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Upper Bounds on the Critical Temperature of the Ising Model on the Pyrochlore Lattice

Gastão A. Braga · F. C. Sá Barreto · Jander P. Santos

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Abstract A procedure, based on exact relations for the spin-spin correlation function and on rigorous correlation inequalities, is presented and used to obtain upper bounds for the critical temperature of the Ising model on the three dimensional pyrochlore lattice. The exact relations for the correlation functions are constructed from clusters of spins that retain the characteristics of the full model

Keywords Ising model · Pyrochlore lattice · Upper bounds on critical temperature

1 Introduction

The Ising model with nearest-neighbor pair interactions is one of the most extensively studied systems in statistical mechanics, see for instance [1, 2]. Since Onsager's solution to the model on a square lattice [3], many different techniques have been developed to deal with more sophisticated models or lattices others than square. Even so, no analytic solution is known for the Ising model on dimensions bigger

than two where perturbative and numerical simulations are heavily employed to study physical properties of the model. In this paper, we use correlation inequalities to decouple interactions up to a minimum building block that retains the properties of the original lattice. We then determine upper bounds to the model's critical temperature T_c which gives theoretical support to the numerical computations of T_c .

Critical temperatures are dimension and lattice dependent. More recently, statistical mechanics on the pyrochlore lattice, and on its two dimensional counterpart Kagomé lattice, have been attracting a lot of attention: In soft condensed matter, it leads to superfrustration and to the possibility of theoretically realizing a spin liquid, a possible new state of matter [4–6]; in crystal engineering, colloidal Kagomé lattices are used as a substrate to forming superstructures from designed building blocks of organic molecules [7].

The aim of the present work is to obtain rigorous upper bounds for the critical temperature of the spin 1/2 ferromagnetic Ising model with nearest-neighbor pair interaction on the pyrochlore lattice, see Fig. 1. Our bounds are obtained from an exact spin-spin correlation function identity and on an iterative procedure ignited by rigorous spin-spin correlation inequalities. The method itself is inspired on applications of the Simon–Lieb inequality [8, 9], and it is based upon Griffiths [10, 11] and Newman's [11–13] inequalities for ferromagnetic models. Similar ideas have been applied earlier to the standard Ising model [14, 15], for the spin $S = 1$ Blume–Emery–Griffiths model [16, 17], both on a square lattice, and for the transverse Ising model [18]. In a forthcoming paper, we intend to apply the present procedure to the Potts model [19] and to models which show frustration [4–6], specifically the antiferromagnetic Ising model on the Kagomé lattice. For this case, one has to rely on rigorous inequalities for antiferromagnetic interaction models [20].

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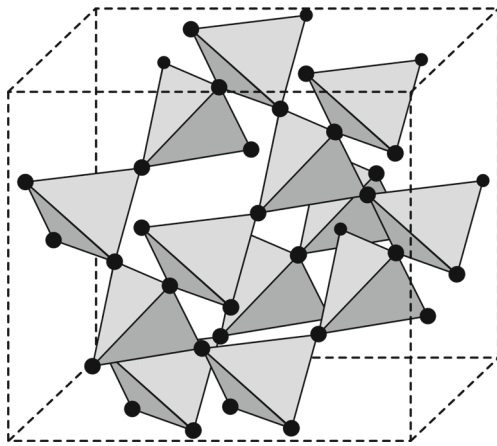


Fig. 1 The Pyrochlore lattice

In words, the method may be described as follows: starting from an identity for the spin-spin correlation, an iterative procedure leads to the exponential decay of correlations (equivalently to a finite correlation length) if a certain condition on the temperature is satisfied. Then, we find, according to our estimates, the lowest temperature up to which the correlation length is finite thus obtaining an upper bound on the critical temperature. The result that comes out is numerically comparable to other approximate (mean/effective field) calculations with the advantage of providing rigorous bounds for the true critical temperature. When one has to rely on an approximate description of the major aspects of the physical phenomena, the effective field type calculations play an important role among the various theoretical methods. On the other hand, correlation inequalities combined with exact identities are useful in obtaining rigorous results in statistical mechanics.

The paper is divided as follows: In Section 2, we derive the correlation identities having as building block a cluster of four spin sites sited on the vertices of a tetrahedron, see Fig. 2. The cluster retains the characteristics of the pyrochlore lattice. In Section 3, we use the identities to obtain mean and effective field approximations which will be denoted by MFA and EFA, respectively. Next, in Section 4, we apply the identities to obtain an equation that expresses the spin-spin correlation function $\langle S_0 S_l \rangle$ as a sum of higher order spin-spin correlations. Using Griffiths' [10, 11] and Newman's inequalities [11–13] to decouple correlations, we replace the above mentioned equation by an inequality of the following type:

$$\langle S_0 S_l \rangle \leq \left[\sum_{\{j:|j|\leq k\}} \alpha_j(T) \right] \langle S_j S_l \rangle, \quad (1)$$

