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Ground-state and magnetocaloric properties of a coupled spin–electron double-tetrahedral chain (exact study at the half filling)

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ABSTRACT

Ground-state and magnetocaloric properties of a double-tetrahedral chain, in which nodal lattice sites occupied by the localized Ising spins regularly alternate with triangular clusters half filled with mobile electrons, are exactly investigated by using the transfer-matrix method in combination with the construction of the Nth tensor power of the discrete Fourier transformation. It is shown that the ground state of the model is formed by two non-chiral phases with the zero residual entropy and two chiral phases with the finite residual entropy $S = Nk_{\mathrm{B}} \ln 2$. Depending on the character of the exchange interaction between the localized Ising spins and mobile electrons, one or three magnetization plateaus can be observed in the magnetization process. Their heights basically depend on the values of Landé g-factors of the Ising spins and mobile electrons. It is also evidenced that the system exhibits both the conventional and inverse magnetocaloric effect depending on values of the applied magnetic field and temperature.

1. Introduction

The magnetocaloric effect (MCE), which is defined as the temperature change (i.e., as the cooling or heating) of a magnetic system due to the application of an external magnetic field, has a long history in cooling applications at various temperature regimes [1]. Since the first successful experiment of the adiabatic demagnetization performed in 1933 [2], the MCE represents the standard technique for achieving the extremely low temperatures [3]. In this regard, theoretical predictions and descriptions of materials showing an enhanced MCE create real opportunities for the effective selection of the construction for working magnetic-refrigeration devices. Of particular interest is the investigation of the MCE in various one-dimensional (1D) quantum spin models [4–17] and several coupled spin–electron systems [18–21]. The reason lies in a possibility of obtaining exact analytical or numerical results as well as in a potential use of these models for the explanation of MCE data measured for real magnetic compounds. In particular, 1D models may give correct quantitative description of many real magnetic compounds when appropriate scaling of material parameters are taken into account [10,22–25].

In general, the MCE is characterized by the isothermal entropy change (ΔS_T) and/or by the adiabatic temperature change (ΔT_{ad}) upon the magnetic field variation. Depending on sings of these magnetocaloric potentials, the MCE can be

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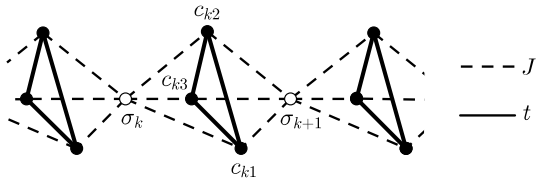

Fig. 1. A part of the spin–electron system on a double-tetrahedral chain. Empty circles denote nodal lattice sites occupied by the localized Ising spins, while the full circles forming triangular clusters are available to mobile electrons.

either conventional ($\Delta S_T < 0$, $\Delta T_{ad} > 0$) or inverse ($\Delta S_T > 0$, $\Delta T_{ad} < 0$). In the former case, the system cools down when the magnetic field is removed adiabatically, while in the latter case it heats up. Whether the conventional MCE or the inverse MCE is present basically depends on the particular magnetic arrangement in the system [26–28]. Namely, the former phenomenon can be observed in regular ferromagnets or paramagnets, while the latter one can be detected in ferrimagnetic and antiferromagnetic materials. Moreover, coexistence of the above phenomena is also possible. Both conventional and inverse MCE can be found in magnetic systems with rich structure of the ground-state phase diagram, in particular, in various 1D models [4–21], some multilayers [29] or even some finite structures [30–32].

