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Research articles

Highly macroscopically degenerated single-point ground states as source of specific heat capacity anomalies in magnetic frustrated systems

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ABSTRACT

Anomalies of the specific heat capacity are investigated in the framework of the exactly solvable antiferromagnetic spin-$1/2$ Ising model in the external magnetic field on the geometrically frustrated tetrahedron recursive lattice. It is shown that the Schottky-type anomaly in the behavior of the specific heat capacity is related to the existence of unique highly macroscopically degenerated single-point ground states which are formed on the borders between neighboring plateau-like ground states. It is also shown that the very existence of these single-point ground states with large residual entropies predicts the appearance of another anomaly in the behavior of the specific heat capacity for low temperatures, namely, the field-induced double-peak structure, which exists, and should be observed experimentally, along with the Schottky-type anomaly in various frustrated magnetic system.

1. Introduction

The Schottky-type anomaly in the behavior of the specific heat capacity, i.e., the appearance of the second peak of the specific heat capacity at low temperatures, is experimentally and theoretically observed feature of various frustrated systems. Typical examples are the magnetic systems on the geometrically frustrated lattices with kagome, triangular, or pyrochlore structure (see, e.g., Refs. [1–20], as well as references cited therein). A clear theoretical explanation of this phenomenon is a nontrivial task due to the fact that there does not exist any exactly solvable and, at the same time, physically relevant spin model on real two- or three-dimensional lattices with the presence of the magnetic field based on which it would be possible to understand fundamentally and explain exactly this intriguing phenomenon. In this respect, let us note that even the simplest classical ferromagnetic or antiferromagnetic spin-$1/2$ Ising model is exactly solvable on two-dimensional regular lattices only in zero external magnetic field (see, e.g., Refs. [21–23] and references cited therein).

However, there exists an interesting and important class of lattices, namely, the so-called Husimi-type recursive lattices [24–26], which take into account basic geometrical structure of regular two- or three-dimensional lattices (see, e.g., Refs. [27–29] and references cited therein) and on which various classical spin models can be solved exactly even in the presence of the external magnetic field [30–32]. It is worth mentioning that such models on suitable recursive lattices are able to describe basic properties of real systems at least qualitatively. Therefore, very often, they are appropriate for fundamental understanding of various peculiarities observed by real experiments as well as by numerical simulations.

In this respect, in the present paper, we intend to give a natural explanation of the origin of the Scottky-type anomaly in the behavior of the specific heat capacity in the framework of an exactly solvable antiferromagnetic spin-$1/2$ Ising model in the presence of the nonzero external magnetic field on a geometrically frustrated recursive lattice. As we shall see, the existence of the exact solution of the model allows us to identify the source of the Shottky-type anomaly in specific heat capacity at low temperatures as well as to predict another peculiarity in the behavior of the specific heat capacity directly connected to the Schottky-type anomaly. We shall show that the crucial role for the very existence of various anomalies in the behavior of the specific heat capacity in geometrically frustrated magnetic systems is played by the formation of highly macroscopically degenerated single-point ground states in such systems when temperature tends to zero, which are formed on the borders between various plateau-like ground states and which have well-defined unique thermodynamic properties.

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Finally, although our conclusions are based on the exact analysis of an classical antiferromagnetic spin system, it is worth mentioning that even classical spin models often represent a very good approximation of real frustrated systems (see, e.g., Refs. [5,15,19]).

2. Entropy and residual entropies of the antiferromagnetic spin-1/2 Ising model on the tetrahedron recursive lattice

Thus, consider the antiferromagnetic spin-1/2 Ising model in the presence of the external magnetic field described by the Hamiltonian

$$\mathcal{H} = -J\sum_{\langle ij\rangle} s_i s_j - H\sum_i s_i, \tag{1}$$

on the corner-sharing tetrahedron recursive lattice with coordination number $z = 6$ (see the left figure in Fig. 1) which represents an appropriate approximation of real three-dimensional pyrochlore lattice (see the right figure in Fig. 1) and which takes into account its basic geometric structure responsible for strong geometric frustration (see Ref. [32] for all details). In Hamiltonian (1), each variable s_i acquires one of two possible values $\pm 1, J < 0$ is the nearest-neighbor antiferromagnetic interaction parameter, and H represents the external magnetic field. In addition, the first sum runs over all nearest-neighbor spin pairs and the second sum runs over all spin sites.

As was shown in Ref. [32], the model is quite exceptional due to the fact that it belongs into the rather restricted set of antiferromagnetic spin models which are exactly solvable even in the presence of the magnetic field. In Ref. [32], it was proven that the model exhibits exactly one unique solution for all values of the model parameters and the explicit form of the solution was found. Besides, a detailed analysis of the magnetic properties of the model was performed together with the analysis of the system of all ground states. From the phenomenological point of view, one of the most important results obtained in Ref. [32], which is also the key point for our present analysis, is the proof of the existence of the so-called single-point ground states, which are realized for some exact values of the external magnetic field, along with the well-known standard plateau ground states. Note that the existence of the single-point ground states was exactly proven for the first time in Refs. [30] in the framework of the antiferromagnetic model on the kagome-like recursive lattice and latter also on geometrically frustrated one-dimensional systems [33,34]. It is worth mentioning that the process of formation of the single-point ground states is very often visible in real experiments, e.g., in the behavior of the magnetization curves (see, e.g., Refs. [11,12]).

