M_0)^{2\beta}}. \quad (15)$$

Function $M_0(b)$ is represented graphically in Fig. 2 (curve *1*). At $T > 0$, spontaneous magnetization appears for a concentration exceeding the value of $b_K = b_c(1+\eta)/(1-\eta) = b_c\coth(K)$ [4] (curves *2* and *3* in Fig. 2).

In domain III in Fig. 1, the ground state of the system is not ferromagnetic, which, as noted above, rules out the application of Eqs. (13) or (14) in this domain. At the boundary between domains I and III (line *2* in Fig. 1) at $T \to 0$, magnetization M tends to value

$$\tilde{M}_0 = \frac{1-y^q}{1+y^q},$$

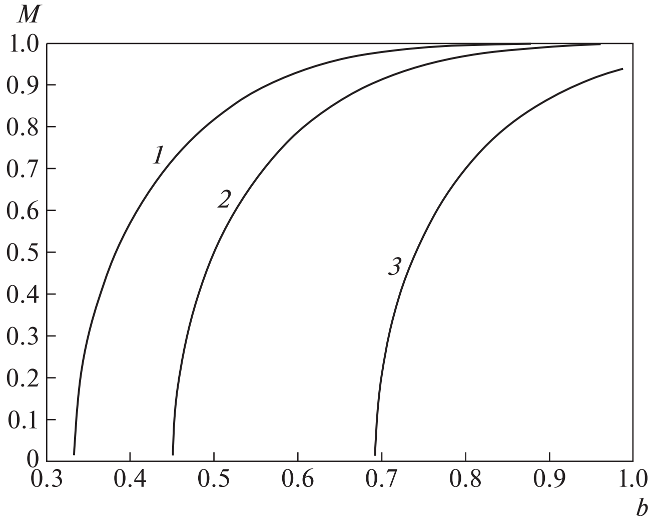

Fig. 2. Spontaneous magnetization of a diluted Ising ferromagnet on the Bethe lattice (q = 4) as a function of the concentration of magnetic atoms (or bonds): (curve *1*) η = 0; (*2*) η = 0.15, and (*3*) η = 0.35 ($\eta = \exp(-2K)$).

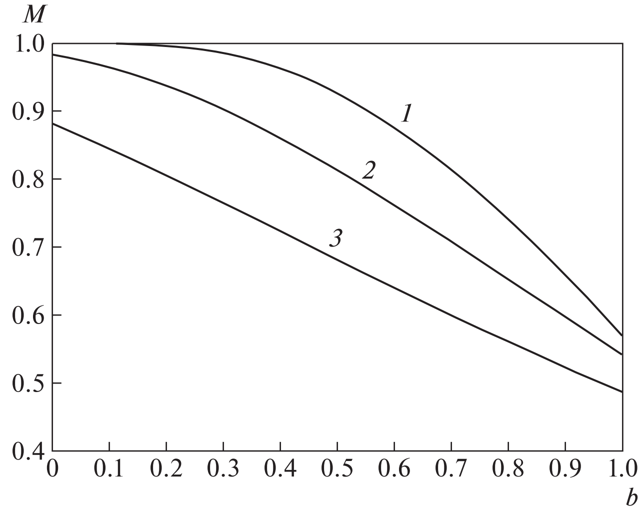

Fig. 3. Magnetization of a diluted Ising antiferromagnet on the Bethe lattice (q = 4) in external field $H = -qJ$ as a function of the concentration of magnetic atoms (or bonds): (curve *1*) $\eta = \infty$, (*2*) $\eta = 10/3$, and (*3*) $\eta = 2$ ($\eta = \exp(-2K)$).

where y can be determined from equation

$$(2-b)y^q + y - b = 0. \tag{16}$$

Function $\tilde{M}_0(b)$ is shown graphically in Fig. 3 (curve *1*). For $q = 2$ and $b = 1$ (i.e., for the 1D Ising chain without nonmagnetic dilution), Eq. (16) gives the result coinciding with that obtained in [9]. For $T > 0$, the magnetization on line *2* in Fig. 1 decreases monotonically upon an increase in concentration b as well as in temperature T (curves *2* and *3* in Fig. 3); i.e., neither concentration nor temperature phase transitions occur in this region.