In the present paper, we will consider a double-tetrahedral chain, in which nodal lattice sites occupied by the localized Ising spins regularly alternate with triangular clusters with the dynamics described by the Hubbard model. Note that this 1D spin–electron model can be rigorously solved by two distinct analytical approaches regardless of a number of mobile electrons in triangular clusters. The first approach is the standard transfer-matrix technique [33–35], which is rather straightforward but applicable only to 1D systems. The second one lies in a combination of the generalized decoration–iteration mapping transformation [36–39] with the well known analytical results for the partition function of the spin-1/2 Ising chain in a presence of the longitudinal magnetic field [33–35]. As has been shown in our recent works [19–21], the coupled spin–electron double-tetrahedral chain provides an excellent prototype model with a rather complex ground state, which allows a rigorous theoretical investigation of the MCE in a vicinity of the first-order phase transitions at non-zero magnetic fields. Last but not least, it is valuable to mention the copper-based polymeric chain $Cu_3Mo_2O_9$, which represents a possible experimental realization of the double-tetrahedral chain structure [40–44].

The paper is organized as follows. In the following two Sections 2 and 3, the model under investigation is defined and the corresponding Hilbert space is organized for an exact analytical diagonalization of the block Hamiltonian. Subsequently, a particular ground-state analysis of the model is realized by using a complete set of eigenvalues of the block Hamiltonian. Sections 4 and 5 deal with the method used for rigorous analytical solution of the partition function and the most interesting numerical results for the magnetization, entropy and magnetocaloric properties of the model. Finally, the most significant findings are briefly summarized in Section 5.

2. Spin–electron double-tetrahedral chain

Let us consider a magnetic system on a double-tetrahedral chain composed of N nodal lattice sites occupied by localized Ising spins and N triangular clusters available to three mobile electrons. The magnetic structure of the considered 1D model is schematically illustrated in Fig. 1. Assuming interactions between the nearest neighboring lattice sites, the on-site Coulomb repulsion $U > 0$ between two mobile electrons of opposite spins at the same lattice site and the effect of a longitudinal magnetic field B on magnetic particles, the total Hamiltonian of the model reads

$$H = -t\sum_{\langle i,j\rangle}\sum_{s\in\{\uparrow,\downarrow\}}\left(c_{i,s}^{\dagger}c_{j,s}+c_{j,s}^{\dagger}c_{i,s}\right)+\frac{J}{2}\sum_{\langle j,k\rangle}\left(n_{j,\uparrow}-n_{j,\downarrow}\right)\sigma_k^z+U\sum_j n_{j,\uparrow}n_{j,\downarrow}$$
$$-\frac{g_e\mu_{\mathrm{B}}B}{2}\sum_j\left(n_{j,\uparrow}-n_{j,\downarrow}\right)-g_I\mu_{\mathrm{B}}B\sum_k\sigma_k^z. \quad (1)$$

Above, the summation $\langle i,j\rangle$ runs over lattice sites forming triangular clusters, while the summation $\langle j,k\rangle$ runs over lattice sites of triangular clusters and the nearest-neighboring nodal lattice sites. The operators $c_{i(j),s}^{\dagger}$, $c_{i(j),s}$ represent usual fermionic creation and annihilation operators for mobile electrons occupying the $i(j)$th lattice site with the spin $s\in\{\uparrow,\downarrow\}$, respectively, $n_{j,s}=c_{j,s}^{\dagger}c_{j,s}$ is the number operator of the mobile electron at the jth lattice site and σ_k^z labels the Ising spin localized at the kth nodal lattice site. The hopping parameter $t>0$ takes into account the kinetic energy of mobile electrons delocalized over triangular clusters and J stands for the Ising-type coupling between mobile electrons and their nearest Ising neighbors. Finally, the last two terms in (1) represent the Zeeman's energies of the mobile electrons and the localized Ising spins, respectively, in a presence of the applied magnetic field B. The quantity μ_{B} is a Bohr magneton and g_e, g_I denote g-factors of the mobile electrons and the localized Ising spins, respectively.

For further calculations, it is advisable to think of the considered model as a system of N interacting double-tetrahedrons whose common vertices are occupied by the localized Ising spins, while others are available for mobile electrons. In this regard, the total Hamiltonian (1) can be written as a sum of N block Hamiltonians $H=\sum_{k=1}^{N}H_k$, where each block