A non-isotropic Antiferromagnetic Spin Chains in a Transverse Field: Reentrant Behavior of the Staggered Magnetization

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We investigate one-dimensional $S = 1/2$ and $S = 1$ antiferromagnetic quantum spin chains with easy-axis anisotropies in a transverse field. We calculate both the uniform $m$ magnetization and the staggered $m$ magnetization, using a variant of the density matrix renormalization group method. We find that the staggered magnetizations exhibit reentrant behavior as functions of the transverse field, where the competition between the classical Neel order and the quantum fluctuations plays an important role. We also discuss the critical behavior associated with the staggered magnetizations.

1. INTRODUCTION

Recently, magnetization processes of one-dimensional (1D) quantum spin systems have been attracting much interest from both theoretical and experimental viewpoints. Particularly, various types of field-induced critical behavior in the magnetization processes, such as a square-root behavior associated with the excitation gap, the magnetization plateau, the cusplike singularities, etc., have been investigated intensively. In most of these theoretical analyses of the magnetization processes, the external field is supposed to be applied in the longitudinal direction. For the case of a system having an anisotropy, however, the magnetic properties of the system may be essentially different, depending on whether the external field is applied in the transverse or longitudinal directions. In this paper, we wish to make a quantitative analysis for the magnetic properties of antiferromagnetic quantum spin chains with easy-axis anisotropies in a transverse field.

In analyzing an anisotropic model in the transverse magnetic field, an essential point is that the total $S^z$ of the system is not a conservative quantity, since the symmetry of the model is reduced to be $Z_2$. Then, the property of the system is characterized with the staggered magnetization. For example, the appearance of the staggered magnetization is known for the $S = 1/2$ XXZ spin chain in the Ising limit, while the isotropic $XXZ$ model has no Neel order. The anisotropy favors the classical Neel order, whereas the transverse field term induces a quantum fluctuation in addition to the usual XY term. What we are interested in here is how the system behaves between the Ising limit and the isotropic limit. We discuss the physics developed by the competition between the anisotropy and the quantum fluctuations, based on quantitative calculations of the staggered magnetization.

For the purpose of computing the magnetization curves, we employ the product wave function renormalization group (PW FRG) method, which is a variant of the density matrix renormalization group (DMRG) method. The PW FRG is successfully applied to various types of the magnetization processes and further it can treat a system without the total $S^z$ conservation efficiently. We calculate the staggered magnetization in the easy-axis direction and the uniform $m$ magnetization in the transverse one, for the infinite-length chains. Here, it should be noted that the lack of the total $S^z$ conservation makes the exact diagonalization study difficult for the anisotropic models in the transverse field.

For the $S = 1/2$ XXZ chain, we find the reentrant behavior of the staggered magnetization, which is partially supported by the exact results at some special parameters. We further discuss the $S = 1$ XXZ spin chain and the $S = 1$ Heisenberg spin chain with the single-ion anisotropy, where the existence of the Haldane gap makes the physics of the system more fruitful. We verify that the phase transitions are second at the lower critical field and the higher critical one. The former field is associated with the Haldane gap, and the latter can be connected with the saturation field of the isotropic case adiabatically. We also discuss the critical behavior characterized by the staggered magnetizations.

This paper is organized as follows: In §II, we describe the $S = 1/2$ XXZ spin chain in a transverse field. In §III, we consider the $S = 1$ quantum spin chains with the XXZ-type anisotropy (§III-A) and the single-ion anisotropy (§III-B). The last section is devoted to the summary.

