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Random Bond Ising Model in Self-Avoiding Walk Approximation

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Free energy of random bond Ising model is analysed by high-temperature expansion in self-avoiding walk approximation. Conditions of instability of the paramagnetic state are determined through the convergence criterion of the random high-temperature series. Critical concentrations for the loss of the long-range magnetic order are determined for different 2d and 3d lattices.

Методами высокотемпературных разложений в приближении путей без пересечений исследуется свободная энергия модели Изинга со случайными обменными связями. Из определения порогов сходимости случайных высокотемпературных рядов найдены условия неустойчивости парамагнитного состояния. Для различных двумерных и трехмерных решеток определены критические концентрации, при которых происходит разрушение дальнего магнитного порядка.

1. Introduction

In recent years there has been considerable interest in the properties of disordered magnetic systems [1], and in particular the random bond Ising model was actively studied [2 to 10]. We have the situation in mind of the Ising lattice with antiferromagnetic bonds distributed with concentration c, and ferromagnetic bonds — with concentration $1 - c$. In this model the important concept of frustration has been formulated for the first time [2, 5, 7, 9]. One of the basic (and not yet completely solved) problems in this model is the structure of its phase diagram [3 to 6, 8 to 10] and, especially, the value of the critical concentration c_1^* of the antiferromagnetic bonds, at which ferromagnetism in the system disappears. These problems have been analysed by different methods, from numerical simulation [3 to 5] and renormalization group [4, 8] to relatively simple variants of molecular-field approximation for disordered systems [6, 10].

In this paper these problems are studied by a simple method based upon the convergence criterion of the high-temperature expansion for the Ising model in the self-avoiding walk approximation, used previously for regular systems by Domb [11]. Our approach is based in part on the previous work by one of the authors [12], where the convergence of a similar random series had been considered related to the problem of electron localization in disordered systems. The main attractive feature of our method is its simplicity, as well as the similarity of the obtained results, to those of more refined approaches. This leads us to believe in a rather high accuracy of these results. At the same time we are able to analyse some of more general cases than those considered before by different authors.

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2. High-Temperature Expansion for the Free Energy in the Self-Avoiding Walk Approximation

Consider an Ising lattice described by the Hamiltonian

$$H = -\sum_{\langle ij \rangle} J_{ij}\sigma_i\sigma_j \,, \tag{1}$$

where the exchange interaction J_{ij} of the nearest neighbours takes random values, $\sigma_i = \pm 1$ is an Ising spin. The distribution function of exchange interactions is factorized over the bonds on the lattice,

$$\mathcal{P}\{J_{ij}\} = \prod_{\langle ij \rangle} P(J_{ij}) \,, \tag{2}$$

where

$$P(J_{ij}) = c\,\delta(J_{ij} - J_B) + (1 - c)\,\delta(J_{ij} - J_A) \,. \tag{3}$$

Here $J_A > 0$ is the "ferromagnetic" exchange integral, $J_B < 0$ is the "antiferromagnetic" exchange integral, $0 \leq c \leq 1$ is the concentration of antiferromagnetic bonds.

The partition function of the system can be represented as usual in the following form [13]:

$$\begin{aligned} Z\{\beta\} &= \sum_{\{\sigma\}} [\exp \sum_{\langle ij \rangle} K_{ij}\sigma_i\sigma_j] = \\ &= \sum_{\{\sigma\}} [\prod_{\langle ij \rangle} (\cosh K_{ij})\,(1 + w_{ij}\sigma_i\sigma_j)] \,, \end{aligned} \tag{4}$$

where $w_{ij} = \tanh K_{ij}$, $K_{ij} = \beta J_{ij}$, $\beta = 1/T$, T is the temperature. High-temperature expansion is the expansion in powers of w_{ij}. The coefficient of the N-th power of w_{ij} consists of all possible products of N pairs of $\sigma_i\sigma_j$. Because of $\sum_{\{\sigma\}} \sigma_i = 0$; $\sum_{\{\sigma\}} \sigma_i^2 = \sum_{\{\sigma\}} 1 = 1$, this coefficient can be represented by a closed polygon on the lattice [13] (Fig. 1). Every bond on the graph represents a factor $\tanh K_{ij}$ and each bond appears only once. At each vertex of the graph only an even number of bonds can meet.