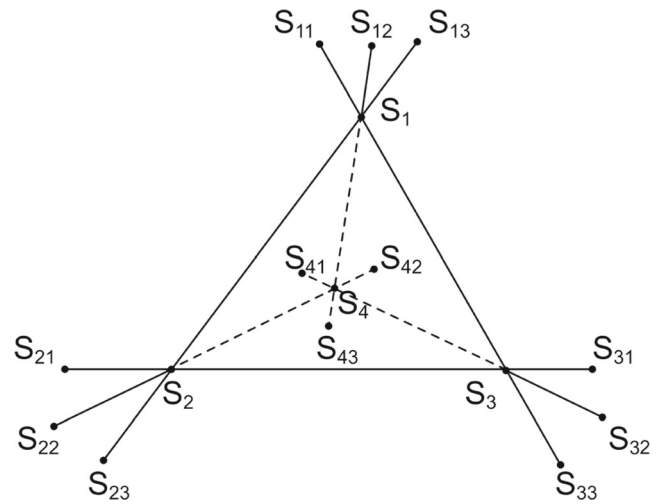


Fig. 2 The vertices of a tetrahedron forming a pyrochlore cluster of four sites

which, when iterated, leads to the exponential decay of spin-spin correlations whenever

$$\sum_{\{j:|j|\leq k\}} \alpha_j(T) < 1.$$

Defining \bar{T}_c so that $\sum_{\{j:|j|\leq k\}} \alpha_j(\bar{T}_c) = 1$, it comes out that the critical temperature T_c must satisfy the bound $T_c < \bar{T}_c$.

2 Derivation of Correlation Identities

We consider a three dimensional box $\Lambda \subset K^3$, where K^3 is the three dimensional pyrochlore lattice, see Fig. 2. Lattice sites will be denoted by letters i, j, \dots and, sometimes, by numbers $1, 2, \dots$. The Hamiltonian for the Ising model with nearest neighbor pair interaction and free boundary conditions on Λ is given by

$$H_\Lambda = -J \sum_{ij} S_i S_j, \quad (2)$$

where the sum is over $i, j \in \Lambda$ with $\|i - j\| = 1$, $S_i = -1, +1$ and $J > 0$ is the exchange constant between nearest neighbor sites. Finite volume expectations, denoted by

$$\langle \cdot \rangle_\Lambda = \frac{\sum_{\{S\}} \cdot e^{-\beta H_\Lambda}}{\sum_{\{S\}} e^{-\beta H_\Lambda}}, \quad (3)$$

where $\beta \equiv 1/kT$ and the sum is over spin configurations in Λ , will be used for computations. Infinite volume limits $\langle \cdot \rangle \equiv \lim_{k \rightarrow \infty} \langle \cdot \rangle_{\Lambda_k}$, for a sequence $\{\Lambda_k\}$ of nested volumes $\Lambda_k \subset \Lambda_{k+1}$, are obtained as a straightforward application of Griffiths first and second inequalities. In what follows, we will take $\beta = 1$ or, equivalently, replace βJ by J .

We look for a representation formula for the spin-spin correlation function $\langle S_i S_l \rangle$ in terms of higher order correlations $\langle S_i S_j \cdots S_k S_l \rangle$ which will allow us to estimate exponential decay rates, as a function of J , as $\|i - l\| \rightarrow \infty$. The identity thus obtained is a generalization of Callen's identity [21] and it will be used latter on for an iteration procedure. The framework presented below applies to the expectations $\langle S_i F(\{S\}) \rangle$, $i = 1, 2, 3, 4$, where F is a spin configuration function supported on finite subsets of K^3 whose distance to i is at least 3. In what follows, we consider a tetrahedron cluster of four sites which retains the main aspects of the pyrochlore lattice, see Fig. 2. We first deduce the representation formula for a single spin correlation $\langle S_i \rangle$, and then we generalize it for multi-spin correlations $\langle S_i F(\{S\}) \rangle$.

For $i = 1, 2, 3, 4$, see Fig. 2, define the single spin Hamiltonian

$$H_i = -J(S_1 S_2 + S_1 S_3 + S_1 S_4 + S_2 S_3 + S_2 S_4 + S_3 S_4) - J \left(\sum_{i=1}^4 S_i \sum_{j=1}^3 S_{ij} \right), \quad (4)$$

where the sum j is over the neighbors of i , and write $H_\Lambda = H_i + H'_\Lambda$, where $H'_\Lambda \equiv H_\Lambda - H_i$. Consequently, $\exp[-H_\Lambda] = \exp[-(H_i + H'_\Lambda)] = \exp[-H_i] \exp[-H'_\Lambda]$ and it is straightforward to obtain the relation

$$\langle S_i \rangle = \left\langle \frac{\sum_{\{S_1, \dots, S_4\}} S_i e^{-H_i}}{\sum_{\{S_1, \dots, S_4\}} e^{-H_i}} \right\rangle. \quad (5)$$