4. RESULTS OF CALCULATION

Let us now calculate the free energy and entropy of a diluted Ising magnet on the Bethe lattice using their expressions (9) and (10) in the pseudo-chaotic approximation. In relation (9), we pass to variable x,

$$\frac{f(x_0,K)}{qkT} = -\frac{1}{2}bK - x_0 + \int\limits_{x_0}^{\infty}(M(x)-1)dx \tag{17}$$

using relation $dx = dw - \beta dz = dw - \beta(\operatorname{arctanh}(M))'dM$, we obtain

$$\frac{f(x_0,K)}{qkT} = -\frac{1}{2}bK - x_0 + \int\limits_{w_0}^{\infty}(M(w)-1)dw$$
$$-\beta\int\limits_{M_0}^{1}(M-1)(\operatorname{arctanh}(M))'\,dM$$

or (discarding subscript "0" after integration)

$$\frac{f(w,K)}{qkT} = -\frac{1}{2}Kb - x + w - \psi(w)$$
$$-\beta\ln(1+M) - \left(1-\frac{b}{2}-\beta\right)\ln 2.$$

Using equality $w - x = \beta\operatorname{arctanh}(M)$, we can finally write

$$\frac{f(w,K)}{qkT} = -\frac{1}{2}Kb - \psi(2) - \frac{\beta}{2}\ln(1-M^2)$$
$$-\left(1-\frac{b}{2}-\beta\right)\ln 2. \tag{18}$$

For $b = 1$, this expression can be reduced to

$$\frac{f(w,K)}{kT} = -\frac{qK}{2} + \frac{1}{2}(q-2)\ln(2\cosh(2w) + 2\eta)$$
$$-\frac{1}{2}(q-1)\ln(1 + 2\eta\cosh(2w) + \eta^2),$$

which coincides (after a passage to the corresponding variables) with the result obtained in [1] for a pure magnet on the Bethe lattice. Since specific free energy f for $T \to 0$ coincides with specific energy u_0 of the ground state, we obtain from relation (18)

$$u_0 = \frac{1}{2}bqJ - \lim_{T\to 0}\left(qkT\psi(w) + \frac{\beta}{2}qkT\ln(1-M^2)\right). \tag{19}$$

Evaluating the limit in this expression, we can show that in domains I and II (see Fig. 1) and on their boundary *1*, we have

$$u_0 = -\frac{1}{2}nqJ - |H|,$$

i.e., the ground-state energy coincides with the minimal possible energy $u_{\min}$ per atom. In [10], the quantitative measure of frustration, which is defined as

$$p_f = \frac{u_0 - u_{\min}}{u_{\max} - u_{\min}}, \quad (20)$$

was used, where $u_{\max} = -u_{\min}$. Therefore, at all internal points of domains I and II and line *1* on the phase diagram (see Fig. 1), measure (20) equals zero. It will be shown below, however, that the entropy on line *1* differs from zero at $T \to 0$ if $b \neq 1$. On lines *2* and *3* of the diagram, we obtain, using relation (19),

$$u_0 = qJ\left(1 - \frac{b}{2}\right),$$

$$u_{\min} = qK\left(1 + \frac{b}{2}\right).$$

which, in accordance with relation (20), gives

$$p_f = \frac{b}{b+2}. \quad (21)$$

Thus, in accordance with this criterion, the system turns out to be frustrated at boundaries *2* and *3* of the diagram in Fig. 1, and relation (21) assumes the maximal value equal to 1/3 for a pure magnet ($b = 1$).

We can now obtain the entropy of the diluted magnet by differentiating free energy (19) with respect to temperature or directly by formula (8):

$$s(H_0, T) = -\int_{H_0}^{\infty} \frac{\partial M(H,T)}{\partial T} \partial H.$$

Passing to variables x and K and considering that

$$\frac{\partial x}{\partial T} = -\frac{x}{T}, \quad \frac{\partial K}{\partial T} = -\frac{K}{T},$$

we obtain

$$\frac{s(x_0, K)}{qk} = \int_{x_0}^{\infty} \left(X\frac{\partial M}{\partial x} + K\frac{\partial M}{\partial K}\right)dx = (I_1 + I_2)\Big|_{x_0}^{\infty}, \quad (22)$$

$$I_1 = \int X\frac{\partial M}{\partial x}dx, \quad I_2 = \int K\frac{\partial M}{\partial K}dx;$$

$$I_1 = \int W\frac{\partial M}{\partial x}\partial x - \beta\int \operatorname{arctanh}(M)\frac{\partial M}{\partial x}\partial x$$

or

$$I_1 = (1-b)w\tanh(w) + \frac{bw\sinh(2w)}{\cosh(2w)+\eta} - \psi(w)$$
$$-\frac{\beta}{2}((1+M)\ln(1+M) + (1-M)\ln(1-M)).$$