The expansion of $Z\{\beta\}$ consists of all possible polygons (including unconnected ones) constructed on the lattice by these rules. In the lowest orders in N most of these graphs are just self-avoiding walks (SAW) on the lattice. (Cf. Fig. 1 a to c for $N = 8$.)

The logarithm of the partition sum (4),

$$\ln Z\{\beta\} = \sum_{\langle ij \rangle} \ln \cosh K_{ij} + \ln \sum_{\{\sigma\}} \prod_{\langle ij \rangle} (1 + w_{ij}\sigma_i\sigma_j) \,, \tag{5}$$

can also be expressed as an expansion in powers of w_{ij} [11]. This expansion consists only of connected graphs, which can be represented by the closed paths on the lattice, starting and ending in the given lattice site. However, in this case the graphs are not

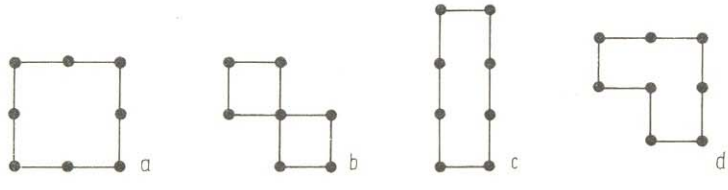

Fig. 1. Examples of graphs in the expansion of $Z\{\beta\}$ for $N = 8$

so simple as in the case of the partition function. In particular, every bond can appear several times, though again only an even number of bonds can meet at each vertex. This graphs can be classified over the so-called cyclomatic number $C = l - p + 1$ [11], where l is the number of the lines in the graph (multiple bonds are calculated as one), p is the number of vertices. The class corresponding to $C = 1$ consists of graphs topologically equivalent to the closed SAW's (which can be traced several times, however). Examples of such graphs are given in Fig. 2 a to c. In Fig. 2d we show the graph with $C = 2$ (the so-called 0-topology [11]). Our approximation neglects all the graphs with $C > 1$, thus we take into account only the graphs topologically equivalent to the closed SAW's.

Then we get

$$\ln \tilde{Z}\{\beta\} = \ln Z\{\beta\} - \sum_{\langle ij \rangle} \ln \cosh K_{ij} =$$

$$= \sum_N \sum_i \sum_{\Gamma_N^i} \frac{1}{N} w_{ij} w_{jk} \ldots w_{li} -$$

$$- \frac{1}{2} \sum_N \sum_i \sum_{\Gamma_{N/2}^i} \frac{2}{N} w_{ij}^2 w_{jk}^2 \ldots w_{li}^2 + \frac{1}{3} \sum_N \sum_i \sum_{\Gamma_{N/3}^i} \frac{3}{N} w_{ij}^3 w_{jk}^3 \ldots w_{li}^3 + \ldots \tag{6}$$

Here the products of w_{ij}, w_{ij}^2, ... etc, are taken along all possible SAW's Γ_N^i of N steps, $\Gamma_{N/2}^i$ of $N/2$ steps (but with two bonds on each step) etc., starting and ending in the i-th site. The structure of the expansion (6) is clear from (5) and the expansion of $\ln(1 + x) = x - 1/2x^2 + 1/3x^3 - 1/4x^4 + \ldots$ The extra combinatorial factors $1/N$ for the contribution of Γ_N^i, $2/N$ for the contribution of $\Gamma_{N/2}^i$, etc. are due to the fact that the initial vertex i of Γ_N^i can be chosen arbitrarily among N vertices of Γ_N^i, among $N/2$ vertices for $\Gamma_{N/2}^i$, etc.

