Hidden Order and Dimerization Transition in $S = 2$ Chains

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We study ground state properties of the $S = 2$ quantum antiferromagnetic chain with a bond alternation

$$H = \sum_j [1 + \delta (-1)^j] \mathbf{S}_j \cdot \mathbf{S}_{j+1},$$

by a Quantum Monte Carlo calculation. We find that the hidden $Z_2 \times Z_2$ symmetry is broken for $0.3 < |\delta| < 0.5$ while it is unbroken in the other regions. This confirms the successive dimerization transitions first predicted by Affleck and Haldane. Our result shows that these transitions can be understood in terms of the hidden $Z_2 \times Z_2$ symmetry breaking, as was discussed using the Valence-Bond-Solid states. Furthermore, we find that the behavior of the generalized string correlation is qualitatively very similar to that in the Valence-Bond-Solid states, including the location of zeroes as a function of the angle parameter.

KEYWORDS: quantum spin chain, Haldane gap, bond-alternation, hidden order, dimerization

Much effort has been devoted to examining Haldane’s conjectured\footnote{E-mail: yamanaka@kodama.issp.u-tokyo.ac.jp} on the difference between quantum antiferromagnetic chains with integer and half-odd-integer spins. These studies also found several interesting phenomena besides the original conjecture. One of them is the successive transitions induced by a bond alternation. Consider the Hamiltonian

$$H = \sum_j [1 + \delta (-1)^j] \mathbf{S}_j \cdot \mathbf{S}_{j+1},$$

where $\delta$ represents the strength of the bond-alternation ($-1 \leq \delta \leq 1$). The standard spin-$S$ Heisenberg antiferromagnetic chain corresponds to $\delta = 0$. When $\delta = \pm 1$, this Hamiltonian reduces to that of isolated dimers. Affleck and Haldane\footnote{** Present address: Department of Applied Physics, University of Tokyo, Bunkyo-ku, Tokyo 113.} made an interesting prediction: there are critical transition points in $-1 < \delta < 1$ for spin $S$. (See also ref.\footnote{*** E-mail: oshikawa@physics.ubc.ca} They mapped the model\footnote{**** E-mail: miya@temp.ess.sci.osaka-u.ac.jp} into an $O(3)$ non-linear sigma model with a topological term defined by the Lagrangian

$$\mathcal{L} = \frac{1}{2g} \left( \partial_{\mu} \varphi \right) \left( \partial_{\nu} \varphi \right) + \alpha \frac{g}{8\pi} \epsilon^{\mu\nu\alpha\beta} \left( \partial_{\mu} \varphi \times \partial_{\nu} \varphi \right),$$

where $\varphi$ is a three-component vector field with the constraint $\varphi^2 = 1$. The parameters are related to those of the original model as follows:

$$v = 2S \sqrt{1 - \delta^2}, \quad g = \frac{2}{S^2 \sqrt{1 - \delta^2}}, \quad \alpha = 2\pi S (1 + \delta),$$

where $v$ denotes the spin-wave velocity, which corresponds to the “speed of light” in the relativistic field theory. Thus the topological angle $\alpha$ depends on the bond-alternation parameter $\delta$. When $\delta$ is changed from $-1$ to $1$, $\alpha$ changes from $-4\pi S$ to $4\pi S$. It was argued that the above model has a massless (critical) point for $\alpha = \pi$ (mod $2\pi$), namely $2S$ critical points are expected in model\footnote{E-mail: yamanaka@kodama.issp.u-tokyo.ac.jp} for $-1 < \delta < 1$.

There is another (more intuitive) argument\footnote{E-mail: oshikawa@physics.ubc.ca} based on a class of exactly solvable spin chains – Valence-Bond-Solid (VBS) models.\footnote{E-mail: miya@temp.ess.sci.osaka-u.ac.jp} We can introduce VBS states with various degrees of dimerization. For $S = 2$, each spin can be constructed by symmetrization of four spin-1/2’s and we can consider VBS-type states as shown in fig. 1. In general, $2S + 1$ states can be constructed for spin $S$. If we assume that the ground state of the Hamiltonian\footnote{E-mail: yamanaka@kodama.issp.u-tokyo.ac.jp} belongs to the same phase as one of these states, and that there are phase transitions between them, there should be $2S$ phase transitions as expected in the field-theory argument.

However, both approaches are based on some assumptions or approximations and thus the prediction should be verified by, for example, a numerical calculation. In addition, the concept of the order parameter is lacking in these arguments. How can we distinguish the phases which correspond to “different numbers of valence bonds”? For $S = 1$, den Nijs and Rommelse\footnote{E-mail: yamanaka@kodama.issp.u-tokyo.ac.jp} found that a kind of non-local order parameter characterizes the Haldane gap phase. (See also ref.\footnote{E-mail: oshikawa@physics.ubc.ca} Kennedy and Tasaki\footnote{E-mail: miya@temp.ess.sci.osaka-u.ac.jp} revealed that this den Nijs-Rommelse string order parameter measures a hidden $Z_2 \times Z_2$ symmetry breaking. One of us extended this idea in ref.\footnote{E-mail: yamanaka@kodama.issp.u-tokyo.ac.jp} to general integer spin, and found that the VBS states can be (partly) distinguished by the hidden $Z_2 \times Z_2$ symmetry breaking. Namely, it was found that the symmetry is
broken (unbroken) when the number of valence bonds is odd (even). Thus the dimerization transitions can be understood as hidden $Z_2 \times Z_2$ symmetry breaking, if the VBS picture is correct. (See fig. 1.)