II. THE $S = 1/2$ CASE

The $S = 1/2$ XXZ chain is one of the most fundamental models among spin chains of $S = 1/2$. In this section, we consider the XXZ chain in a transverse field. We write the Hamiltonian $H$ as

$$H = J \sum_i S_i^x (S_{i+1}^x S_i^z),$$

(1)
where $S_i$ is the component of the $S = 1/2$ spin operator at $i$-th site, and $\gamma$ is the strength of the transverse field. The exchange coupling constant in easy-plane ($xy$-plane) is denoted by $J_x$, and that of the easy-axis ($x$-axis) direction by $J_y$. We have set $g = 1$ (g: g-factor, $\hbar$: Bohr magneton) for simplicity. In this section, we discuss the system in the range $0 < J_x < 1$ with $J_y = 1$.

The magnetic property of the Hamiltonian \cite{1} has been studied for several years \cite{2,3}. Particularly, it should be remarked that there is a special value of the transverse field called a disorder point, where the ground state is written down analytically \cite{1,6}. In addition, Mori et al. have discussed how the excitation structure of eq. \cite{3} is affected by the transverse field \cite{4,5}. However, the full magnetization process for general parameters of eq. \cite{3} has not been calculated quantitatively, except for the exactly solved cases $J_y = 0$ (the Ising model in a transverse field) and $J_y = 1$ (the Heisenberg model).

In the following, we calculate the uniform magnetization in $x$-direction $M_x = \sum \langle S_i^x \rangle$ and the staggered magnetization in $z$-direction $M_{st} = \sum \langle S_i^z \rangle$ by using the PW FRG method. Here we note that it is useful to consider the rotation of spins at every two sites (for example, at every even sites):

$$U \exp \{ \sum_{\langle ij \rangle} i S_i^x \};$$

since we can calculate the staggered magnetization as the uniform magnetization in the transformed system $H' = U^\dagger H U$. We have confirmed that the computed results for the transformed model agree with the staggered magnetization calculated directly for eq. \cite{3}.

Before proceeding to the detailed analysis of the $XXZ$ chain, we consider the Ising model in a transverse field (ITF) \cite{yamada,4}: (a) the uniform magnetization $M_x$ and (b) the staggered magnetization $M_{st}$. The exact solutions of $M_x$ and $M_{st}$ are denoted by the solid lines.

![FIG. 1. The PW FRG results (represented by ) for the Ising model in a transverse field: (a) the uniform magnetization $M_x$ and (b) the staggered magnetization $M_{st}$. The exact solutions of $M_x$ and $M_{st}$ are denoted by the solid lines.](image1)

![FIG. 2. The PW FRG results for the $S = 1/2$ XXZ spin chain with various $J_x$: (a) the uniform magnetization $M_x$ and (b) the staggered magnetization $M_{st}$. The $M_x$ curves correspond to $J_x = 0, 0.2, 0.4, 0.6, 0.8, 1$ from left to right. The $M_{st}$ curves correspond to $J_x = 0, 0.2, 0.4, 0.6, 0.8, 1$ from left to right. The symbol indicates the disorder point.](image2)
In Fig. 3, we display the PW FRG results of the magnetization in the x direction $M_x$ for $J_k = 0, 0.2, 0.4, 0.6, 0.8, 1$ and the staggered magnetization $M_{st}$ for $J_k = 0, 0.2, 0.4, 0.6, 0.8$. In Figs 3(a) and (b), the $M_x$ grows monotonically as the field is increased, whereas in Fig. 3(b), the staggered magnetization $M_{st}$ for $J_k > 0.4$ exhibits the reentrant behavior. This reentrant behavior can be explained qualitatively in terms of the competition between the classical Néel order and two kinds of quantum fluctuations. In the low-field region, the system is under the influence of the quantum fluctuation from the XY-term $J_k S_x S_{x+1}^x + S_{y+1}^y (0 < J_k < 1)$, while, in the high-field region, the effect of the transverse-field becomes dominant. Although both of them can decrease the classical Néel order, the staggered magnetization is rather enhanced in the middle-field region. This enhancement implies that the two quantum fluctuations compete with each other rather than reduce the Néel order. This picture is consistent with the shape changes of the static structure factor in the transverse-field, as was reported in Ref. 1.

