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Magnetization distribution in a spin ladder-shaped quantum nanomagnet

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ABSTRACT

The quantum nanomagnets show interesting site-dependent magnetic properties as a function of the temperature and the external magnetic field. In the paper we present the results of calculations for a finite quantum spin ladder with two legs, consisting of 12 spins $S = 1/2$, with open ends. We describe our system with isotropic quantum Heisenberg model and perform exact numerical diagonalization of the Hamiltonian to use canonical ensemble approach. Our analysis focuses on the site-dependent magnetization in the system, presenting magnetization distributions for various interaction parameters. We discuss extensively the temperature and magnetic field dependences of individual site magnetizations. The interesting behaviour, with pronounced non-uniformity of magnetization across the ladder, is found.

1. Introduction

The quantum magnetic nanosystems exhibit numerous non-trivial properties [1,2]. Although the zero-dimensional nature of such systems excludes the presence of the typical phase transitions expected in infinite systems, yet a range of interesting phenomena specific to this class of objects can be observed instead. On the one hand, such nanomagnets can be experimentally realized either chemically, as molecular magnets [3–5], or by assembling them on the surface atom by atom [6]. On the other hand, their finite size enables the application of the most powerful (but computationally demanding) method for theoretical studies - the exact diagonalization, which yields an entirely physically correct picture, free from any artefacts even for fully quantum models [7–9]. These facts should be supplemented with observation that nanomagnets can carry huge potential for applications in information storage and processing, both at classical level [10–12] and at quantum level [13–17]. As a consequence, the studies of nanomagnetic systems are strongly motivated. This motivation seems to peak at the finite chain-like and ladder-shaped systems, which recently attract particular experimental attention [11,12]. Although the theoretical studies of finite systems were mainly aimed at extrapolation to infinite, one-dimensional cases [18–20], yet also chains and ladders of finite length are interesting by themselves (to mention, for example, the presence of nontrivial edge states) [21–25].

It should be emphasized that the finite, zero-dimensional nanomagnets exhibit lack of translational symmetry, so that all the physical quantities which are defined for single spins can be expected to be site-dependent. This contrasts with the behaviour of the infinite systems, where the symmetry of the magnetic ordering does not lead usually to such non-uniformity. Therefore, nanomagnets offer a particularly interesting opportunity to investigate the highly non-uniform systems. Especially, the magnetization can be expected to depend on the considered site, so that the study of the magnetization distribution is of primary importance. The local magnetization can be characterized experimentally with atomic-resolved methods [26–32] and experimental studies focused on the magnetization distribution [33–35] can be mentioned. Moreover, the non-uniformity of magnetization can influence the functioning of any nanomagnet-based device or even serve as a basis for its design. The modeling of site-dependent magnetization as a function of the temperature and external magnetic field for cluster-like systems appears therefore well motivated and valuable, especially if based on the exact approach. We can mention that the theoretical studies of magnetization distribution (performed with either exact or approximate methods) are known in the literature both for zero-dimensional magnets [36] as well as for other non-uniform systems, like, for example, thin films [37–39]. Also the thermodynamics of magnetic clusters was subject of several computational works exploiting the exact (or close to exact) approaches, involving both ‘classical’, Ising-based systems [40–45] as well as highly non-trivial quantum Heisenberg systems [40,46,7,47–56].

In view of the mentioned facts, the aim of our paper is to perform an exact study of the site-dependent magnetization of a selected ladder-shaped, finite nanomagnet. In particular, we would like to uncover the evolution of the magnetization distribution as a function of the temperature and the external magnetic field. The study is aimed at supplementing and developing the previous ground-state results [57]

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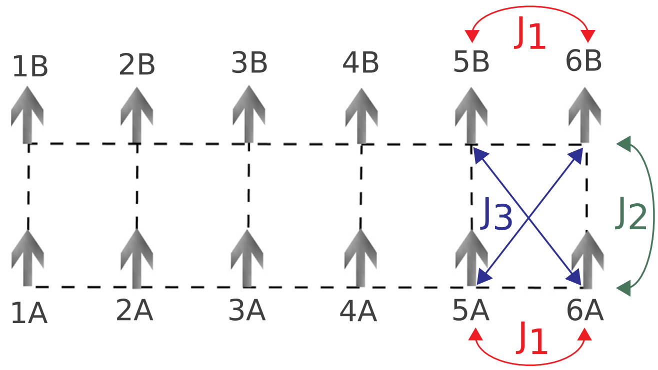

Fig. 1. A schematic view of the system of interest – a quantum nanomagnet being a finite two-legged ladder. The spins $S = 1/2$ are labelled with the index of leg (A or B) and the position in the leg (1–6). The interactions between the spins are depicted schematically.

obtained for a two-legged spin ladder composed of 12 spins. It should be emphasized here that our system of interest lacks translational symmetry because of the open ends of both chains (legs of the ladder). The effect of various intra- and interleg interactions of either ferro- or antiferromagnetic sign and different magnitudes will be characterized. Some further discussion concerning the selection of the system of interest can be found in the Section 4.

