Physics Letters A 378 (2014) 1773–1779

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Entropy of spin clusters with frustrated geometry

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ARTICLE INFO

Article history:
Received 15 October 2013
Received in revised form 16 April 2014
Accepted 24 April 2014
Available online 10 May 2014
Communicated by R. Wu

Keywords:
Ising antiferromagnet
Triangular lattice
Spin cluster
Geometrical frustration
Residual entropy

ABSTRACT

Geometrically frustrated clusters of Ising spins of different shapes on a triangular lattice are studied by exact enumeration. The focus is laid on the ground-state energy and residual entropy behaviors as functions of the cluster shape and size, as well as the spin value. Depending on the cluster shape, the residual entropy density in approach to the thermodynamic limit can either vanish or remain finite and the dependence can be decreasing, increasing or non-monotonic. Nevertheless, the relative entropies normalized by the respective thermodynamic limit values turn out to be little sensitive to the spin value. Attention is drawn to magnetocaloric properties of systems of selected cluster shapes.

1. Introduction

The effect of geometrical frustration in spin systems is a subject of intensive investigations. One of the simplest such models is a triangular lattice Ising antiferromagnet (TLIA) with spin $s = 1/2$, which shows no long-range ordering at any finite temperature [1,2]. TLIA is fully frustrated and the ground state (GS) is highly degenerated with non-vanishing entropy [1]. The lack of order is due to large ground-state degeneracy, nevertheless, the latter can be lifted by various perturbations, such as an external magnetic field [3–6] or selective dilution [7,8]. The degeneracy can also be removed in case of finite lattices and certain types of boundary conditions [9,10]. By increasing the lattice size to infinity the ground-state entropy in the thermodynamic limit is recovered only if the boundary conditions giving maximum degeneracy are considered [10,11]. For example, if the lattice has a shape of a rhombus the ground state is non-degenerate (unique up to a global spin inversion) for any lattice size and thus the entropy density vanishes in the thermodynamic limit [12]. Millane et al. [13,14] have investigated the dependence of the entropy density on different boundary conditions on finite triangular domains for which the ground states do not admit a dimer covering and found that it can vary between zero and maximal value. Therefore, the present model is a good example of the intricate relationship between finite (zero-dimensional) spin clusters, their shapes and the residual entropy in the infinite (two-dimensional) volume limit. It is also worth mentioning that the present frustrated spin clusters have been successfully applied to model the array of myosin filaments in higher vertebrate muscle pack, imagined by electron microscopy [15,16]. The latter contains of order a few hundred filaments surrounded by amorphous material (therefore must be modeled by a finite lattice with free boundaries), which adopt two orientations that are distributed with short-ranging order. Such a system can be described by the antiferromagnetic Ising model on a finite triangular lattice.

Several studies [17–21] have shown that the ground-state properties of TLIA can be significantly affected by the spin value s. For sufficiently large s even a long-range order can occur as a result of the presence of so-called free spins (their state does not affect the energy), the degeneracy of which then outweighs the degeneracy of the disordered phase [19]. Naturally, one can expect that the spin value can also affect the ground-state energies and degeneracies of finite clusters of different shapes. To our best knowledge the character of such dependence has not been studied yet.

In the present paper we consider geometrically frustrated Ising spin-s ($s = 1/2, 1$ and $3/2$) clusters of various shapes and sizes with free boundaries and study effects of the shape, size and the spin value on the ground-state energy and residual entropy. In particular, we are interested in how these quantities can be influenced by minimal manipulation in the clusters' shapes, such as removal of a small number of vertices. We study their behavior for different s on approach to the respective thermodynamic limits, which for $s > 1/2$ are obtained by Monte Carlo simulations [21].

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http://dx.doi.org/10.1016/j.physleta.2014.04.063

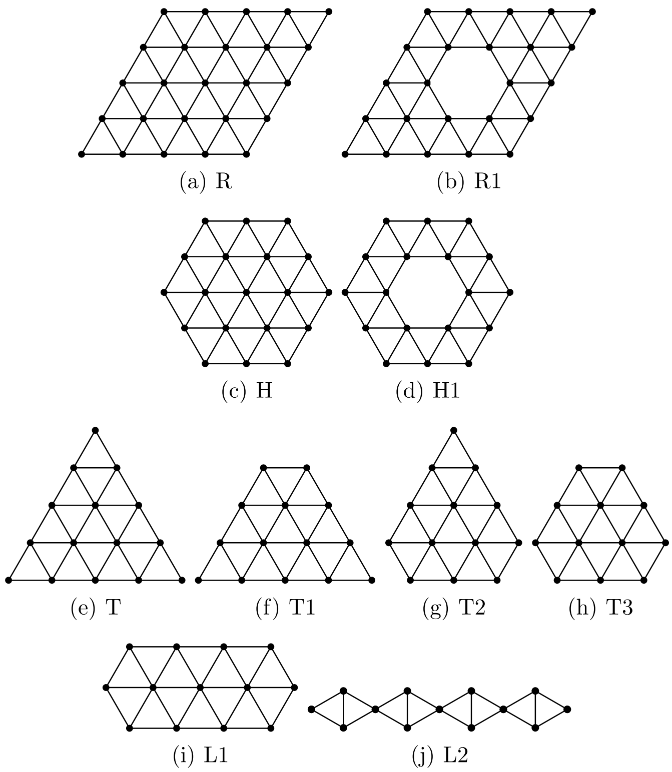

Fig. 1. Various clusters derived from the rhombus with the side length $L = 5$: (a) rhombus (R), (b) rhombus without the central spin (R1), (c) hexagon (H), (d) hexagon without the central spin (H1), (e) triangle (T), triangles with (f) one (T1), (g) two (T2) and (h) three (T3) vertices removed, ladder-like structures consisting of the spins along (i) the main diagonal (L1) and (j) the antidiagonal (L2) of the rhombus (a).