However, the hidden $Z_2 \times Z_2$ symmetry is not sufficient for full characterization of all possible VBS states. Also it cannot be applied to half-odd-integer spin chains. As an attempt to overcome these problems, a generalized string order was proposed. In a dimerized state, the generalized string order depends on how the limit is taken. Here we choose the definition

$$O_{\text{string}}^a(\theta) = \lim_{|k-j| \to \infty} \left\langle S_{2j+1}^x \exp \left( i\theta \sum_{l=(2j+1)}^{2k} S_l^z S_{2k+1}^z \right) \right\rangle.$$  

(4)

This reduces to the Néel order for $\theta = 0$, and to the den Nijs-Rommelse string order for $\theta = \pi$, which is related to the hidden $Z_2 \times Z_2$ symmetry breaking for integer spin.

It was found that the generalized string order parameter in the $(n,m)$-VBS state (with $n$ valence bonds between sites $2j$ and $2j+1$ and $m$ between $2j+1$ and $2j+2$) is given by a polynomial of $z = e^{i\theta}$ as

$$O_{\text{string}}^a(\theta) = \left| f_{n,m}(e^{i\theta}) \right|^2,$$  

(5)

where $f$ is given by

$$f_{n,m}(z) = \frac{n + m + 2}{2(n+2)(n+1)} \sum_{k=0}^n (2k-n)z^k.$$  

(6)

We note that $O_{\text{string}}^a$ is not the same for $(n,m)$- and $(m,n)$-VBS states. The order parameter defined as eq. (4) in the $(n,m)$-VBS state is equal to an order parameter in the $(m,n)$-VBS state with a slightly different definition. It was proved that the $n$-th order polynomial $f_{n,m}$ has $n$ simple roots on the unit circle. Thus the generalized string order has $n$ zeroes as a function of $\theta$ in $0 \leq \theta < 2\pi$. It was conjectured that this property is generic for the partially dimerized phases. We also note that $O_{\text{string}}^a(\theta) = O_{\text{string}}^a(2\pi - \theta)$ and it is always real.

For $S = 1$, the presence of the critical transition point has been numerically established by several authors. Recently Yajima and Takahashi studied the $S = 3/2$ case and confirmed the presence of the transitions. They also measured the generalized string order parameter at $\theta = \pi$ (this is not related to the hidden symmetry for half-odd-integer spin) and found the behavior consistent with the above VBS picture. For $S = 2$, the Heisenberg point ($\theta = 0$) was studied by several authors, and the behavior of the string order parameter was found to be consistent with the VBS picture. Tonegawa numerically calculated the energy gap of the model with the next-nearest-neighbour couplings.

In this paper, we study the ground state properties of the $S = 2$ chain with the Hamiltonian more thoroughly by the Quantum Monte Carlo method, with particular emphasis on the hidden order and the hidden symmetry breaking.

We performed a world-line Quantum Monte Carlo calculation using the Lie-Trotter-Suzuki product formula with checker-board decomposition. That is, we made an approximation to the partition function $Z$ for temperature $T$ as $Z_n = \text{Tr}[e^{-H_A/(nT)}e^{-H_B/(nT)}]$. Here we choose $H_A = \sum_{j=\text{odd}} V_j$, $H_B = \sum_{j=\text{even}} V_j$ and $V_j = |1 + \delta(-1)^j | S_j \cdot S_{j+1}$. The approximate partition function $Z_n$ approaches the true partition function $Z$ as $n \to \infty$. We chose a heat-bath algorithm. While we prepared global flips along the chain direction, we did not use global flips along the Trotter direction and restricted the calculation to the $\sum S_z = 0$ subspace, in order to study the ground state. We used the periodic boundary condition. For most of the calculation we took $T = 0.04$ and $n = 96$, which turned out to be sufficiently close to the extrapolation $T \to 0$ and $n \to \infty$.

We measured the generalized string correlation (5) at $\theta = \pi/20 \ (n = 0, 1, \ldots, 20)$. We assumed the $L$ dependence of the correlation function at distance $L/2$ to be

$$\left\langle S_{0}^x \exp \left( i\theta \sum_{l=0}^{L/2-1} S_l^z S_{L/2}^z \right) \right\rangle \approx A + B \exp (-CL).$$  

(7)

We made a least-square fit of our data for system size $L(=40, 60, 80)$ with the above formula and checked the stability of the extrapolation for different choices of the system size ($L = 40, 50, 60, 70, 80$).

