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FREE ENERGY, ENTROPY, AND MAGNETIZATION OF A ONE-DIMENSIONAL ISING MODEL OF A DILUTED MAGNET

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We consider a one-dimensional Ising model (chain) with the the nearest-neighbor interaction and with a random nonmagnetic dilution. We find the exact free energy of such a chain as a function of the impurity concentration, temperature, and the external magnetic field. In the case of antiferromagnetic interaction in the chain, we find the specific magnetization, the mean value of the product of neighboring spins, and the entropy as functions of these parameters. We study the residual system entropy.

Keywords: Ising model, diluted antiferromagnetic, magnetic frustration

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1. Introduction

It is known[1], [2] that the critical behavior of diluted or amorphous magnets can differ significantly from the behavior of magnets with a translational lattice symmetry. However, even for simple models of magnets with dilution, for example, for the Ising model with nonmagnetic impurities, it is impossible to construct the exact solution for flat or three-dimensional lattices. Therefore, one-dimensional models of magnets were often considered [3]–[6].

In this paper, we obtain an exact solution of the one-dimensional Ising model with fixed, randomly located (frozen) nonmagnetic impurities. This exact solution is based on representing the partition function of the diluted chain as a product of the partition functions of isolated segments of the chain with different lengths. To calculate the partition functions of these segments, we use the method of a nonsymmetric transfer matrix [3], in contrast to the method used in [6].

In the one-dimensional Ising model, there is no phase transition at a finite temperature [3]; for any dilution, the one-dimensional Ising chain with the nearest-neighbor interaction decomposes into decoupled finite-length segments of magnetic atoms. In other words, there are no magnetic or concentration transitions in the diluted one-dimensional Ising model. But at low concentrations of magnetic atoms or bonds (that are below the percolation threshold [1]), the diluted Ising model on any lattice is also a collection of finite fragments of this lattice, and finding thermodynamic averages reduces, one way or another, to averaging over the ensemble of such finite fragments.

The aim of this paper is to calculate the free energy of the diluted Ising chain at any values of the external magnetic field, concentration of magnetic bonds, and temperature, and for any value of the exchange interaction constant. In addition, we study the magnetic, thermodynamic, and frustrating properties of this model.

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2. Partition function of the one-dimensional Ising model with the nonmagnetic dilution

We consider a one-dimensional Ising magnet (chain) with the nearest-neighbor interaction. We assume that some bonds are accidentally disrupted, for example, by fixed nonmagnetic impurities, such that there is a probability b that atoms at neighboring sites are magnetically coupled and the probability $1-b$ that they are not. In the case of such a dilution, the chain is divided into segments of magnetic atoms with different lengths, which are separated by nonmagnetic bonds. The partition function of such a chain of length N is given by

$$Z_N = Z_1^{N_1} \times Z_2^{N_2} \times \cdots \times Z_m^{N_m}, \tag{1}$$

where N_n is the number of segments with the lengths n, Z_n is the partition function of such a segment, and $N = \sum nN_n$. The free energy at the temperature T per magnetic atom is $f = -kT(\ln Z_N)/N$, where k is the Boltzmann constant. From (1), we obtain

$$-\frac{f}{kT} = \sum_n \frac{nN_n}{N}\frac{\ln Z_n}{n}.$$

As $N \to \infty$, the ratio nN_n/N tends to p_n, the probability that an arbitrarily taken magnetic atom belongs to a segment of n spins. Hence, as $N \to \infty$,

$$-\frac{f}{kT} = \sum_n p_n \frac{\ln Z_n}{n}. \tag{2}$$

It is obvious that $p_n = nb^{(n-1)}(1-b)^2$, and we calculate the partition function for the segment of n Ising spins $\sigma_1, \sigma_2, \ldots, \sigma_n$ as

$$Z_n = \sum_{\sigma_1,\ldots,\sigma_n} \exp\left(K\sum_i^{n-1}\sigma_i\sigma_{i+1} + h\sum_i^n \sigma_i\right) = \Phi_n(+1) + \Phi_n(-1), \tag{3}$$

where

$$\Phi_n(\sigma_n) = \sum_{\sigma_1,\ldots,\sigma_{n-1}} \exp\left(K\sum_i^{n-1}\sigma_i\sigma_{i+1} + h\sum_i^n \sigma_i\right).$$

Here, $K = J/kT$ (J is the exchange integral (exchange energy)), T is the temperature, and $h = H/kT$ (H is the external field). These dimensionless parameters have a clear meaning: K is the ratio of the exchange interaction energy to the thermal one, and h is the ratio of the spin–external-field interaction energy to thermal energy.

