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Unusual field-induced transitions in exactly solved mixed spin-(1/2, 1) Ising chain with axial and rhombic zero-field splitting parameters ☆

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ABSTRACT

The mixed spin-(1/2, 1) Ising chain with axial and rhombic zero-field splitting parameters in the presence of the longitudinal magnetic field is exactly solved within the framework of decoration-iteration transformation and transfer-matrix method. Our particular emphasis is laid on an investigation of the influence of the rhombic term, which is responsible for an onset of quantum entanglement between two magnetic states $S_k^z = \pm 1$ of the spin-1 atoms. It is shown that the rhombic term gradually destroys a classical ferrimagnetic order in the ground state and simultaneously causes diversity in magnetization curves including intermediate plateau regions, regions with a continuous change in the magnetization as well as several unusual field-induced transitions accompanied with magnetization jumps. Another interesting findings concern with an appearance of the round minimum in the temperature dependence of susceptibility times temperature data, the double-peak zero-field specific heat curves and the enhanced magnetocaloric effect. The temperature dependence of the specific heat with three separate maxima may also be detected when driving the system through the axial and rhombic zero-field splitting parameters close enough to a phase boundary between the ferrimagnetic and disordered states and applying sufficiently small longitudinal magnetic field.

1. Introduction

Over the last few decades, exactly solved one-dimensional quantum spin models [1–3] have attracted considerable research interest as they may describe subtle quantum phenomena to emerge in real magnetic materials without a danger of over-interpretation, which is inherent to any approximative treatment. The present work is devoted to an exact study of the mixed spin-(1/2, 1) Ising chain model, which accounts both for the axial zero-field splitting (AZFS) as well as the rhombic zero-field splitting (RZFS) parameter in the presence of the applied longitudinal magnetic field. It is worthy of notice that the special limiting case of this model system in the absence of the external magnetic field has been proposed and exactly solved by Wu et al. [4–6] using the rigorous procedure based on the Jordan–Wigner transformation [7] (see Refs. [8–10] for related works on this subject). However, it has been recently shown by the present authors [11] that the exact results obtained by Wu et al. [4,5] can also be recovered by another independent way by making use of the transfer-matrix method. The foremost advantage of the formulation based on the transfer-matrix method lies in the fact that this rigorous method may be even applied in the presence of the non-zero longitudinal magnetic field. The main purpose of this work is therefore to investigate the effect of longitudinal field on magnetic properties of the mixed spin-(1/2, 1) Ising chain with both AZFS and RZFS parameters.

Before proceeding to an exact calculation for the investigated model system, let us briefly comment on an experimental motivation of our study. It is noteworthy that there exist several heterometallic molecular-based compounds with a magnetic structure, which can be properly described as one-dimensional chain of alternating spin-1/2 and spin-1 metal ions. Among the most common examples of the one-dimensional mixed spin-(1/2, 1) chains one could mention

- $CuNi(EDTA)\cdot 6H_2O$ [12],
- $CuNi(pbaOH)(H_2O)_3\cdot nH_2O$ [13],
- $CuNi(pba)(D_2O)_3\cdot 2D_2O$ [14],
- $PPh_4[Ni(pn)_2][Fe(CN)_6]\cdot H_2O$ [15],
- $\{Pr(bet)_2(H_2O)_3Fe(CN)_6\}$ [16],
- $\{Ru(acac)_2(CN)_2\}\{Ni(dmphen)(NO_3)\}$ [17].

Even though the vast majority of aforementioned polymeric compounds should be preferentially regarded as experimental representatives of the mixed-spin quantum Heisenberg chain rather than the mixed-spin Ising chain, it is the authors' hope

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that our exact analytical results for the mixed spin-(1/2, 1) Ising chain may provide a deeper insight into several important vestiges of real physical behavior and explain some experimental results at least at a qualitative level. Besides, one should also expect that the theoretical description based on the mixed spin-(1/2, 1) Ising chain may be quite appropriate for those heterometallic coordination polymers, where at least one from both constituent magnetic ions possesses a rather high magnetic anisotropy. It should be stressed that the magnetic behavior of this type has been recently found in two heterometallic complexes containing highly anisotropic rare-earth ions [18–20].

