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STATISTICAL

Some Upper Bounds for the Critical Temperature for Ising Model with Four-spin Interactions

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Abstract Upper bounds for the critical temperature of Ising models with different types of four-spin interactions on honeycomb and square lattices, which act only between the nearest-neighbor sites or to the nearest- and next-nearest-neighbor sites in addition to the conventional pair interactions, are obtained, using an exact relation for the two-spin correlation functions and rigorous inequalities for the spin correlation functions.

Keywords Classical spin models · Critical couplings · Rigorous results

1 Introduction

The Ising model with nearest-neighbor pair interactions is one of the most extensively studied systems in statistical mechanics. Some rigorous solutions have been given for this model for certain two-dimensional lattices. In this work, we will focus our attention to the Ising models where we will also consider four-spin interactions in addition to the conventional nearest-neighbor pair interactions. In general, the four-spin interaction added to the nearest-neighbor pair interactions can be used to describe reentrant phase diagrams and tricritical behavior. For the Ising model with a four-spin interaction in addition to the conventional nearest-neighbors pair interactions, a few exact solutions have also been obtained for special lattices [1]. These four-spin interaction models are also connected with the eight vertex model [2, 3], which exhibits nonuniversal critical behavior [4]. Experimentally, the models with multispin interactions have been used to describe various physical systems [5–10].

Theoretically, the effect of the multispin interaction on critical properties of various models has been studied within various methods [1, 2, 11–20]. Among the various theoretical methods, the effective field (EFT)-type calculations play an important role when one has to rely on an approximate description of the major aspects of the physical phenomena. Very recently, few authors [21–26] have applied the effective field-type theories, including mean-field calculations, to the Ising model with various types of four-spin interactions and to the Blume–Capel and Blume–Emery–Griffiths models [27, 28]. The four-spin interaction models, as shown in the references, can be applied to study ferroelectric models [3], collinear-ordered two-sublattice magnets [9], fcc binary alloys [5], and liquid bilayers [8]. Also important is its effect on the critical behavior of Ising models [15, 16].

On the other hand, correlation inequalities combined with exact identities are useful in obtaining rigorous results in statistical mechanics. Among the various questions that are resolved by them, one is the decay of correlation functions. The decay of correlation functions gives information about the critical couplings of the statistical mechanical models. In this work, starting from correlation identities for the Ising model with

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two- and four-spin interactions and using correlation inequalities, we obtain rigorous upper bounds for the critical temperature. Upper bounds for the critical temperature $\overline{T}_c$, for Ising and multicomponent spin systems have been obtained by showing, for $T > T_c$, the exponential decay of the two-point function [29–31]. Spin correlation inequalities and their iteration have been used by Brydges et al. [30], Simon [31], and Lieb [32]. The inequality used in Ref. [32] and its iteration can, in principle, be applied to obtain a sequence of temperatures that converge to the critical temperature. This procedure has been applied for the standard Ising model [33] and for the spin $S = 1$ BEG model [34, 35].

The aim of the present work is to obtain rigorous upper bounds for the critical couplings of the spin-1/2 model with nearest-neighbor pair interactions and four-spin interactions in two-dimensional lattices. The method we will employ is based on an exact two-point correlation function identity and rigorous inequalities for the correlation functions. Thus, our results are rigorous upper bounds for the critical temperature of the model. The results are comparable to others calculations with the advantage of representing rigorous limits for the true critical temperature.

In Section 2, we present the derivation of the correlation identities for the Ising model with nearest-neighbor pair interactions and four-spin interactions [24, 25, 27, 28]. In Section 3, we apply these identities to the $z = 3$ and $z = 4$ planar lattices. We will use models that have been used before [19, 25, 26] for the four-spin interactions. Next, in Section 4, we apply the correlation inequalities to these identities to obtain the upper bounds for T_c.

The procedure to improve this bound for the nearest-neighbor pair interactions and four-spin interaction Ising model is as follows: starting from a two-point correlation function identity, a generalization of Callen's identity [36] for this model [1], and using Griffiths first and second inequalities (Griffiths I, II) [37–39] and Newman's inequalities [38, 40], we establish the inequality for the exact equation of the two-point function, $< S_0 S_l >$, as

$$< S_0 S_l > \leq \sum_j a_j < S_j S_l >, \quad 0 \leq a_j \leq 1, \tag{1}$$

which when iterated [31], implies exponential decay for $T > T_c$. Griffiths's, Newman's, and Lebowitz's inequalities have been generalized to systems with interactions involving an arbitrary number of spins [38, 41, 42]. The results for the planar models honeycomb ($z = 3$) and square ($z = 4$) lattices are presented.

