A novel intermediate phase in $S = 2$ antiferromagnetic chains with uniaxial anisotropy

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Abstract

We study ground state properties of the $S = 2$ quantum antiferromagnetic chain with a uniaxially anisotropic Hamiltonian: $H = \sum_j [S_j \cdot S_{j+1} + D(S_j^z)^2]$ by a Monte Carlo calculation. While it has been reported that a string order parameter vanishes exponentially at the isotropic Heisenberg point ($D = 0$), we found it tends to remain finite in the thermodynamic limit around $D = 1.2$. This implies that the model for $S = 2$ has a novel intermediate phase between the Haldane phase and the large-$D$ phase, as was anticipated from the earlier argument based on the Valence-Bond-Solid picture.

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Since Haldane predicted [1,2] a qualitative difference between quantum antiferromagnetic chains with integer and half-odd-integer spins, much work has been devoted to examine his prediction. Now it is widely believed based on many theoretical, numerical and experimental studies. (For a review, see [3]). In the present letter, we report numerical results which indicate that integer spin chains with \( S > 1 \) exhibit much richer structures than expected, and are still full of fascinating surprises.

Exactly solvable models of integer spin chains, which exhibit the properties predicted by Haldane, were introduced by Affleck, Kennedy, Lieb and Tasaki [4]. It was found that the exact ground state — Valence-Bond-Solid (VBS) state — of the above model with \( S = 1 \) possesses two peculiar properties: the presence of edge states in a finite open chain, and the existence of a hidden antiferromagnetic order. The hidden antiferromagnetic order can be measured by the den Nijs-Rommelse string order parameter [5]

\[
\mathcal{O}_{str}^\alpha = \lim_{|i-j| \to \infty} \langle S_i^\alpha \exp \left( i\pi \sum_{i \leq k < j} S_k^\alpha \right) S_j^\alpha \rangle. \tag{1}
\]

Later it was argued [5–11] that the above two properties are characteristic to general \( S = 1 \) chains which are in the Haldane phase including the standard \( S = 1 \) Heisenberg model. Kennedy and Tasaki [12] showed that these properties can be viewed as consequences of spontaneous breakdown of a hidden \( Z_2 \times Z_2 \) symmetry.

One of us (M.O.) [13] extended the notion of hidden \( Z_2 \times Z_2 \) symmetry to chains with arbitrary integer spin. Earlier, Affleck and Haldane [14] made a field theory argument to predict that the quantum antiferromagnetic chain with a bond alternation undergoes \( 2S \) successive phase transitions when the magnitude of the alternation is changed. Based on VBS-type models, he argued in [13] that breaking of the hidden \( Z_2 \times Z_2 \) symmetry is important in these successive dimerization transitions. Moreover, he conjectured unexpected successive transitions in integer \( S > 1 \) quantum antiferromagnetic chains with uniaxial anisotropy.

We summarize the conjecture for \( S = 2 \) below. Let us consider a quantum spin chain with the Hamiltonian

\[
H = \sum_j [JS_j \cdot S_{j+1} + D(S_j^z)^2]. \tag{2}
\]

We take \( J \) as the unit of energy and put it unity hereafter. For \( S = 1 \), the phase structure has been thoroughly investigated [12,15,16]. A finite region in \( D \) including the Heisenberg point (\( D = 0 \)) belongs to the Haldane phase which is characterized by a spontaneous breakdown of the hidden \( Z_2 \times Z_2 \) symmetry. When \( D \) is sufficiently large, it belongs to a different phase called the large-\( D \) phase, in which the hidden symmetry is unbroken.

For \( S = 2 \), the ground state at the isotropic Heisenberg point (\( D = 0 \)) is expected to be similar to the \( S = 2 \) VBS state (Fig. [1]). In this state, the den Nijs-Rommelse string order parameter [1] is exactly evaluated [13] to be zero; the hidden \( Z_2 \times Z_2 \) symmetry is unbroken here. When \( D \to \infty \), the ground state tends toward the simple tensor product state with \( S^z = 0 \) for each site. The hidden symmetry is also unbroken in this state and this is similar to the large-\( D \) phase for \( S = 1 \). However, in an intermediate range of \( D \), the ground state may become similar to the incomplete VBS-type state as in Fig. [4]. Here
the hidden symmetry is shown [13] to be broken. From the symmetry argument we expect that there exist a new “intermediate-$D$ phase” between the Haldane phase and the large-$D$ phase for $S = 2$, in contrast to the well-established two phases for $S = 1$ (Fig. 3).

On the other hand, the validity of the VBS-model description is not clear for $S > 1$. While the VBS-model provides a simple way of understanding the difference between integer and half-odd-integer spins, the Hamiltonian of the model contains many extra terms when $S > 1$. Actually a bosonization argument [17] concludes that the qualitative feature of the phase diagram of an anisotropic Heisenberg-type model is universal for any integer spin, against the above conjecture.

