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Ground-state magnetic properties of spin ladder-shaped quantum nanomagnet: Exact diagonalization study

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The paper presents a computational study of the ground-state properties of a quantum nanomagnet possessing the shape of a finite two-legged ladder composed of 12 spins $S = 1/2$. The system is described with isotropic quantum Heisenberg model with nearest-neighbour interleg and intraleg interactions supplemented with diagonal interleg coupling between next nearest neighbours. All the couplings can take arbitrary values. The description of the ground state is based on the exact numerical diagonalization of the Hamiltonian. The ground-state phase diagram is constructed and analysed as a function of the interactions and the external magnetic field. The ground-state energy and spin-spin correlations are extensively discussed. The cases of ferro- and antiferromagnetic couplings are compared and contrasted.

1. Introduction

Low-dimensional systems attract increasing attention of solid state physicists. The most intensive studies focus on various nanostructures and within this class a considerable attention is paid to magnetic nanosystems [1–3]. The principal motivation for studies of the smallest nanostructured magnetic systems is the possibility of arranging them within bottom-up approach from single atoms of surfaces [4–6]. This approach allows the design and engineering of artificial nanomagnets with high precision. Moreover, their properties can also be carefully characterized at the nanoscale [7–11]. What is crucial, the geometry [12] and underlying magnetic interactions in such systems [13–16] can be tuned to achieve the desired characteristics. It has been demonstrated that the nanomagnets arranged of single atoms can serve as memory devices, what proves the high potential for applications [5,6]. Moreover, the nanomagnetic systems are also hoped to be useful for quantum computations [17], to mention, for example, spin clusters representing the qubits [18,19]. This route is particularly promising when based on molecular nanomagnets [20–24]. The mentioned facts serve as a strong motivation for theoretical studies of a variety of nanomagnetic systems.

One of the interesting classes of such systems is nanomagnets possessing the shape of spin ladder with finite length. This structure was the subject of experimental interest in Ref. [6] and built a prototypical memory device. It should be mentioned that major attention in the literature is paid to infinite spin ladders with various number of legs, constituting one-dimensional systems [25–29]. In that context the notion of Haldane gap and the dependence of excitations on spin magnitude and the number of legs in the ladder should be mentioned [25]. However, highly interesting properties can be shown also by the finite systems themselves. Although the magnetic ordering is excluded in such structures, yet they can exhibit interesting magnetic phases and cross-overs between them. Among the studies of such zero-dimensional structures, the works based on exact methods should be especially mentioned [27,30–44]. It is worth emphasizing that rigorous and exact numerical solutions are, so far, available only for a very limited class of models (especially when the quantum version is considered) [45–47].

In order to explore the magnetic properties of the finite structures, it is first vital to examine their ground states, taking into account various possible interactions between the spins as well as the external magnetic field. This is the aim of the present paper, in which we investigate a nanomagnet being a two-legged finite spin ladder with 12 spins $S = 1/2$. For this purpose we select an approach based on exact diagonalization, which provides an approximation-free picture of the physics of the studied system. The further parts of the paper contain a detailed description of the system in question, the theoretical approach and the review of the obtained results.

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2. Theoretical model

The system of interest in the present study is a nanomagnet having the shape of a finite ladder with two (equivalent) legs. The schematic view of the system is presented in Fig. 1. It consists of $N = 12$ quantum spins $S = 1/2$, coupled with isotropic, Heisenberg-like interactions. Therefore, it is described with the following quantum Hamiltonian:

$$\mathcal{H} = -J_1\sum_{\langle i,j\rangle}\mathbf{S_i}\cdot\mathbf{S_j} - J_2\sum_{\langle i,j\rangle}\mathbf{S_i}\cdot\mathbf{S_j} - J_3\sum_{\langle\langle i,j\rangle\rangle}\mathbf{S_i}\cdot\mathbf{S_j} - H\sum_{i} S_i^z. \qquad (1)$$

The operator $\mathbf{S_i} = (S_i^x, S_i^y, S_i^z)$ denotes a quantum spin $S = 1/2$, located at site labelled with i ($i = 1, \dots, 12$), with $S_i^\alpha = \sigma^\alpha/2$, where σ^α is the appropriate Pauli matrix and $\alpha = x, y, z$ is the direction in spin space. Moreover, the product $\mathbf{S_i}\cdot\mathbf{S_j} = S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z$. The exchange integral between nearest-neighbour spins in the same leg of the ladder amounts to J_1, while the interactions between the ladder legs are denoted by J_2 for nearest neighbours (rung interactions) and J_3 for next-nearest neighbours (crossing interactions); see the scheme Fig. 1. All the exchange integrals J_1, J_2, J_3 are allowed to take arbitrary values, both positive (ferromagnetic) and negative (antiferromagnetic). The external magnetic field acting in z direction in spin space is introduced by H.