2 Derivation of the Correlation Identity

We write the hamiltonian for the Ising model with two- and four-spin interactions, as

$$H = -\sum_{ij} J_{ij} S_i S_j - \sum_{ijkl} K_{ijkl} S_i S_j S_k S_l, \tag{2}$$

where $S_i = -1, +1$, $J_{ij} > 0$ is the exchange constant between pairs of nearest neighbors and K_{ijkl} is the coupling between any four spins in the lattice. For any lattice there usually exists more than one possibility for the choice of the four-spin interaction. We will use three different models for the four-spin interaction, to be described later.

We present the deduction of a generalization of Callen's identity for the model which has been obtained previously by Saber [24]. In order to calculate the expectation value of S_i we write $H = H_i + H'$, where

$$H_i = -S_i \Big(\sum_j J_{ij} S_j - \sum_{jkl} K_{ijkl} S_j S_k S_l \Big). \tag{3}$$

Here j,k,l are neighbors of i and H' corresponds to the Hamiltonian of the rest of the lattice. Consequently $[H_i, H'] = 0$ and we can write $e^{-\beta H} = e^{-\beta(H_i + H')} = e^{-\beta H_i} e^{-\beta H'}$. It is straightforward to obtain the relation,

$$< S_i > = \left\langle \frac{Tr_i e^{-\beta H_i} S_i}{Tr_i e^{-\beta H_i}} \right\rangle \tag{4}$$

Explicitly operating the trace over site i, $Tr_i(.) = \sum_{S_i}(.)$, we get

$$<S_i> \;=\; \left\langle \tanh \left(\beta \sum_j J_{ij} S_j + \beta \sum_{jkl} K_{ijkl} S_j S_k S_l \right) \right\rangle. \tag{5}$$

By using the differential operator defined by the following relations,

$$e^{\lambda \nabla_1} f(x_1, x_2, x_3, x_4)$$
$$= f(x_1 + \lambda, x_2, x_3, x_4), \quad \nabla_1 = d/dx_1. \tag{6}$$

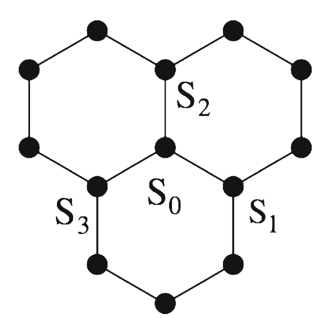

Fig. 1 Honeycomb lattice with nearest-neighbor pair interactions and four-spin interactions

Similar definitions for $e^{\lambda\nabla_j}f(x_1,x_2,x_3,x_4)$ and $j=2,3,4$. Noticing that $S_i^2=1$, we have

$$e^{\gamma S_i}=\cosh(\gamma)+S_i\sinh(\gamma). \tag{7}$$

Applying (6) and (7), one can easily rewrite (5), which is exact, in the form

$$<S_i> = \left\langle \prod_j \left[\cosh(J_{ij}\nabla)+S_j\sinh(J_{ij}\nabla)\right] \times \prod_{jkl}\left[\cosh(K_{ijkl}\nabla)+S_j\sinh(K_{ijkl}\nabla)\right]\right\rangle \times \tanh(\beta x)|_{x=0}. \tag{8}$$

Let us use the site $i=0$ as a reference and let $F(S)$ be any function of the spin variables, except S_0. The following expression is also exact:

$$<F(S)S_0> = \left\langle (F(S))\prod_j \left[\cosh(J_{ij}\nabla)+S_j\sinh(J_{ij}\nabla)\right] \times \prod_{jkl}\left[\cosh(K_{ijkl}\nabla)+S_j\sinh(K_{ijkl}\nabla)\right]\right\rangle \times \tanh(\beta x)|_{x=0}, \tag{9}$$

where j, k, and l are neighbors of 0.

