

Thermodynamic description of the Ising antiferromagnet on a triangular lattice with selective dilution by a modified pair-approximation method

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The pair-approximation method is modified in order to describe systems with geometrical frustration. The Ising antiferromagnet on a triangular lattice with selective dilution (Kaya-Berker model) is considered and a self-consistent thermodynamic description of this model is obtained. For this purpose, the Gibbs free energy as a function of temperature, concentration of magnetic atoms on the selected sublattice, and external magnetic field is derived. In particular, the phase diagram is constructed and a comparison of different methods is presented. The thermodynamic quantities are discussed in the context of their physical validity, and the improvement in the description introduced by the modified method is emphasized.

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I. INTRODUCTION

Although frustrated spin systems have been studied in the literature for over six decades, they still present a challenging problem for theorists [1–21]. During recent years the interest in theoretical studies of such systems has still been increasing [22–41]. This interest mainly concerns the low-dimensional frustrated magnets which exhibit an intriguing interplay between order and disorder and can reveal the existence of new magnetic phases. In turn, the theoretical efforts stimulate the search for the experimental realization of such systems. For instance, in response to theoretical demand, frustrated triangular lattices have been synthesized in some layered magnets [16,18,32,38,42–45].

The theoretical studies of low-dimensional frustrated systems have included such structures as triangular [1,2,6,8,9,11,14,17,24,27,30,31,35,37,40,41], honeycomb [19,25,26,29], square [13,20,36], triangular-square [3], kagome [10,11,46], pyrochlore [10], pentagonal [33], and Shastry-Sutherland lattice [34], and others [47]. Apart from several exact results [1,6,13,33,34,39], most of them have been obtained by the approximate methods, for example, the constant coupling method [10], the Green function technique [23], the spin waves approach [27], cluster theory [8,25,41], the hard-spin mean-field (HSMF) method [7,9], effective field theory (EFT) [24,31], and Monte Carlo (MC) simulations [3,14,19,20,35–37,40,48,49].

The classical frustrated spin system is an antiferromagnetic Ising model with spin $S = 1/2$ on a triangular lattice with nearest-neighbor (NN) interactions. This model has been solved exactly by Wannier [1], who has shown that no long-range ordering exists there at any temperature $T > 0$. For $T = 0$ the long-range correlation function has been studied in Ref. [50] showing its algebraic decay with distance as

$\propto 1/\sqrt{r}$. On the other hand, the triangular lattice can also be understood as the planar, hexagonal centered lattice [6]. When the central atoms from each hexagon are removed we obtain a pure honeycomb lattice. In turn, the honeycomb lattice with antiferromagnetic NN interactions has no frustration and reveals antiferromagnetic ordering.

According to the above observation, Kaya and Berker [9] proposed a model in which the atoms in centers of hexagons are randomly diluted. Such a model presents an intermediate situation between a fully frustrated (disordered) triangular lattice and an unfrustrated honeycomb lattice with antiferromagnetic order. Namely, in the Kaya-Berker (K-B) model the system can be decomposed into three interpenetrating lattices A , B , and C . The situation is schematically presented in Fig. 1. We assume that sublattice C is randomly diluted with concentration $0 \leq p \leq 1$. In particular, for $p = 0$, we obtain a pure hexagonal lattice composed of A and B atoms only, whereas for $p = 1$, when all sites C are occupied by magnetic atoms, the system presents an ideal triangular lattice. Thus, the occurrence of selective dilution on the C sublattice presents an interesting situation, where the magnetic ordering emerges when the p parameter decreases. It is worth noticing that, when the concentration p is large enough ($p \geq 1/2$), a decrease of p means an increase of structural disorder, so this phenomenon can be regarded as a structural analog of the “order by disorder” effect.

One of the first results for the K-B model, which was originally described in the frame of the HSMF method [9], was prediction of the critical concentration p_c for the diluted lattice, below which the system develops long-range ordering. In the first approximation this concentration amounts to $p_c = 0.958$, whereas in the further approximation $p_c = 0.875$. The last result has recently been confirmed by EFT calculations [31], with an astonishing accuracy of three digits. In order to explain this agreement, one can show on the basis of Ref. [51] that EFT (which was introduced some time ago by Honmura and Kaneyoshi [52]) is formally equivalent to the HSMF method

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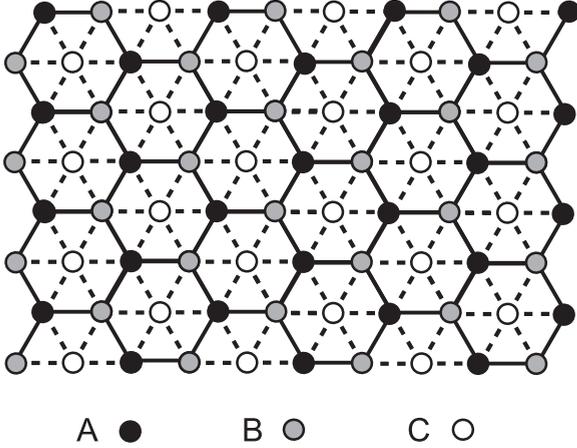


FIG. 1. A schematic presentation of the triangular lattice consisting of three sublattices A , B , and C . Sublattice C is randomly diluted with concentration p .

in its further approximation. On the other hand, EFT is also equivalent to the first Matsudaira approximation [53,54]. It has also been shown that the HSMF method is equivalent to an improved mean-field theory [55,56], which is nothing more than EFT. So, the coincidence of the results for p_c , yielded by the HSMF method and EFT, becomes a rather obvious consequence. On the other hand, MC studies of the K-B model predict, at least in the region $0 \leq p \leq 0.95$, that the antiferromagnetic ordering exists on A and B sublattices, and for $p = 0.95$ the critical temperature is still high (about 40% of its maximal value for $p = 0$) [14].

In the view of above results, the value of p_c , and even its existence, remains unsettled. It is worth noticing that the existence of $p_c < 1$ would imply the existence of the interval $p_c < p < 1$ in which no ordering takes place at $T = 0$. On the other hand, for $p = 1$, i.e., for a pure triangular lattice, it follows from the Wannier paper [1] that the system may order at $T = 0$ with no costs of energy. This conclusion was also confirmed in Ref. [12]. The ordered state at $T = 0$ corresponds to the following sublattice magnetizations: $m_A = 1/2$, $m_B = -1/2$, and $m_C = 0$, where A , B , and C are arbitrarily chosen sublattices. In the context of these results, the existence of the gap for $p_c < p < 1$, where no ordering takes place, would be difficult to explain. This issue motivated us to study, by means of another method, whether $p_c < 1$ in the K-B model exists.

We apply the pair-approximation (PA) method in the frame of the cluster variational approach. The method is based on the cumulant expansion for the entropy [57] when the second-order cumulants are taken into account and higher-order cumulants are neglected. This approach has already been applied for the low-dimensional Ising [58] and Heisenberg [59] systems, including structural disorder [60]. The advantage of the PA method over the molecular field approximation (MFA) has been discussed there. It is worth noticing that, contrary to MFA, the PA method takes into account nearest-neighbor spin-pair correlation functions which incorporate important fluctuations. Recently, the method was also applied for the ferromagnetic analog of the K-B model, without frustration [61]. However, for the frustrated system

considered here the method should be adopted with some necessary modification, which is explained in the theoretical section.

