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Magnetocaloric Properties of an Ising Antiferromagnet on a Kagome Lattice

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Owing to a high degree of geometrical frustration an Ising antiferromagnet on a kagome lattice is known to exhibit no long-range ordering at any temperature, including the ground state. Nevertheless, at low temperatures it shows a strongly correlated, highly fluctuating regime known as a cooperative paramagnet or classical spin liquid. In the ground state it is characterized by a macroscopic degeneracy which translates to a relatively large value of the residual entropy. It has been shown that the presence of a macroscopic degeneracy associated with geometrical frustration below the saturation field can facilitate an enhanced magnetocaloric effect, which can exceed that of an ideal paramagnet with equivalent spin by more than an order of magnitude. In the present study we investigate magnetic and magnetocaloric properties of the Ising antiferromagnet on a kagome lattice by Monte Carlo simulation. In particular, we calculate the entropy of the system using the thermodynamic integration method and evaluate quantities which characterize magnetocaloric effect, such as the isothermal entropy and adiabatic temperature changes in a varying magnetic field. It is found that the Ising antiferromagnet on a kagome lattice shows the most interesting magnetocaloric properties at low temperatures and moderate magnetic fields, suggesting that its potential can be used in technological applications for low-temperature magnetic refrigeration.

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1. Introduction

The phenomenon of geometrical frustration in magnetic systems is closely related to the geometry of the lattice, which does not allow to fully satisfy all the interactions between its spins [1]. The effects of frustration are rich and still not well-understood. Previous research suggests that the field-induced adiabatic temperature change is significantly larger for such systems [2] than for their non-frustrated counterparts, which makes them better candidates for magnetic refrigeration using the magnetocaloric effect (MCE). MCE can be characterized by the change of the magnetic entropy in response to variation of the magnetic field. The Ising antiferromagnet on a kagome lattice (IAKL) is a great example of a highly frustrated system, which was extensively studied in the past [1, 3–5]. The kagome lattice consists of corner-sharing triangles (Fig. 1) and its elementary cell is shaped like the "Star of David". The exact solution for the Ising model on the kagome lattice was found in 1951 by Syozi [3]. He discovered that in the ferromagnetic case the system shows a phase transition at the critical temperature which is slightly lower than that of the square lattice. Nevertheless, the antiferromagnetic case shows no critical behavior at any temperature. It is also known that the density of a residual entropy of IAKL is $0.5018k_{\mathrm{B}}$ [4], which is larger than that of the triangular lattice ($0.3231k_B$) [6]. The ground state energy per spin was calculated by Kano and Naya [4] and it is $-2J$ in the ferromagnetic ($J > 0$) case and $2J/3$ in the antiferromagnetic ($J < 0$) case, where J is the exchange interaction constant. In this paper, magnetocaloric properties of IAKL in the presence of an external magnetic field are explored by means of Monte Carlo simulation.

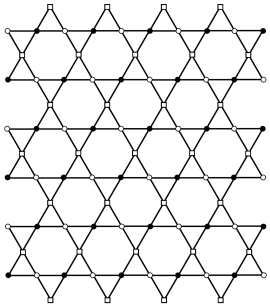

Fig. 1. The kagome lattice is a tripartite lattice and can be divided into three sublattices — denoted by ○, ● and □.

2. Model

The Hamiltonian of the studied system is given by

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_{i=1}^{N} \sigma_i, \tag{1}$$

where the first summation goes over the nearest neighbors, the second sum goes over each spin, N is the total number of spins, $\sigma_i = \pm 1$ is the Ising spin variable and h is the external magnetic field. In order to introduce frustration, interactions between neighboring spins were chosen to be antiferromagnetic ($J < 0$).