The outline of the present paper is as follows. In the following Section 2, we will shed light on the basic steps of our exact calculation for the investigated model system. Section 3 deals with the discussion of the most interesting results obtained for the phase diagrams and basic thermodynamic quantities. Finally, some concluding remarks are given in the Section 4.

2. Exact solution of the mixed-spin Ising chain

Let us consider the mixed spin-(1/2, 1) Ising chain with AZFS and RZFS parameters in the presence of the longitudinal external magnetic field. Suppose that the linear chain consists of the alternating spin-1/2 and spin-1 atoms, whereas the former spin-1/2 atoms constitute the sublattice A and the latter spin-1 atoms form the sublattice B. The total Hamiltonian of the system can be written as a sum of three parts

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_{ex} + \hat{\mathcal{H}}^{(1)}_{zfs} + \hat{\mathcal{H}}_{zee}, \tag{1}$$

which account for the nearest-neighbor Ising interaction, AZFS and RZFS terms acting on the spin-1 atoms and the magnetostatic (Zeeman's) energy of the spin-1/2 and spin-1 atoms in the applied longitudinal magnetic field

$$\hat{\mathcal{H}}_{ex} = -J\sum_{k=1}^{N}\hat{S}^z_k(\hat{\sigma}^z_k+\hat{\sigma}^z_{k+1}), \tag{2}$$

$$\hat{\mathcal{H}}^{(1)}_{zfs} = -D\sum_{k=1}^{N}(\hat{S}^z_k)^2 - E\sum_{k=1}^{N}[(\hat{S}^x_k)^2-(\hat{S}^y_k)^2], \tag{3}$$

$$\hat{\mathcal{H}}_{zee} = -H_A\sum_{k=1}^{N}\hat{\sigma}^z_k - H_B\sum_{k=1}^{N}\hat{S}^z_k. \tag{4}$$

Above, $\hat{\sigma}^z_k$ and $\hat{S}^\alpha_k(\alpha = x,y,z)$ denote standard spatial components of the spin-1/2 and spin-1 operators, respectively, N denotes a total number of spins from each sublattice and the periodic boundary condition $\sigma_{N+1}\equiv\sigma_1$ is imposed for simplicity. The parameter J stands for the Ising interaction between nearest-neighboring spin-1/2 and spin-1 atoms, whereas the terms D and E label the AZFS and RZFS parameters acting on the spin-1 atoms only. Last, two Zeeman's terms H_A and H_B describe the influence of longitudinal magnetic field on the spin-1/2 and spin-1 atoms from the sublattices A and B, respectively.

Before proceeding further, it is worthwhile to remark that there exist several equivalent representations of the zero-field splitting Hamiltonian $\hat{\mathcal{H}}^{(1)}_{zfs}$ given by Eq. (3). As a matter of fact, one may for instance prove one-to-one correspondence between $\hat{\mathcal{H}}^{(1)}_{zfs}$ and the effective spin Hamiltonian with three different single-ion anisotropy parameters D^x, D^y and D^z

$$\hat{\mathcal{H}}^{(2)}_{zfs} = -D^x\sum_{k=1}^{N}(\hat{S}^x_k)^2 - D^y\sum_{k=1}^{N}(\hat{S}^y_k)^2 - D^z\sum_{k=1}^{N}(\hat{S}^z_k)^2. \tag{5}$$

The Hamiltonians $\hat{\mathcal{H}}^{(1)}_{zfs}$ and $\hat{\mathcal{H}}^{(2)}_{zfs}$ differ from one another just by unimportant constant term, because the mapping relations $D = D^z-(D^x+D^y)/2$ and $E = (D^x-D^y)/2$ establish a precise equivalence between the Hamiltonians (3) and (5) (see Ref. [11] for more details). It should also be noticed that the particular case of the Hamiltonian $\hat{\mathcal{H}}^{(2)}_{zfs}$ with $D^y=0$ has been considered by Wu et al. [4] in their recent work. However, it has been shown in our preliminary report [11] that the Hamiltonian $\hat{\mathcal{H}}^{(1)}_{zfs}$ with one less free parameter is much more appropriate for the interpretation of obtained exact results compared with the Hamiltonian $\hat{\mathcal{H}}^{(2)}_{zfs}$ and thus, this more convenient definition of the zero-field-splitting Hamiltonian will be used throughout the rest of this paper.