2. Theoretical model

The study is devoted to the system being a spin ladder with two legs of finite length, consisting in total of $N = 12$ quantum spins $S = 1/2$ [57]. Fig. 1 presents a schematic view of the investigated nanomagnet. Each spin is labelled with an index of a leg (A or B) as well as the position in the leg ($i,j = 1,...,6$). The interactions between the spins are isotropic in spin space and described with Heisenberg model, with the exchange integrals explained in Fig. 1. The system is ruled by the following Hamiltonian:

$$\mathcal{H} = -J_1\left(\sum_{\langle iA,jA\rangle} \mathbf{S}_{iA}\cdot\mathbf{S}_{jA} + \sum_{\langle iB,jB\rangle} \mathbf{S}_{iB}\cdot\mathbf{S}_{jB}\right) - J_2\sum_{\langle iA,jB\rangle} \mathbf{S}_{iA}\cdot\mathbf{S}_{jB} - J_3\sum_{\langle\langle iA,jB\rangle\rangle} \mathbf{S}_{iA}\cdot\mathbf{S}_{jB} - H\left(\sum_{iA} S^z_{iA} + \sum_{iB} S^z_{iB}\right). \tag{1}$$

The intraleg coupling between nearest neighbours is denoted by J_1, whereas analogous interleg (rung) coupling amounts to J_2. In addition, interleg (crossing) interactions between second neighbours are denoted by J_3. The external magnetic field, defining the z direction in spin space, is equal to H. The spin operators $\mathbf{S} = \left(\frac{1}{2}\sigma^x, \frac{1}{2}\sigma^y, \frac{1}{2}\sigma^z\right)$ are composed of appropriate Pauli matrices.

The Hamiltonian (Eq. (1)) and all the other quantum operators related to the system in question can be expressed as the matrices of the size 4096×4096. The exact numerical diagonalization of the Hamiltonian yields the eigenvalues ϵ_k and eigenvectors $|\psi_k\rangle$. On such basis, within the canonical ensemble approach, the statistical sum for the system in question can be expressed as

$$\mathscr{Z} = \sum_k \exp(-\beta\,\epsilon_k), \tag{2}$$

where $\beta = (k_B T)^{-1}$, with k_B denoting the Boltzmann constant. Also the thermal average value of an arbitrary quantum operator $\boldsymbol{A}$ can be directly determined from the formula:

$$\langle \boldsymbol{A}\rangle = \frac{1}{\mathscr{Z}}\sum_k \langle\psi_k|\,\boldsymbol{A}\,|\psi_k\rangle \exp(-\beta\,\epsilon_k). \tag{3}$$

In the present paper the quantity of particular interest is the magnetization. The magnetization at j-th site can be expressed with the following operator:

$$\boldsymbol{m}_j^z = \bigotimes_i \left(\frac{1}{2}\delta_{i,j}\,\boldsymbol{\sigma}^z + (1-\delta_{i,j})\boldsymbol{I}_2\right). \tag{4}$$

The symbol $\otimes$ denotes the Kronecker (external) product, while $\delta_{i,j}$ is the Kronecker delta. The operator $\boldsymbol{\sigma}^z$ is the appropriate Pauli matrix and $\boldsymbol{I}_2$ is identity matrix of the size 2×2. The total magnetization of the system is expressed as the following sum:

$$\boldsymbol{m}_T^z = \sum_j \mathbf{m}_j^z. \tag{5}$$

The key quantities studied in the present paper are: the average total magnetization $m_T^z = \langle \boldsymbol{m}_T^z\rangle$ and the average magnetizations for individual sites of the nanomagnet, $m_j^z = \langle \boldsymbol{m}_j^z\rangle$. The numerical results concerning their behaviour as a function of the temperature and external magnetic field will be extensively analysed in the next section of the paper.

3. Numerical results and discussion

All the results of numerical calculations presented in this section were obtained using Wolfram Mathematica software [58]. The discussed diagrams concern in general the dependence of magnetization on the temperature and the magnetic field for the system in question, for a representative selection of the interaction parameters between the spins. For the investigated range of parameters, no site-dependent magnetization was found to depend on the leg index (A or B) and only the dependence on the position in the leg was observed.

Let us commence the analysis from the dependence of the total magnetization of the system on the temperature and magnetic field, which is shown in Fig. 2(a) for the case of $J_1 < 0$ and $J_2 > 0$. The density plot allows additionally to trace the contours of constant magnetization vs. both thermodynamic variables – T and H. The values lay between 0 and 6, where the value of 0 is achieved for $H = 0$ and arbitrary temperature and 6 means the magnetic saturation. The points in which numerous contours tend to merge at the ground state ($T = 0$) correspond to the subsequent critical magnetic fields at which the total magnetization changes its value discontinuously. Such behaviour is presented in Fig. 2(a) in our previous work (Ref. [57]) and the values of critical magnetic field shown there are consistent with the limiting behaviour seen in Fig. 2(a) in the present work. At finite temperatures, it is evident that the total magnetization always increases with an increasing magnetic field. However, analysis of the isolines of constant magnetization supports the statement that in some range the magnetization increases with the increasing temperature and then falls down, reaching some local maximum. In some narrow ranges also a minimum and maximum or two maxima separated by a minimum or a plateau can exist (as evidenced by the detailed analysis of the data).

After a brief analysis of the total magnetization, let us focus the attention on the particular position in the ladder. Namely, in Fig. 2(b) we present the temperature and magnetic field dependence of the magnetization for the sites in ladder labelled with 2 and 5 (see Fig. 1 for explanation). In such case it is seen that the magnetization can reach both positive values and negative values (in some area of the diagram for low temperatures and magnetic fields, limited with a bold contour). It follows that the magnetization for temperatures low enough drops down when the magnetic field increases and then crosses the zero value and increases further. Therefore, a non-monotonous behaviour is predicted at sufficiently low temperatures. In addition to extrema achieved as a function of the magnetic field for constant temperature also extrema as a function of the temperature for fixed magnetic field can be expected.

The occurrence of antiparallel orientation of spins at the sites 2 and 5 with respect to the other spins, promoted by external magnetic field,

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