Let us now proceed to analysis of details in the magnetization curve. In the zero transverse-field $x$ axis, the staggered magnetization is calculated exactly:

$$M_{st} = \frac{1}{2} \left( 1 + \frac{q^{2k}}{1 + q^{2k}} \right); \quad (5)$$

where $q = 1 = J_k$, $1 = J_k^2$. By comparing the PW FRG results with the exact values of eq. (5), we have confirmed that the obtained data for $J_k > 0$ agree with the exact values in 5 digits, within the numbers of the retained bases $m = 88$.

There is another special value of a transverse-field called disorder point where the ground state can be calculated analytically. The disorder-point field $J_D$ is given by:

$$J_D = \frac{q}{2 - 2 J_k (J_k + 1)}; \quad (6)$$

and the exact values of the magnetizations are obtained as:

$$M_x = \frac{1}{2} \left( J_k + 1 \right); \quad (7)$$

and

$$M_{st} = \frac{1}{2} \left( J_k + 1 \right); \quad (8)$$

In Figs 3(a) and (b) we have plotted the disorder point with the open circles, which are consistent with the curves calculated by the PW FRG.

Here we remark that we can obtain an inequality:

$$M_{st} > 0, M_{st} = J_D; \quad (9)$$

for $J_k > 0.3$, by comparing eq. (3) and eq. (8). This inequality guarantees the reentrant behavior of the staggered magnetization analytically in the range $J_k > 0.3$. A precise numerical calculation of $M_{st}$ (using maximum $m = 30$) illustrates that the reentrant behavior emerges for $J_k = 0.3984$.

We next discuss the critical behavior of eq. (9). The critical field is defined by the field at which the staggered magnetization vanishes. Since the symmetry of the system is $Z_2$, the universality class is expected to be the two-dimensional (2D) classical Ising one, where the staggered magnetization behaves as:

$$M_{st} (x) \sim (a) \quad \text{for } x < a; \quad (10)$$

with $x = 1 = 8$. For the case of $J_k = 0$, we can see $x = 1 = 8$ from the exact solution of the equation easily. For $0 < J_k < 1$, we have checked the eq. (10) with the PW FRG result of the staggered magnetization. For example, we show the plot of $-M_{st}^x$ for $J_k = 0.8$ in Fig. 3, where we see the good linearity of the plotted data. We have performed the fitting of $M_{st} = A (a - x)^{0.8}$ with fitting parameters $A$, $x$, and then obtained the exponent $0.124; 0.124$ and $0.125$, for $J_k = 0.4; 0.6$ and $0.8$, respectively. These values are consistent with $x = 1 = 8$.

Thus, we have verified that the universality class of the XXZ model at the critical transverse-field is the 2D Ising one.

![Fig. 3. The check of linearity of the $-M_{st}^x$ curve in the case of $J_k = 0.8$ near the critical field. The good linearity (see eq. (10)) can be seen.](image)

### III. S = 1 Cases

In this section, we consider the $S = 1$ XXZ spin chain and the $S = 1$ Heisenberg spin chain with a single-ion anisotropy. In contrast to the $S = 1$ XXZ model, the $S = 1$ chains with small anisotropies have the Halban gap. Then it is an interesting problem to clarify how the Halban gap emerges the competition between the classical Néel order and the transverse-field.
A. The $S = 1 \times 1 \times 2$ model

In this subsection, we consider the $S = 1 \times 1 \times 2$ spin chain, whose Hamiltonian is written as

$$H = \sum_i [J_x S_i^x S_{i+1}^x + S_i^y S_{i+1}^y] + J_z S_i^z S_{i+1}^z$$

where $S_i^z$ is the component of the $S = 1$ spin operator at $i$-th site. In this section, we take $J_x = 1$ and vary $J_z$ in $J_x = 1$, for the later convenience.

