



The second order phase transitions of the Ising model on tetrahedron recursive lattices: Exact results



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ABSTRACT

We investigate the ferromagnetic spin-1/2 Ising model on the so-called tetrahedron recursive lattices with arbitrary coordination numbers. First, the concept of the tetrahedron recursive lattice is introduced which can be considered as the simplest but effective approximation of real tetrahedron lattices which takes into account their basic geometric properties. An explicit analytic formula for exact determining of the values of the critical temperatures of the second order phase transitions simultaneously on all tetrahedron recursive lattices is derived. In addition, an exact explicit expression for the spontaneous magnetization on the simplest tetrahedron recursive lattice with the coordination number $z = 6$ is also found.

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1. Introduction

During last two decades a great interest has been devoted to the experimental investigation of the magnetic properties of various pyrochlore oxides $A_2B_2O_7$, where A is a rare-earth ion and B is usually a transition metal (see, e.g., Ref. [1] and references cited therein). In such systems both A and B sites separately form tetrahedron lattices and, at the same time, either or both sublattices can be magnetic and exhibit ferromagnetic or anti-ferromagnetic type of interaction. Another example of systems exhibiting the tetrahedron structure are the so-called spinels AB_2O_4 with transition metal ions (see, e.g., Ref. [2–4] and references cited therein). The magnetic systems on lattices with tetrahedron structure are nowadays extremely interesting, especially due to the fact that elementary building blocks of these lattices (tetrahedrons) consist of four triangles with common edges and therefore are subject to geometric magnetic frustration [5] when an anti-ferromagnetic model on such kind of lattices is considered (see, e.g., Refs. [1,6,7] as well as references cited therein).

However, from theoretical point of view, it is well known that only rather restricted set of even classical statistical mechanical magnetic models (e.g., ferromagnetic or anti-ferromagnetic Ising or Ising-like models) on real lattices can be solved exactly. All of them are one-dimensional or two-dimensional models in zero external magnetic field (see, e.g., Ref. [8] and references cited

therein). On the other hand, at the moment there does not exist any such model on a real three-dimensional lattice that would be exactly solvable. Of course, being the three-dimensional structure, this conclusion is also valid for the models on the tetrahedron lattices. Therefore, for systematic theoretical investigation of various physical properties of such systems it is necessary to use some kind of approximation. In this situation, when an exact solution of a given model on the tetrahedron lattice does not exist, there are in principle two basic possibilities to proceed in the investigation of the studied problem. First of them is to investigate a more simplified model on the same lattice (e.g., to study the corresponding mean-field model). The second possibility is to study the same model but on an approximative lattice (e.g., on the corresponding recursive lattices in analogy with the Bethe or Husimi lattices) which takes into account basic properties of the real lattice and, at the same time, on which the original model can be analyzed and solved in an exact analytical form or, at least, can be exactly analyzed by using numerical methods. Here, it is important to note that physical results obtained by using an adequate recursive lattice are usually much more better, i.e., they are much more closer to real systems, than the corresponding results obtained by using the mean-field approximation (see, e.g., discussions given in Refs. [9–11] and references cited therein).

In this respect, for example quite recently it was shown that the anti-ferromagnetic Ising model in the presence of the external magnetic field on the simplest pure Husimi lattice, which is the simplest possible approximation of the kagome lattice that takes into account geometric frustration [12], can be solved exactly in fully analytic form [13]. The existence of this solution allows

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authors of Ref. [13] to carry out complete analysis of all possible ground states of the model.

In the present Letter, we shall introduce the corresponding effective and suitable approximation of the real tetrahedron lattices by the so-called tetrahedron recursive lattices, on which various classical statistical mechanical models can be studied exactly at least by using the method of recursion relations.

Thus, the aim of the present Letter is twofold. First, the concept of the tetrahedron recursive lattice is exactly defined and the ferromagnetic spin-1/2 Ising model on this lattice is described and analyzed in the form of the corresponding recursion relations. Second, the efficiency of the approximation is demonstrated on the analysis of the second order phase transitions. In this respect, an exact analytic expression for the positions of the critical temperatures for arbitrary tetrahedron recursive lattices is derived. The value of the critical temperature on the simplest tetrahedron recursive lattice with coordination number $z = 6$ (the recursive lattice which is the most interesting from the phenomenological point of view) is compared to the critical temperature on the real tetrahedron lattice obtained by using the high-temperature series expansion technique [14,15] (which is usually considered as very close to the exact value for the critical temperature on the tetrahedron lattice). As we shall see the difference between these two values of the critical temperature is surprisingly very small (the relative difference is only 4.5% of the value obtained by the high-temperature series expansion technique). This nontrivial result demonstrates the fact that we can suppose that the analysis of various models on the tetrahedron recursive lattices will be rather precise not only at the qualitative level but also it can give rather precise quantitative results.

In addition, an exact analytic expression for the spontaneous magnetization of the ferromagnetic spin-1/2 Ising model on the tetrahedron recursive lattice with the coordination number $z = 6$ is also found.