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3. Method

The standard Metropolis algorithm was used. At each Monte Carlo (MC) step a new state σ_i' is proposed for a selected spin σ_i and the new configuration is accepted with the probability $p(\sigma_i \to \sigma_i') = \min\{1, \exp(-\beta \mathrm{d}E)\}$, where $\beta = 1/(k_\mathrm{B}T)$ is the inverse temperature and $\mathrm{d}E$ is the energy difference between the proposed and the old configuration. When the algorithm makes a MC trial for each spin, we say that a MC sweep was completed. From the simulation, we directly obtain the energy per spin $e = \langle \mathcal{H} \rangle / (|J|N)$, from Eq. (1), and the magnetization per spin $m = \langle M \rangle / N$, where $M = \sum_{i=1}^{N} \sigma_i$ and $\langle \dots \rangle$ denotes a thermal average. However, the entropy, which we are interested in, cannot be calculated directly from the MC simulation. Nevertheless, it can be obtained as a function of the inverse temperature by utilizing the thermodynamic integration method (TIM) [7] as

$$S(\beta) = N \ln(2s+1) + \beta E(\beta) - \int_0^\beta E(\beta') \mathrm{d}\beta', \qquad (2)$$

where the spin number s is in our case $1/2$ and $E = Ne$. MCE is characterized by the following quantities: the adiabatic temperature change ΔT_{ad} and the isothermal entropy change ΔS_iso. For a fixed temperature T and the change of the field from h_1 to h_2, ΔS_{iso} is defined as:

$$\Delta S_\mathrm{iso}(h_2 - h_1, T) = S(h_2, T) - S(h_1, T). \qquad (3)$$

Similarly, in adiabatic condition with the entropy S the corresponding temperature change ΔT_ad from T_1 to T_2 can be calculated as

$$\Delta T_\mathrm{ad}(h_2 - h_1, S) = T_2(h_2) - T_1(h_1). \qquad (4)$$

4. Results and discussion

Throughout the paper we set $J = -1$ and $k_\mathrm{B} = 1$. For each temperature 4×10^5 MC sweeps were used to calculate physical quantities after discarding another 10^5 for thermalization. For smaller values of the field $h = 0$, 0.1, 0.2, 0.3, 0.4, and 0.5, simulations were performed on the lattice with 50×50 cells (7500 spins in total). The inverse temperature was chosen in the range $\beta \in \langle 0, 50 \rangle$. Values of β were denser in a low-temperature region to increase the precision of TIM. Additional simulations were performed on a smaller lattice with 20×20 cells (1200 spins in total) for larger values of the field $h = 1$, 2, 3, 4, and 5. In the absence of the field, our simulation yielded the ground state (GS) energy close to the value $e = -2/3$ (see Fig. 2a), which is in a good agreement with the exact value [4]. The energy corresponds to each elementary triangle having two spins up and one down or vice versa, with no ordering among them — the spin liquid state. In the presence of the external magnetic field, the GS energy is lowered by a Zeeman term proportional to the field's strength.

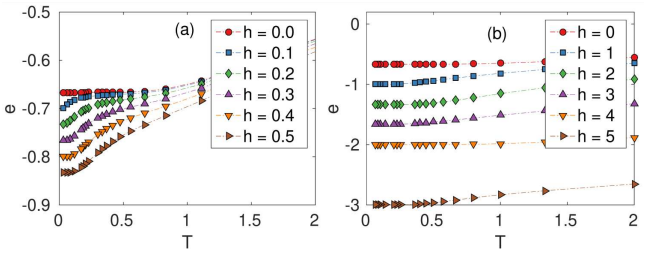

Fig. 2. Energy per spin for various values of the field h.

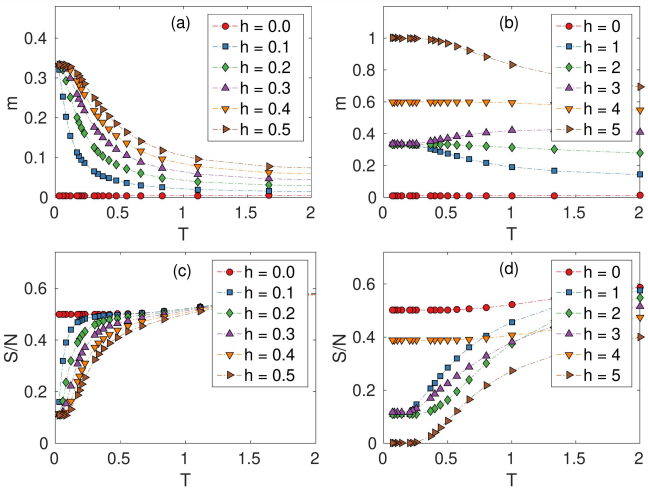

Fig. 3. Magnetization per spin and entropy density for various values of the field h.