The modified PA method proposed here yields the Gibbs free energy of the system, which is a function of temperature, external field, and number of particles (spins). Next, from the expression for the Gibbs energy all thermodynamic quantities can be derived. Thus, the modified PA method gives the possibility of a complete thermodynamic description of the frustrated system in an approximate but fully self-consistent way.

The paper is organized as follows: In the theoretical part a foundation of the PA method is outlined and its application for frustrated systems is explained in detail. In the following section the numerical calculations are presented in the figures and discussed. The results concern all basic thermodynamic properties which are obtained from minimization of the Gibbs energy. In particular, the phase diagram and the existence of critical concentration p_c is discussed in the context of other methods. In the last section a summary of the results is presented and some final conclusions are drawn.

II. THEORETICAL MODEL

A. General formulation

We consider the Ising model with spins $S_{i_\alpha} = \pm 1/2$ arranged on the triangular lattice with antiferromagnetic NN interactions. The i th lattice site belongs to the sublattice $\alpha = A, B, C$, and the random dilution of the selected sublattice (C) is assumed. The Hamiltonian can be presented as follows:

$$\mathcal{H} = -J \sum_{i_A, j_B} S_{i_A} S_{j_B} - J \sum_{j_B, k_C} S_{j_B} S_{k_C} \xi_{k_C} - J \sum_{i_A, k_C} S_{i_A} S_{k_C} \xi_{k_C} - h \left(\sum_{i_A} S_{i_A} + \sum_{j_B} S_{j_B} + \sum_{k_C} S_{k_C} \xi_{k_C} \right), \quad (1)$$

where $J \leq 0$ is the NN antiferromagnetic exchange interaction, h stands for the external field, and $\xi_{k_C} = 0, 1$ is the random occupation operator. The configurational mean value of ξ_{k_C} , $\langle \xi_{k_C} \rangle_r = p$ presents a fraction of occupied sites (concentration of magnetic atoms) on the C sublattice.

In general, the Gibbs energy G can be presented as

$$G = \langle \mathcal{H} \rangle - ST, \quad (2)$$

where $\langle \mathcal{H} \rangle$ is the enthalpy and S presents the entropy of the system. The enthalpy (which is the averaged Hamiltonian containing the external field term) is of the form

$$\langle \mathcal{H} \rangle = -NJ(c_{AB} + pc_{BC} + pc_{AC}) - \frac{1}{3}Nh(m_A + m_B + pm_C). \quad (3)$$

In Eq. (3) N denotes the total number of lattice sites in the triangular lattice (which is equal to the number of NN lattice site pairs in two sublattices). The thermal mean values are written in shortened notation as $c_{AB} = \langle S_{i_A} S_{j_B} \rangle$, $c_{BC} = \langle S_{j_B} S_{k_C} \rangle$, and $c_{AC} = \langle S_{i_A} S_{k_C} \rangle$ and denote three NN correlation functions (for occupied lattice sites), whereas $m_\alpha = \langle S_{i_\alpha} \rangle$

($\alpha = A, B, C$) denote three sublattice magnetizations per (occupied) lattice site. Assuming that occupation operators are independent of the Ising spins, Eq. (3) is exact for the model in question.

As a general approach, the entropy can be expressed in a series of cumulants [57]. In the PA method only first- and second-order cumulants are taken into account. Thus, the entropy can be approximately presented as follows:

$$S = \frac{N}{3}(\sigma_A + \sigma_B + p\sigma_C) + N(\sigma_{AB} - \sigma_A - \sigma_B) + Np(\sigma_{BC} - \sigma_B - \sigma_C) + Np(\sigma_{AC} - \sigma_A - \sigma_C), \quad (4)$$

where σ_α ($\alpha = A, B, C$) are the single-site entropies and $\sigma_{\alpha\beta}$ ($\alpha \neq \beta = A, B, C$) are the entropies of NN pairs. Expression (4) for the entropy can be rewritten in a more convenient form:

$$S = N[\sigma_{AB} + p(\sigma_{BC} + \sigma_{AC}) - (\frac{2}{3} + p)(\sigma_A + \sigma_B) - \frac{5}{3}p\sigma_C]. \quad (5)$$

The single site and pair entropies can be found from their definitions:

$$\sigma_\alpha = -k_B \text{Tr}_{i_\alpha}(\rho_{i_\alpha} \ln \rho_{i_\alpha}) \quad (6)$$

and

$$\sigma_{\alpha\beta} = -k_B \text{Tr}_{i_\alpha j_\beta}(\rho_{i_\alpha j_\beta} \ln \rho_{i_\alpha j_\beta}), \quad (7)$$

where ρ_{i_α} and $\rho_{i_\alpha j_\beta}$ are the single-site and pair density matrices, respectively. For spins 1/2 these matrices are given by the expressions:

$$\rho_{i_\alpha} = \frac{1}{2} + 2m_\alpha S_{i_\alpha} \quad (8)$$

($\alpha = A, B, C$; $S_{i_\alpha} = \pm \frac{1}{2}$), and

$$\rho_{i_\alpha j_\beta} = \frac{1}{4} + m_\alpha S_{i_\alpha} + m_\beta S_{j_\beta} + 4c_{\alpha\beta} S_{i_\alpha} S_{j_\beta} \quad (9)$$

($\alpha \neq \beta = A, B, C$), respectively. Let us remark that decoupling of correlations, $c_{\alpha\beta} \approx m_\alpha m_\beta$, is equivalent to factorization of the pair matrices, $\rho_{i_\alpha j_\beta} \approx \rho_{i_\alpha} \rho_{j_\beta}$, and leads to the approximation $\sigma_{\alpha\beta} \approx \sigma_\alpha + \sigma_\beta$. This is equivalent to the molecular field approximation method, in which expression (4) for the entropy contains only the first, additive term [58]. As discussed in Ref. [58], the single-site density matrices are

normalized,

$$\text{Tr}_{i_\alpha} \rho_{i_\alpha} = 1, \quad (10)$$

and the pair density matrices can be reduced:

$$\text{Tr}_{j_\beta} \rho_{i_\alpha j_\beta} = \rho_{i_\alpha}. \quad (11)$$

The matrices given by Eqs. (8) and (9) satisfy the relationships for the thermodynamic mean values:

$$m_\alpha = \langle S_{i_\alpha} \rangle = \text{Tr}_{i_\alpha} (S_{i_\alpha} \rho_{i_\alpha}) \quad (12)$$

and

$$c_{\alpha\beta} = \langle S_{i_\alpha} S_{j_\beta} \rangle = \text{Tr}_{i_\alpha j_\beta} (S_{i_\alpha} S_{j_\beta} \rho_{i_\alpha j_\beta}). \quad (13)$$

With the help of the density matrices (8) and (9) the single-site (6) and pair (7) entropies can be expressed as

$$\sigma_\alpha = -k_B \left(\frac{1}{2} + m_\alpha \right) \ln \left(\frac{1}{2} + m_\alpha \right) - k_B \left(\frac{1}{2} - m_\alpha \right) \ln \left(\frac{1}{2} - m_\alpha \right) \quad (14)$$

($\alpha = A, B, C$), and

$$\sigma_{\alpha\beta} = -k_B \rho_{\alpha\beta}^{++} \ln \rho_{\alpha\beta}^{++} - k_B \rho_{\alpha\beta}^{+-} \ln \rho_{\alpha\beta}^{+-} - k_B \rho_{\alpha\beta}^{-+} \ln \rho_{\alpha\beta}^{-+} - k_B \rho_{\alpha\beta}^{--} \ln \rho_{\alpha\beta}^{--} \quad (15)$$