It is possible to write recursive relations for $\Phi_n(\sigma)$; it is convenient to represent them in matrix form

$$\begin{pmatrix}\Phi_n(+1)\\ \Phi_n(-1)\end{pmatrix} = \mathbf{V}\begin{pmatrix}\Phi_{n-1}(+1)\\ \Phi_{n-1}(+1)\end{pmatrix}, \tag{4}$$

where

$$\begin{pmatrix}\Phi_1(+1)\\ \Phi_1(-1)\end{pmatrix} = \begin{pmatrix}e^h\\ e^{-h}\end{pmatrix}, \qquad \mathbf{V} = \begin{pmatrix}e^{(K+h)} & e^{-K+h)}\\ e^{(-K-h)} & e^{(K-h)}\end{pmatrix},$$

i.e., $\mathbf{V}$ is a nonsymmetric transfer matrix [3]. Thus,

$$\begin{pmatrix}\Phi_n(+1)\\ \Phi_n(-1)\end{pmatrix} = \mathbf{V}^{n-1}\begin{pmatrix}e^h\\ e^{-h}\end{pmatrix}. \tag{5}$$

3. Thermodynamic functions of the diluted Ising chain

If the magnet free energy is known as a function of the temperature T, the external field H, and the exchange energy J, then it is possible to express the magnetization $m = \langle\sigma_i\rangle$, the internal energy u, the entropy s, and the average value of the product of neighboring spins $v = \langle\sigma_i\sigma_{i+1}\rangle$ (per one magnetic atom) as [7]

$$m = -\frac{\partial f}{\partial H}, \qquad u = -T^2\frac{\partial}{T}\left(\frac{f}{T}\right), \qquad s = -\frac{\partial f}{\partial T}, \qquad v = -\frac{\partial f}{\partial J}. \tag{6}$$

Passing to the variables K and h and setting $\alpha = -f/kT = \lim_{N\to\infty}\frac{\ln Z_N}{N}$, we obtain

$$m = \frac{\partial\alpha}{\partial h}, \qquad v = \frac{\partial\alpha}{\partial K}, \qquad \frac{s}{k} = \alpha - (hm + Kv), \qquad u = -kT(hm + Kv). \tag{7}$$

The eigenvalues λ_1 and λ_2 of the matrix $\mathbf{V}$ are found from the corresponding characteristic equation

$$\lambda_{1,2} = e^K\cosh h \pm R, \qquad R = \sqrt{e^{2K}\cosh h + e^{-2K}}, \tag{8}$$

which shows that they are the same as those of the symmetrized transfer matrix of the Ising chain [3]. Calculating the eigenvectors of $\mathbf{V}$ corresponding to the eigenvalues λ_1 and λ_2n and constructing the diagonalizing matrix $\mathbf{R}$ from them, we represent $\mathbf{V}$ in the form

$$\mathbf{V} = \mathbf{R}\begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix}\mathbf{R}^{-1}.$$

We also represent the matrices $\mathbf{R}$ and $\mathbf{R}^{-1}$ in trigonometric form

$$\mathbf{R} = \begin{pmatrix}\cos\varphi_1 & -\sin\varphi_2\\ \sin\varphi_1 & \cos\varphi_2\end{pmatrix}, \qquad \mathbf{R}^{-1} = \frac{1}{\Delta}\begin{pmatrix}\cos\varphi_1 & \sin\varphi_2\\ -\sin\varphi_1 & \cos\varphi_2\end{pmatrix},$$

where φ_1 and φ_2 belong to the interval from 0 to $\pi/2$ and are defined by the conditions

$$\tan\varphi_1 = \lambda_1 e^{K-h} - e^{2K}, \qquad \cot\varphi_2 = e^{2K} - \lambda_2 e^{K-h}, \qquad \Delta = \cos(\varphi_1 - \varphi_2). \tag{9}$$