The instability of the paramagnetic phase is determined by the convergence criterion of the high-temperature expansion (6) [11, 13]. In the regular case $w_{ij} = w_{jk} = \ldots = w = \tanh \beta J$ and the problem reduces to the convergence criterion of the series [11],

$$\ln \tilde{Z}\{\beta\} \approx \sum_N a_N w^N , \tag{7}$$

where

$$a_N = p(N) - \tfrac{1}{2} p(N/2) + \tfrac{1}{3} p(N/3) + \ldots , \tag{8}$$

$$p(N) = \frac{1}{N} U_N ,$$

and U_N is the number of the closed SAW's of N steps on the lattice, associated with the given site. It is known [11, 14] that for $N \gg 1$ $U_N \approx N^{-h} \mu^N$ $(h > 0)$, where μ is

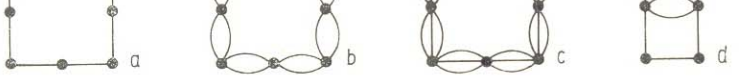

Fig. 2. Examples of graphs in the expansion of $\ln Z\{\beta\}$

the so-called connectivity constant of the lattice. Then it is obvious that for $N \gg 1$ only the first term in (8) is relevant (because of $\mu > \mu^{1/2} > \mu^{1/3} \ldots$) and the series in (7) diverges if $\mu w = \mu \tanh \beta J \geqq 1$. The equality determines the critical temperature [11]. The error of the SAW-approximation in regular case is $\approx 3\%$ for the 3d lattices, and $\approx 10\%$ for the 2d lattices [11].

3. Convergence Criterion of the Random High-Temperature Series

In a disordered system the high-temperature expansion (6) is a random series and its convergence must be treated statistically. It is generally accepted [1] that this expansion must be averaged over (2) and (3) and considered as representing the observable free-energy of the system. However, first of all we shall consider the convergence of the series (6) in the sense of convergence in probability, as it is done in localization theory [15, 16]. Our analysis will be similar to that used in [12].

First of all let us consider qualitatively the case of $J_A = -J_B$ and $c = 1/2$ in (3). Now only the terms with odd powers of w_{ij} on the bonds in (6) are random (in sign !). Consider the first series in (6). In the N-th order in w_{ij} it consists of terms $\sim \mu^N$, corresponding to the number of SAW's Γ_N^i, and the sign of each of them is absolutely random for $c = 1/2$ (positive and negative bonds are equally probable). Then from the obvious analogy with the one-dimensional Brownian motion it is clear, that the modulus of this term for $N \gg 1$ is of the order of $\mu^{N/2} w^N$, where $w = \tanh \beta J_A = \tanh \beta |J_B|$. The limit of convergence of the series is then determined by $\mu^{1/2} w = 1$, and this coincides by the way with the limit of convergence of the second (non-random) series in (6): there are terms $\sim \mu^{N/2}$, each contributing a factor of w^N. Only the first two terms in (6) are relevant due to $\mu > \mu^{1/2} > \mu^{1/3}$, etc. Note, that the *average* of the first term in (6) is exactly equal to zero for $c = 1/2$, $J_A = |J_B|$, and the convergence of the averaged high-temperature series is determined by the second term in (6). We shall demonstrate that this is the general property of the high-temperature series for the random bond Ising model. The possibility of a singularity in the high-temperature expansion for this model at $\mu^{1/2} w = 1$ for $c = 1/2$, $J_A = -J_B$ was first noted by Domb [17] (see, however, [19]).