3 Honeycomb Lattice

In this section, we study the honeycomb lattice. Let S_0 denote the center spin and S_1, S_2, and S_3 denote the nearest neighbors spins of site 0 (shown in Fig. 1). Defining $F(S)=S_r$, we obtain from (9), after a straightforward calculation, the following exact relation for the two-spin correlation function $<S_0S_r>$,

$$<S_0S_r> = A\sum_j <S_jS_r> + B<S_1S_2S_3S_r>, \tag{10}$$

where $j=1,2,3$ are neighbor sites of 0, and

$$A=\frac{1}{4}\left[\tanh(3\beta J+\beta K)+\tanh(\beta J-\beta K)\right] \tag{11}$$

and

$$B=\frac{1}{4}\left[\tanh(3\beta J+\beta K)-3\tanh(\beta J-\beta K)\right]. \tag{12}$$

Using Griffiths II in the second term of the previous equation, $<S_1S_2S_3S_r> \geq <S_1S_r><S_2S_3>$, and noticing that $A>0$ and $B<0$, we get,

$$<S_0S_r> \leq A\sum_j <S_jS_r> - |B|\,(<S_1S_r><S_2S_3>). \tag{13}$$

We obtain,

$$<S_0S_r> \leq \sum_j a_j <S_jS_r> \tag{14}$$

where $a_j=3A-|B|<S_2S_3>_{1D}$. We have bound the resulting two-point function occurring in the previous results, (13), from below with the two-point function of a one-dimensional infinite chain (which follows from Griffiths II). In other words, we have used the fact that $<S_iS_j> \geq <S_iS_j>_{1D}$ (the subscript 1D denotes the correlation between S_i and S_j on a one-dimensional chain), which follows from the second Griffiths inequality. The two-point function of the one-dimensional infinite chain of the nearest-neighbor pair interaction Ising model, i.e., $<S_2S_3>_{1D}$ is the exact spin correlation function separated by two sites, given by,

$$<S_2S_3>_{1D} = \tanh^2\beta J. \tag{15}$$

4 Square Lattice

In this section, we study the four-spin interaction on the square lattice using three different models (denoted by A, B, and C). Model A is similar to that used in the honeycomb lattice, and models B and C have been studied before [16, 19, 25, 26]. Let S_0 denote the center spin; S_1, S_2, S_3, and S_4 denote the nearest-neighbor spins of site 0; and S_5, S_6, S_7, and S_8 denote the next-nearest neighbors of site 0 (in Fig. 2, we show the square lattice with two- and four-spin interactions). The four-spin interaction in model A couples any three nearest neighbor sites of the center site 0; in other words, we consider $S_0S_1S_2S_3$, $S_0S_2S_3S_4$, $S_0S_3S_4S_1$, and $S_0S_4S_1S_2$. The four-spin interaction in model B couples any four next-nearest neighbor sites of the vertices of all unit squares; or, we consider $S_0S_1S_2S_5$, $S_0S_2S_3S_6$, $S_0S_3S_4S_7$, and $S_0S_1S_4S_8$. In model C, only the spins on the vertices of alternate unit squares are coupled with four-spin interaction, or $S_0S_1S_2S_5$ and $S_0S_3S_4S_7$. We also consider the nearest-neighbor pair interaction.

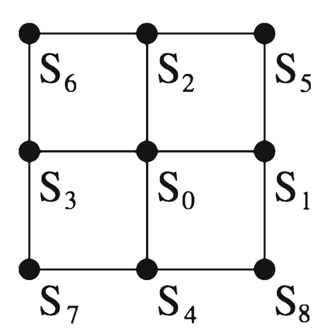

Fig. 2 Square lattice with nearest-neighbor pair interactions and four-spin interactions

As before, defining $F(S) = S_r$, we obtain from (9), after a straightforward calculation, the following exact relations for the two-spin correlation function $<S_0 S_r>$, for the three models defined in the preceding paragraph.

(a) Model A:

$$<S_0 S_r> = A \sum_j <S_j S_r> + B \sum_{jkl} <S_j S_k S_l S_r>, \tag{16}$$

where $j, k, l = 1, 2, 3, 4$ are neighbor sites of 0, and

$$A = \frac{1}{8} [\tanh(4\beta J + 4\beta K) + 2 \tanh(2\beta J - 2\beta K)] \tag{17}$$

and

$$B = \frac{1}{8} [\tanh(4\beta J + 4\beta K) - 2 \tanh(2\beta J - 2\beta K)] \tag{18}$$