Hence we find the partition function Z_n for a segment of n spins in the form

$$\begin{aligned} Z_n &= \lambda_1^{n-1}(A_1 + A_2\delta^{n-1}), \qquad \delta = \frac{\lambda_2}{\lambda_1},\\ A_1 &= \frac{1}{\Delta}(e^h\cos\varphi_2 + e^{-h}\sin\varphi_2)(\cos\varphi_1 + \sin\varphi_1),\\ A_2 &= \frac{1}{\Delta}(e^h\sin\varphi_1 - e^{-h}\cos\varphi_1)(-\cos\varphi_2 + \sin\varphi_2). \end{aligned}$$

Expressions for the coefficients $A_{1,2}$ can be simplified using (8) and (9):

$$A_{1,2} = \cosh h \pm \frac{1 + e^{2K}(\sinh h)^2}{Re^K}. \tag{10}$$

The free energy of the entire system (per one atom) is

$$f = -kT\left(b\ln\lambda_1 + (1-b)^2\sum_{n=0}^{\infty} b^n\ln(A_1 + A_2\delta^n)\right). \tag{11}$$

At $h = 0$, the calculations are significantly simplified. The transfer matrix $\mathbf{V}$ becomes symmetric, and its eigenvectors, orthogonal. The eigenvalues are $\lambda_1 = 2\cosh K$ and $\lambda_2 = 2\sinh K$. Free energy (11) becomes

$$f_0 = -kT(b\ln\cosh K + \ln 2). \tag{12}$$

This result (12) can be obtained directly using the high-temperature representation of the partition function of a diluted Bethe lattice (in particular, of a linear chain) in the framework of the Kramers–Wannier duality [3]. We use the representation of the partition function of the Ising magnet in the form

$$Z_N = (\cosh K)^{N_b} \sum\left(\prod(1 + \sigma_i\sigma_j \tanh K)\right),$$

where the summation is performed over all N lattice spins, and the product, over N_b bonds. Because there are no closed paths in any Bethe lattice, we obtain

$$\frac{\ln Z_N}{N} = \frac{N_b}{N}\ln(\cosh K) + \ln 2,$$

which is equivalent to (12) at $N_b/N = b$.

Thus, the thermodynamic functions of the diluted Ising chain are given by formulas (7) with

$$\alpha = b\ln\lambda_1 + (1-b)^2\sum_{n=0}^{\infty} b^n \ln\left((1+\delta^n)\cosh K + (1+\delta^n)\frac{1 + e^{2K}(\sinh h)^2}{Re^K}\right), \tag{13}$$

where $\delta = \lambda_2/\lambda_1$, the values of $\lambda_{1,2}$ and R are found from (8), and in differentiating with respect to h and K, we must use the formulas

$$\frac{\partial\delta}{\partial h} = -2\frac{e^K\sinh K}{R}\delta, \qquad \frac{\partial\delta}{\partial K} = 2\frac{e^K\sinh K}{R}\frac{e^{-2K}}{e^{2K} - e^{-2K}}\delta.$$

4. Results and conclusions

Formulas (7) and (13) allow calculate the thermodynamic functions for any diluted Ising chain in the cases $J > 0$ and $J < 0$, i.e., for the ferromagnetic and antiferromagnetic interaction types. In what follows, we restrict ourself to considering only the antiferromagnetic case $J < 0$, because the system then has the most interesting properties [8], [9]. In Fig. 1, we plot the specific magnetization $m = \langle\sigma_i\rangle$ (curve I) as a function of the external field (in the units of $|J|$) for $J < 0$. The plot is constructed for the low temperature $|K| = 25$, because the "stepwise" character of the dependence $m(H)$ can be clearly seen for such temperatures; the steps are smoothed as the temperature increases. As $T \to 0$, the behavior of the magnetization $m(H)$ can be found directly from expressions obtained from (7) and (13) by passing to the corresponding limit. However, it is easy to understand what the values and positions of the steps in Fig. 1 are by considering the magnetization in the ground state. The first step on curve I corresponds to the field $H \in (0; |J|)$. We recall that the diluted chain is regarded as an ensemble of linear fragments of magnetic atoms of the lengths n contained in that ensemble with the probability p_n; accordingly, for the diluted chain, all specific quantities are calculated as averages over such an ensemble with the weights $p_n = nb^{n-1}(1-b)^2$. Therefore, for the field $H \in (0; |J|)$, the contribution to the magnetization of the ground state of fragments with even lengths n is zero, and the fragments with odd lengths have the average ground-state magnetization $1/n$ (per fragment atom). Therefore, on the first step of curve I, the magnetization m_1 is

$$m_1 = \sum_{k=0}^{\infty}\frac{p_{2k+1}}{2k+1} = (1-b)^2\sum_{k=0}^{\infty} b^{2k} = \frac{1-b}{1+b}. \tag{14}$$