We see the ratio on the r.h.s. of (5) as a function of $a_i \equiv J \sum_{j=1,2,3} S_{ij}$, $i = 1, \dots, 4$ and denote it by $f(a_1, a_2, a_3, a_4)$. Observe that it can be explicitly computed, see Appendix A.1. Since f is an analytic function of the a_i 's then

$$f(a_1 + \lambda, a_2, a_3, a_4) = \sum_{n=0}^{\infty} \frac{[\nabla_1^n f](a_1, a_2, a_3, a_4)}{n!} \lambda^n, \quad (6)$$

where $\nabla_1 = \frac{\partial}{\partial a_1}$ and we may make use of the following differential operator representation formula [22]

$$[e^{\lambda \nabla_1} f](a_1, a_2, a_3, a_4) = f(a_1 + \lambda, a_2, a_3, a_4), \quad (7)$$

with similar representations for $e^{\lambda \nabla_i} f(a_1, a_2, a_3, a_4)$, $i = 2, 3, 4$. Since the ∇ 's commute among themselves, we obtain that (5) can be rewritten as

$$\langle S_i \rangle = \left[\left\langle \prod_{i=1}^4 \prod_{j=1}^3 e^{(J S_{ij}) \nabla_i} \right\rangle \cdot f \right] (0, 0, 0, 0), \quad (8)$$

or, after using that $S^2 = 1$ and $S^3 = S$,

$$\langle S_i \rangle = \left[\left\langle \prod_{i=1}^4 \prod_{j=1}^3 (\cosh(J \nabla_i) + S_{ij} \sinh(J \nabla_i)) \right\rangle \cdot f \right] \times (0, 0, 0, 0), \quad (9)$$

where $[\cosh(\lambda \nabla_1) f](a_1, a_2, a_3, a_4) = [f(a_1 + \lambda, a_2, a_3, a_4) + f(a_1 - \lambda, a_2, a_3, a_4)]/2$ and similarly for $\sinh(\lambda \nabla_1) f$. More generally, let $F(\{S\})$ be a function of spin configurations supported on finite subsets of K^3 whose distance to i is at least 3. Then

$$\begin{aligned} \langle S_i F(\{S\}) \rangle &= \left[\left\langle F(\{S\}) \prod_{i=1}^4 \prod_{j=1}^3 (\cosh(J \nabla_i) + S_{ij} \sinh(J \nabla_i)) \right\rangle \cdot f \right] \times (0, 0, 0, 0), \end{aligned} \quad (10)$$

where f is given by (25) in Appendix A.1, $i = 1, 2, 3, 4$ and the j 's are neighbors of i . Equation (10) is our starting point. We use it in 3 section to obtain mean and effective field approximations. Both of them provide us with an estimate of the critical temperature. In Section 4, we use (10) to obtain an identity which, together with correlation inequalities, provide us with rigorous upper bounds on the critical temperature. We then compare this result with the ones obtained by MF and EF approximations.

3 Mean Field and Effective Field Approximations

The MFA is obtained from (8) by ignoring spin-spin correlations, i.e., by assuming that the identity $\langle \prod_i S_i \rangle = \prod_i \langle S_i \rangle$ holds true which, of course, is only an approximation. Therefore, from (8), we obtain that

$$\langle S_i \rangle = m = \left[\prod_{i=1}^4 e^{3Jm \nabla_i} f \right] (0, 0, 0, 0) \quad (11)$$

which, after applying the differential operators to f , leads to the MF equation

$$m = f(3Jm, 3Jm, 3Jm, 3Jm), \quad (12)$$

where f is given in Appendix A.1. So, explicitly we get

$$m = \frac{e^{6J} \sinh 12Jm + 4 \sinh 6Jm}{e^{6J} \cosh 12Jm + 4 \cosh 6Jm + 3e^{-2J}} \quad (13)$$

For small m , (13) reduces to $m \approx am + bm^3$. Expanding the hyperbolic functions, we get the explicit expressions for a and b ,

$$m = \left(3Je^{6J} + 3J - \frac{1}{4}e^{6J} - \frac{3}{4}e^{-2J} \right) m + (72J^3e^{6J} - 18J^2e^{6J} - 18J^2 + 18J^3)m^3 \quad (14)$$

We obtain for $a = 1$, the value of J_c^{MFA} ,

$$J_c^{MFA} = 0.18699498. \quad (15)$$

We remark that the above value is not the 1-site MFA value of $J_c = 1/6 = 0.1666$ which turns out to be equal to the value obtained for the $z = 6$ cubic lattice.