($\alpha \neq \beta = A, B, C$), respectively. In Eq. (15) we introduced the following abbreviated notation:

$$\begin{aligned} \rho_{\alpha\beta}^{++} &= \frac{1}{4} + \frac{1}{2}m_\alpha + \frac{1}{2}m_\beta + c_{\alpha\beta}, \\ \rho_{\alpha\beta}^{+-} &= \frac{1}{4} + \frac{1}{2}m_\alpha - \frac{1}{2}m_\beta - c_{\alpha\beta}, \\ \rho_{\alpha\beta}^{-+} &= \frac{1}{4} - \frac{1}{2}m_\alpha + \frac{1}{2}m_\beta - c_{\alpha\beta}, \\ \rho_{\alpha\beta}^{--} &= \frac{1}{4} - \frac{1}{2}m_\alpha - \frac{1}{2}m_\beta + c_{\alpha\beta}. \end{aligned} \quad (16)$$

Taking into account the above formulas and Eq. (2), the Gibbs energy per lattice site, expressed in $|J|$ units, can be written in the final form:

$$\begin{aligned} \frac{G}{N|J|} &= c_{AB} + p(c_{AC} + c_{BC}) \\ &- \frac{1}{3} \frac{h}{|J|} (m_A + m_B + pm_C) - \frac{k_B T}{|J|} \frac{S}{Nk_B}, \end{aligned} \quad (17)$$

where the dimensionless entropy per lattice site is in the form of

$$\begin{aligned} \frac{S}{Nk_B} &= -\rho_{AB}^{++} \ln \rho_{AB}^{++} - \rho_{AB}^{+-} \ln \rho_{AB}^{+-} - \rho_{AB}^{-+} \ln \rho_{AB}^{-+} - \rho_{AB}^{--} \ln \rho_{AB}^{--} \\ &- p [\rho_{AC}^{++} \ln \rho_{AC}^{++} + \rho_{AC}^{+-} \ln \rho_{AC}^{+-} + \rho_{AC}^{-+} \ln \rho_{AC}^{-+} + \rho_{AC}^{--} \ln \rho_{AC}^{--}] \\ &- p [\rho_{BC}^{++} \ln \rho_{BC}^{++} + \rho_{BC}^{+-} \ln \rho_{BC}^{+-} + \rho_{BC}^{-+} \ln \rho_{BC}^{-+} + \rho_{BC}^{--} \ln \rho_{BC}^{--}] \\ &+ \left(\frac{2}{3} + p \right) \left[\left(\frac{1}{2} + m_A \right) \ln \left(\frac{1}{2} + m_A \right) + \left(\frac{1}{2} - m_A \right) \ln \left(\frac{1}{2} - m_A \right) \right] \\ &+ \left(\frac{2}{3} + p \right) \left[\left(\frac{1}{2} + m_B \right) \ln \left(\frac{1}{2} + m_B \right) + \left(\frac{1}{2} - m_B \right) \ln \left(\frac{1}{2} - m_B \right) \right] \\ &+ \frac{5}{3} p \left[\left(\frac{1}{2} + m_C \right) \ln \left(\frac{1}{2} + m_C \right) + \left(\frac{1}{2} - m_C \right) \ln \left(\frac{1}{2} - m_C \right) \right] \end{aligned} \quad (18)$$

and $\rho_{\alpha\beta}^{\pm\pm}$ are given by Eqs. (16).

B. Modification of the PA method for the system with geometrical frustration

From the general formulation, the Gibbs energy given by Eq. (17) is a function of six variational parameters: m_A , m_B , m_C , c_{AB} , c_{AC} , and c_{BC} . In the conventional approach within PA, the Gibbs energy in equilibrium corresponds to the minimum with respect to all these parameters, which are treated equally. However, in the case of geometrical frustration such treatment leads to wrong (unphysical) results since the correlations $c_{\alpha\beta}$ are not fully independent parameters [8]. As a consequence, the ground-state energy is incorrect and the entropy is negative in the low-temperature region. In order to improve on the method, we propose its modification for the Gibbs energy calculation. The modified method is based on the assumption that the correlations involving frustrated spins should be partly decoupled. Namely, let us assume that the spin S_{k_C} is frustrated in the k site of the selected lattice C . Then, m_A , m_B , m_C , and c_{AB} can further be treated as independent parameters; however, the correlations c_{AC} and c_{BC} , which involve the frustrated spin S_{k_C} , are not independent of the rest of parameters and should be treated in a more complex way. First of all, let us observe that in a given triangle (i_A, j_B, k_C) , the spin S_{k_C} is frustrated only when the spins S_{i_A} and S_{j_B} take the antiparallel orientation. The probability x of such a situation can be estimated as follows:

$$x = \rho_{AB}^{+-} + \rho_{AB}^{-+} = \frac{1}{2} - 2c_{AB}. \quad (19)$$

In the rest of states (i.e., when the spins S_{i_A} and S_{j_B} are parallel) the spin S_{k_C} is not frustrated in this triangle. This type of (unfrustrated) situation occurs with the probability $1 - x$, where

$$1 - x = \rho_{AB}^{++} + \rho_{AB}^{--} = \frac{1}{2} + 2c_{AB}. \quad (20)$$

Therefore, for the correlations c_{AC} and c_{BC} we propose the following approximation:

$$c_{AC} \approx x \langle S_{i_A} S_{k_C} \rangle'' + (1 - x) \langle S_{i_A} S_{k_C} \rangle' \quad (21)$$

and

$$c_{BC} \approx x \langle S_{j_B} S_{k_C} \rangle'' + (1 - x) \langle S_{j_B} S_{k_C} \rangle', \quad (22)$$

respectively. For the case when the spins S_{i_A} and S_{j_B} are parallel, both correlations involving spin S_{k_C} must be equal; therefore, $\langle S_{i_A} S_{k_C} \rangle' = \langle S_{j_B} S_{k_C} \rangle' = c'$, and c' can be treated as a new variational parameter, in addition to m_A , m_B , m_C , and c_{AB} . On the other hand, for the frustrated states of S_{k_C} , the correlations $\langle S_{i_A} S_{k_C} \rangle''$ and $\langle S_{j_B} S_{k_C} \rangle''$ should be decoupled as follows:

$$\langle S_{i_A} S_{k_C} \rangle'' \approx \langle S_{i_A} \rangle'' \langle S_{k_C} \rangle = \langle S_{i_A} \rangle'' m_C \quad (23)$$

and

$$\langle S_{j_B} S_{k_C} \rangle'' \approx \langle S_{j_B} \rangle'' \langle S_{k_C} \rangle = \langle S_{j_B} \rangle'' m_C, \quad (24)$$

where $\langle S_{i_A} \rangle''$ (and $\langle S_{j_B} \rangle''$) denote the conditional averages, i.e., the averages when the neighboring spins S_{j_B} and S_{i_A} are antiparallel, respectively. These mean values can be calculated with the help of the two normalized probabilities, ρ_{AB}^{+-}/x and ρ_{AB}^{-+}/x , as follows:

$$\langle S_{i_A} \rangle'' = \frac{1}{x} \left(\frac{1}{2} \rho_{AB}^{+-} - \frac{1}{2} \rho_{AB}^{-+} \right) = \frac{1}{2x} (m_A - m_B) \quad (25)$$

and

$$\langle S_{j_B} \rangle'' = \frac{1}{x} \left(\frac{1}{2} \rho_{AB}^{-+} - \frac{1}{2} \rho_{AB}^{+-} \right) = \frac{1}{2x} (m_B - m_A). \quad (26)$$

Thus, for the correlations c_{AC} and c_{BC} we obtain the following approximation:

$$c_{AC} \approx \frac{1}{2} (m_A - m_B) m_C + \left(\frac{1}{2} + 2c_{AB} \right) c' \quad (27)$$

and

$$c_{BC} \approx \frac{1}{2} (m_B - m_A) m_C + \left(\frac{1}{2} + 2c_{AB} \right) c'. \quad (28)$$

This approximation contains partial decoupling, but also introduces a new variational parameter c' for the correlations containing unfrustrated states of S_{k_C} . Substituting Eqs. (27) and (28) into the Gibbs energy (17) [and entropy (18)] we can describe our frustrated system with no risk of getting unphysical solutions. The equilibrium for the Gibbs energy is obtained for five variational parameters only, whose values should be restricted to the following physical ranges: $-1/2 \leq m_\alpha \leq 1/2$ ($\alpha = A, B, C$), and $-1/4 \leq (c_{AB}, c') \leq 1/4$.