The Heisenberg point: The generalized string order $A$ obtained by the fitting (5) and the result (5) for the $S = 2$ VBS state are shown in fig. 2. Their qualitative behaviors are very similar. In particular, they have zeroes at $\theta = 0, \pi$. The former corresponds to vanishing Néel order and the latter means that the hidden $Z_2 \times Z_2$ symmetry is unbroken. These results are in agreement with the VBS picture and also with previous numerical calculations at the Heisenberg point.

The generalized string order has its maximum value at a point near $\theta = \pi/2$. The dependence of the generalized string order on $\theta$ was studied in a short chain by Hatsugai. The long-range order at $\theta = \pi/2$ was confirmed numerically in refs. 19 and 20. Here we emphasize that the generalized string order is non-vanishing for $\theta \neq 0, \pi$, in agreement with the result (5) for the VBS state. We observed a similar result at $\delta = 0.05$.

The intermediate phase: We show the Néel and the den Nijs-Rommelse string correlation functions at $\delta = 0.4$ in fig. 3. The Néel correlation decays faster than that at the Heisenberg point. Due to the bond-alternation, the den Nijs-Rommelse string correlation has an oscillating part. Besides the oscillating part, it seems to have a long-range order. This means that the hidden $Z_2 \times Z_2$ symmetry is broken. We show the extrapolated results in fig. 4 together with the result (5) for the partially dimerized VBS state. The result again agrees (qualitatively) with that of the VBS state. At $\theta = \pi$ (den Nijs-Rommelse string order) there is no longer zero and instead we see another zero in $0 < \theta < \pi$. By symmetry, there are three zeroes in $0 < \theta < 2\pi$ in agreement with the conjecture in ref. 16. It is somewhat surprising that not only the number of zeroes, but also the location of the zeroes in $\theta$ seems to coincide with the VBS result. For $\delta = 0.3$ and 0.5 we obtained similar results to that for $\delta = 0.4$.

The dimerized phase: Next we consider $\delta = 0.6$. As
shown in fig. 5, both the Néel correlation and the den Nijs-Rommelse string correlation decay to zero. The latter means that the hidden $Z_2 \times Z_2$ symmetry is unbroken. We show the extrapolated results in fig. 6, together with the result [3] for the completely dimerized state. Their behaviors agree well. In particular, the locations of zeroes seem to agree again. For $\delta = 0.7$ and 0.8, we observed similar behaviors to that for $\delta = 0.6$ (but more similar to the result for the completely dimerized state, as expected).

To summarize, we measured the generalized string correlation in the $S = 2$ spin chain with a bond-alternation [1] by the Quantum Monte Carlo method. We observed that there are three phases in $0 < \delta < 1$, confirming the prediction by Affleck and Haldane. The hidden $Z_2 \times Z_2$ symmetry is broken only in the intermediate phase. This is consistent with the VBS picture of the transitions. Hence the transitions can be understood as hidden $Z_2 \times Z_2$ symmetry breaking. From this argument, it would be natural to expect that the transitions belong to the same $c = 1$ universality class as in the $S = 1$ case. This argument is again consistent with the field-theory prediction by Affleck and Haldane.

Furthermore, we found that the behaviors of the generalized string order in those phases are quite similar to those in the VBS-type state. In particular, the locations of the zeroes seem to agree. It might be possible to determine the underlying mechanism for this phenomenon. (For example, the zeroes may be related to some unknown hidden symmetries.)

Our result shows that the region $0 \leq \delta \leq 0.05$ belongs to the $S = 2$ Haldane phase, $0.3 \leq \delta \leq 0.5$ to the intermediate phase, and $0.6 \leq \delta \leq 1$ to the dimerized phase. Thus the transition points should be located in the regions $0.05 < \delta < 0.3$ and $0.5 < \delta < 0.6$. However, in these regions, the correlation length seems to grow and hence we could not make reliable extrapolation and could not estimate the transition points more precisely.

From eq. (3) we can obtain the field-theory prediction for the transition points: $\delta = 0.25$ and $\delta = 0.75$. The latter is clearly inconsistent with our result $0.5 < \delta < 0.6$. (The value was not consistent with the numerical result for $S = 1$ [1] and for $S = 3/2$ [3].) In general, we cannot expect that the field theoretical argument gives the quantitatively precise location of the critical point. However, the qualitative prediction of the occurrence of the phase transition and the description of the critical behavior are reliable.

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**Fig. 1**

Hidden Symmetry

unbroken

broken

unbroken

**Fig. 2**

Generalized string order (delta=0)

Extrapolated Result

VBS

**Fig. 3**

(a) Neel correlation (delta=0.4)

(b) String correlation (theta=pi, delta=0.4)

**Fig. 4**

Generalized string order (delta=0.4)

Extrapolated Result

(3,1)-VBS

**Fig. 5**

(a) Neel correlation (delta=0.6)

(b) String correlation (theta=pi, delta=0.6)

**Fig. 6**

Generalized string order (delta=0.6)

Extrapolated Result

Complete Dimer [(4,0)-VBS]