To evaluate I_2, we pass in this integral to variable w. Then

$$I_2 = K\int \frac{\partial M}{\partial K}dw = -\frac{bK\eta}{\cosh(2w)+\eta}.$$

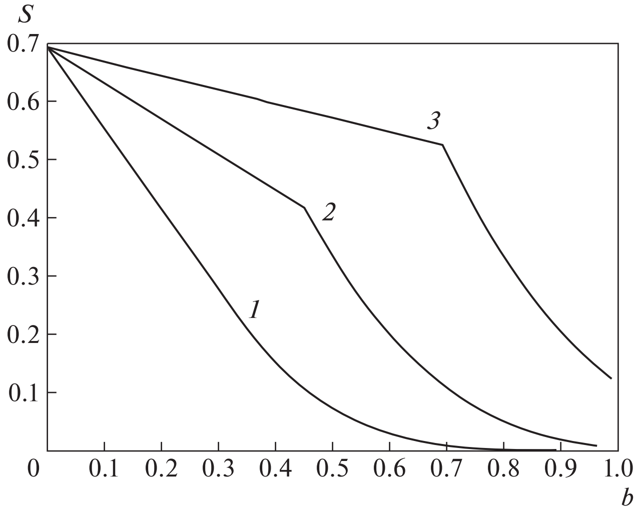

Fig. 4. Entropy of a diluted Ising ferromagnet on the Bethe lattice ($q = 4$) in zero external field as a function of concentration of magnetic atoms (bonds): (curve *1*) $\eta = 0$; (*2*) $\eta = 0.15$, and (*3*) $\eta = 0.35$ ($\eta = \exp(-2K)$).

Therefore, the specific entropy of a diluted magnet can be calculated as

$$\frac{s(x,K)}{qk} = \left(1 - \frac{b}{2} - \beta\right)\ln(2) - I, \quad (23)$$

where

$$I = (1-b)w\tanh(w) + \frac{b(w\sinh(2w) - K\eta)}{\cosh(2w)+\eta} - \psi(n)$$
$$-\frac{\beta}{2}((1+M)\ln(1+M) + (1-M)\ln(1-M)).$$

It follows from relation (23) that at all internal points of domains I and II on the phase diagram (see Fig. 1), the entropy vanishes at $T = 0$.

For $H = 0$ ($x = 0$), parameter w equals zero if

$$b < b_K = b_c\frac{(1+\eta)}{(1-\eta)}.$$

In this case, the entropy is given by

$$\frac{s(0,K)}{k} = \left(1 - \frac{qb}{2}\right)\ln(2)$$
$$+\frac{qb}{2}\left(\ln(1+\eta) - \frac{\eta\ln(\eta)}{1+\eta}\right).$$

If, however, $b > b_K$, the entropy as a function of the concentration of magnetic atoms can be calculated using expressions (13) and (23) as follows:

$$\frac{s(0,K)}{k} = \left(1 - \frac{qb(w)}{2}\right)\ln(2) - qI(w),$$

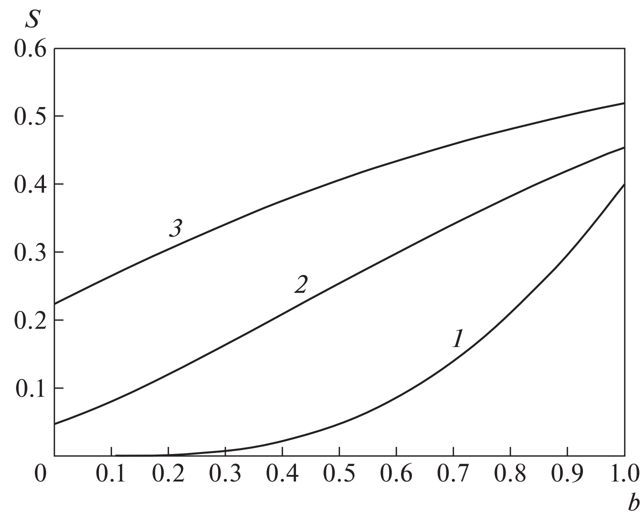

Fig. 5. Entropy of a diluted Ising antiferromagnet on the Bethe lattice ($q = 4$) in external field $H = -qJ$ as a function of the concentration of magnetic atoms (or bonds): (curve *1*) $\eta = \infty$, (*2*) $\eta = 10/3$, and (*3*) $\eta = 2$ ($\eta = \exp(-2K)$).