C. Thermodynamic properties and the variational equations

The complete and self-consistent thermodynamic description can be obtained from the basic equation for the Gibbs potential (17) with the help of Eqs. (27) and (28). Since the Gibbs energy is a function of the external field h and temperature T , the first derivatives lead to the results

$$\frac{1}{N} \left(\frac{\partial G}{\partial h} \right)_T = -\frac{1}{3} (m_A + m_B + p m_C) = -m, \quad (29)$$

where m is the averaged magnetization per lattice site, and

$$\left(\frac{\partial G}{\partial T} \right)_h = -S, \quad (30)$$

where S is the entropy [given in the form of Eq. (18)]. It is worth noticing that formulas (29) and (30) are only satisfied together with the necessary extremum conditions:

$$\frac{\partial G}{\partial m_\alpha} = 0 \quad (31)$$

($\alpha = A, B, C$),

$$\frac{\partial G}{\partial c_{AB}} = 0, \quad (32)$$

and

$$\frac{\partial G}{\partial c'} = 0 \quad (33)$$

(provided $|c'| \leq 1/4$). Equations (31)–(33) form a set of five variational equations from which the variational parameters can be obtained. The detailed form of these equations for $h = 0$ is presented in the Appendix. When solving such equations it should be controlled whether the solutions fall into the physical ranges $-1/2 \leq m_\alpha \leq 1/2$ ($\alpha = A, B, C$), $-1/4 \leq c_{AB} \leq 1/4$, and $-1/4 \leq c' \leq 1/4$. If for a certain parameter this is not the case, we should assume the value of that parameter at the edge of the physical range, where the Gibbs energy reaches its minimum. In such a case, when the variational parameter is constant at the edge, the corresponding

variational equation should be ignored. This objection mainly concerns Eq. (33) in the low-temperature region, and the consequences are discussed in the next section in more detail.

As far as other thermodynamic properties are concerned, they can be obtained from the second derivatives of the Gibbs energy. For instance, the isothermal susceptibility is given by

$$\chi_T = N \left(\frac{\partial m}{\partial h} \right)_T = - \left(\frac{\partial^2 G}{\partial h^2} \right)_T. \quad (34)$$

In turn, the magnetic contribution to the specific heat at constant field h can be found from the relationship

$$C_h = T \left(\frac{\partial S}{\partial T} \right)_h = -T \left(\frac{\partial^2 G}{\partial T^2} \right)_h. \quad (35)$$

Since the whole theory is self-consistent, the specific heat can also be calculated in an equivalent way:

$$C_h = \left(\frac{\partial \langle \mathcal{H} \rangle}{\partial T} \right)_h, \quad (36)$$

where $\langle \mathcal{H} \rangle$ is the enthalpy given by Eq. (3). Equivalency of Eqs. (35) and (36) requires that calculations of the entropy must be consistent with calculations of the correlation function. The numerical results and their detailed analysis are presented in the next section.

III. NUMERICAL RESULTS AND DISCUSSION

We start the numerical analysis from the ground state. At $T = 0$ the entropic part in the Gibbs energy is unimportant and only enthalpy (the mean value of the Hamiltonian) determines the thermodynamic potential. Therefore, the ground-state phase diagram can be determined exactly. By analysis of the enthalpy minimum in five-dimensional space, in the range of concentration $0 < p < 1$ and $h = 0$, we found that the sublattice magnetizations in the ground state take the values $m_A = 1/2$, $m_B = -1/2$, and $m_C = 0$ (or, symmetrically, $m_A = -1/2$, $m_B = 1/2$, and $m_C = 0$). At the same time, the correlation parameters in this regime are $c_{AB} = -1/4$ and $c' = -1/4$. The absence of magnetization on C sublattice is due to the fact that the frustrated spins S_{k_C} can take the values $\pm 1/2$ with the same probability. For $h/|J|$ belonging to the range $0 < h/|J| < 1.5$, magnetization in the ground state is given by $m_A = 1/2$, $m_B = -1/2$, and $m_C = 1/2$ (or $m_A = -1/2$, $m_B = 1/2$, and $m_C = 1/2$). At $h/|J| = 1.5$ the spin-flip transition takes place, and for $1.5 < h/|J| < 3$ the ground state is characterized by $m_A = 1/2$, $m_B = 1/2$, and $m_C = -1/2$. The next spin reversal on the C sublattice is observed for $h/|J| = 3$, leading to the uniform magnetization $m_A = 1/2$, $m_B = 1/2$, and $m_C = 1/2$ when $h/|J| > 3$. At $h/|J| = 1.5$ and $h/|J| = 3$ the coexistence of neighboring phases takes place.

For $p = 1$ the situation becomes more complex, because for $h = 0$ and $T = 0$ each triangle consisting of NN spins is sixfold degenerated [62]. From the analysis of enthalpy at this point we found that two distinct kinds of states can coexist with the same energy. One is the ordered state, in which two sublattices have opposite magnetizations, and the magnetization of the third sublattice is equal to zero. This state can be considered a continuation of the situation which occurs for $0 < p < 1$ and can be characterized by the parameters

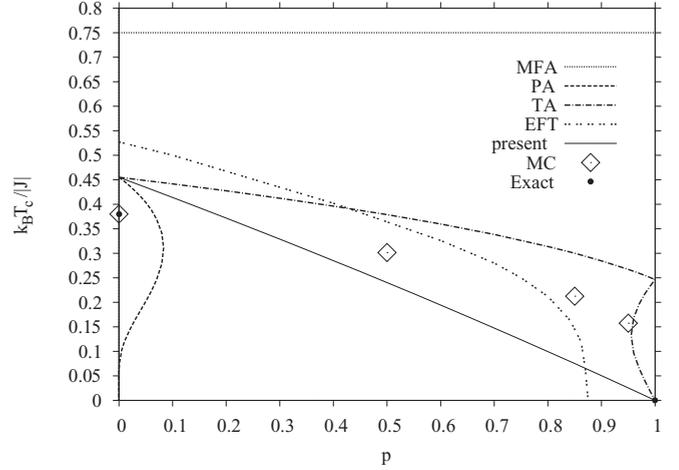


FIG. 2. Dependence of critical temperature $k_B T_c / |J|$ on concentration p . A comparison of different methods is presented.