Consider now the general case of distribution (2) and (3). Let us analyse the modulus of the N-th order term in the first series in (6). Obviously we have

$$|\ln \tilde{Z}^{(N)}\{\beta\}| = |\sum_{\Gamma_N} w_A^{N - n_{\Gamma_N}} (-w_B)^{n_{\Gamma_N}}| = w_A^N |\sum_{\Gamma_N} (-a)^{n_{\Gamma_N}}| \equiv w_A^N |X_N| , \tag{9}$$

where n_{Γ_N} is the number of negative bonds on the path Γ_N, $a = w_B/w_A$, $w_A = \tanh \beta J_A$, $w_B = \tanh \beta |J_B|$. The probability of n_{Γ_N} is given by the binomial distribution

$$P_N(n_{\Gamma_N}) = \frac{N!}{n_{\Gamma_N}!(N - n_{\Gamma_N})!} c^{n_{\Gamma_N}} (1 - c)^{N - n_{\Gamma_N}} . \tag{10}$$

Then it is easy to find

$$\begin{aligned} \langle (-a)^{n_{\Gamma_N}} \rangle &= (1 - c - ca)^N , \\ \langle (-a)^{2n_{\Gamma_N}} \rangle &= (1 - c + ca^2)^N \end{aligned} \tag{11}$$

and the dispersion of an isolated term in (9) is equal to

$$\langle (-a)^{2n_{\Gamma_N}} \rangle - \langle (-a)^{n_{\Gamma_N}} \rangle^2 = (1 - c + ca^2)^N - (1 - c - ca)^{2N} . \tag{12}$$

Let us estimate the most probable value of $|X_N|$ by $\langle X_N^2\rangle^{1/2}$. The dispersion of the sum of independent random variables equals the sum of dispersions of isolated terms in the sum. Thus, supposing independence (for $N \gg 1$) of terms $\sim \mu^N$ in X^N we get

$$\langle X_N^2\rangle - \langle X_N\rangle^2 \approx \mu^N[(1-c+ca^2)^N - (1-c-ca)^{2N}] . \tag{13}$$

Use now

$$\langle X_N\rangle \approx \mu^N\langle(-a)^{n\Gamma_N}\rangle = \mu^N(1-c-ca)^N \tag{14}$$

to get

$$\langle X_N^2\rangle \approx \mu^N[(1-c+ca^2)^N - (1-c-ca)^{2N}] + \mu^{2N}(1-c-ca)^{2N} . \tag{15}$$

Independence of contributions from the different paths Γ_N is crucial for our analysis. Obviously some of $\sim \mu^N$ paths have some parts in common. We suppose, that this leads to correlations negligible in the limit of $N \to \infty$.

The convergence condition for the first series in (6) is given now by

$$w_A \lim_{N\to\infty} \langle X_N^2\rangle^{1/2N} < 1 \tag{16}$$

and the critical temperature is determined by the equation

$$w_A \lim_{N\to\infty} \left\{\mu^{2N}\left(1-c-c\frac{w_B}{w_A}\right)^{2N} + \mu^N\left[\left(1-c+c\frac{w_B^2}{w_A^2}\right)^N - \right.\right.$$

$$\left.\left. -\left(1-c-c\frac{w_B}{w_A}\right)^{2N}\right]\right\}^{1/2N} = 1 . \tag{17}$$

In particular, for $a = w_B/w_A = 1$, i.e. $|J_B| = J_A = J$, we have

$$w \lim_{N\to\infty} \{\mu^{2N}(1-2c)^{2N} + \mu^N[1-(1-2c)^{2N}]\}^{1/2N} = 1 . \tag{18}$$

From (18) we get

$$\mu^{1/2} w = 1 \tag{19}$$

or $c_1^* < c < c_2^*$ and

$$\mu w\,|1-2c| = 1 \tag{20}$$

for $c < c_1^*$, $c > c_2^*$, where the critical concentrations $c_{1,2}^*$ are determined by the equation $\mu(1-2c)^2 = 1$ and are

$$c_{1,2}^* = \frac{1}{2} \mp \frac{1}{2\sqrt{\mu}} . \tag{21}$$

Table 1

lattice	square	honeycomb	s.c.	b.c.c.
$\tilde{\mu}$	2.6390	1.8484	4.6826	6.5288
μ	2.4142	1.7321	4.5840	6.4032
c_1^*	0.1782	0.1201	0.2665	0.3024
c_2^*	0.8218	0.8799	0.7335	0.6976