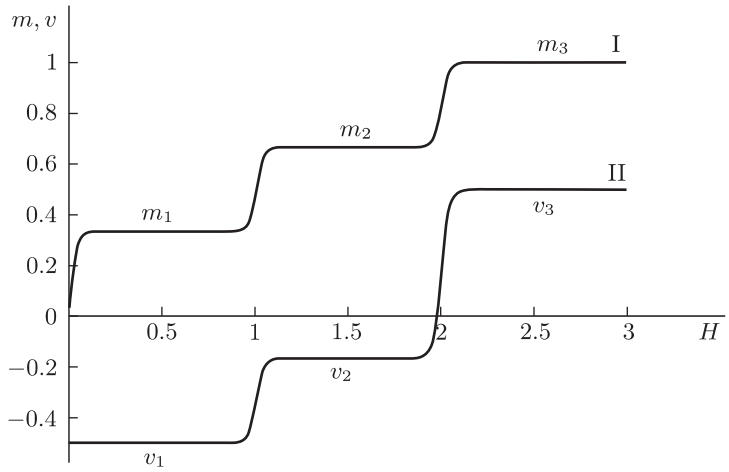

Fig. 1. Dependence of dimensionless specific values of $m = \langle\sigma_i\rangle$ (curve I) and $v = \langle\sigma_i\sigma_{i+1}\rangle$ (curve II) on the external magnetic field H (in units of $|J|$) at $b = 0.5$.

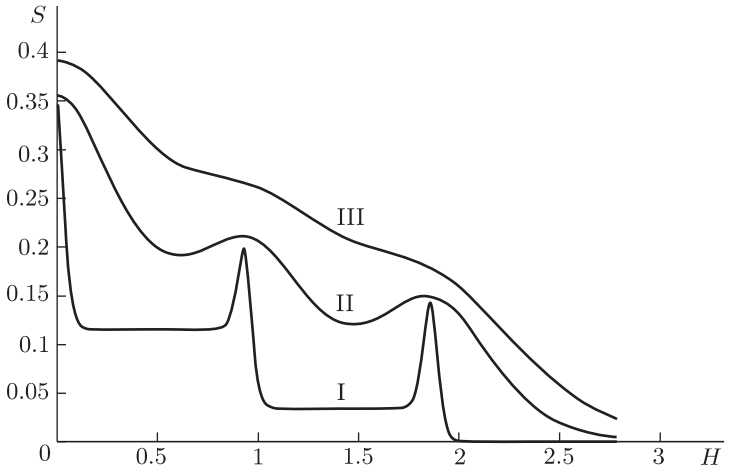

Fig. 2. Dependence of the specific entropy (in units of the Boltzmann constant k) on the external magnetic field H (in units of $|J|$) for different temperatures at $b = 0.5$ for $kT = |J|/25$ (curve I), $kT = |J|/3$ (curve II), and $kT = |J|/2$ (curve III).

The second step of curve I corresponds to external field values in the interval $H \in (|J|; 2|J|)$. The magnetization m_2 on this step can be calculated if we recall that in this range of fields, the contribution to the ground-state magnetization is made by fragments with both odd and even lengths:

$$m_2 = \frac{1-b}{1+b}(1+2b). \tag{15}$$

The third step of curve I corresponds to $H > 2|J|$. In this range, all spins are oriented in the field direction; consequently, the magnetization in the ground state is $m_3 = 1$. Arguing similarly, we can appropriately interpret the steps on curve II, which shows the dependence of $v = \langle\sigma_i\sigma_{i+1}\rangle$ on the external field at low temperatures. On the first step of this curve, the value of v_1 corresponds to $H \in [0; |J|)$ and is $v_1 = -b$. We have $v_2 = b(1-3b)/(1+b)$ for $H \in (|J|; 2|J|)$ and $v_3 = b$ for $H > 2|J|$.