$m_A = 1/2$, $m_B = -1/2$, $m_C = 0$, $c_{AB} = -1/4$, $c_{AC} = 0$, and $c_{BC} = 0$. The ordered state vanishes discontinuously when $T > 0$. Another state, which coexists in the ground-state point ($p = 1$, $h = 0$, $T = 0$), is the disordered state. It is characterized by the parameters $m_A = 0$, $m_B = 0$, $m_C = 0$, $c_{AB} = -1/12$, $c_{AC} = -1/12$, and $c_{BC} = -1/12$. This disordered state extends over nonzero temperatures $T > 0$. For $p = 1$ and $0 < h/|J| < 3$ the ground state is ordered and is characterized by two sublattices oriented in parallel to the external field and one antiparallel. At $h/|J| = 3$ the spin-flip transition takes place and for $h/|J| > 3$ all three sublattices have magnetizations oriented in parallel with the field.

Furthermore, we concentrate on the numerical calculations of thermodynamic quantities for $h = 0$ in the whole concentration range $0 \leq p \leq 1$ and arbitrary T . The most intriguing problem concerns the existence of phase transitions. In Fig. 2 we illustrate the phase transition (Néel) temperature vs concentration p . The ordered state presents a continuation of the phase existing in the ground state and is characterized by $m_A = -m_B$ and $m_C = 0$. Such a solution has also been found by MC simulations [14]. Various curves and markers in Fig. 2 correspond to different methods. The exact results (marked by bold points) have been found for $p = 0$ and $p = 1$ as $k_B T_c / |J| = 1/(2 \ln(2 + \sqrt{3})) \approx 0.3797$ [63] and $k_B T_c / |J| = 0$ [1], respectively. MC results are marked by diamond symbols [14]. For $p = 0$, a good agreement of the MC result with the exact solution can be noted.

It should also be mentioned that in case of a honeycomb lattice, as well as for other two-dimensional (2D) lattices, high-temperature series-expansion (HTSE) method [64] gives the critical temperature which is practically exact. Other approximate methods are not so accurate. For instance, the thermodynamic perturbation theory [65] gives for a honeycomb lattice the result $k_B T_c / |J| = 0.43$ (for $S = 1/2$) in the fourth approximation, which is slightly better than the Bethe result (0.4551). However, in the sixth approximation the method developed in Ref. [65] gives 0.481, which is worse than the value estimated in the fourth approximation. For this reason such a theory cannot be recommended for a honeycomb lattice as a systematic approach. One of the recent results for

the critical temperature of a honeycomb lattice was obtained by correlated cluster mean-field (CCMF) theory [66]. The value obtained there was ≈ 0.398 . Also a short overview of other approximate methods can be found in Ref. [66]. However, none of these methods have been applied for the Kaya-Berker model with geometrical frustration.

It has been known that the MC method is difficult to apply for this model for $0 < p < 1$ in the low-temperature region, where the spins can be frozen and the algorithm becomes trapped in the vicinity of a local free energy minimum [14]. For $0 < p < 1$ this difficulty is attributed to the glassy behavior of spins S_{k_c} [14]. It should be mentioned that the spin-glass state does not occur for $p = 1$ (i.e., for a pure triangular lattice) [67] and MC methods have been successful there for relatively low temperatures [48,49]. However, for $0 < p < 1$, some analytical methods, which are able to overcome this difficulty, are still desired. The most crude description, which neglects fluctuations, is given by the MFA and is depicted by the horizontal dotted line at $k_B T_c/|J| = 0.75$. It is obvious that such a method cannot be accepted for frustrated systems. A much better description is provided by EFT [31] (marked by the double-dotted line), which, as discussed in the Introduction, is equivalent to HSMF theory in further approximation [9]. In such a case the critical concentration $p_c = 0.875$ is predicted, below which the system becomes ordered. In turn, application of the PA method in its conventional formulation (with six variational parameters) gives the reentrant magnetism (dashed curve) and unphysical result, since no ordering is predicted for all p . It is worth a mention that for ferromagnetic systems, without frustration, the PA method gives usually better results than EFT, as for example discussed in Ref. [61].

We are aware that the PA method in its usual, unmodified formulation for frustrated systems overestimates NN correlation functions in low temperatures, which leads to improper ground-state energy and negative entropy. Therefore, we first tried to develop the triangle approximation (TA) according to the general cluster variational method (CVM) for the Ising systems [68]. In the case of TA we deal with 12 variational parameters. In some testing calculations for the triangular lattice with ferromagnetic interactions we obtained the Curie temperature $k_B T_c/|J| = 1/(2 \ln(5/3)) \approx 0.9788$, which is not far from the exact result $k_B T_c/J = 1/\ln 3 \approx 0.9102$ [63]. However, for the frustrated model with antiferromagnetic interactions the result of the TA method (marked by the dash-dotted line in Fig. 2) is still unsatisfactory. In particular, the reentrant magnetism is found near $p = 1$, and for $p = 1$ the ordered phase extends up to $k_B T_c/|J| = 0.2464$. It is expected that further approximations within the systematic CVM will improve on the results; however, the number of variational parameters then increases (for instance, there would be 21 parameters in the hexagonal approximation) and the method developed in Ref. [68] becomes intractable in practice.

Taking into account the above problems, we decided to modify the PA method in order to obtain a simplified but still qualitatively correct description of the model. The result for T_c is shown in Fig. 2 as a solid curve. For $p = 0$ we obtained $k_B T_c/|J| = 1/(2 \ln 3) \approx 0.4551$, i.e., the same value as for the ferromagnetic case [61], and identical with the Bethe

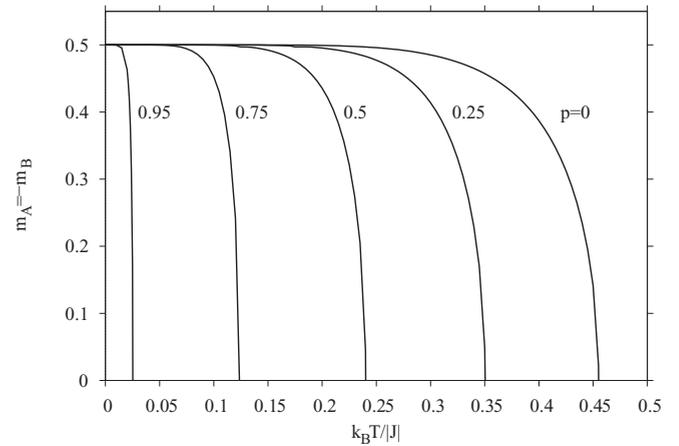


FIG. 3. Sublattice spontaneous magnetizations $m_A = -m_B$ vs dimensionless temperature $k_B T/|J|$. Different curves correspond to various concentrations p .

result $k_B T_c/|J| = 1/[2 \ln(z/(z-2))]$ for NN number $z = 3$. On the other hand, for $p = 1$ the exact Wannier result $T_c = 0$ is recovered. It follows from the present method that the ordered phase exists in the full range of $0 \leq p \leq 1$, whereas for $p = 1$ and $T = 0$ it coexists with the disordered phase.

In Fig. 3 the sublattice spontaneous magnetizations $m_A = -m_B$ are shown vs temperature. Magnetization of the diluted sublattice C amounts to $pm_C = 0$ for all temperatures. Different curves correspond to various concentrations p . For $T = 0$ the sublattice magnetization is constant vs p and reaches its saturated value $m_A = 1/2$ ($m_B = -1/2$), which is in agreement with the ground state. This result differs from that obtained by EFT [31], where the magnetization at $T = 0$ depends on concentration. For $p \rightarrow 1$ a jump of magnetization from the value $1/2$ to 0 signals the first-order phase transition.

