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.

Keywords: D. exchange and superexchange, D. phase transitions

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 ($p(S - M^z) = \text{integer}$) 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, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 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

$$\hat{H} = J \sum_i^{N/2} [S_{2i-1}^z S_{2i}^z + \delta S_{2i}^z S_{2i+1}^z] + \sum_j^N [D(S_j^z)^2 - h S_j^z], \quad (1)$$

where $S^z = \pm\frac{1}{2}, \pm\frac{3}{2}$ 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

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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 "... $\frac{3}{2}, -\frac{3}{2}, -\frac{3}{2}, \frac{3}{2}, \dots$ " or "... $-\frac{3}{2}, \frac{3}{2}, \frac{3}{2}, -\frac{3}{2}, \dots$ " as $\delta < 0$. However, it will become an ideal Néel phase (NP) with two-period spin configurations "... $\frac{3}{2}, -\frac{3}{2}, \frac{3}{2}, -\frac{3}{2}, \dots$ " or "... $-\frac{3}{2}, \frac{3}{2}, \frac{3}{2}, -\frac{3}{2}, \dots$ " 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 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 $\tau \rightarrow \infty$. 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

$$|\psi\rangle = \text{Tr} \left[\prod_{i=1}^{N/4} \Lambda^a \Gamma_{4i-3}^a \Lambda^b \Gamma_{4i-2}^b \Lambda^c \Gamma_{4i-1}^c \Lambda^d \Gamma_{4i}^d \right] | \dots, m_{4i-3}, m_{4i-2}, m_{4i-1}, m_{4i}, \dots \rangle. \quad (2)$$

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 $(4i-3, \dots, 4i)$. $\Lambda^{a \sim d}$ 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

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

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

Figure 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.

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, a NP II, an alternating Néel phase (ANP), a polarized phase (PP) I, a PP II, and an alternating polarized phase (APP), respectively. In detail, the NP I has the spin configuration “ $\dots \frac{3}{2}, -\frac{3}{2}, \frac{3}{2}, -\frac{3}{2}, \dots$ ”, but the NP II has the spin configurations “ $\dots \frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, \dots$ ”. The spin configuration of the ANP is “ $\dots \frac{3}{2}, -\frac{1}{2}, \frac{3}{2}, -\frac{1}{2}, \dots$ ”, and that of the APP becomes “ $\dots \frac{3}{2}, \frac{1}{2}, \frac{3}{2}, \frac{1}{2}, \dots$ ”. The PP I has the spin configuration “ $\dots \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \dots$ ”, and the PP II has the spin configuration “ $\dots \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \dots$ ”. It is found that the ANP and the PP I belong to the same magnetization plateau ($M^z=\frac{1}{2}$) but have different spin structures. It is the same for the NP I and II, which have different magnetization structures but belong to the same $M^z=0$ plateau. According to the different magnetization structures, the phase boundaries on $h=2D+3J$, $h=J$, $h=2D+J$, $h=-2D+3J$, $h=3J$, and $D=J$ are determined explicitly. It must be noted that the phase transition line at $D=J$ (the solid blue line in Fig. 2), which can not be recognized by the magnetization calculations, is exactly determined by the magnetization structure.

To determine the phase boundaries, the ground-state energy per site ($e_i = \frac{1}{N} \sum_{i=1}^N \langle \hat{H} \rangle$) of the uniform ($\delta=1$) AF ($J>0$) Ising chain is calculated. The ground-state energies per site of the NP I and II can be calculated by $e_i = [\frac{9}{4}(D-J)]$ and $[\frac{1}{4}(D-J)]$, respectively. And, that of the ANP and the APP are $[\frac{5}{4}D - \frac{3}{4}J - \frac{1}{2}h]$ and $[\frac{5}{4}D + \frac{3}{4}J - h]$, respectively. The ground-state energies per site of the PP I and II can be calculated by

Figure 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.

$e_i = [\frac{9}{4}(D+J) - \frac{3}{2}h]$ and $[\frac{1}{4}(D+J) - \frac{1}{2}h]$, respectively. Therefore, energy level crossings can be observed on all the phase boundaries (figures are not shown here), which indicate phase transitions take place. It means that the phase boundaries can also be determined by the energy level crossings.

3.2. AF-F bond-alternating Ising chain

Then, we discuss the phase diagram and magnetization structures of the spin- $\frac{3}{2}$ AF-F bond-alternating Ising chain. Similar to the AF case, the average magnetization M^z is also calculated with varying D and h . As shown in Fig. 3, four distinctive magnetization plateaus, i.e., $M^z=0$, $\frac{1}{2}$, 1, and $\frac{3}{2}$, are observed, which is similar to that of the AF case shown in Fig. 1. The main difference is that the $M^z=\frac{1}{2}$ and 1 plateaus can be induced when $D/J>0.5$. As $D/J<0.5$, only the $M^z=0$ and $\frac{3}{2}$ plateaus are observed. Furthermore, the boundary between the $M^z=0$ and $\frac{3}{2}$ plateaus is always $h/J=1.5$, which is independent of the single-ion anisotropy.