Using Griffiths II in the second term of the previous equation, $<S_j S_k S_l S_r> \geq <S_j S_r><S_k S_l>$, and noticing that $A > 0$ and $B < 0$, we get,

$$<S_0 S_r> \leq \sum_j \big[A <S_j S_r> - |B| (<S_j S_r><S_2 S_3>_{1D}) \big]. \tag{19}$$

We obtain

$$<S_0 S_r> \leq \sum_j a_j <S_j S_r>, \tag{20}$$

where $a_j = 4A - 4|B|<S_2 S_3>_{1D}$ and, as before, we bound the resulting two-point function occurring in the previous result, (19), from below with the two-point function, separated by two sites of the one-dimensional infinite chain of the nearest-neighbor pair interaction Ising model. i.e, $<S_2 S_3>_{1D}$ [see (15)].

(b) Model B:

$$\begin{aligned}<S_0 S_r> = {} & A \sum_j <S_j S_r> + B \sum_{jkl} <S_j S_k S_l S_r> \\ & + C \sum_{jkl} <S_j S_k S_l S_m S_n S_r> \\ & + D \sum_{jkl} <S_j S_k S_l S_m S_n S_o S_p S_r>, \end{aligned} \tag{21}$$

where $j, k, l, m, n, o, p = 1, 2, 3, 4, 5, 6, 7, 8$ are nearest-neighbor and next-nearest-neighbor sites of 0, and the coefficient A is given by the equality

$$\begin{aligned} A = \frac{1}{16} \big[& \tanh(4\beta J + 4\beta K) + 3 \tanh(4\beta J + 2\beta K) \\ & + \tanh(4\beta J - 2\beta K) - 2 \tanh(2\beta K) \\ & - \tanh(4\beta K) + 3 \tanh(4\beta J) \\ & + \tanh(2\beta J + 4\beta K) + 4 \tanh(2\beta J + 2\beta K) \\ & + 6 \tanh(2\beta J) + 4 \tanh(2\beta J - 2\beta K) \\ & + \tanh(2\beta J - 4\beta K) \big], \end{aligned} \tag{22}$$

B, by the equality

$$\begin{aligned} B = \frac{1}{16} \big[& 6 \tanh(2\beta K) + \tanh(4\beta K) \\ & + 7 \tanh(4\beta J + 4\beta K) + 7 \tanh(4\beta J + 2\beta K) \\ & - 3 \tanh(4\beta J) - 3 \tanh(4\beta J - 2\beta K) \\ & - 3 \tanh(2\beta J + 4\beta K) - 4 \tanh(2\beta J + 2\beta K) \\ & - 2 \tanh(2\beta J) - 4 \tanh(2\beta J - 2\beta K) \\ & - 3 \tanh(2\beta J - 4\beta K) \big], \end{aligned} \tag{23}$$

C, by the equality

$$\begin{aligned} C = \frac{1}{16} \big[& - 6 \tanh(2\beta K) + \tanh(4\beta K) \\ & + 7 \tanh(4\beta J + 4\beta K) - 7 \tanh(4\beta J + 2\beta K) \\ & - 3 \tanh(4\beta J) + 3 \tanh(4\beta J - 2\beta K) \\ & + 3 \tanh(2\beta J + 4\beta K) - 4 \tanh(2\beta J + 2\beta K) \\ & + 2 \tanh(2\beta J) - 4 \tanh(2\beta J - 2\beta K) \\ & + 3 \tanh(2\beta J - 4\beta K) \big], \end{aligned} \tag{24}$$

and D, by the equality

$$\begin{aligned} D = \frac{1}{16} \big[& \tanh(4\beta J + 4\beta K) \\ & - 3 \tanh(4\beta J + 2\beta K) - \tanh(4\beta J - 2\beta K) \\ & + 2 \tanh(2\beta K) - tanh(4\beta K) + 3 \tanh(4\beta J) \\ & - \tanh(2\beta J + 4\beta K) + 4 \tanh(2\beta J + 2\beta K) \\ & - 6 \tanh(2\beta J) + 4 \tanh(2\beta J - 2\beta K) \\ & - \tanh(2\beta J - 4\beta K) \big]. \end{aligned} \tag{25}$$

The coefficients A and C are >0 and <0, respectively, for all values of K up to $K = 2J$; $B < 0$ for values of K up to $K = 0.4J$, and $D > 0$ is very small compared to A. Therefore, within those limits, we can use Griffiths II in the second term (B term), $<S_j S_k S_l S_r> \geq <S_j S_r><S_k S_l>$, and Newman's inequality