The EFA is obtained by developing the products on the r.h.s. of (9) and assuming: (1) m is positive and small; (2) as above, we make the approximation $\langle \prod_i S_i \rangle = \prod_i \langle S_i \rangle$. Since m is small, we ignore powers of m bigger than one, i.e., the product $\langle \prod_i S_i \rangle = m^k$ will be assumed zero if $k \geq 2$ so that we may neglect correlations of two or more spins when expanding the above mentioned products. We end up with the identity

$$\begin{aligned} \langle S_i \rangle &= m \\ &= 3m \sum_{i=1}^4 \left[\cosh^2(J\nabla_i) \sinh(J\nabla_i) \prod_{l \neq i} \cosh^3(J\nabla_l) \cdot f \right] \\ &\quad \times (0, 0, 0, 0), \end{aligned} \quad (16)$$

where the sum is over nearest neighbors of i ($i = 1, 2, 3, 4$) and the factor of 3 is due to the contribution from each of the three neighbors of each i . One can check that the above sum is independent of i , leading to the identity $1 = 12A_1$, where A_1 is given in Appendix A.2. Equation $1 = 12A_1$ is satisfied if $J = 0.20999$. Therefore, we obtain

$$J_c^{EFA} = 0.20999. \quad (17)$$

4 Bounds for the Correlation Function and Critical Coupling

In this section, we show that $J_c \geq 0.21380$ can be put on rigorous grounds as a lower bound for J_c , the inverse critical temperature for the Ising model on the pyrochlore lattice.

We replace F by S_r in (10) and we expand the product on the r.h.s. of (10). The geometric setting is the one in Fig. 2. We end up with a representation for $\langle S_i S_r \rangle$ which is rewritten as a sum over higher order correlation functions. Observe that at most 12 spin variables can be correlated in this way. Also, due to spin flip symmetry, only correlations

with an even number of spins are present in this expansion. Denoting by S_{ab} the spin variable S_b which is the nearest neighbor of S_a through the bond ab (a and b stands for the sites i, j, \dots), see Fig. 2, we get

$$\begin{aligned} \langle S_i S_r \rangle &= \sum_{ij} A_n \langle S_{ij} S_r \rangle + \sum_{ij, ik, il} B_n \langle S_{ij} S_{ik} S_{il} S_r \rangle \\ &+ \sum_{ij, ik, \dots, in} C_n \langle S_{ij} S_{ik} S_{il} S_{im} S_{in} S_r \rangle \\ &+ \sum_{ij, ik, \dots, ip} D_n \langle S_{ij} S_{ik} S_{il} S_{im} S_{in} S_{io} S_{ip} S_r \rangle \\ &+ \sum_{ij, ik, \dots, is} E_n \langle S_{ij} S_{ik} S_{il} S_{im} S_{in} S_{io} S_{ip} S_{iq} S_{is} S_r \rangle \\ &+ \sum_{ij, ik, \dots, iu} G_n \langle S_{ij} S_{ik} S_{il} S_{im} S_{in} S_{io} S_{ip} S_{iq} S_{is} S_{it} S_{iu} S_r \rangle, \end{aligned} \quad (18)$$

where, for $i = 1, \dots, 4$, the sums on the r.h.s. of (18) run over nearest neighbor bonds ij, ik, \dots, iu , see Fig. 2. The index n appearing in the coefficients denotes a degeneracy because different pairing of spins generates different multi-spin correlation functions (see Appendix A.2). By degeneracy, we mean that there are different types of terms in each sum in (18), with the same notation (A, B, \dots, G). For example $B_1 \langle S_{11} S_{12} S_{13} S_r \rangle$ is different of the $B_2 \langle S_{11} S_{12} S_{21} S_r \rangle$ (see Fig. 2).

Starting from the above identity, we aim an upper bound for $\langle S_i S_r \rangle$ which will be suitable for iteration. From the explicit representations for A, \dots, G given in Appendix A.2, one can verify numerically that, in the ferromagnetic regime $J > 0$, the coefficients A 's, C 's, and E 's are positive while B 's, D 's, and G 's are negative. The higher order spin correlation functions with negative coefficients (B 's, D 's and G 's) are treated with the use of Griffiths's second inequality $\langle S_{ij} S_{ik} S_{il} S_r \rangle \geq \langle S_{ij} S_r \rangle \langle S_{ik} S_{il} \rangle \geq \langle S_{ij} S_r \rangle \langle S_{ik} S_{il} \rangle$, where $\langle S_{ik} S_{il} \rangle$ is computed on a finite cluster of seven spins in the pyrochlore lattice. This value of $\langle S_{ik} S_{il} \rangle$ is given by $g_2(J)$ in Appendix A.3.