The dependence of the system entropy on the external field is shown in Fig. 2. At low temperatures ($K = 25$) and concentrations differing from 0 or 1, the entropy does not tend to zero as $T \to 0$ if $H \in [0; 2|J|)$

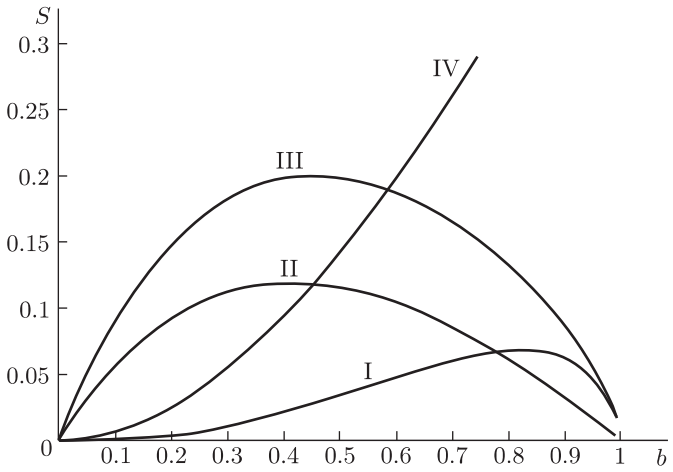

Fig. 3. Dependence of the specific entropy (in units of the Boltzmann constant k) on the concentration of magnetic bonds b in the case of different values of the external field H for $H = 1.5|J|$ (curve I), $H = 0.5|J|$ (curve II), $H = |J|$ (curve III), and $H = 2|J|$ (curve IV).

(curve I in Fig. 2), which means a degeneracy of the ground state of the diluted antiferromagnetic chain in the case of such fields. The degeneracy of low-energy states due to competing interactions in the system is a criterion of frustration [10], [11]. As can be seen from Fig. 2 (curve I), for the system under consideration, local maxima of the residual entropy exist for $H = |J|$ and $H = 2|J|$. However, we note that the ground-state degeneracy in the system of Ising spins is not necessarily related to the presence of competing interactions and can have a simpler "paramagnetic" nature. At $H = 0$, the diluted Ising chain consists of fragments that are not coupled to each other; each of them can be oriented in two ways with the same minimum energy without changing the internal state, which gives the residual specific entropy $s_0 = k(1 - b)\ln 2$. For $H > 0$, this paramagnetic degeneracy disappears completely in the ferromagnetic ($J > 0$) case. In the antiferromagnetic case ($J < 0$), for $H \in (0; |J|)$, the paramagnetic degeneracy is preserved only for fragments with an even number of atoms, which gives the residual specific entropy $s_1 = kb(1 - b)/(1 + b)\ln 2$. In stronger fields ($H \geqslant |J|$), the residual entropy is also related to the degeneracy of the ground states of fragments. The dependence of the entropy on the external field becomes more "smoothed" with increasing temperature and monotonous as the temperature continues to increase (curves II and III in Fig. 2).

The dependence of the residual specific entropy on the concentration of magnetic bonds b is shown in Fig. 3. For all $H \in (0; 2|J|)$, the residual entropy depends nonmonotonically on the concentration (curves I, II, and III in Fig. 3), which can also be observed for diluted frustrated magnets [2]; and for $H = 2|J|$, the residual entropy increases monotonically to $k \ln \frac{1+\sqrt{5}}{2}$ (the logarithm of the golden section) [5], [12] at $b = 1$ (curve IV in Fig. 3).

Although the one-dimensional chain is in a sense a "pathological" case of the Ising model (there is no phase transition at a finite temperature), the above analysis allows advancing some general hypotheses regarding the phase diagram and the residual entropy of the diluted Ising antiferromagnet on an arbitrary lattice with a coordination number q. In any case, irrespective of the degree of nonmagnetic dilution b, the magnetic field $H = q|J|$ must lead to a nonzero residual entropy [12]. But it can be hypothesized that the residual entropy of the diluted Ising antiferromagnet for $b < 1$ is nonzero in the entire range $H \leqslant q|J|$ and attains local maxima at $H = n|J|$, where $n = 1, \ldots, q$.

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