As we shall see in the present paper, the existence of these well-defined single-point ground states, which have unique thermodynamical properties and which play the role of the separating points between neighboring plateau ground states, is responsible and naturally explains all peculiarities in the behavior of the specific heat capacity such as, e.g., the Schottky-type anomaly measured by real experiments as well as theoretically observed in many frustrated systems [1,6,9,13,16,18]. In addition, as we shall show, the existence of highly macroscopically degenerated single-point ground states in comparison to the plateau ground states naturally leads to another typical strong peculiarity in the low-temperature behavior of the specific heat capacity, namely, to the existence of the external-field induced sharp double-peak structure of the specific heat in the vicinity of each single-point ground state.

However, to proceed it is necessary first to investigate the entropy per site as well as to find the residual entropies of all ground states of the model. The entropy per site is standardly defined as follows

$$s = -\frac{\partial f}{\partial T}, \tag{2}$$

where f is the free energy per site of the model which, in our case, has the following explicit form[1]

$$\beta f = -\ln\left(x^3 e^{3h} + 3x^2 e^{h-2K} + 3xe^{-h} + e^{6K-3h}\right) + \frac{1}{2}\ln\left(x^4 e^{4h+6K} + 4x^3 e^{2h} + 6x^2 e^{-2K} + 4xe^{-2h} + e^{6K-4h}\right). \tag{3}$$

Here, $\beta = 1/(k_B T), T$ is the temperature, k_B is the Boltzmann constant, $K = \beta J, h = \beta H$, and x is the exact solution of the corresponding recursion relation (see Ref. [32] for all details) and which can be written in the following explicit from

$$x = -\frac{b}{4a} + A + \frac{1}{2}\left(-4A^2 - B - \frac{C}{A}\right)^{1/2}, \tag{4}$$

where

$$A = \frac{1}{2\sqrt{3}}\left[-B + \frac{1}{a}\left(D + \frac{E}{D}\right)\right]^{1/2}, \tag{5}$$

$$B = \frac{8ac - 3b^2}{4a^2}, \tag{6}$$

$$C = \frac{b^3 - 4abc + 8a^2 d}{8a^3}, \tag{7}$$

$$D = \left[\frac{F + \left(F^2 - 4E^3\right)^{1/2}}{2}\right]^{1/3}, \tag{8}$$

$$E = c^2 - 3bd + 12ae, \tag{9}$$

$$F = 2c^3 - 9bcd + 27b^2 e + 27ad^2 - 72ace, \tag{10}$$

and

$$a = e^{2(3h+K)}, \quad b = e^{4h}\left[3 - e^{2(h+4K)}\right], \tag{11}$$

$$c = 3e^{2(h+K)}\left(1 - e^{2h}\right), \quad d = e^{8K} - 3e^{2h}, \quad e = -e^{2K}. \tag{12}$$

The dependence of the entropy per site on the nonzero reduced temperature and on the absolute values of the external magnetic field is shown explicitly in the left figure in Fig. 2. The entropy is a continuous function of the nonzero temperature as well as of the external magnetic field and a nontrivial system of residual entropies is formed for low enough values of the temperature. The formation of the residual entropies is also shown explicitly in the right figure in Fig. 2 where the behavior of the entropy per site is demonstrated as the function of the temperature for various absolute values of the external magnetic field. The model contains two plateau ground states with absolute values of magnetization $m = 0$ and $|m| = 1/2$ (for magnetization properties of the model see Ref. [32]), which are realized for $|H/J| < 2$ and $2 < |H/J| < 6$, respectively. Their exact residual entropies are $s = \ln(3/2)/2k_B \approx 0.202733\,k_B$ and $s = \ln\left(3\sqrt{3}/4\right)/2\,k_B \approx 0.130812\,k_B$ and their macroscopic degeneracies are[2] $\Omega = (3/2)^{N/2}$ and $\Omega = (3\sqrt{3}/4)^{N/2}$, respectively. It is worth mentioning that our theoretical result for the residual entropy of the plateau ground state with $m = 0$ is in perfect accordance with experimental measurements on the magnetic materials with pyrochlore structure, e.g., such as pyrochlore

[1] Note that the free energy per site of the present model can be derived, e.g., by using the technique discussed in Ref. [35] (see also Ref. [36]).

[2] Note that the macroscopic degeneracy Ω of a given state of the system with total number of sites N is directly related to the total entropy $S = Ns$ as follows: $S = k_B \ln \Omega$. It is, however, necessary to bear in mind that all results have sense only in the limit $N \to \infty$.