The higher order spin correlation functions with positive coefficients (C 's and E 's) are treated by the use of Newman's inequality

$$\langle S_r F \rangle \leq \sum_j \langle S_r S_j \rangle \langle dF/dS_j \rangle,$$

with F equals to the product of four spin variables. For the C 's terms, we bound the six spin correlation by a sum of five terms of the form $\langle S_{11} S_{12} S_{21} S_{22} \rangle \langle S_{ij} S_r \rangle$ and for the E 's terms we bound the ten-spin correlation by a sum of nine terms of the form $\langle S_{11} S_{12} S_{13} S_{21} S_{22} S_{23} S_{31} S_{32} \rangle$.

We proceed and bound from above the four-spin correlations $\langle S_{11}S_{12}S_{21}S_{22} \rangle$ and eight-spin correlations $\langle S_{11}S_{12}S_{13}S_{21}S_{22}S_{23}S_{31}S_{32} \rangle$ by their values obtained on the limit of an infinite magnetic field applied to all lattice spins except the sites involved in the correlation functions, which we call $g_4(J)$ and $g_8(J)$, respectively (Appendix A.3).

Thus, to find an upper bound, taking into account the results discussed in the preceding paragraphs, we analyze each sum on the r.h.s. of (18) as follows:

1. The first sum is over the 12 bonds indexed by pairs $ij = 11, 12, 13, \dots, 41, 42, 43$, see Fig. 2. By symmetry, one concludes that there 12 A_1 coefficients. The last column of Table 1 in Appendix A.2 provides the degeneracy of A_1 . Therefore, the first sum on the r.h.s. of (18) is bounded above by $12A_1 \langle S_{ij}S_r \rangle_{\max}$, where $\langle S_{ij}S_r \rangle_{\max} \equiv \max_{\{ij=12,\dots,44\}} \{\langle S_{ij}S_r \rangle\}$. Finally, in order to get the inequality (1), we define $\alpha_1(J) \equiv 12A_1$;
2. The second term contains three possible coefficients, B_1, B_2 , and B_3 , which multiply a four-spin correlation and there is a multiplicity factor for each one. All three possibilities, together with its corresponding B factor and degeneracy, are listed in Table 1. This implies that the second sum in (18) is bounded above by

$$[(-4|B_1| - 108|B_2| - 108|B_3|) \langle S_{11}S_{12} \rangle] \langle S_{ij}S_r \rangle_{\max}, \quad (19)$$

where $\langle S_{11}S_{12} \rangle = g_2(J)$ and we define $\alpha_2(J) \equiv [(-4|B_1| - 108|B_2| - 108|B_3|)g_2(J)]$;

3. The third term, which is a sum over six-spin correlation functions, one uses Table 1 to count for the multiplicities of the C 's, and we bound from above this term by

$$[5(36C_1 + 108C_2 + 324C_3 + 324C_4) \langle S_{11}S_{12}S_{21}S_{22} \rangle] \times \langle S_{ij}S_r \rangle_{\max}, \quad (20)$$

where $\langle S_{11}S_{12}S_{21}S_{22} \rangle = g_4(J)$ and we define $\alpha_3(J) \equiv [5(36C_1 + 108C_2 + 324C_3 + 324C_4)g_4(J)]$;

4. The fourth term, which is a sum over eight-spin correlation functions, using Table 1, we bound it from above by

$$[(-|36D_1| - 108|D_2| - 324|D_3| - 324|D_4|) \langle (S_{11}S_{12})^3 \rangle] \langle S_{ij}S_r \rangle_{\max}, \quad (21)$$

which leads to the definition of $\alpha_4(J) \equiv [(-|36D_1| - 108|D_2| - 324|D_3| - 324|D_4|) (g_2(J))^3]$;

5. The fifth term, which is a sum over ten-spin correlation functions, using Table 1, we bound it from above by

$$[9(4E_1 + 108E_2 + 108E_3) \langle S_{11}S_{12}S_{13}S_{21}S_{22}S_{23}S_{31}S_{32} \rangle] \times \langle S_{ij}S_r \rangle_{\max}, \quad (22)$$

where $\langle S_{11}S_{12}S_{13}S_{21}S_{22}S_{23}S_{31}S_{32} \rangle = g_8(J)$ and we define $\alpha_5(J) \equiv [9(4E_1 + 108E_2 + 108E_3)g_8(J)]$;

6. The sixth term, which is a sum over 12-spin correlation functions, using Table 1, we bound it from above by

$$[-12|G_1| (\langle S_{11}S_{12} \rangle)^5] \langle S_{ij}S_r \rangle_{\max} \quad (23)$$

and we define $\alpha_6(J) \equiv [-12|G_1| (g_2(J))^5]$.