To uncover more information, the magnetization structures of all the magnetization plateaus are discussed, and the phase diagram including six different phases (see Fig. 4) is determined. The $M^z=\frac{3}{2}$ plateau is found to have spin configuration “ $\dots \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \dots$ ”, therefore it is named as PP II. In the whole $M^z=1$ plateau, the spin configuration “ $\dots \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \dots$ ” is observed, and we call it a stripe polarized phase (SPP). Similar to the AF case, the $M^z=0$ ($M^z=\frac{1}{2}$) is also found to have two different spin configurations.

Figure 3: (Color online) Average magnetization (M^z) of the AF-F bond-alternating ($\delta=-1$) Ising chain with single-ion anisotropy (D). Four distinctive magnetization plateaus, i.e., $M^z=0$, $\frac{1}{2}$, 1, and $\frac{3}{2}$, can be seen.

In detail, “ $\dots \frac{3}{2}, -\frac{3}{2}, -\frac{3}{2}, \frac{3}{2}, \frac{3}{2}, -\frac{3}{2}, -\frac{3}{2}, \frac{3}{2}, \dots$ ” and “ $\dots \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \dots$ ” are observed in the $M^z=0$ plateau region, and we call them the stripe phase (SP) I and the SP II respectively. In the $M^z=\frac{1}{2}$ plateau region, spin configurations “ $\dots \frac{3}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{3}{2}, \frac{3}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{3}{2}, \dots$ ” and “ $\dots \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \dots$ ” are obtained, therefore they are named as an antiferromagnetic stripe phase (ASP) and a PP I. According to their different magnetization structures, we determine the phase boundaries, which are $h=2D + \frac{1}{2}J$, $h=\frac{3}{2}J$, $h=2D - \frac{1}{2}J$, $h=-2D + \frac{5}{2}J$, $h=\frac{1}{2}J$, and $D=J$. It indicates that the $M^z=0$ ($M^z=\frac{1}{2}$) plateau is also divided into two different phases by the boundary $D=J$ (see the solid blue line in Fig. 4).

In addition, the ground-state energies per site of the six phases in the phase diagram (see Fig. 4) are determined to be $[\frac{9}{4}(D - J)]$ (SP I), $[\frac{1}{4}(D - J)]$ (SP II), $[\frac{5}{4}D - \frac{1}{4}J - h]$ (SPP), $[\frac{5}{4}D - J - \frac{1}{2}h]$ (ASP), $[\frac{1}{4}D - \frac{1}{2}h]$ (PP I), and $[\frac{9}{4}D - \frac{3}{2}h]$ (PP II). Furthermore, energy level crossings are also observed on all the phase boundaries, which indicates phase transitions take place there.

3.3. Ferromagnetic Ising chain

Finally, the spin- $\frac{3}{2}$ uniform ($\delta=1$) ferromagnetic ($J<0$) Ising chain is investigated. The average magnetization M^z is shown in Fig. 5, and only two magnetization plateaus ($M^z=\frac{1}{2}$ and $\frac{3}{2}$) are observed. The $M^z=0$ and 1 magnetization plateaus vanish for the ferromagnetic case. Then, the detailed magnetization structures are studied. It is found that the $M^z=\frac{1}{2}$ plateau belong to a PP I with spin configuration “ $\dots \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \dots$ ”, and the $M^z=\frac{3}{2}$ plateau is a PP II with spin configura-

Figure 4: (Color online) Ground-state D - h phase diagram of the AF-F bond-alternating ($\delta=-1$) Ising chain with single-ion anisotropy (D). It includes six different phases: a stripe phase (SP) I, a SP II, an alternating stripe phase (ASP), a polarized phase (PP) I, a PP II, and an stripe polarized phase (SPP). Different phases can be distinguished by their different magnetization structures.

tion “ $\dots \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \dots$ ”. Accordingly, a simple phase diagram is determined and shown in Fig. 6, and the phase boundary between the PP I and II is $h=2D + 2J$. The round-state energies of the PP I and II can be calculated by $e_i = [\frac{9}{4}(D + J) - \frac{3}{2}h]$ and $[\frac{1}{4}(D + J) - \frac{1}{2}h]$ respectively, therefore energy level crossing occurs on the phase boundary.