Entropy vs temperature per occupied lattice site, expressed in Boltzmann constant units, is illustrated in Fig. 4. The number of occupied lattice sites (spins) is denoted by N' , where $N' = N(2+p)/3$, and N is the total number of lattice

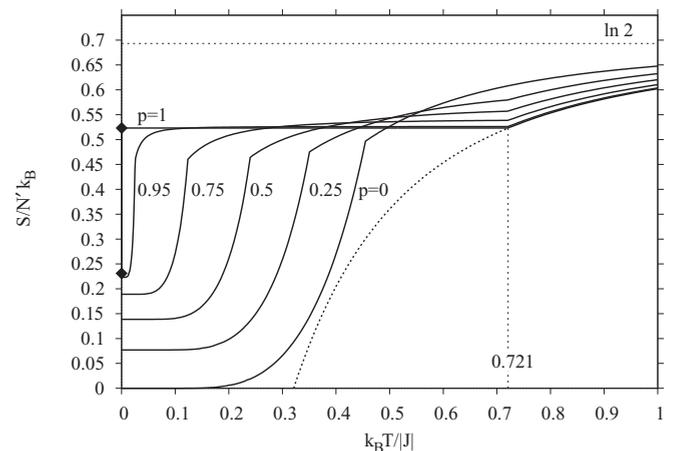


FIG. 4. Entropy $S/N' k_B$ per occupied lattice site, expressed in Boltzmann constant units, vs dimensionless temperature $k_B T/|J|$. Different curves correspond to various concentrations p .

sites. Such normalization of the entropy allows to control its high-temperature limit, which for $T \rightarrow \infty$ amounts to $\ln 2$. As before, various curves correspond to different concentrations p . For $p = 0$ entropy amounts to 0 in the ground (fully ordered, antiferromagnetic) state. On the other hand, for $p = 1$ and $T = 0$ we obtained two values of the residual entropy: $S/N'k_B = (\ln 2)/3 \approx 0.2310$ and $S/N'k_B = 0.5232$. These values are marked by the bold points. A jump of the entropy at ($p = 1, T = 0$) signifies the first-order transition between ordered and disordered phases which have been identified in the ground state.

We also found that for $p = 1$, below the characteristic temperature $k_B T_f/|J| = 0.721$, the entropy practically does not depend on temperature. It is connected with the fact that in this temperature range the correlation c' takes the constant value $c' = -1/4$, which is at the edge of its physical region. Namely, in this case the absolute minimum of the Gibbs energy lies outside the physical region, i.e., for $c' < -1/4$, and therefore Eq. (33) cannot be applied. However, when we restrict the domain of c' to the physical region, i.e., $|c'| \leq 1/4$, the minimal value of the Gibbs energy in this domain exists at $c' = -1/4$. The situation changes for $k_B T/|J| > 0.721$, where the absolute minimum of G falls into the physical region $|c'| \leq 1/4$ and Eq. (33) becomes effective for determination of c' .

We conclude that the kink on the entropy curve at $k_B T_f/|J| = 0.721$ originates from cutting off the unphysical solution for the correlation function c' . It is seen for the entropy because these quantities are interrelated via a minimum condition for the Gibbs energy. In Fig. 4 we also present the unphysical solution for the entropy curve for $p = 1$ (dashed line), which results from the unmodified PA method. This entropy becomes negative for $k_B T/|J| < \approx 0.321$ and reaches its minimum value $S/N'k_B \approx -1.386$ for $T = 0$. However, the negative part of this entropy curve is not presented in the figure. The effect of the kink diminishes when p decreases and for $p = 0$, when the system has no frustration, it does not occur at all. Other kinks on the entropy curves for $p < 1$ which occur in lower temperatures are connected with the second-order phase transitions from antiferromagnetic to paramagnetic phase.

Further results obtained for the entropy are illustrated in Fig. 5 vs concentration p . The upper curve presents entropy at the phase transition (Néel) temperature, whereas the lower curve presents entropy at $T = 0$. An increasing character of the residual entropy vs p is worth noticing. For $p = 1$ two values of entropy (the same as those indicated in Fig. 4) are seen. Since for $p = 1$ we have $T_c = 0$, the entropy jump at this temperature point confirms the existence of first-order phase transitions. The exact Wannier result [69], i.e., $S/N'k_B = 0.32306$, is also depicted in the interval between our two points. It is worth noticing that the recent result obtained from MC simulations gave the value $S/N'k_B = 0.32303$ [70], which is very close to the exact value.

The Gibbs energy curves vs temperature are presented in Fig. 6 for various concentrations p . A monotonously decreasing character of these curves evidences that the entropy [given by Eq. (30)] is positive everywhere. For large temperatures the Gibbs energy becomes linear vs T with the same slope for all curves, which corresponds to the saturation value of the entropy, as indicated in Fig. 4. The Gibbs energy is a smooth

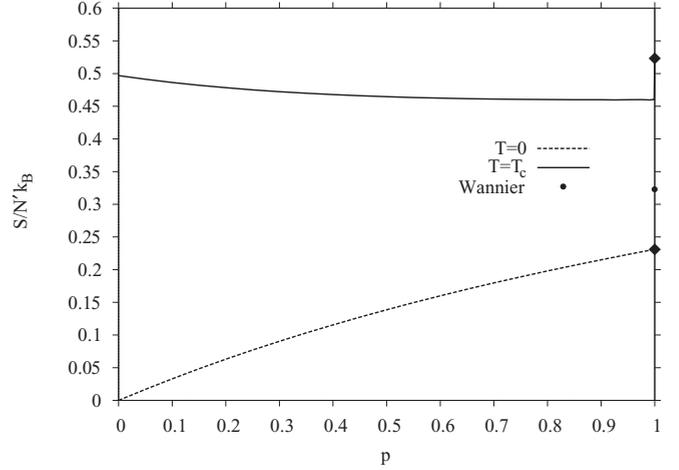


FIG. 5. Entropy $S/N'k_B$ per occupied lattice site, expressed in Boltzmann constant units, vs concentration p . Upper curve corresponds to entropy at critical temperature $T = T_c$, whereas lower curve presents the residual entropy at $T = 0$.

function vs temperature, without any kinks for $T > 0$ which would signal the first-order phase transition. At $T = 0$, for all concentrations the Gibbs energy is the same.

In Fig. 7 the NN correlation functions c_{AB} are presented vs temperature for various concentrations p . For $p = 1$, similarly to entropy, the correlations are constant below the characteristic temperature $k_B T_f/|J| = 0.721$, and for $T = 0$ a jump of correlation function is seen between $-1/4$ value (for ordered phase) and $-1/12$ value for the disordered state. The analogous jump is seen in Fig. 8, where the NN correlation functions $c_{AC} = c_{BC}$ are presented. In this case a jump from the value $-1/12$ (for disordered phase) to 0 (for ordered state) takes place. It can be noted from Figs. 7 and 8 that for $T = 0$ the mean correlation per pair, $(c_{AB} + c_{AC} + c_{BC})/3$, is equal to $-1/12$ for both states, and its absolute value amounts to one-third of the value for the ferromagnetic case. The same result was also pointed out by Wannier [1] in his exact solution.