In this letter, we numerically examine the existence of the conjectured intermediate phase in the $S = 2$ chain with the Hamiltonian (2). Before presenting our results, we briefly summarize previous studies on the $S = 2$ spin chain. Numerical confirmation of the Haldane’s conjecture for the $S = 2$ Heisenberg model ($D = 0$) is done by several authors [18–21]. All the results support the Haldane’s conjecture: the energy gap above the ground state is finite and the spin correlation function decays with a finite correlation length. Furthermore, Meshkov [20] and Nishiyama et al. [21] examined the den Nijs-Rommelse string correlation function at the Heisenberg point. They found that the string order seems exponentially vanishing; the hidden $Z_2 \times Z_2$ symmetry is unbroken there. Instead, Nishiyama et al. found a modified string order parameter [13] remains finite. (See also [22]). These results qualitatively coincides with the properties of the $S = 2$ VBS state.

Let us also note that it is trivial that the hidden $Z_2 \times Z_2$ symmetry is unbroken at $D = \infty$. In addition, applying the rigorous perturbation theory by Kennedy and Tasaki [12], it can be stated rigorously that the symmetry is unbroken for sufficiently large but finite $D$.

Thus we concentrate to find a hidden $Z_2 \times Z_2$ symmetry breaking in some finite value of $D$. We performed a world-line Quantum Monte Carlo calculation [23] using the Lie-Trotter-Suzuki product formula with the checker-board decomposition [24]. That is, we made an approximation to the partition function $Z$ for temperature $T$ as

$$Z_n = \text{Tr}[\exp(-H_A/(nT)) \exp(-H_B/(nT))^n].$$

(3)

Here we choose $H_A = \sum_{j=\text{odd}} V_j$, $H_B = \sum_{j=\text{even}} V_j$ and $V_j = S_j \cdot S_{j+1} + D(S_j^z + S_{j+1}^z)^2$. The approximate partition function $Z_n$ approaches to the true partition function $Z$ as $n \to \infty$. We made calculations for several values of finite $n$, and then extrapolate the results to $n \to \infty$. Inserting the sum of complete set of bases, the decomposed formula (3) can be interpreted as a classical spin system with a four-body interaction. Monte Carlo flips for each plaquette were performed with a heat-bath algorithm. Although we also prepared global flips along the chain direction, the acceptance ratio becomes very small when the system size is large (over 100). For the study of the ground state, we did not use global flips along the Trotter direction and restricted the calculation into the $\sum S^z = 0$ subspace.

Scanning several values of $D$ by preliminary calculations, we have chosen $D = 1.2$ as a candidate for a point in the intermediate phase. We calculated spin chains with a periodic boundary condition up to the system size $L = 160$. We investigate the quantities at low enough temperature, below which the correlation function is temperature independent. For actual calculation we take $T = 0.04$ for $L \leq 140$ and $T = 0.02$ for $L = 160$. The Trotter numbers $n$ used for the calculation were 48, 64, 72, 80 and 96 for $L \leq 140$ and 96, 128, 144 and 192 for $L = 160$. 
Typical data are obtained as follows. To reduce the effect of the autocorrelation, the measurements were done in every 10 Monte Carlo Steps (MCS). In each configuration, we chose 800 points as positions of \( i \) from the classical spin lattice of size \( L \times 2n \). For each point, we scan \( j \) to the chain direction to measure the den Nijs-Rommelse string correlation function (in \( z \)-axis)

\[
\langle S_i^z \exp(i\pi \sum_{i \leq k < j} S_k^z)S_j^z \rangle,
\]

and the \( S^z \) correlation function \( \langle S_i^z S_j^z \rangle \) as functions of \( j - i \). We performed the measurement during \( 1 \sim 5 \times 10^6 \) MCS, after \( 1 \times 10^6 \sim 9 \times 10^6 \) MCS of thermalization.

Error bars are calculated from the standard deviation of averages during each \( 1 \times 10^4 \) MCS. The dependence on the Trotter number is extrapolated by the least square method with the formula

\[
A(n) = A_0 + A_1/n^2,
\]

where \( A(n) \) is a physical quantity for the Trotter number \( n \) and \( A_0 \) and \( A_1 \) are the unknown constants (fitting parameters). We have checked that the extrapolation is stable under different choices of Trotter numbers or inclusion of the \( A_2/n^4 \) term.

In Fig. 4 we show the extrapolated correlation functions for system sizes \( L = 80, 100, 120, 140 \) and 160. The expected antiferromagnetic part in \( S^z \) correlation is dominant only for nearest few sites and decays very rapidly. Actually, in the figure the major part of the \( S^z \) correlation function is not antiferromagnetic. It is rather a negative correlation which can be explained by the sum rule \( \sum_j S_j^z = 0 \) in the ground state. Anyway, the \( S^z \)-correlation (or Néel correlation) decays to zero. On the other hand, the den Nijs-Rommelse string correlation seems to show a plateau at a finite positive value around 0.001.