4. Discussions and conclusions

By the iTEBD algorithm, the magnetization of the spin- $\frac{3}{2}$ bond-alternating Ising chain with single-ion anisotropy was investigated. Three cases, i.e., ($J>0$, $\delta=1$), ($J>0$, $\delta=-1$), and ($J<0$, $\delta=1$), have been discussed in detail. The case ($J<0$, $\delta=-1$), which has not been dealt with in the present paper, belongs to a F-AF alternating chain and has the same ground-state properties as that of the AF-F alternating chain ($J>0$, $\delta=-1$). For these classical models, the ground-state states of all the phases are found to be some matrix direct product states (with only one nonzero diagonal element ($\Lambda_1=1$)).

Magnetization plateaus including their detailed magnetization structures and ground-state phase diagrams of the three cases mentioned above have been explicitly determined. Especially, for the case ($J>0$, $\delta=1$), a phase transition line at $D=J$, which divides the $M^z=0$ ($M^z=\frac{1}{2}$) plateau into two phases, was detected by the spin configurations and ground-state energy. It must be noted that such a transition line ($D=J$) was not be recognized by the average magnetization previously [29]. Further-

Figure 5: (Color online) Average magnetization (M^z) of the uniform ($\delta=1$) ferromagnetic ($J<0$) Ising chain. It includes two magnetization plateaus, i.e., $M^z=\frac{1}{2}$ and $\frac{3}{2}$.

Figure 6: (Color online) Ground-state D - h phase diagram of the uniform ($\delta=1$) ferromagnetic ($J<0$) Ising chain. It includes two different phases, i.e., a polarized phase (PP) I and a PP II, which have different magnetization structures.

more, a similar phase transition line at $D=J$, which divides the $M^z=0$ ($M^z=\frac{1}{2}$) plateau into two phases, was also detected in the AF-F alternating case ($J>0$, $\delta=-1$). It is found that the system behaves like a $S=\frac{1}{2}$ Ising chain as the single-ion anisotropy becomes strong enough, for example, the PP I in Figs. 2, 4, and 6, the NP II in Fig. 2, and SP II in Fig. 4. However, it exhibits $S=\frac{3}{2}$ Ising characters as the magnetic field becomes strong enough but the single-ion anisotropy is too weak (see the PP II in Figs. 2, 4, and 6, the NP I in Fig. 2, and the SP I in Fig. 4). In the intermediate regions with moderate h and D , the system shows $S=\frac{1}{2}$ and $S=\frac{3}{2}$ alternating characters; for instance, the ANP and APP in Fig. 2 and the ASP and SPP in Fig. 4.

As mentioned above, only the $M^z=\frac{1}{2}$ and $\frac{3}{2}$ plateaus can be observed in the magnetization of the spin- $\frac{3}{2}$ antiferromagnetic Heisenberg chain with single-ion anisotropy [26, 27], and the $M^z=\frac{1}{2}$ plateau vanishes absolutely as the single-ion anisotropy is too weak ($D < 0.93$). Furthermore, the $M^z=0$ and 1 plateaus can not be observed in this quantum case, which is due to the effects from the XY-planar interactions [28]. In other words, strong quantum fluctuations will destroy the formation of both $M^z=0$ and 1 plateaus. Three cases investigated in the present paper are absolutely classical and without any quantum fluctuations, therefore distinctive and stable $M^z=0$ and 1 plateaus are easily induced. Our numerical results show that the single-ion anisotropy plays a key role in the formation of $M^z=\frac{1}{2}$ and 1 plateaus in the present model.

It must be noted that, for the classical cases, the magnetization structures actually can be replaced by the nearest-neighbor (NN) correlations. For instance, the NN correlation of the PP I phase is $\langle S_i^z S_{i+1}^z \rangle = \frac{1}{4}$, but that of the PP II and APP phases become $\frac{9}{4}$ and $\frac{3}{4}$ respectively. For the SP I and the SP II phases, their NN correlations on odd- and even-bonds have alternating signs “ $\dots -\frac{9}{4}, \frac{9}{4}, \dots$ ” and “ $\dots -\frac{1}{4}, \frac{1}{4}, \dots$ ”, respectively. The NN correlations ($\langle S_i^z S_{i+1}^z \rangle$) of the NP I, the NP II, and the ANP phases are $-\frac{9}{4}$, $-\frac{1}{4}$, and $-\frac{3}{4}$, respectively. In the four-period SPP and ASP phases, four-period NN correlations are also observed, which are “ $\dots \frac{3}{4}, \frac{1}{4}, \frac{3}{4}, \frac{9}{4}, \dots$ ” and “ $\dots -\frac{3}{4}, \frac{1}{4}, -\frac{3}{4}, \frac{9}{4}, \dots$ ”, respectively. It is obvious that these NN correlations can also be used to reveal their corresponding magnetic structures of all the phases.

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