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Phase diagram and magnetization structures of spin-$\frac{3}{2}$ bond-alternating Ising chains with single-ion anisotropy

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ABSTRACT

By the infinite time-evolving block decimation (iTEBD) algorithm, the magnetization process of the spin-$\frac{3}{2}$ bond-alternating Ising chain with single-ion anisotropy (D) is investigated. Magnetization plateaus including detailed magnetization structures of three different cases are uncovered, and three rich ground-state phase diagrams are explicitly determined. Especially, for the uniform antiferromagnetic case, a phase transition line at $D=J$, which divides the $M^z=0$ ($M^z=\frac{1}{2}$) plateau into two phases, are detected by the magnetization structure and the ground-state energy, and a updated phase diagram is proposed. Such a transition line was not recognized by the average magnetization previously. A same transition line ($D=J$) is also detected in the phase diagram of the antiferromagnetic-ferromagnetic alternating case. Magnetization plateaus are found to be easily induced for the classical Ising systems without quantum fluctuations, and the single-ion anisotropy plays a key role in the formation of $M^z=\frac{1}{2}$ and 1 plateaus in the present model.

1. Introduction

Magnetization plateau with constant magnetization [1] is a novel macroscopic quantum phenomenon in low-dimensional spin systems. To our knowledge, magnetization plateaus in one-dimensional (1D) spin systems can be induced by dimerization, frustration, single-ion anisotropy, periodic field and so on. Precisely, a necessary condition ($p(S-M^z)=$integer) for the appearance of magnetization plateau in spin chains was proposed by Oshikawa et al. [2]. The S represents the magnitude of spins, and M^z denotes the average magnetization. The p is the period of the ground state. Magnetization plateaus have attracted considerable attention [3–27] in the past decades. Among them, the existence of magnetization plateau in big spin ($S\geq 1$) chains with single-ion anisotropy is an interesting issue. For example, $M^z=\frac{1}{2}$ plateaus were observed in the spin-1 antiferromagnetic Heisenberg bond-alternating chain with single-ion anisotropy [25] and the spin-$\frac{3}{2}$ antiferromagnetic Heisenberg chain with single-ion anisotropy [26,27]. However, except for the fully polarized phase ($M^z=\frac{3}{2}$), no other plateaus can be realized in the spin-$\frac{3}{2}$ antiferromagnetic Heisenberg chain when the single-ion anisotropy is too weak ($D<0.93$). It was argued that the XY-planar interactions make the magnetization curve smooth and even destroys the other two plateaus of $M^z=0$ and 1 which exist in the Ising model with single-ion anisotropy [28]. In addition, four distinctive magnetization plateaus ($M^z=0$, $\frac{1}{2}$, 1, and $\frac{3}{2}$) were observed in the spin-$\frac{3}{2}$ antiferromagnetic Ising chain with single-ion anisotropy [29].

Besides the single-ion anisotropy, we think that the bond-alternation may also induce rich ground states. In the present paper, we would like to investigate spin-$\frac{3}{2}$ bond-alternating Ising chains with single-ion anisotropy and under an external magnetic field, which is described by

$$\hat{H}=J\sum_{i}^{N/2}[S_{2i-1}^{z}S_{2i}^{z}+\delta S_{2i}^{z}S_{2i+1}^{z}]+\sum_{j}^{N}[D(S_j^z)^2-hS_j^z], \qquad (1)$$

where S^z ($S^z=\pm\frac{1}{2}, \pm\frac{3}{2}$) denotes the z component of a spin-$\frac{3}{2}$ operator, and N is the length of the spin chain. J and $J\delta$ denote the nearest-neighbor couplings on odd and even bonds respectively, where δ represents the strength of the bond-alternation. D and h are the single-ion anisotropy and the external magnetic field, respectively. It is obvious that the ground state of such a model with ($J>0$ and $D=h=0$) should be an ideal stripe phase (SP) with four-period spin configurations "$\cdots\frac{3}{2}, -\frac{3}{2}, -\frac{3}{2}, \frac{3}{2}, \cdots$" or "$\cdots -\frac{3}{2}, \frac{3}{2}, \frac{3}{2}, -\frac{3}{2}, \cdots$" as $\delta<0$. However, it will become an ideal Néel phase (NP) with two-period spin configurations "$\cdots\frac{3}{2}, -\frac{3}{2}, \frac{3}{2}, -\frac{3}{2}, \cdots$" or "$\cdots -\frac{3}{2}, \frac{3}{2}, -\frac{3}{2}, \frac{3}{2}, \cdots$" as $\delta>0$. It means the $\delta=0$ is the transition point separating the ideal SP and NP. In fact, several typical models can be described by the Hamiltonian in Eq. (1). For instance, when $J>0$ and $\delta=1$, it becomes the uniform antiferromagnetic Ising model which was investigated by Chen et al. previously [29]. But, it