Although, in the present Letter we investigate only the ferromagnetic spin-1/2 Ising model on the tetrahedron recursive lattices the technique can be simply extended on the models with higher spin values as well as on the models with different kind of interactions, e.g., on the models with anti-ferromagnetic interactions or multisite interactions. We suppose that nontrivial and, at the same time, exact results can be obtained here. We intend to analyze these phenomenologically interesting models in near future.

2. The spin-1/2 Ising model on the tetrahedron recursive lattices

We consider the ferromagnetic spin-1/2 Ising model on the so-called *tetrahedron recursive lattices*. By definition, a *tetrahedron tree* is a connected graph build up solely by elementary tetrahedrons, in which, firstly, every line lies exactly on one tetrahedron, secondly, equal number of tetrahedrons, $q \geq 2$, are connected in each inner site of the graph (i.e., the coordination number of each inner site is $z = 3q$), and, thirdly, every closed cycle lies within single tetrahedron. Then, the *tetrahedron recursive lattice* is obtained in the same way as, e.g., the Bethe lattice is defined from the corresponding Cayley tree (see, e.g., Ref. [8]), i.e., we suppose that we are located deep inside of the graph, where all sites are equivalent to each other (see Fig. 1). Thus, the Hamiltonian of the model is

$$\mathcal{H} = -J \sum_{(ij)} s_i s_j - H \sum_i s_i, \quad (1)$$

where each variable s_i acquires one of the two possible values $\pm 1/2$, $J > 0$ is the nearest-neighbor ferromagnetic interaction parameter, and H is the external magnetic field. In Eq. (1), the first sum runs over all nearest-neighbor spin pairs and the second sum runs over all spin sites.

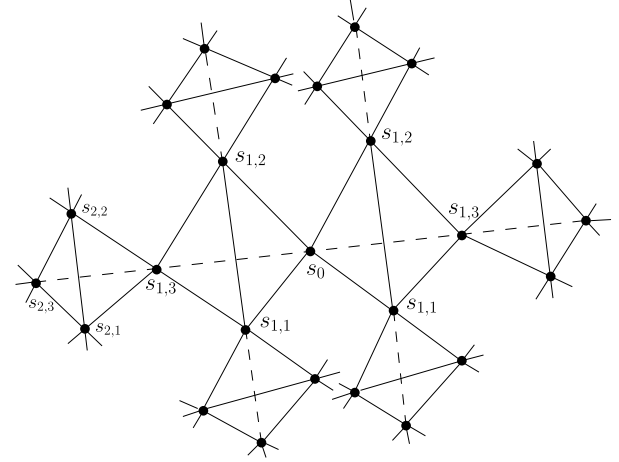


Fig. 1. The tetrahedron recursive lattice with $q = 2$. Site denoted as s_0 is taken to be the central site. The points on the lattice denoted as $s_{1,i}$, $i = 1, 2, 3$, form the first layer of the tetrahedron recursive lattice, etc.

Standardly, the partition function of the model given by Hamiltonian (1) has the following general form

$$Z \equiv \sum_s \exp(-\beta \mathcal{H}) = \sum_s \exp\left(K \sum_{(ij)} s_i s_j + h \sum_i s_i\right), \quad (2)$$

where $\beta = 1/(k_B T)$, T is the temperature, k_B is the Boltzmann constant, $K = \beta J$, and $h = \beta H$. The sum over s in Eq. (2) means the summation over all possible spin configurations on the lattice.

The ferromagnetic model given by Hamiltonian (1) on the tetrahedron recursive lattice with arbitrary q can be studied numerically by using the method of recursion relations in the same way as, e.g., in the case of the Bethe lattices (see, e.g., Ref. [8]). Let us describe it briefly.

If the tetrahedron recursive lattice is cut in the site 0 (see Fig. 1), then the corresponding graph splits into q disconnected identical pieces (subgraphs) and the partition function (2) can be rewritten as follows

$$Z = \sum_{s_0} \exp(h s_0) [g_n(s_0)]^q, \quad (3)$$

where functions $g_n(s_0)$ for $s_0 = 1/2$ and $-1/2$ can be expressed in the form of recursion relations, namely,

$$g_n(s_0) = \sum_{s_{1,1}, s_{1,2}, s_{1,3}} \exp\left\{K [s_0(s_{1,1} + s_{1,2} + s_{1,3}) + s_{1,1}s_{1,2} + s_{1,1}s_{1,3} + s_{1,2}s_{1,3}] + h \sum_{l=1}^3 s_{1,l}\right\} \times \prod_{l=1}^3 [g_{n-1}(s_{1,l})]^{q-1}. \quad (4)$$

It is supposed that the tetrahedron recursive lattice has n layers and $s_{1,l}$, $l = 1, 2, 3$ represent the spin variables of sites which lie on shell 1 (see Fig. 1).

However, from calculational point of view, it is appropriate to rewrite the recursion relations (4) for $g_n(s_0)$ into the form of recursion relations for their ratios

$$x_n(i, t) = g_n(s_0^i) / g_n(s_0^t), \quad i = 0, 1, \quad (5)$$

where $s_0^i = 1/2 - i$ is introduced for possible values of the spin variable and the integer t can be chosen arbitrary from two possible values 0 and 1. The choice is completely free. But once one of

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