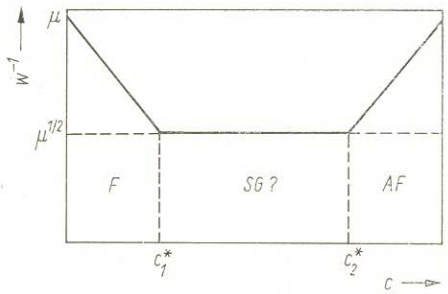

Fig. 3. Phase diagram for the case of $J_A = |J_B|$, F ferromagnetic region, AF antiferromagnetic region, SG spin-glass region (?)

Note, that the result (19) simply means that in the concentration interval $c_1^* < c < c_2^*$ all terms $\approx \mu^N$ in X_N are random in sign (with equal probability!).

For the numerical estimates we use the constant μ which is not the connectivity constant of the lattice, as it should be done in the SAW approximation [11, 14], but instead we use an "Ising constant" μ, which determines the exact critical temperature for the regular case by the relation $\mu w = 1$ [11]. This assures the matching with the regular case for $c = 0;1$, and we hope that such an approximation takes into account qualitatively the role of graphs with cyclomatic number $C > 1$, neglected above. As was noted before (it can be seen also from Table 1, where $\tilde{\mu}$ denotes now the connectivity constant), this leads to a rather small change of the results, diminishing slightly the critical temperature. Critical concentrations $c_{1,2}^*$ determined for different lattices are given in Table 1. We assume, that these concentrations correspond to the loss of the long-range ferromagnetic and antiferromagnetic order in the system. The phase diagram is shown in Fig. 3.

In the general case of $w_A \neq w_B$ we obtain from (17)

$$\mu^{1/2}\{(1-c)\, w_A^2 + c w_B^2\}^{1/2} = 1 \tag{22}$$

for $c_1^* < c < c_2^*$, and

$$\mu\,|(1-c)\, w_A - c w_B| = 1 \tag{23}$$

for $c < c_1^*$ and $c > c_2^*$, where the critical concentrations $c_{1,2}^*$ are determined by the roots of the equation

$$1 - c + c\frac{w_B^2}{w_A^2} = \mu\left(1 - c - c\frac{w_B}{w_A}\right)^2 . \tag{24}$$

In Table 2 we give critical concentrations $c_{1,2}^*$ for different lattices and ratios w_A/w_B. In Fig. 4 the phase diagram of the system for $w_A \neq w_B$ is shown.

Consider finally the case of $w_B \to 0$, $w_A \neq 0$, i.e. the percolation limit. In this case we obtain from (17)

$$\mu(1-c)\, w_A = 1 \tag{25}$$

for $c < c^*$, where

$$c^* = 1 - \mu^{-1} \equiv 1 - \tilde{c}^* . \tag{26}$$

For $c > c^*$ the critical temperature is zero, thus $\tilde{c}^* = 1/\mu$ is the critical concentration of the percolation transition, i.e. the critical concentration of the ferromagnetic bonds for the appearance of the long-range ferromagnetic order. In Table 3 we give the values of $\tilde{c}^*$ for the different lattices according to (26), as well as the exact critical