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becomes an antiferromagnetic-ferromagnetic (AF-F) bond-alternating Ising chain as $\delta=-1$. Furthermore, a uniform ferromagnetic Ising chain is formed as $J<0$ and $\delta=1$. It is natural to expect that these cases will have richer phase diagrams and complicated magnetization structures when both the single-ion anisotropy and the bond-alternation are taken into account.

In the present paper, magnetization processes of these cases mentioned above with single-ion anisotropy will be discussed. As shown below, very rich phase diagrams and magnetization structures will be uncovered. Especially, some plateau states with the same magnetization are found to have different microscopic magnetic structures. In detail, both $M^z=0$ and $\frac{1}{2}$ plateaus are found to consist of two different phases with different magnetic structures. It means that the magnetization is a macroscopic quantity, and incapable of distinguishing states with the same magnetization but different microscopic magnetization structures. Based on the magnetization diagram suggested by Chen et al. [29] and the magnetization structures, an updated phase diagram including six different phases will be obtained.

2. Numerical method

The infinite time-evolving block decimation (iTEBD) method [30] is applied to obtain the ground state of the Hamiltonian (see Eq. (1)). The iTEBD algorithm is an efficient numerical method based on the infinite matrix-product state (iMPS) representation, and can deal with systems in the thermodynamic limit. An imaginary time evolution operator $\exp(-\tau\hat{H})$ is acted on an arbitrary initial state $|\psi_0\rangle$, and $\exp(-\tau\hat{H})|\psi_0\rangle$ will converge to the ground state $|\psi_g\rangle$ in the limit $\tau\to\infty$. As a variational state, the initial state in the algorithm should be adopted in a proper way to avoid orthogonality for such a classical model without flipping terms. Practically, a very small $\delta\tau$ is adopted for each evolution step, hence the operator $\exp(-\delta\tau\hat{H})$ can be expanded into a sequence of two-site gates $U^{[i,i+1]}$ through the Suzuki-Trotter decomposition. The initial step $\delta\tau$ is set to be 10^{-1}, and then diminished to 10^{-8} gradually. In order to describe the possible four-period ground states, four-period wavefunctions should be adopted. In the framework of the iMPS, a four-period wavefunction of one-dimensional quantum system reads

$$|\psi\rangle=\mathrm{Tr}\left[\prod_{i=1}^{N/4}\Lambda^a\Gamma^a_{4i-3}\Lambda^b\Gamma^b_{4i-2}\Lambda^c\Gamma^c_{4i-1}\Lambda^d\Gamma^d_{4i}\right]|\ldots,m_{4i-3},m_{4i-2},m_{4i-1},m_{4i},\ldots\rangle. \quad (2)$$

The m_{4i-3}, m_{4i-2}, m_{4i-1}, and m_{4i} are local spin physical indices, and $\Gamma^{a\sim d}$ are 3-index tensors on sites $(4i-3,\cdots,4i)$. $\Lambda^{a\sim d}$ are χ by χ (χ is the cut-off bond dimension) diagonal matrices. For the classical cases discussed in the present paper, their ground states are all matrix direct product states, therefore a very small χ ($\chi>1$) is enough to obtain reliable results. In the following calculations, the cut-off bond dimension χ is set to be 30, which is large enough to obtain reliable results.