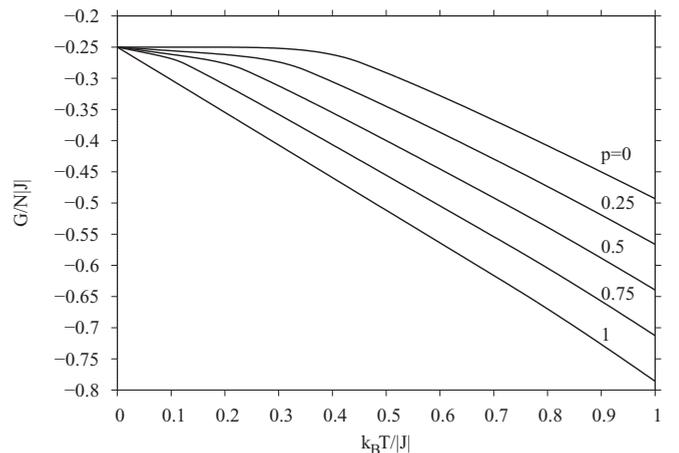


FIG. 6. Gibbs energy $G/N|J|$ per lattice site, expressed in $|J|$ units, vs dimensionless temperature $k_B T/|J|$. Different curves correspond to various concentrations p .

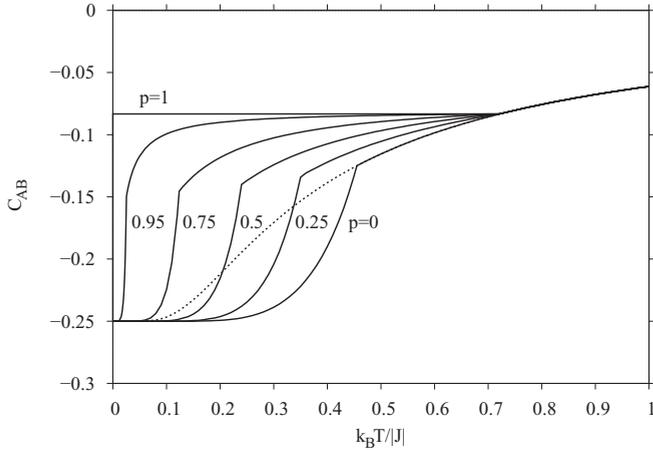


FIG. 7. Nearest-neighbor correlation function c_{AB} vs dimensionless temperature $k_B T/|J|$. Different curves correspond to various concentrations p .

In Figs. 7 and 8 by dashed curves we denote the unphysical solutions for the correlation functions for $p = 1$. Both curves tend to $-1/4$ value for $T = 0$; however, in Fig. 8 only a part of the curve is shown. These curves result from the unmodified PA method and correspond to the unphysical entropy (presented by the dashed curve in Fig. 4). The ground-state energy for such a solution (for $p = 1$) amounts to $-3/4|J|$ per spin and is three times lower than the exact ground-state energy [1], as well as the value obtained in the modified PA method.

A decreasing character of the $c_{AC} = c_{BC}$ curves in Fig. 8, when T increases in the range $0 < k_B T/|J| \leq 0.721$, has no influence on the sign of magnetic specific heat, since the total internal energy, and entropy, are monotonously increasing functions of temperature. Thus, the specific heat is positive everywhere.

The specific heat can be conveniently calculated from Eq. (35) and the results are presented in Fig. 9. In this figure, apart from the pronounced peaks corresponding to the Néel temperatures, small jumps can be noted for $k_B T_f/|J| = 0.721$.

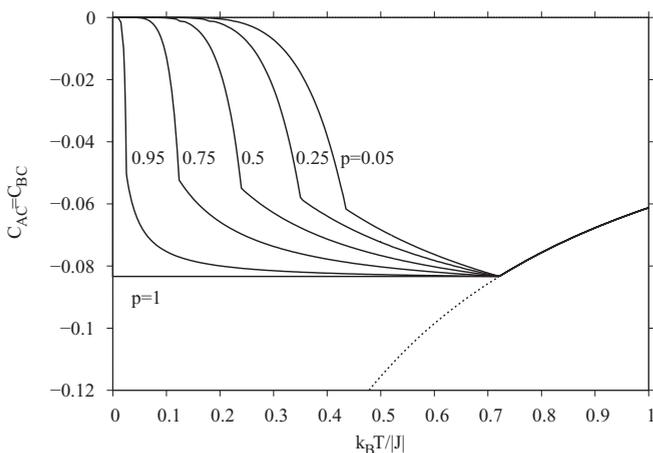


FIG. 8. Nearest-neighbor correlation functions $c_{AC} = c_{BC}$ vs dimensionless temperature $k_B T/|J|$. Different curves correspond to various concentrations p .

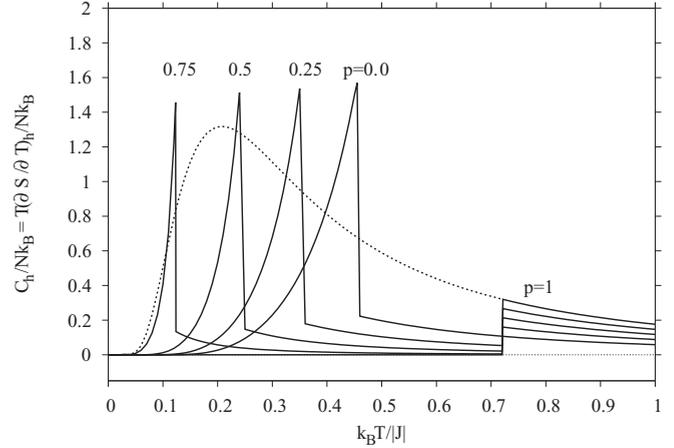


FIG. 9. Magnetic specific heat C_h/Nk_B per lattice site, expressed in Boltzmann constant units, vs dimensionless temperature $k_B T/|J|$. Different curves correspond to various concentrations p .

Again, these jumps result from the entropy (or correlation function) kinks presented in Figs. 4, 7, and 8. In Fig. 9, by dashed curve, we present also the specific heat for $p = 1$, when the correlation functions are not limited to the physical range, i.e., are calculated within the unmodified PA method. Such specific heat shows a broad maximum whose magnitude is comparable with the peaks at the phase transitions presented in this figure for $p < 1$. We are aware that the broad maximum of the paramagnetic specific heat has also been found in MC simulations [14], in accordance with the exact results for a triangular lattice [1]. However, in the modified PA method only a tail of this peak is present as a physical solution, whereas the main part has been cut off in order to obtain self-consistent thermodynamics (and to avoid unphysical entropy—see dashed line in Fig. 4). It is interesting to note here that a similar double-peak structure of the magnetic specific heat has been found in the triangular antiferromagnet NiGa_2S_4 [16].