Putting the above information together, we may replace the identity (18) by the inequality

$$\langle S_iS_r \rangle \leq \left[\sum_v \alpha_v(J) \right] \langle S_{j_{\max}}S_r \rangle. \quad (24)$$

The above procedure can now be iterated and the exponential decay of correlations will follow as long as the condition $\sum_v \alpha_v(J) < 1$ is satisfied. We recall that the critical value $J_c^{EFA} = 0.20999$, see (17), was obtained under the condition $\alpha_1(J) = 1$. The condition $\alpha_1(J) + \dots + \alpha_6(J) = 1$ leads that $J_c \geq 0.21380$, i.e., spin-spin correlations decay exponentially with the distance as long as $J < 0.21380$.

5 Final Comments

We have determined for the Ising model on a pyrochlore lattice a spin correlation function identity from a finite cluster of spins which has the symmetries of the lattice. The mean-field and the effective field approximations for the critical temperature were obtained. The upper bounds on the critical temperature were also determined, giving $(J_c)^{\text{bounds}} = 0.21380$. This value should be compared to the Monte Carlo estimate of the critical temperature for the ferromagnetic case, which is $J = 0.25$ [6]. We mention that $(J_c)^{\text{bounds}} > (J_c)^{EFA} > (J_c)^{MFA}$ and that the critical value (J_c) of the Ising model on the pyrochlore lattice must satisfy the inequality $(J_c) \geq (J_c)^{\text{bounds}}$. The importance of the present results lies in the fact that they are rigorous. They were obtained after using correlation inequalities to a finite sum representation formula for the spin-spin correlation function. For this reason, they provide rigorous upper bounds for the model critical temperature. As mentioned in the introduction, this procedure will be used by us to study the antiferromagnetic Ising model in the Kagomé lattice, which shows frustration. It can also be applied to other models such as the Blume–Capel spin one model or the Potts model on the Kagomé lattice for which recent results [23] are available. We intend to do this in the future.

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Appendix Pyrochlore Lattice Calculations

A.1 An Expression for $f(a_1, a_2, a_3, a_4)$

In this section, we give an explicit representation formula for

$$f(a_1, a_2, a_3, a_4) = \left\langle \frac{\sum_{\{S_1, S_2, S_3, S_4\}} S_i e^{-\beta H_i}}{\sum_{\{S_1, S_2, S_3, S_4\}} e^{-\beta H_i}} \right\rangle,$$

where H_i is the local Hamiltonian (4) seen as a function of $a_i \equiv J \sum_{j=1,3} S_{ij}$, $i = 1, \dots, 4$. A straightforward computation leads to the identity

$$\begin{aligned} f(a_1, a_2, a_3, a_4) = & [\cosh(6J - a_1 - a_2 - a_3 - a_4) \\ & + \sinh(6J - a_1 - a_2 - a_3 - a_4) \\ & + \sinh(a_1 - a_2 - a_3 - a_4) \\ & - \sinh(a_1 - a_2 + a_3 + a_4) \\ & - \sinh(a_1 + a_2 - a_3 + a_4) \\ & - \sinh(a_1 + a_2 + a_3 - a_4) \\ & - \cosh(6J + a_1 + a_2 + a_3 + a_4) \\ & - \sinh(6J + a_1 + a_2 + a_3 + a_4)] \\ & / [-2 \cosh(a_1 - a_2 + a_3 + a_4) \\ & - 2 \cosh(a_1 + a_2 - a_3 + a_4) \\ & - \cosh(6J - a_1 - a_2 - a_3 - a_4) \\ & - \sinh(6J - a_1 - a_2 - a_3 - a_4) \\ & - 2 \cosh(a_1 - a_2 - a_3 - a_4) \\ & - \cosh(2J + a_1 + a_2 - a_3 - a_4) \\ & + \sinh(2J + a_1 + a_2 - a_3 - a_4) \\ & - \cosh(2J + a_1 - a_2 + a_3 - a_4) \\ & + \sinh(2J + a_1 - a_2 + a_3 - a_4) \\ & + \sinh(2J + a_1 - a_2 - a_3 + a_4) \\ & - \cosh(2J - a_1 + a_2 + a_3 - a_4) \\ & + \sinh(2J - a_1 + a_2 + a_3 - a_4) \\ & - \cosh(2J - a_1 - a_2 + a_3 + a_4) \\ & + \sinh(2J - a_1 - a_2 + a_3 + a_4) \\ & - \cosh(6J + a_1 + a_2 + a_3 + a_4)] \end{aligned}$$

$$\begin{aligned} & - \sinh(6J + a_1 + a_2 + a_3 + a_4) \\ & - \cosh(2J - a_1 + a_2 - a_3 + a_4) \\ & + \sinh(2J - a_1 + a_2 - a_3 + a_4) \\ & - \cosh(2J + a_1 - a_2 - a_3 + a_4) \\ & - 2 \cosh(a_1 + a_2 + a_3 - a_4)]. \end{aligned} \quad (25)$$

Comment: Beyond the single-site cluster theory, the complexity of the algebra rapidly increases and one must thus resort to the use of a computer for the determination of the expansion coefficients on the right hand side of (5). The calculations were developed using an algebraic computation software.