In Fig. 4, we show the staggered magnetization $M_x$ and the uniform magnetization $M_z$. Each curve corresponds to $J_x = 1.5, 1.4, 1.3, 1.2, 1.15, 1.1, 1.05$ from top to bottom. The open circle represents the disorder point for each $J_x$.

In Fig. 4, we show the staggered magnetization $M_x$ and the uniform magnetization $M_z$. The maximum number of the retained bases in the DMRG calculation is $m = 70$. In the figures, we plot the disorder points for the $S = 1 \times 1 \times 2$ model, which is given by

$$M_x = \frac{2}{1 + J_z} \quad \text{and} \quad M_z = \frac{J_x}{J_z + 1}$$

with the disorder-point exponents $d_{p} = 2 + \frac{J_x}{2(1 + J_z)}$. We can see that they are in good agreement with the DMRG results. When the anisotropy is not so big ($J_z < 1.18$), the Haldane state is maintained up to the critical value of the transverse $M_x$, where the phase transition occurs accompanying the spontaneous staggered order (Fig. 4 (b)). As $J_x$ is increased above $c_1$, the staggered magnetization grows rapidly. However, as is further increased, $M_x$ turns to decrease and finally vanishes at the higher critical field $c_2$. In Fig. 4 (a), we show the uniform magnetization $M_x$, where the anisotropy effect seems not to be significant. However, a notable point for this uniform magnetization is that $M_x$ has a small but finite value below the critical field $c_1$, in contrast to the isotropic case where $M_x$ is exactly zero below $c_1$. In a real experiment, it may be inportant to distinguish such a behavior of $M_x$ from the finite temperature effect.

As $J_z$ is increased, the lower-critical field $c_1$ becomes small and thus the region of the Haldane phase shrinks (see Fig. 4(a)). When $J_z$ is increased above the critical value of the anisotropy $J_z < 1.18$, the spontaneous staggered magnetization appears at the zero transverse field and $M_x$ is observed.

For $J_x < J_z$, the staggered magnetization exhibits the week resonant behavior, which is similar to the $S = 1/2$ case. In the $J_x > 1$ limit, the system becomes to the $S = 1$ version of the Ising model in a transverse field, without the resonance of $M_x$.

In Fig. 5, we show the staggered magnetizations for the $S = 1 \times 1 \times 2$ model: (a) $S = 1 \times 1 \times 2$ chain with $J_x = 1.2$ near the higher critical field $c_1$ and (b) $S = 1 \times 1 \times 2$ chain with $J_x = 1.1$ near the lower critical field $c_1$.

Let us next discuss the critical behavior at $c_1$ and $c_2$, which are also expected to belong to the 2D Ising universality class. In Figs. 5 (a) and (b), we show the plot of $M_x$ near the critical exponents $c_1$ and $c_2$, respectively. In these figures, we can recognize the good linearity. Near the lower critical field $c_1$, we have estimated the critical exponent as $\delta_1 = 0.126$ for $J_z = 1.1$. Also near the higher
the staggered order in the 2D Ising model, as well. However it is difficult to estimate the exponent with a direct calculation, since the expected value \( \beta = 0 \) (log) is too weak to be detected numerically.

B. S = 1 Heisenberg model with a single-ion anisotropy

For the case of the \( S = 1 \) quantum spin chains, we can consider the single-ion-type crystal eld as an origin of the anisotropy, which is actually observed in the real compounds. The Hamiltonian is given by

\[
H = S_1 \cdot S_1 + D \sum_i (S_i^z)^2 - J \sum_i S_i^x.
\]

If \( D < 0 \), the D-term \( \sum_i (S_i^z)^2 \) stabilizes \( 1^\text{st} \) spins equivalently and hence the D-term is expected to make the similar effect to the previous XXZ-type anisotropy. In the following, we thus consider \( D < 0 \) region, where the staggered order in the \( z \)-direction is induced. The phase boundary of this model is investigated by Sakai and Takahashi, using the exact diagonalization up to 14 sites. However the magnetization curve of this model has not been calculated yet.

