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Research articles

Magnetization process and magnetocaloric effect in geometrically frustrated Ising antiferromagnet and spin ice models on a 'Star of David' nanocluster

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ABSTRACT

Magnetic and magnetocaloric properties of geometrically frustrated antiferromagnetic Ising (IA) and ferromagnetic spin ice (SI) models on a nanocluster with a 'Star of David' topology, including next-nearest-neighbor (NNN) interactions, are studied by an exact enumeration. In an external field applied in characteristic directions of the respective models, depending on the NNN interaction sign and magnitude, the ground state magnetization of the IA model is found to display up to three intermediate plateaus at fractional values of the saturation magnetization, while the SI model shows only one zero-magnetization plateau and only for the antiferromagnetic NNN coupling. A giant magnetocaloric effect is revealed in the IA model with the NNN interaction either absent or equal to the nearest-neighbor coupling. The latter is characterized by abrupt isothermal entropy changes at low temperatures and infinitely fast adiabatic temperature variations for specific entropy values in the processes when the magnetic field either vanishes or tends to the critical values related to the magnetization jumps.

1. Introduction

Molecular nanomagnets, composed of a finite number of interacting spins (spin cluster) magnetically decoupled from their environment, in recent decades have attracted considerable attention [1–3]. They can be found in many real materials but nowadays they can also be artificially designed in a highly controlled manner [4–6]. In spite of their simplicity, such zero-dimensional magnetic structures are still of theoretical interest as they can provide an excellent opportunity to examine fundamental magnetic interactions, in case of small clusters, as well as possibilities to explore novel many-body quantum states and quantum phenomena, in case of larger clusters. From the practical point of view, they can find applications in data storage, quantum computing and molecule-based spintronics devices [7,8]. It has also been demonstrated that molecular nanomagnets can potentially show a very large magnetocaloric effect (MCE) at low temperatures (for an overview, see, e.g., [9]) and are thus attractive materials for a magnetic cooling technology.

Even larger MCE can be achieved by the presence of degenerate or low-lying spin states that can be induced, for example, by frustration. It has been theoretically concluded that the field-dependent efficiency of a geometrically frustrated magnet can exceed that of an ideal paramagnet with equivalent spin by more than an order of magnitude [10,11] and experimentally supported by the results obtained for the geometrically frustrated Fe_{14} [12,13] and Ga_7 [14] molecular nanomagnets. Besides the enhanced MCE, an effect of frustration has been demonstrated to lead to a variety of other unusual magnetic properties, such as non-collinear ground states, magnetization plateaus and magnetization jumps [15,16]. Some of these properties have been studied on small antiferromagnetic Ising spin clusters [17] or more complex nanoparticles [18–22], focusing on the magnetization process. More recently investigations have been extended also to geometrically frustrated antiferromagnetic Ising spin clusters of different shapes and sizes on a triangular lattice [23–25] as well as to the clusters of the shapes of regular polyhedra (Platonic solids) [26,27], focusing on both the magnetization and the adiabatic demagnetization processes. In both frustrated systems it was shown that the magnetization process (number and height of the magnetization plateaus) as well as the adiabatic demagnetization process (magnetocaloric properties) strongly depend on the cluster geometry. Several shapes displaying enhanced (giant) MCE were identified. We note that modern techniques enable syntheses of molecular magnets of various structures, thus providing opportunity for the selected systems showing giant MCE to be practically used in technological applications.

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In the present study we focus on the magnetic and magnetocaloric properties of two geometrically frustrated spin systems: antiferromagnetic Ising (IA) and ferromagnetic spin ice (SI) models, including the effect of both the nearest-neighbor (NN) and the next-nearest-neighbor (NNN) interactions, localized on a nanocluster of a 'Star of David' shape (Fig. 1). The latter is the elementary cell of a kagomé lattice, which, based on the residual entropy as a measure of frustration, is considered to be the most frustrated lattice with no long-range ordering at any temperature [28]. We note that very recently a family of single-molecule magnets with the 'Star of David' topology has been synthesized and their magnetocaloric properties have been investigated [29]. Our study shows that both IA and SI systems display favorable magnetocaloric properties. Nevertheless, particularly fast cooling rates to ultra low temperatures at small fields were observed in the former system, which makes it a good candidate for application as an efficient low-temperature refrigerator.