3. Phase diagram and magnetization structures

3.1. AF Ising chain

First, we investigate the case with $J>0$ and $\delta=1$ (see Eq. (1)), which is a uniform AF spin-$\frac{3}{2}$ Ising chain. The average magnetization defined as

$$M^z=\frac{1}{N}\sum_{i=1}^{N}\langle S^z_i\rangle \quad (3)$$

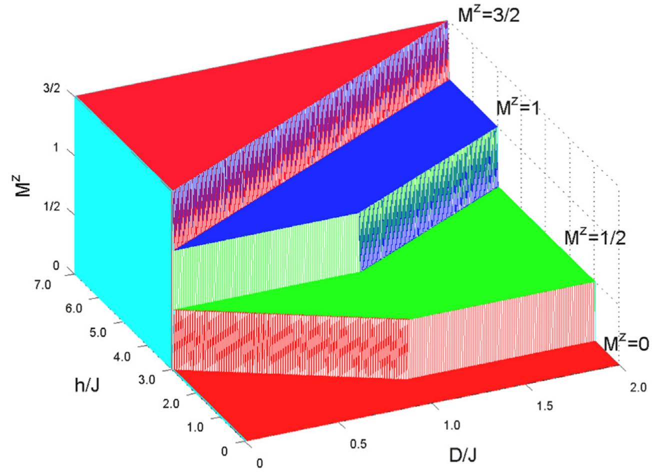

Fig. 1. (Color online) Average magnetization (M^z) of the uniform ($\delta=1$) AF ($J>0$) Ising chain with single-ion anisotropy (D). Four magnetization plateaus, i.e., $M^z=0$, $\frac{1}{2}$, 1, and $\frac{3}{2}$, can be clearly observed.

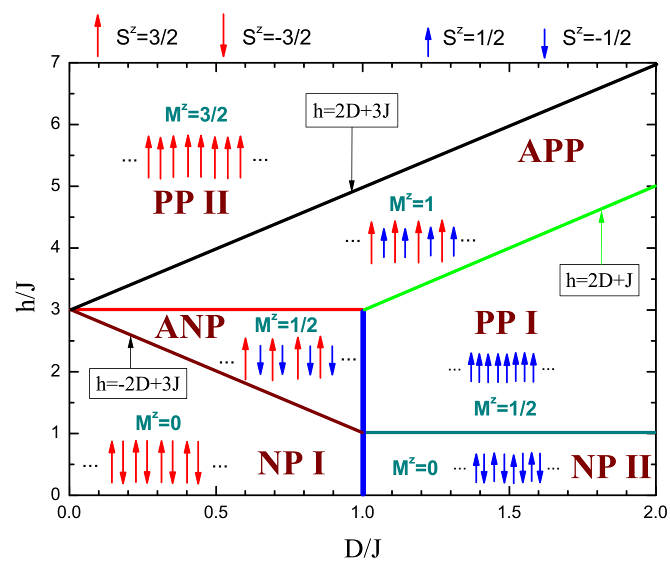

Fig. 2. (Color online) Ground-state *D*-*h* phase diagram of the uniform AF Ising chain. It includes six different phases: a Néel phase (NP) I, a NP II, an alternating Néel phase (ANP), a polarized phase (PP) I, a PP II, and an alternating polarized phase (APP). Different phases can be distinguished by their different magnetization structures.

is calculated, and a *D*-*h* magnetization diagram is plotted in Fig. 1. From Fig. 1, four magnetization plateaus, i.e., $M^z=0$, $\frac{1}{2}$, 1, and $\frac{3}{2}$, can be clearly observed. As the anisotropy vanishes ($D=0$), only two plateaus ($M^z=0$ and $\frac{3}{2}$) separated by $h/J=3.0$ exist. However, all the four plateaus can be induced by the increasing magnetic field once the single-ion anisotropy is switched on. The width of the $M^z=0$ ($M^z=1$) plateau becomes wider and wider with increasing D as $D/J<1.0$, but the widths of both plateaus become independent of the single-ion anisotropy as $D/J>1.0$. In addition, the $M^z=\frac{1}{2}$ plateau becomes wider and wider with increasing D. These magnetization plateaus including their boundaries are consistent with that suggested previously by the classical Monte Carlo method [29].

As argued above, the average magnetization is incapable of uncovering the microscopic magnetization structures. Therefore, we calculate the detailed magnetization structures of all the magnetization plateau states. According to the magnetization structures, a rich phase diagram including six phases is uncovered (see Fig. 2). The six ground states are named as a Néel phase (NP) I,