A.2 Coefficients A_n, \dots, G_n of the Pyrochlore Lattice

To determine the coefficients $\Lambda_n \equiv \{A_n, \dots, G_n\}$, appearing in (18), we define,

$$\Lambda_n \equiv \mathcal{F}(\mathcal{S}_j \mathcal{C}_j) \cdot f(a_1, a_2, a_3, a_4) \Big|_{(0,0,0,0)},$$

where f is given by (25) and \mathcal{F} is a symbolic operation to be specified in the second column of Table 1 for the different multi-spin correlation functions. The operators \mathcal{S}_i and \mathcal{C}_i , defined by $\mathcal{S}_i \equiv \sinh(J\nabla_i)$ and $\mathcal{C}_i \equiv \cosh(J\nabla_i)$, $i = 1, 2, 3, 4$, are directly connected to the spin variables appearing in the multi-spin correlation functions in (18).

Remark: In (18), each pairing of spins generates a different multi-spin correlation function. This gives rise to a degeneracy and by this word we mean that different k-spin correlation functions have the same coefficient. For example, the spin correlation function $\langle S_{11} S_{12} S_{13} S_r \rangle$ has a coefficient B_1 , as shown in Table 1, which was obtained from the operation $[(\mathcal{S}_1^3 \mathcal{C}_2^3 \mathcal{C}_3^3 \mathcal{C}_4^3) \cdot f](0, 0, 0, 0)$. There are four spin correlation functions which have the coefficients constructed by the same operation $[(\mathcal{S}_1^3 \mathcal{C}_2^3 \mathcal{C}_3^3 \mathcal{C}_4^3) \cdot f](0, 0, 0, 0)$. This number of identical coefficients is obtained by combinatorial analysis. The degeneracy (λ_n) associated with each coefficient of (18) is given by the numbers $\sum a_n, \dots, \sum g_n$. For example, for the three coefficients B , the degeneracy is given by,

$$\sum_{ij, \dots} b_n = \left(\frac{12!}{(12-p)!p!} \right) = 220,$$

where $p = 3$ is the number $(k-1)$ of the spin variables appearing in the k-spin correlation function, in this case $k = 4$.

We provide in Table 1 the multi-spin correlation functions $\langle S_{ij} \dots S_r \rangle$, the generating operators $\mathcal{F}(\mathcal{S}_j \mathcal{C}_j)$, the associated coefficients Λ_n , and the degeneracy of each term λ_n , of (18).

Table 1 Multi-spin correlation function, generating operators, coefficients, and degeneracy

Multi-spin correlation function	Generating operators	Coefficients	Degeneracy
$\langle S_{ij} \dots S_r \rangle$	$\mathcal{F}(S_j C_j)$	Λ_n	λ_n
$\langle S_{11} S_r \rangle$	$S_1 C_1^2 C_2^3 C_3^3 C_4^3$	A_1	12
$\langle S_{11} S_{12} S_{13} S_r \rangle$	$S_1^3 C_2^3 C_3^3 C_4^3$	B_1	4
$\langle S_{11} S_{12} S_{21} S_r \rangle$	$S_1^2 C_1 S_2 C_2^2 C_3^3 C_4^3$	B_2	108
$\langle S_{11} S_{21} S_{31} S_r \rangle$	$S_1 C_1^2 S_2 C_2^2 S_3 C_3^3 C_4^3$	B_3	108
$\langle S_{11} S_{12} S_{13} S_{21} S_{22} S_r \rangle$	$S_1^3 S_2^2 C_2 C_3^3 C_4^3$	C_1	36
$\langle S_{11} S_{12} S_{13} S_{21} S_{31} S_r \rangle$	$S_1^3 S_2 C_2 S_3 C_3^2 C_4^3$	C_2	108
$\langle S_{11} S_{12} S_{21} S_{22} S_{31} S_r \rangle$	$S_1^2 C_1 S_2^2 C_2 S_3 C_3^2 C_4^3$	C_3	324
$\langle S_{11} S_{12} S_{21} S_{31} S_{41} S_r \rangle$	$S_1^2 C_1 S_2 C_2^2 S_3 C_3^2 S_4 C_4^2$	C_4	324
$\langle S_{11} S_{12} S_{13} S_{21} S_{22} S_{23} S_{31} S_r \rangle$	$S_1^3 S_2^3 S_3 C_3^2 C_4^3$	D_1	36
$\langle S_{11} S_{12} S_{13} S_{21} S_{22} S_{31} S_{32} S_r \rangle$	$S_1^3 S_2^2 C_2 S_3^2 C_3 C_4^3$	D_2	108
$\langle S_{11} S_{12} S_{13} S_{21} S_{22} S_{31} S_{41} S_r \rangle$	$S_1^3 S_2^2 C_2 S_3 C_3^2 S_4 C_4^2$	D_3	324
$\langle S_{11} S_{12} S_{21} S_{22} S_{31} S_{32} S_{41} S_r \rangle$	$S_1^2 C_1 S_2^2 C_2 S_3^2 C_3 S_4 C_4^2$	D_4	324
$\langle S_{11} S_{12} S_{13} S_{21} S_{22} S_{23} S_{31} S_{32} S_{33} S_r \rangle$	$S_1^3 S_2^3 S_3^3 C_4^3$	E_1	4
$\langle S_{11} S_{12} S_{13} S_{21} S_{22} S_{23} S_{31} S_{32} S_{41} S_r \rangle$	$S_1^3 S_2^3 S_3^2 C_3 S_4 C_4^2$	E_2	108
$\langle S_{11} S_{12} S_{13} S_{21} S_{22} S_{31} S_{32} S_{41} S_{42} S_r \rangle$	$S_1^3 S_2^2 C_2 S_3^2 C_3 S_4^2 C_4$	E_3	108
$\langle S_{11} S_{12} S_{13} S_{21} S_{22} S_{23} S_{31} S_{32} S_{33} S_{41} S_{42} S_r \rangle$	$S_1^3 S_2^3 S_3^3 S_4^2 C_4$	G_1	12