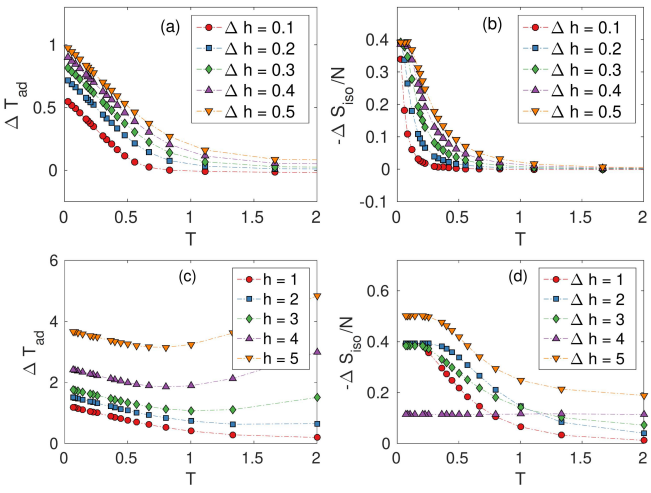

Fig. 4. Adiabatic temperature change and isothermal entropy change for various values of the field change Δh.

In the zero field, the system being antiferromagnetic, has zero magnetization (Fig. 3a). In the presence of a small field, we observe in GS 1/3 plateau which persists up to $h = 4$. Right at the $h = 4$ the magnetization jumps to the value $m = 3/5$ (Fig. 3b) and for $h > 4$,

the system reaches the fully saturated state with $m = 1$. This behavior is also reflected in the entropy density (see Fig. 3c,d), which is in the zero field equal to the theoretical value 0.5018 [4]. Small fields partially lift the degeneracy and the entropy density reaches the value 0.109 (which is close to the value mentioned in Ref. [8]). At the saturation field $h = 4$, the entropy density is equal to 0.3878 and for $h > 4$ it becomes zero.

In addition to the previous quantities, the isothermal entropy change $\Delta S_{\rm iso}$ and the adiabatic temperature change $\Delta T_{\rm ad}$ were calculated from Eqs. (3) and (4), respectively. We chose $h_1 = 0$ and $h_2 > 0$. From Fig. 4 one can see that MCE is the most prominent in the region of low temperatures. Even a small change of the field can lead to a large change of $\Delta S_{\rm iso}$ and $\Delta T_{\rm ad}$. The entropy change has the largest value $-\Delta S_{\rm iso}^{\rm max}/N = 0.3911$ for small fields ($h < 4$), for $h = 4$ it is $-\Delta S_{\rm iso}^{\rm max}/N = 0.1142$, and for $h > 4$ its value is $-\Delta S_{\rm iso}^{\rm max}/N = 0.5019$. This suggests that IAKL could be used for magnetic refrigeration in a low-temperature region. Similarly, the adiabatic temperature change $\Delta T_{\rm ad}$ has the most interesting behavior in the low-temperature region (Fig. 4a,c). If the field is increased (decreased), the temperature of the system under adiabatic conditions increases (decreases) proportional to the field's strength.

5. Summary

We have investigated magnetic and magnetocaloric properties of the Ising antiferromagnet on a kagome lattice by Monte Carlo simulation. A thermodynamic integration method allowed us to indirectly calculate the magnetic entropy and thus obtain relevant quantities characterizing magnetocaloric effect, such as the isothermal entropy and adiabatic temperature changes in a varying magnetic field. We found that the model shows favorable magnetocaloric properties at very low temperatures even in relatively small applied magnetic fields, which makes this system a promising candidate to be used for low-temperature magnetic refrigeration.

Acknowledgments

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