$$b(w) = \frac{\sinh(b_c w)}{\sinh(w)} \frac{\cosh(2w) + \eta}{(1-\eta)\cosh((1+b_c)w)},$$

$$M(w) = \tanh((1+b_c)w).$$

Figure 4 shows the curves describing the specific entropy (in the units of k) as a function of the concentration of magnetic atoms (bonds) at different temperatures. Curve *1* is the entropy of the ground state ($T = 0$). Curves *2* and *3* are the entropies for the values of temperature parameter $\eta = \exp(-2J/kT)$ equal to 0.15 and 0.35, respectively. For $b = 0$, when the system is a paramagnet in zero external magnetic field, the entropy at any temperature is equal to ln(2), while for $b > 0$, it decreases monotonically with increasing b. At $T > 0$, the entropy as a function of concentration b exhibits a discontinuity of the first derivative for $b = b_K$ (curves *2* and *3* in Fig. 4). At $T = 0$, these is no such a discontinuity (curve *1* in Fig. 4).

In accordance with criterion (20), on line *1* of the diagram of state (see Fig. 1), the system is not frustrated. However, the authors of [11] believe that the state in which the entropy differs from zero at $T = 0$ can be treated as frustrated. If we follow this criterion, the system on line *1* (see Fig. 1) is frustrated for $b < 1$.

Let us consider the entropy on lines *2* and *3* of the diagram in Fig. 1. On line *2*, condition $K + x = 0$ holds. Taking this condition into account, we find the limit (23) for $T \to 0$, which after some transformations can be written in form

$$\tilde{S}_0 = \frac{bq}{2}\ln\frac{b}{y} + \left(1 - \frac{2-b}{2}q\right)\ln\frac{2-y}{2-b}, \quad (24)$$

where y can be determined from Eq. (16). Figure 5 shows graphically function $\tilde{S}_0(b)$ (curve *1*).

For $b = 1$ and $q = 2$, we have

$$\tilde{S}_0 = \ln\frac{\sqrt{5}+1}{2}.$$

which coincides with the result of calculation in [9], in which the transfer matrix method has been used for a 1D spin chain. The same figure show the concentration dependences of the entropy for nonzero values of temperature (curves *2* and *3* in Fig. 5).

5. CONCLUSIONS

Thus, the account for nonmagnetic dilution into the pseudo-chaotic approximation [4] makes it possible to calculate not only the concentration dependence of the magnetization (see Figs. 2 and 3), but also the entropy (see Figs. 4 and 5) and the free energy of a diluted magnet on an arbitrary Bethe lattice. Analysis of the concentration dependence of the entropy shows that for $J > 0$ and $H = 0$ (line *1* in the diagram in Fig. 1) and at zero temperature, the entropy differs from zero, decreases with increasing b, and has no discontinuity of the first derivative with respect to b (curve *1* in Fig. 4) in the entire concentration range. However, at a nonzero temperature, there exists a discontinuity of the first derivative for $b = b_K$ (i.e., for the value of b corresponding to the emergence of spontaneous magnetization).

Our calculations show (see Fig. 4) that even at $T = 0$ (curve *1*), the entropy on line *1* does not vanish, which, according to some authors [9, 11], can be treated as the criterion of frustration of the system. It should be noted, however, that the nonzero value of the ground-state entropy in zero external field in this case is of the "paramagnetic" origin: upon the nonmagnetic dilution, isolated spin "islands" appear in the system, which can change their spontaneous magnetization in the absence of a change in energy. According to frustration criterion (20) [10], which is equal to zero on line *1* for any b, the state of the system in this region cannot be treated as frustrated.

If $J < 0$ (antiferromagnetic exchange interaction), but the external field is $H = -qJ$ (line *2* on the diagram in Fig. 1), the system is frustrated in the sense of a nonzero value of the residual entropy (curve *1* in Fig. 5) as well as in the sense of criterion (20). In this domain, there are neither concentration phase transitions nor temperature phase transitions.

CONFLICT OF INTERESTS

The authors declare that there is no conflict of interests.

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