Now, let us turn our attention to the main points of the method, which enables an exact treatment of the investigated quantum spin chain. First, the total Hamiltonian (1) can be rewritten as the sum of Zeeman's term for all spin-1/2 atoms from the sublattice A and the sum of site Hamiltonians

$$\hat{\mathcal{H}} = \sum_{k=1}^{N}\hat{\mathcal{H}}_k - H_A\sum_{k=1}^{N}\hat{\sigma}^z_k, \tag{6}$$

whereas each site Hamiltonian $\hat{\mathcal{H}}_k$ involves all the interaction terms including the kth spin-1 atom from the sublattice B

$$\hat{\mathcal{H}}_k = -E_k\hat{S}^z_k - D(\hat{S}^z_k)^2 - E[(\hat{S}^x_k)^2-(\hat{S}^y_k)^2] \tag{7}$$

with $E_k = J(\hat{\sigma}^z_k+\hat{\sigma}^z_{k+1})+H_B$. Because the Hamiltonians (7) at different sites commute, i.e. $[\hat{\mathcal{H}}_i,\hat{\mathcal{H}}_j]=0$ is valid for each $i\neq j$, the partition function can be partially factorized and consequently rewritten in the form

$$\mathcal{Z} = \sum_{\{\sigma_k\}}\prod_{k=1}^{N}\exp\left[\frac{\beta H_A}{2}(\hat{\sigma}^z_k+\hat{\sigma}^z_{k+1})\right]\mathrm{Tr}_{S_k}\exp(-\beta\hat{\mathcal{H}}_k) = \sum_{\{\sigma_k\}}\prod_{k=1}^{N}\mathcal{Z}_k, \tag{8}$$

where $\beta = 1/(k_BT)$, k_B is Boltzmann's constant, T is the absolute temperature, Tr_{S_k} means a trace over degrees of freedom of the kth spin-1 atom from the sublattice B and the symbol $\sum_{\{\sigma_k\}}$ denotes a summation over all possible configurations of the spin-1/2 atoms from the sublattice A. The crucial step of our exact procedure represents calculation of the expression $\mathrm{Tr}_{S_k}\exp(-\beta\hat{\mathcal{H}}_k)$. For this purpose, it is useful to rewrite the site Hamiltonian (7) into the usual matrix representation

$$\langle k_i|\hat{\mathcal{H}}_k|k_j\rangle = \begin{pmatrix} -E_k-D & 0 & -E \\ 0 & 0 & 0 \\ -E & 0 & E_k-D \end{pmatrix}, \tag{9}$$

using the standard basis of ket vectors $|k_j\rangle = |\pm 1\rangle, |0\rangle$ $(j=1-3)$ corresponding to the three possible spin states $S^z_k = \pm 1,0$ of the kth spin-1 atom from the sublattice B. The straightforward diagonalization of the site Hamiltonian yields the following eigenenergies and eigenvectors:

$$\lambda_{k1} = -D-\sqrt{E_k^2+E^2}, \quad |\psi_{k1}\rangle = \cos\left(\frac{\varphi_k}{2}\right)|1\rangle + \sin\left(\frac{\varphi_k}{2}\right)|-1\rangle,$$

$$\lambda_{k2} = 0, \quad |\psi_{k2}\rangle = |0\rangle,$$

$$\lambda_{k3} = -D+\sqrt{E_k^2+E^2}, \quad |\psi_{k3}\rangle = \sin\left(\frac{\varphi_k}{2}\right)|1\rangle + \cos\left(\frac{\varphi_k}{2}\right)|-1\rangle, \tag{10}$$

with the mixing angle φ_k defined through the relation $\varphi_k = \arctan(E/E_k)$. It is worth mentioning that the eigenenergies listed in the set of Eq. (10) can readily be used for calculating the expression $\mathrm{Tr}_{S_k}\exp(-\beta\hat{\mathcal{H}}_k)$ and moreover, the analytical form of the site partition function $\mathcal{Z}_k$ then immediately implies a possibility of performing the generalized decoration-iteration transformation [21–24]

$$\mathcal{Z}_k = \exp\left[\frac{\beta H_A}{2}(\sigma^z_k+\sigma^z_{k+1})\right]\left[1+2\exp(\beta D)\cosh\left(\beta\sqrt{E_k^2+E^2}\right)\right]$$