2. Model and methods

The spin-s Ising model on a lattice with triangular geometry can be described by the Hamiltonian

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

where the spins on the ith lattice site are allowed to take $2s+1$ values: $s_i = -s, -s+1, \ldots, s-1, s$. The summation $\langle i, j \rangle$ runs over nearest-neighbor sites and $J < 0$ is an antiferromagnetic exchange interaction parameter. The lattice is considered to consist of a finite number of spins arranged in clusters of various shapes, as shown in Fig. 1. For such relatively small clusters it is possible to fully explore the state space, exactly determine ground states and calculate some quantities of interest, such as the internal energy and the entropy. In order to understand the effects of different shapes and sizes of the finite clusters it is interesting to compare the obtained results with those for the thermodynamic limit, i.e., for an infinite lattice. The latter can be obtained from Monte Carlo (MC) simulation data and the residual (ground state) entropy can be determined by the thermodynamic integration method [22,23].

2.1. Exact enumeration

Considering the Hamiltonian (1) and for simplicity putting $J = -1$, a zero-temperature energy can be expressed as

$$E = \sum_{\langle k,l \rangle} s_k s_l, \tag{2}$$

where the summation $\langle k, l \rangle$ runs over the nearest neighbors s_k and s_l on the considered cluster. Ground-state (GS) spin configurations $\mathbf{s}_{\mathrm{GS}} = \{s_1, \ldots, s_N\}$, where N is a number of spins in the cluster, can be found as configurations[1] that minimize the energy functional $f(\mathbf{s}) \equiv E$, i.e.:

$$\mathbf{s}_{\mathrm{GS}} = \arg\min_{\mathbf{s}} f(\mathbf{s}). \tag{3}$$

We record the minimum energy per spin $E/N \equiv f(\mathbf{s}_{\mathrm{GS}})/N$ and from the obtained number of GS configurations W, we calculate the entropy per spin $S/N = \ln W/N$ (we put the Boltzmann constant $k_B = 1$).

3. Results

3.1. Spin $s = 1/2$

The ground-state configurations of finite clusters, their energies and degeneracies are expected to depend on the shapes and sizes of the clusters [12–14]. The exact results presented in Table 1 demonstrate how the respective quantities for different cluster shapes change with the increasing cluster size for spin $s = 1/2$. For better visual presentation, as well as relation of the obtained values with that expected in the infinite lattice, we show the following plots: In Fig. 2(a) we plot the reduced internal energies per spin E/s^2N and in Fig. 2(b) the reduced entropy S/S_{inf}, where $S_{inf} = 0.3231$ represents the exact Wannier value of the infinite system [1,25], as functions of the spin numbers N. Thus, in the thermodynamic limit of $N \to \infty$ the quantities E/s^2N are expected to approach the value of -1 and S/S_{inf} the value of 1 [1].

The respective values for the original rhombic (R), hexagonal (H) and triangular (T) shapes correspond to those presented in Ref. [12][2] for the chosen cluster sizes. With the increasing size, all the energies seem to approach the infinite limit value of -1. In order to convincingly show that the thermodynamic limit value for the energy density of each cluster shape approaches the same value of -1, we followed the same procedure as presented in Ref. [12] for the ground-state energy determination of the respective finite clusters and then we took the infinite volume limit. In particular, we decomposed the respective finite clusters, consisting of N spins, to individual triangles covering the entire cluster and estimated the lower bound of the ground-state energy such a way that each triangle has two favorable (antiparallel) pair interactions and if there are edges not coved by the triangles then we also considered them to be favorable. Then we found such a configuration and explicitly expressed its ground-state energy as a function of the cluster edge length n in the respective finite clusters. Following the above procedure one obtains the following expressions (see Ref. [12]): $N = n^2$ and $E = -(n^2 - 1)$ for R shape, $N = 3n(n-1) + 1$ and $E = -3n(n-1)$ for H shape, $N = n(n+1)/2$ and $E = -n(n-1)/2$ for T shape. Analogically, we extended these considerations also to L1 and L2 shapes and for both obtained the same expressions: $N = 3n + 1$ and $E = -3n$. Note that the edge length n for the shapes R, H and T is the same as L shown in Fig. 1, i.e., $n = 5 = L$, however, for L1 and L2 shapes $n = 4 \neq L$. Then, it is easy to see that by taking the infinite volume limit of E/N, we obtain the same energy density value of -1 for each cluster shape. The reduced entropies of T and H shapes seem to approach the value of 1, i.e. the respective entropy densities of the clusters appear to approach that for the thermodynamic limit,[3] which sug-

[1] There are in total $(2s+1)^N$ configurations to be considered.

[2] Actually, the values of S/S_{inf} slightly deviate, since in Ref. [12] incorrect value of $S_{inf} = 0.3383$ was used.

[3] For H shape the increasing character of the entropy density only shows up for larger cluster sizes, as demonstrated in Ref. [12] for H cluster and also confirmed by our MC simulations for both H and H1 clusters with the side length up to $L = 15$, i.e., $N = 169$ and 168 spins, respectively (not shown).