In the present study, the interest is focused on the ground-state properties of the system, at zero temperature. In order to perform the description, the full Hamiltonian (Eq. (1)) is constructed in a form of a matrix (of the size $2^N \times 2^N = 4096 \times 4096$) and diagonalized numerically [48]. This procedure yields the eigenvalues E_k and eigenvectors $|\psi_k\rangle$ (which can be degenerate). Among the eigenenergies, the ground-state energy E_0 is selected, with eigenvectors $|\psi_0^p\rangle$, where $p = 1, \dots, d$ and d is the degeneracy. At the zero temperature, each of the degenerate ground states is equally probable. Therefore, the ground-state average of the arbitrary quantum operator A can be evaluated on the basis of the following formula: $\langle A\rangle = \frac{1}{d}\sum_{p=1}^{d}\langle\psi_0^p|A|\psi_0^p\rangle$. The observable of special interest is here the total z component of spin of the nanomagnet, with the average value of $S_T = \langle\sum_{i=1}^{N} S_i^z\rangle$. In that context, another quantum number can be defined, namely the total spin quantum number, defined by $\widetilde{S}_T\left(\widetilde{S}_T + 1\right) = \langle\sum_{i=1}^{N}\mathbf{S}_i^2\rangle$. Further important quantities are spin-spin correlation functions $c_{ij}^{\alpha\beta} = \langle S_i^\alpha S_j^\beta\rangle$, where $\alpha, \beta = x, y, z$.

The presented theoretical formalism serves as a basis for numerical calculations of the crucial ground-state properties of the studied nanomagnet, which will be discussed in the following section of the paper.

3. Numerical results and discussion

All the calculations presented in this section rely on the exact numerical diagonalization of the system Hamiltonian (Eq. (1)) performed with the Mathematica software [48]. The discussion will be subdivided into subsections related to the key characteristics of the ground state.

3.1. Ground-state phase diagram

Let us commence the analysis from the investigation of the ground-state phase diagram for the system in the external magnetic field. The phases correspond here to various values of the z component of the total spin, denoted by S_T. The phase diagram presenting the stability areas for phases with different values of S_T as a function of $J_2/|J_1|$ and the magnetic field $H/|J_1|$ is shown in Fig. 2, for different values of $J_3/|J_1|$. The cases of antiferromagnetic $J_1 < 0$ and ferromagnetic $J_1 > 0$ are shown separately, as the absolute value $|J_1|$ is taken as the convenient energy to normalize other quantities. Let us analyse first the diagram for $J_1 < 0$ and $J_3/|J_1| = 0.0$ [Fig. 2(a)]. At $J_2 = 0.0$ we deal with a pair of non-interacting finite spin chains, so the total spins take only even values. Introducing a finite, non-zero interaction J_2 restores the presence of the phases with all possible spins. What is interesting, for strongly antiferromagnetic J_2 the phase boundaries linearize and have identical slopes. This can be explained due to the fact that in the limit of dominant J_2 coupling the critical fields do not depend on J_1 (but only on J_2 itself). On the other hand, for strongly ferromagnetic J_2 the critical fields $H/|J_1|$ cease to depend on J_2. Let us mention that the diagram bears some resemblance to Fig. 2 in Ref. [27], where the two-legged finite ladder was studied with the aim of characterizing an infinite system.

If the antiferromagnetic crossing inter-leg interaction J_3 is switched on [as shown in Fig. 2(b)], the ladder legs are no longer non-interacting for $J_2 = 0.0$. As a consequence, for the full range of exchange integrals J_2 we pass through all the states with spins $0, \dots, 6$ when the magnetic field increases. However, close to some critical values of J_2 (slightly decreasing with the considered spin) the phases with odd spins are suppressed. The limiting behaviour of the diagram for strongly ferromagnetic and strongly antiferromagnetic coupling J_2 remains similar to the case of $J_3 = 0.0$.

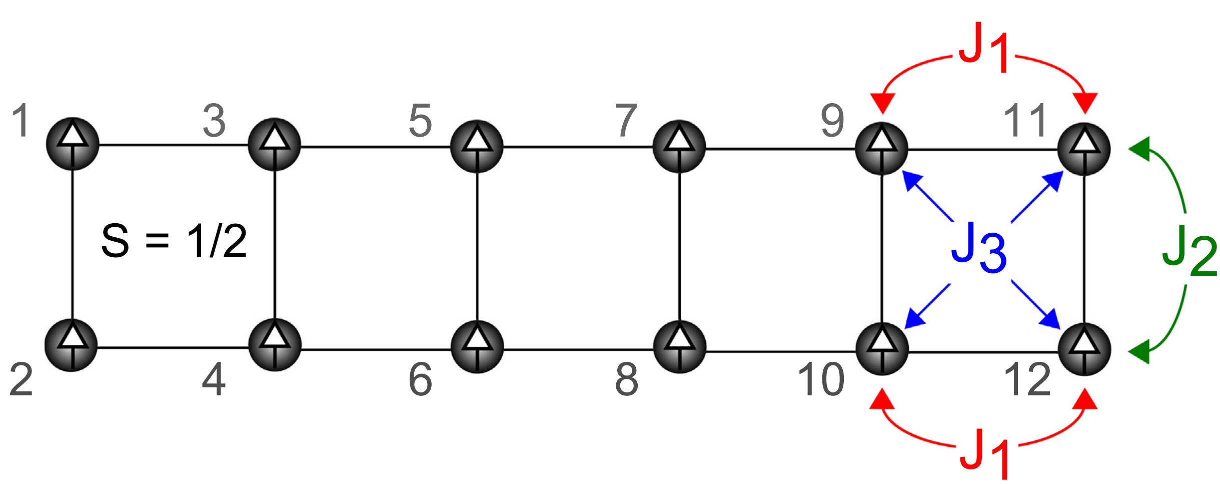

Fig. 1. A schematic view of the quantum nanomagnet composed of 12 spins $S = 1/2$, having a shape of finite two-legged ladder. The exchange integrals between the spins are depicted schematically.