In the last figure (Fig. 10) the initial magnetic susceptibility (for $h = 0$) is shown vs temperature for various concentrations

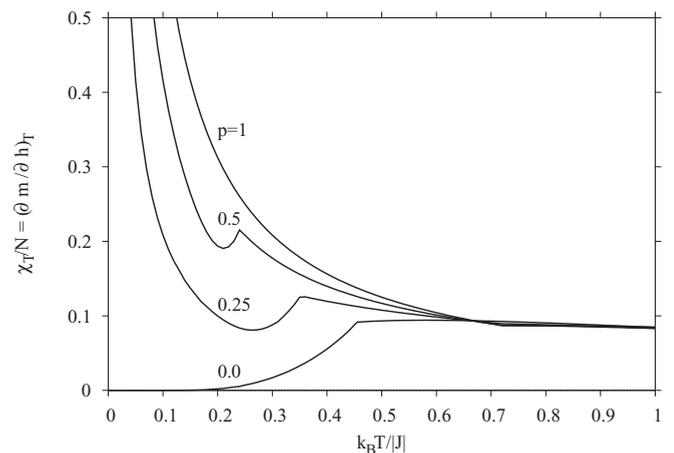


FIG. 10. Magnetic isothermal susceptibility χ_T/N per lattice site vs dimensionless temperature $k_B T/|J|$. Different curves correspond to various concentrations p .

p . In this case only the finite peaks connected with the phase transition (Néel) temperature are seen. For $p > 0$ the susceptibility diverges at $T = 0$, which is connected with the rapid rearrangement of the ground state from $m_A = -m_B = 1/2$ and $m_C = 0$ configuration (for $h = 0$) to the configuration characterized by $m_A = -m_B = 1/2$ and $m_C = 1/2$, which occurs for $0 < h/|J| < 3/2$. Moreover, a divergence of χ_T for $p = 1$ and $T = 0$, and lack of peak for $T > 0$, confirms the phase transition in the ground state for a triangular antiferromagnet, in accordance with previous discussion. It can be noted from Figs. 9 and 10 that both specific heat and susceptibility curves present a correct thermodynamic behavior in the limits $T \rightarrow 0$ and $T \rightarrow \infty$.

IV. SUMMARY AND FINAL CONCLUSIONS

In this paper we modified the PA method in order to adopt it for frustrated systems. The Kaya-Berker model presents an ideal benchmark for testing the method, since the degree of frustration is controlled by the dilution parameter p . Moreover, the exact solutions in the limits $p = 0$ and $p = 1$ are known. Figure 2 illustrates that the results are extraordinarily sensitive to the approximate methods. The occurrence of unphysical solutions for $0 < p < 1$, or the lack of complete thermodynamic description, are the main problems in all former analytical approaches. The MC simulations are very useful; however, in the frustrated systems they are difficult to perform in the low-temperature region.

The present method, although relatively simple and based on the approximate Gibbs energy, gives a physically correct description of all thermodynamic quantities in a frustrated system. It allows to eliminate the unphysical solutions which result from the unmodified PA method. In particular, the modified PA method gives a qualitatively correct phase diagram as well as the exact energy and magnetization of the ground state in the full (p, h) space (Sec. III). An important finding is that the critical temperature tends to zero when $p \rightarrow 1$. This is contrary to HSMF and EFT methods, however, in agreement with the tendency seen from the MC and exact Wannier result [1]. It has also been shown that the ordered phase for $h = 0$, characterized by $m_A = -m_B$ and $m_C = 0$, corresponds to the minimum of modified Gibbs potential, and such a phase is in agreement with MC results.

In conclusion, the modified PA method gives a physically correct description of the Kaya-Berker model. The results are most accurate in low temperatures ($T \leq T_c$) and, in particular, are exact in the ground state. Taking into account the completeness of the method, the description of the model is better than that obtained by any other analytical method used to date. A price for this completeness is a less accurate description for higher temperatures ($T > T_c$), consisting in cutting off the paramagnetic maximum of specific heat and flattening of entropy and correlation functions. However, such a cutting off was necessary in order to obtain self-consistent thermodynamics in all temperatures and to eliminate the unphysical solutions. It should be noted that an example of similar radical cutting off has already been known in thermodynamics: the Maxwell construction for van der Waals

equation of state. The flattening of the entropy and correlation function for $T_c < T < T_f$ appears to be most spectacular for a triangular lattice ($p = 1$), since $T_c \rightarrow 0$ and the $T_c - T_f$ distance is the longest. This effect of flattening vanishes gradually with increase of dilution.

From the analysis of the above results it becomes obvious that the occurrence of the characteristic temperature, $k_B T_f/|J| = 0.721$, for which such quantities as the correlation functions, or entropy, present a kink, is an artifact of the approximation. Fortunately, this effect occurs in the paramagnetic region, far above the critical temperatures, and has no destructive influence on the low-temperature behavior (i.e., in the most interesting regime) and on the ground state where the method is most accurate. It is also worth mentioning that in the limit $T \rightarrow \infty$, where entropy saturates, we again obtain correct thermodynamic behavior of all calculated quantities.

As a final remark, we hope that the presented approach can also be useful for investigations of other spin systems with geometrical frustrations.

APPENDIX: THE VARIATIONAL EQUATIONS FOR $h = 0$

In order to obtain the detailed form of variational equations without external field ($h = 0$) one should note that the spontaneously ordered phase is characterized by $m_A = -m_B \equiv m$ and $m_C = 0$. Then, Eqs. (31) reduce to $\partial G/\partial m = 0$. For the sake of simplicity we introduce a short notation:

$$\begin{aligned} R_1 &\equiv \rho_{AB}^{++} = \frac{1}{4} + c_{AB}, & R_2 &\equiv \rho_{AB}^{+-} = \frac{1}{4} + m - c_{AB}, \\ R_3 &\equiv \rho_{AB}^{-+} = \frac{1}{4} - m - c_{AB}, & R_4 &\equiv \rho_{AB}^{--} = \frac{1}{4} + c_{AB}, \end{aligned} \quad (\text{A1})$$

and

$$\begin{aligned} A_1 &\equiv \rho_{AC}^{++} = \rho_{BC}^{--} = \frac{1}{4} + \frac{1}{2}m + \left(\frac{1}{2} + 2c_{AB}\right)c', \\ A_2 &\equiv \rho_{AC}^{+-} = \rho_{BC}^{-+} = \frac{1}{4} + \frac{1}{2}m - \left(\frac{1}{2} + 2c_{AB}\right)c', \\ A_3 &\equiv \rho_{AC}^{-+} = \rho_{BC}^{+-} = \frac{1}{4} - \frac{1}{2}m - \left(\frac{1}{2} + 2c_{AB}\right)c', \\ A_4 &\equiv \rho_{AC}^{--} = \rho_{BC}^{++} = \frac{1}{4} - \frac{1}{2}m + \left(\frac{1}{2} + 2c_{AB}\right)c'. \end{aligned} \quad (\text{A2})$$

With the help of the above coefficients the equilibrium condition $\partial G/\partial m = 0$ takes the form of

$$\ln\left(\frac{R_2}{R_3}\right) + p \ln\left(\frac{A_1 A_2}{A_3 A_4}\right) = 2\left(\frac{2}{3} + p\right) \ln\left(\frac{1/2 + m}{1/2 - m}\right). \quad (\text{A3})$$

In turn, from Eq. (32) we obtain

$$\frac{|J|}{k_B T} (1 + 4pc') = 4pc' \ln\left(\frac{A_2 A_3}{A_1 A_4}\right) + \ln\left(\frac{R_2 R_3}{R_1 R_4}\right), \quad (\text{A4})$$

and Eq. (33) leads to the result

$$\frac{|J|}{k_B T} = \ln\left(\frac{A_2 A_3}{A_1 A_4}\right). \quad (\text{A5})$$

Equations (A3)–(A5) form a set of three variational equations for m , c_{AB} , and c' . However, Eq. (A5) should be used only if $|c'| \leq 1/4$. If this is not the case, according to the discussion presented in the theoretical section (Sec. II C), we should assume $c' = -1/4 = \text{const}$. Then, only two variational equations [Eqs. (A3) and (A4)] are effective. It has been

checked by the direct numerical calculation of the Gibbs functional that such a choice of m , c_{AB} , and c' minimizes

the Gibbs energy in the physical range of these parameters, whereas $h = 0$.

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