Table 2

lattice		square	honeycomb	s.c.	b.c. c.
$w_B/w_A = 1.5$	c_1^*	0.1234	0.0810	0.1920	0.2214
	c_2^*	0.7595	0.8344	0.6517	0.6098
$w_B/w_A = 2.0$	c_1^*	0.0912	0.0587	0.1465	0.1713
	c_2^*	0.7135	0.8004	0.5928	0.5476
$w_B/w_A = 2.5$	c_1^*	0.0705	0.0446	0.1163	0.1375
	c_2^*	0.6785	0.7743	0.5485	0.5008
$w_B/w_A = 3.0$	c_1^*	0.0562	0.0350	0.0950	0.1135
	c_2^*	0.6508	0.7536	0.5138	0.4646

concentrations for the bond percolation [14]. From these results one may estimate the accuracy of our approach, but one must also remember that classical percolation is relevant for $T = 0$, i.e. strictly speaking it cannot be analysed on the basis of high-temperature expansions.

Our results up to now were obtained from the convergence in probability criterion for the first series in (6) (which consists of terms of random signs). Now we show that the same results follow also from the analysis of the convergence of the series for the *average* of $\ln \tilde{Z}\{\beta\}$,

$$\langle \ln \tilde{Z}\{\beta\} \rangle = \sum_N \sum_i \sum_{\Gamma_N^i} \frac{1}{N} \langle w_{ij} w_{jk} \dots w_{li} \rangle_{\Gamma_N^i} - \\ - \frac{1}{2} \sum_N \sum_i \sum_{\Gamma_{N/2}^i} \frac{2}{N} \langle w_{ij}^2 w_{jk}^2 \dots w_{li}^2 \rangle_{\Gamma_{N/2}^i} + \dots \tag{27}$$

The averaging can be performed directly with the help of (10). Analogously to (11) we get

$$\langle w_{ij} w_{jk} \dots w_{li} \rangle_{\Gamma_N^i} = w_A^N \left(1 - c - c \frac{w_B}{w_A}\right)^{N/2}, \tag{28}$$

$$\langle w_{ij}^2 w_{jk}^2 \dots w_{li}^2 \rangle_{\Gamma_{N/2}^i} = w_A^N \left(1 - c + c \frac{w_B^2}{w_A^2}\right)^{N/2}.$$

Then the limit of convergence for the first series in (27) is

$$\mu \, |(1 - c) \, w_A - c w_B| = 1 \tag{29}$$

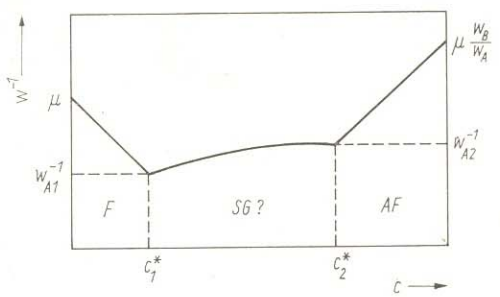

Fig. 4. Phase diagram for the case of $J_A < |J_B|$. Notatiosn are the same as in Fig. 3. $1/w_{A1,2} = (1/2)\,[\sqrt{4\mu a + (1 - a^2)} \pm (1 - a)]$; $a = w_B/w_A$

Table 3

lattice	square	honeycomb	s.c.	b.c.c.
$\tilde{c}^* = 1/\mu$	0.4142	0.5773	0.2181	0.1561
c^* [14]	0.5000	0.6527	0.2470	0.1780

and for the second series it is given by

$$\mu^{1/2}\{(1-c)\, w_A^2 + c w_B^2\}^{1/2} = 1 \,. \tag{30}$$

These coincide with (23) and (22), respectively. The convergence of the whole series for $\langle \ln \tilde{Z}\{\beta\}\rangle$ is determined by (29) for $c < c_1^*$, $c > c_2^*$, and by (30) for $c_1^* < c < c_2^*$, where $c_{1,2}^*$ are determined from the condition of equivalence of (29) and (30), which coincides with (24). It is easy to see that the neglected terms of (27) (with triple and other multiple bonds) are irrelevant, because the corresponding series converge if (29) and (30) are satisfied.