A.3 Correlation functions $g_2(J)$, $g_4(J)$, and $g_8(J)$ of the pyrochlore lattice

The correlation functions of two spin occurring in (19), (21) and (23), denoted by $g_2(J)$, were exactly computed on a finite cluster of seven spins in the pyrochlore lattice, calculated in the cluster constituted by the spins S_1 , S_2 , S_3 , S_4 , S_{11} , S_{12} , and S_{13} (see Fig. 2), i.e., the hamiltonian used in the calculations contains only those spins and their interactions. It is given by,

$$g_2(J) = \frac{e^{12J} - 4e^{-2J} + 4e^{6J} - 3e^{-4J} + 2e^{4J}}{e^{12J} + 8e^{6J} + 6e^{4J} + 16 + 24e^{-2J} + 9e^{-4J}}. \quad (26)$$

The four-spin correlation function occurring in (20), denoted by $g_4(J)$, was exactly determined on the limit of an infinite magnetic field applied to all lattice spins except the spins S_1 , S_2 , S_3 , S_4 , S_{11} , S_{12} , S_{13} , S_{21} , and S_{22} (see Fig. 2). All other spins of the lattice have been assigned value $S = 1$.

The hamiltonian used in the calculations contains only the above mentioned spins and their interactions. The value of $g_4(J)$ is given by

$$g_4(J) = [5e^{6J} - 16e^{10J} + e^{-26J} - 8e^{-14J} - 2e^{-22J} + 2e^{-10J} + 7e^{-2J} + 3e^{-6J} + 3e^{-18J} + 4e^{2J} + 2e^{22J} + 2e^{30J} - 6e^{14J} + 2e^{18J} + e^{42J}] / [101e^{6J} + 120e^{10J} + e^{-26J} + 64e^{-14J} + 6e^{-22J} + 114e^{-10J} + 247e^{-2J} + 131e^{-6J} + 19e^{-18J} + 132e^{2J} + 18e^{22J} + 10e^{30J} + 18e^{14J} + 42e^{18J} + e^{42J}] \quad (27)$$

The eight-spin correlation function occurring in (22), denoted by $g_8(J)$ was exactly determined on the limit of an infinite magnetic field applied to all lattice spins except the spins S_1 , S_2 , S_3 , S_4 , S_{11} , S_{12} , S_{13} , S_{21} , S_{22} , S_{23} , S_{31} , and S_{32} .

(see Fig. 2) with similar comments on the hamiltonian as in the preceding paragraph. The value of $g_8(J)$ is given by

$$g_8(J) = [-77e^{6J} - 71e^{10J} - 11e^{-26J} + e^{-30J} - 12e^{-14J} + 36e^{-22J} - 7e^{-10J} + 46e^{-2J} + e^{54J} + 27e^{-6J} - 33e^{-18J} + 11e^{2J} - 10e^{22J} + 2e^{30J} - 21e^{26J} + 89e^{14J} + 28e^{18J} + 4e^{34J} - 3e^{42J}]/[369e^{14J} + 264e^{18J} + e^{54J} + 1031e^{-6J} + 259e^{-18J} + 21e^{-26J} + e^{-30J} + 564e^{-14J} + 108e^{-22J} + 27e^{26J} + 13e^{42J} + 24e^{34J} + 1017e^{-10J} + 1434e^{-2J} + 687e^{6J} + 885e^{10J} + 1179e^{2J} + 234e^{22J} + 74e^{30J}].$$

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