**Fig. 6.** The PW FRG results for the \( S = 1 \) Heisenberg model with the single-ion anisotropy: (a) the uniform magnetization \( M_x \), and (b) the staggered magnetization \( M_{st} \). In Fig. (a), the curves correspond to \( D = 0, 0.4, 0.8, 1.2, 1.4 \), and \( 1.6 \) from left to right. In Fig. (b), the curves correspond to \( D = 0, 0.35, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, \) and \( 1.7 \) from top to bottom.

In Fig. 6, we show the uniform magnetization \( M_x \) and the staggered magnetization \( M_{st} \). We can see that they exhibit the similar behavior to that of the \( S = 1 \) XXZ model. For \( 0.3 < D < 0 \), the system has the staggered order between the two critical elds \( c_1 \) and \( c_2 \). In \( c_1 \), the system is in the Haldane phase, but the uniform magnetization \( M_x \) has a finite value due to the lack of the total-\( S^z \) conservation law. As \( D \) is decreased, \( c_1 \) becomes small and finally vanishes at the critical value of the anisotropy \( D_c' = 0.3 \), which is consistent with \( D_c = 0.29 \) calculated by Sakalet al. As \( D \) is decreased further, the staggered magnetization appears at the zero transverse eld, and then the reentrant behavior of the staggered magnetization can be seen.

Next, we plot \( M_{st}^0 \) near the critical eld in Fig. 7, where the good linearity can be seen. For example, the estimated critical exponent at the lower-critical eld is \( \beta = 0.127 \) for \( D = 0.15 \), and the one at the higher critical eld is \( \beta = 0.142 \) for \( D = 0.45 \) and \( 0.45 \) respectively. These values are also consistent with the universality class of the 2D Ising model.
FIG. 7. Critical behavior of the staggered magnetizations for \( S = 1 \) Heisenberg model with the single-ion anisotropy of \( D = 0.15 \): (a) near the higher critical \( \varepsilon \) and (b) near the lower critical \( \varepsilon \).

IV. SUMMARY

In this paper, we have considered the one-dimensonal quantum spin chains with the easy-axis anisotropy in the transverse magnetic \( \varepsilon \). We have calculated the staggered magnetization \( M_{\text{xx}} \) in the \( z \) direction and the uniform magnetization \( M_{\text{x}} \) along the \( x \) direction precisely, using a variant of the DMRG (the PF FRG method). For the \( S = 1 \) XXZ chain, we have shown that the \( M_{\text{xx}} \) exhibits the remnant behavior when \( J_0 \) = 0.3984, where the competition between the classical Néel order and the quantum fluctuations from the transverse \( \varepsilon \) and the \( X Y \)-term plays an important role. We have also discussed the critical behavior associated with the staggered magnetization and verified that the universality class of the model is the two-dimensional classical Ising one.

For the \( S = 1 \) XXZ model and the \( S = 1 \) Heisenberg model with a single-ion anisotropy, we have shown that, if the anisotropies are not big \((J_y < 1d \; or \; D < 0.3)\), the system has the staggered order between the lower critical \( \varepsilon \) associated with the Haldane gap \((\varepsilon_1)\) and the higher one connected to the saturation \( \varepsilon \) of the isotropic case \((\varepsilon_2)\). When the anisotropies are big, the staggered order appears at the zero transverse \( \varepsilon \) with the remnant behavior, which is similar to that of the \( S = 1 \) XXZ model. We have also investigated the critical behavior at \((\varepsilon_1, \varepsilon_2)\), by estimating the exponent \( \gamma \). As a result, we have verified that they are consistent with the class of the 2D classical Ising model.

In the actual one-dimensional compound, various types of the anisotropy can be considered. When analyzing the magnetization processes of such matters, we believe that the present results are useful.

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