Thus the convergence criterion for the averaged high-temperature expansion leads to exactly the same results as the convergence in the probability criterion. During the averaging we were not using the assumption of statistical independence of different paths Γ_N (for $N \gg 1$), and the result obtained confirms the use of this assumption in the analysis of the convergence in probability. The equivalence of both approaches is based in fact on the following theorem [19]: a random series (with independent terms) converges with probability equal to unity, if both the averaged series converge, and the series the terms of which are equal to the dispersions of the terms of the initial series.

4. Discussion

Consider now the physical meaning of the results obtained. Our analysis of the convergence in probability allows one to give a very simple interpretation of these results in terms of distribution of frustrations. It is well known [2, 5, 7, 9] that the model under consideration possesses a local gauge invariance and the statistical mechanics of the model should be expressed in terms of gauge invariant quantities. In our approach this is assured by the closed character of the paths Γ_N^i on the lattice. Consider for simplicity the case of $J_A = |J_B|$ on the square lattice. Then the product of w_{ij}'s along the path Γ_N^i (in the first series in (6)) is equal to

$$w_{ij} w_{jk} \ldots w_{li} = w^N \operatorname{sgn} J_{ij} J_{jk} \ldots J_{li} = w^N \prod_p \Phi_p \,, \tag{31}$$

where [2, 7]

$$\Phi_p = \operatorname{sgn} J_{ij} J_{jk} J_{kl} J_{li} \tag{32}$$

is the product of J_{ij}'s around the elementary plaquette ($\Phi_p = \pm 1$). The product of Φ_p's in (31) is taken over all the plaquettes inside the contour of Γ_N^i. Thus, its sign is positive or negative depending on whether there is an even or odd number of frustrated ($\Phi_p = -1$) plaquettes inside Γ_N^i. As was noted above, for high enough concentration of negative (positive) bonds, greater than $c_1^*(c_2^*)$, the value of $\prod_p \Phi_p$ in (31) is equal to ± 1 with the same probability. This means that in the concentration interval $c_1^* < c < c_2^*$ an odd or an even number of frustrated plaquettes belong to the interior of an arbitrary SAW Γ_N^i ($N \gg 1$) with the same probability. It is natural to assume that in such a situation there is no long-range ferromagnetic or antiferromagnetic order,

which leads to the interpretation of $c^*_{1,2}$ given above. In the previous considerations [2, 5, 7, 9] different aspects of frustration distributions with the variance of c had been discussed, but the interpretation of the instability of long-range order based upon a stochastic parity of frustrated plaquettes inside a closed SAW on the lattice has not been, apparently, given before.

On the basis of our results it seems possible to assume the existence of a spin-glass state in the concentration region $c_1^* < c < c_2^*$, but in fact our approximations are too crude to solve this problem. The SAW-approximation has a tendency to overestimate the critical temperature of the phase transition [11], and also the role of neglected graphs is not very clear in this region (cf. [18]). Our method is based upon the high-temperature expansion and is inapplicable for the discussion of the nature of condensed phases (below the phase-transition line in Fig. 3, 4).

The critical concentrations $c^*_{1,2}$ found above are in good agreement with the results of other authors [3 to 6, 8]. Note, however, that in most of these papers only the case of $J_A = J_B$ was considered for the simplest lattices. Our results coincide with the results of molecular field approximation for the critical temperatures [6] if we replace there the number of nearest neighbours z by the connectivity constant μ and the ratio J/T by $\tanh J/T$, which is typical also for the regular Ising model [11]. However, our results are obtained without any assumptions about the nature of condensed phases, such as an introduction of the Edwards-Anderson order parameter. Note, that the critical concentrations determined above are related to the line of the instability of the paramagnetic state (see Fig. 3, 4), they are naturally different from the similar concentrations for $T = 0$ [6], which cannot be found from the high-temperature expansion. We hope that the accuracy of our results is approximately the same as for the SAW approximation in the regular case [11].

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