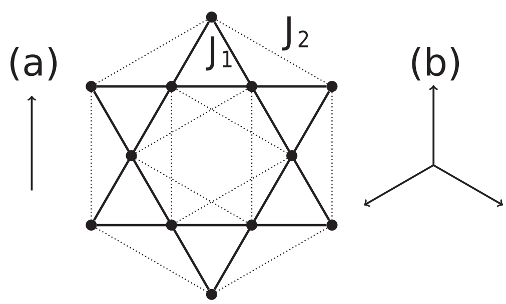

Fig. 1. 'Star of David' nanocluster with NN (solid lines J_1) and NNN (dashed lines J_2) couplings. Local anisotropy axes in the direction of (a) z-axis for IA and (b) elementary triangle axes for SI models.

2. Models

2.1. Ising antiferromagnet

The NNN IA model on the 'Star of David' nanocluster in an external magnetic field can be described by the Hamiltonian

$$\mathcal{H}_{IA} = -J_1\sum_{\langle i,j\rangle}\sigma_i\sigma_j - J_2\sum_{\langle i,k\rangle}\sigma_i\sigma_k - h\sum_i\sigma_i, \tag{1}$$

where $\sigma_i = \pm 1/2$ are the Ising variables on the ith site, the summations $\langle i,j\rangle$ and $\langle i,k\rangle$ run over NN and NNN spin pairs, $J_1 < 0$ is an antiferromagnetic NN exchange interaction parameter, the NNN exchange interaction parameter is restricted to the range $-|J_1| < J_2 < |J_1|$, and h is the external magnetic field. The 'Star of David' cluster consists of 6 corner-sharing triangles with $N = 12$ Ising spins, arranged as shown in Fig. 1. Each of the spins can be in spin-up or spin-down states totaling in 2^{12} possible configurations.

2.2. Spin ice

In the SI model the spins also possess the Ising anisotropy, however, the Ising axes now run through the center of the triangular plaquettes (Fig. 1) and and the interaction between the neighboring spins is ferromagnetic. The Hamiltonian of the corresponding NNN SI model reads

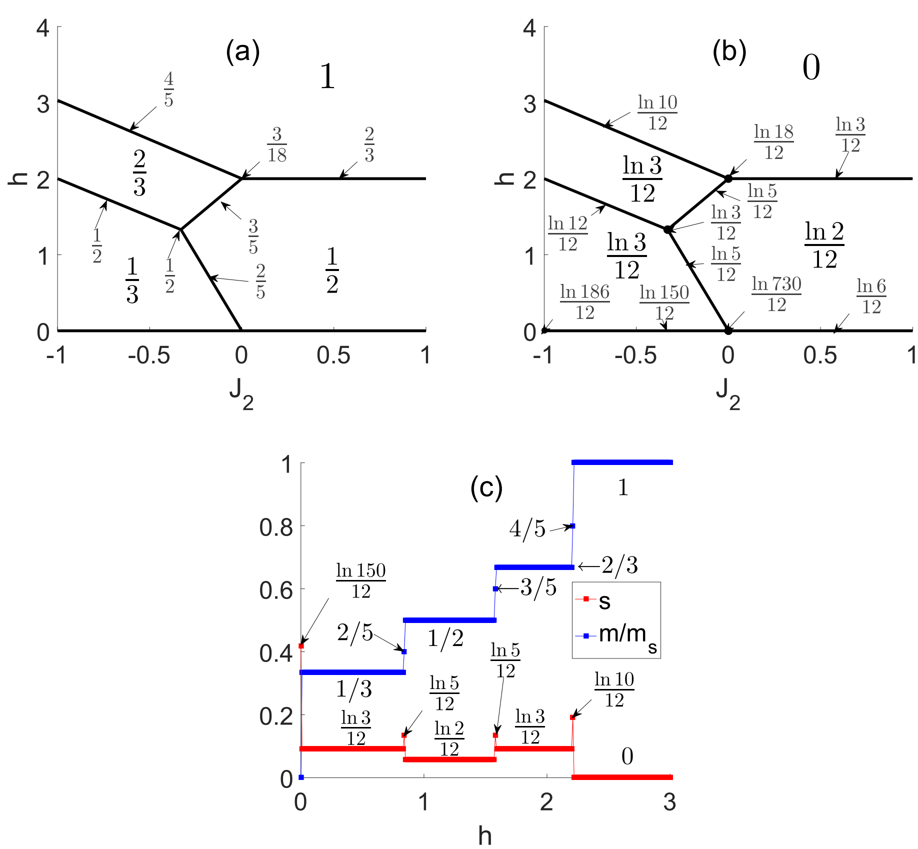

Fig. 2. Ground state (a) normalized magnetization m/m_s and (b) entropy density s of the IA model in the (h, J_2) parameter plane. Values shown in larger font (smaller font with arrows) correspond to the interior (boundaries) of the respective phases. (c) Magnetization and entropy processes, for $J_2 = -0.2$.