($<S_iF> \leq \sum_j <S_iS_j><dF/dS_j>$, where F are polynomials with positive coefficients) in the third (i.e. C) term coupled with Griffiths I ($<S_A> \leq 1$), $<S_jS_kS_lS_mS_nS_r> \leq <S_jS_r>$ of the previous equation, to get that

$$<S_0S_r> \leq \sum_j \big[A<S_jS_r> - |B|(<S_jS_r> < S_2S_3 >_{1D}) + C(<S_jS_r>)\big]. \quad (26)$$

We obtain the inequality

$$<S_0S_r> \leq \sum_j a_j<S_jS_r>, \quad (27)$$

where $a_j = 4A - 4|B|<S_2S_3>_{1D} + 5C$ and $<S_2S_3>_{1D}$ is the exact spin correlation function separated by two sites of the one-dimensional infinite chain of the nearest-neighbor pair interaction Ising model [see (15)].

(c) Model C:

$$<S_0S_r> = A\sum_j <S_jS_r> + B\sum_{jkl} <S_jS_kS_lS_r> + C\sum_{jkl} < S_jS_kS_lS_mS_nS_r >, \quad (28)$$

where $j, k, l, m, n = 1, 2, 3, 4, 5, 6, 7, 8$ are nearest-neighbor and next-nearest-neighbor sites of 0, and

$$A = \frac{1}{16}\big[3\tanh(4\beta J + 2\beta K) - 2\tanh(2\beta K) + \tanh(4\beta J - 2\beta K) + 4\tanh(4\beta J) + 4\tanh(2\beta J + 2\beta K) + 8\tanh(2\beta J) + 4\tanh(2\beta J - 2\beta K)\big], \quad (29)$$

$$B = \frac{1}{8}\big[(5\tanh(4\beta J + 2\beta K) + 2\tanh(2\beta K) - \tanh(4\beta J - 2\beta K) - 4\tanh(2\beta J + 2\beta K) - 4\tanh(2\beta J - 2\beta K)\big], \quad (30)$$

and

$$C = \frac{1}{16}\big[3\tanh(4\beta J + 2\beta K) - 2\tanh(2\beta K) + \tanh(4\beta J - 2\beta K) + 4\tanh(2\beta J + 2\beta K) + 4\tanh(2\beta J - 2\beta K) - 4\tanh(4\beta J) - 8\tanh(2\beta J)\big]. \quad (31)$$

The coefficients A and C are >0 and <0, respectively, for all values of K; $B < 0$ for values of K up to $K = 0.75J$. Therefore, within those limits, we can use Griffiths II in the second term (B term), $<S_jS_kS_lS_r> \geq <S_jS_r><S_kS_l>$, and Newman's inequality ($<S_iF> \leq \sum_j <S_iS_j><dF/dS_j>$, where F are polynomials with positive coefficients) combined with Griffiths I ($<S_A> \leq 1$), in the third (i.e., C) term, $<S_jS_kS_lS_mS_nS_r> \leq <S_jS_r>$ of the previous equation, to get the inequality

$$<S_0S_r> \leq \sum_j \big[A<S_jS_r> - |B|(<S_jS_r><S_2S_3>_{1D}) + 5C(<S_jS_r>)\big]. \quad (32)$$

We obtain

$$<S_0S_r> \leq \sum_j a_j<S_jS_r>, \quad (33)$$

where $a_j = 4A - 4|B| < S_2S_3 >_{1D} + 5C$ and $< S_2S_3 >_{1D}$ is the exact spin correlation function separated by two sites of the one-dimensional infinite chain of the nearest-neighbor pair interaction Ising model [see (15)].

5 Numerical Results

Evaluating numerically the value of T such that $\sum a_j \leq 1$, $a_j > 0$, we obtain, by sufficient condition , the upper bounds for T_c. The equations obtained from these conditions, which are satisfied by T_c, are (14) for $d = 2$, $z = 3$, and (20), (27), and (33) for $d = 2$, $z = 4$ and models A, B, and C, respectively. In Fig. 3, we show the previous equations for kT_c/J, as a function of K/J. In