Because the value is so small, we checked the thermal equilibrium carefully by comparing the results for various length of the thermalization. We also performed a lot of measurement in order to make the statistical error less than 0.0001. We note that the string correlation is always positive, which is contrasted to the oscillating behavior at the Heisenberg point [22].

It seems that the string correlation converges to a finite positive value around 0.001 in the thermodynamic limit, in contrast to the vanishing Néel order. However, there is a subtlety about the presence of the true long-range string order. The string correlation function is fit well with a power-law function

\[
0.12x^{-1.3}
\]

within a range of the distance. It is difficult to distinguish a true long-range order from a power-law decay.

To examine this problem, let us compare the string correlation data with the assumption that the system is in a criticality with the conformal invariance. (See for example [23] for a review. On applications to the finite size scaling of correlations, see [24, 25]) Under the assumption, string correlation corresponds to the two-point correlation function of a spinless primary field \( \phi \) with the conformal weight \( h = \bar{h} \), whose correlation function in an infinite system is given by

\[
\langle \phi(x)\phi(y) \rangle = C/|x - y|^{2h}
\]

where \( C \) is a constant. The equal-time correlation function of the same field in a periodic ring with length \( L \) is given by

\[
\langle \phi(x)\phi(y) \rangle_L = C \left( \frac{\pi}{L} \right)^{2h} \frac{1}{(\sin \pi |x - y|/L)^{2h}}.
\]
Thus the minimum of the correlation function at $|x - y| = L/2$ is given by $C(\pi/L)^{2h}$. In Fig. 2 we plot the value of correlation function at the middle point measured in our Monte Carlo calculation. (We averaged the central 7 - 11 sites for $L \geq 80$.) We compare it with the prediction from the conformal invariance with parameters $C = 0.12$ and $2h = 1.3$, which are determined from the fitting (1). Although the data fit well with the prediction for $L \leq 100$, we see the data deviate upward for $L \geq 120$. This suggests that the string correlation converges to a finite value in the thermodynamic limit, which means the hidden $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry is broken (at least partially) at this point.

We find a similar result for $D = 0.9$ although the string correlation function is smaller than that for $D = 1.2$. This result also supports that the phase diagram for $S = 2$ is different from that for $S = 1$ where there is a single critical point $D = D_c$. Thus we conclude that there exists the conjectured intermediate-$D$ phase with a finite region between the Haldane phase and the large-$D$ phase.

To summarize, we performed a Monte-Carlo calculation on the $S = 2$ quantum antiferromagnetic spin chain with an anisotropy as in eq. (2). We found that, for $D = 1.2$, the den Nijs-Rommelse string order tends to remain finite (at least decays slower than a simple power-law) in contrast to the vanishing Néel order. Together with the previous numerical and rigorous results that the string correlation decays exponentially at the isotropic point $D = 0$ and at sufficiently large $D$, our data shows there is an intermediate phase, which is absent in the corresponding $S = 1$ chain. This confirms the conjecture based on a VBS-type model in Ref. [13].

Our result confirms numerically that, while the presence of the Haldane gap would be universal for all integer spins, the phase diagram of quantum spin chain is not universal among all integer spins and would become more complex as the spin quantum number is increased. It is also suggested that the VBS-model approach would be qualitatively useful even for standard Heisenberg-type models with higher spins, although the quantitative discrepancy increases as spin quantum number $S$ increases.

The fact that the string correlation behaves like a power-law suggests that the system resides near a criticality. Recently it is argued [28] that there is an XY-phase in the finite-$D$ region; this XY-phase like character may be related to the power-law-like behavior of the string correlation. In the present work, however, we found that the string correlation in $z$-axis deviates from a simple power-law, implying the spontaneous breakdown of the hidden $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. This rather suggests that the system is not in a truly gapless XY-phase in the thermodynamic limit. In any case, the intermediate phase studied in this letter can be distinguished from the XY phase in the ferromagnetic region (or equivalently with a negative $S^z_i S^z_{i+1}$ coupling) by the dominance of the string order.

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FIGURES

FIG. 1. The standard VBS state for $S = 2$. A small solid circle denotes a spin-1/2, and a solid line denotes a valence bond (singlet of two spin-1/2). A dotted circle represents the symmetrization of four spin-1/2's at each site to form a spin-2.

FIG. 2. The intermediate-$D$ VBS state for $S = 2$. An up (down) arrow denotes an up (down) spin-1/2. (cf. Fig. 1)

Hidden $Z_2 \times Z_2$ symmetry

$S = 1$

$D_c$

$D$

unbroken

FIG. 3. The established phase structure for $S = 1$, and the conjectured phase structure for $S = 2$ for the Hamiltonian (2).
FIG. 4. Extrapolated correlation functions for system sizes $L = 80, 100, 120$ and $140$ at $D = 1.2$. The string correlation seems to show a plateau at 0.001, while the $S^z$ correlation is vanishing.
FIG. 5. The value of the string correlation function at the middle point as a function of the system size. The straight line is a theoretical prediction assuming the conformal invariance.