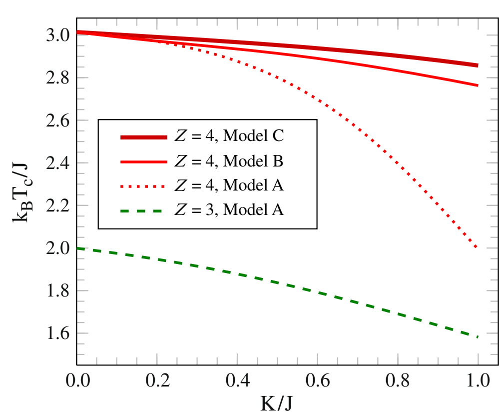

Fig. 3 (Color online) Critical temperature as a function of the four-spin coupling K/J for the honeycomb and square lattices

other words, Fig. 3 shows the dependence of the critical temperature on the four-spin interaction coupling.

The numerical values for $K = 0$, which corresponds to the bilinear Ising model, obtained from this method, are

$$\begin{aligned} d = 2, z = 3: \quad & \frac{kT_c}{J} = 1.99881 \\ d = 2, z = 4, \text{ Models A, B, and C}: \quad & \frac{kT_c}{J} = 3.01399. \end{aligned} \tag{34}$$

For the honeycomb lattice ($z = 3$), this value can be compared with the mean-field (MFA) result ($kT_c/J = 3.0$), the EFT approximation ($kT_c/J = 2.104$), the Bethe–Peierls result ($kT_c/J = 1.804$), and the exact result [43–45] ($kT_c/J = 1.518653$). For the square lattice ($z = 4$), this value can be compared with the MFA result ($kT_c/J = 4.0$), the EFT approximation ($kT_c/J = 3.088$ and $kT_c/J = 3.616$), the Bethe–Peierls result ($kT_c/J = 2.8854$), and the Onsager exact result [46] ($kT_c/J = 2.2691$).

The results in (34), which represent rigorous upper bounds for $K = 0$, improve over the standard mean field results and other effective field results incorporating some correlation [22, 47]. The results for $z = 4$ and $K = 0$ have been previously obtained [33] using the same methodology presented here. The upper bounds, described for the case $K = 0$, will occur for the $K \neq 0$, giving other upper bounds for $T_c(K)$. As can be seen in Fig. 3, the effect of the four-spin coupling in lowering the critical temperature is stronger for model A, followed by model B and model C. As an example, let us calculate the critical temperature for the coupling $K/J = 0.2$. This value is within the limit of validity of (14), (20), (27), and (33).The numerical values of $\frac{kT_c}{J}$ for $K/J = 0.2$ are the following:

$$\begin{aligned} d = 2, z = 3: \quad & \frac{kT_c}{J} = 1.9470 \\ d = 2, z = 4, \text{ Model A}: \quad & \frac{kT_c}{J} = 2.9702 \\ d = 2, z = 4, \text{ Model B}: \quad & \frac{kT_c}{J} = 2.9716 \\ d = 2, z = 4, \text{ Model C}: \quad & \frac{kT_c}{J} = 2.9909 \end{aligned}$$

The importance of the present numerical results lies in the fact that they were obtained using an identity and rigorous inequalities for the two-spin correlation function. For this reason, they represent rigorous upper bounds for the critical temperature.

6 Concluding Remarks

In this work, we have studied the rigorous bounds for the critical temperature of four different planar spin 1/2 models with two- and four-spin interactions. First, we presented the deduction of a correlation identity for the spin correlation functions. We then applied this identity to the honeycomb lattice and to three different four-spin distributions of the planar square lattice to obtain exact identities for the two-spin correlation functions. By means of rigorous correlation inequalities, we studied the decay of the correlation functions. Upper bounds for the critical temperature were obtained by showing , for temperatures greater than the transition temperature, the exponential decay of the correlation functions.

We obtained rigorous results that improve mean field and some EFT-type calculations. This was achieved by the use of an identity for the two-spin correlation function for the model, which is an exact result, and is derived explicitly in the paper, combined with correlation inequalities, which are rigorous and have been obtained by various authors. This is the main advantage of the method—it is rigorous. The numerical results for the critical coupling, which represent the upper bounds, are quite good when compared to other results obtained by approximated methods. Other methods give better numerical results for the critical coupling (more precise results) although not based on rigorous procedures. As a final comment, there is the possibility of using the present method to discuss models with $K < 0$, so that the two- and four-spin interactions compete, with the appearance of a tricritical point. In this case, one has to rely on rigorous inequalities for antiferromagnetic-type interaction models [48].

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