Nonlocal Topological Order in Antiferromagnetic Heisenberg Chains

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(Received 17 July 2002; published 12 February 2003)

We demonstrate the existence of nonlocal topological (string) order in half-integer-spin antiferromagnetic Heisenberg chains on macroscopic scale on the basis of analytical scaling analysis and density matrix renormalization group calculations. Strong numerical evidence leads to a conjecture that chains with $S = (2m - 1)/2$ and m (m = integers) belong to the same topological class defined by the topological angle $\theta/\pi = 1/m$ that plays a role similar to the fictitious gauge field in the fractional quantum Hall effect.

DOI: 10.1103/PhysRevLett.90.067202 PACS numbers: 75.10.Jm, 75.40.Mg

One-dimensional quantum spin chains have been a subject of great interest since the early days of quantum mechanics. Important earlier work includes the Bethe-ansatz solutions [1,2] and the sine-Gordon [3] and bosonization [4] theories on the nearest-neighbor isotropic antiferromagnetic Heisenberg chain (AFHC) with spin $S = 1/2$. It was long assumed that the properties of the $S = 1/2$ AFHC are generic for all spins. However, this notion was challenged in 1983 when Haldane pointed out [5] a fundamental difference between spin chains with integer and half-integer spins. By mapping the Heisenberg spin chains onto the $O(3)$ nonlinear σ model [6] Haldane conjectured that the low-energy excitation spectrum displays a finite energy gap for integer-spin chains. The key to this conjecture is the topological aspects of AFHC that allow integer-spin chains to be treated in the large-S limit in the nonlinear σ-model formalism and have been shown to have finite energy gap and correlation length. Meanwhile the half-integer spin chains cannot be treated in the same formalism and are thought to be generically critical on the basis of the Bethe-ansatz results for $S = 1/2$ and the generalized Lieb-Schultz-Mattis theorem [7,8]. Because of a lack of exact analytic solutions, accurate verification of Haldane's conjecture has come from numerical calculations. These include AFHCs with $S = 3/2$ [9], $S = 1$ [10], and $S = 2$ [11–13]. Numerical efforts for higher spins are hampered by exceedingly small gaps and large correlation lengths which in the limit $S \to \infty$ obey $\Delta(S) \propto S^2 e^{-\pi S}$ and $\xi(S) \propto S^{-1} e^{\pi S}$ [5,6].

A microscopic description of the Haldane state is provided by the valence bond solid (VBS) picture [14] which reproduces essentially all qualitative features of AFHC. A nonlocal string order parameter has been introduced [15] to characterize fundamental topological order in both VBS and AFHC [10,15–17]. Topological order in integer-spin chains has been extensively studied in recent years. For $S = 1$, hidden $Z_2 \times Z_2$ symmetry [18] and end chain states [10,19] have been identified. For $S > 1$, it was proposed that higher topological symmetries would account for the end chain states [20]. Numerical studies on high spin VBS models [21] and AFHCs [11,22] verified the existence of the string order and end chain states. To detect hidden topological order in AFHC with $S > 1$, the original (''ordinary'') string order parameter [15] has been extended [20,21] to include a topological angle θ that serves a role similar to that of the fictitious gauge field in the adiabatic heuristic argument of the fractional quantum Hall effect (FQHE) [16,23–26]. The extended string order parameter O_S defined at the peak position $\theta = \pi/S$ measures nonlocal topological order in quantum spin chains with general (integer) spins [16,20,21].

On the other hand, based on the observation of critical (gapless) behavior and a lack of end chain states in the $S = 1/2$ AFHC, it is widely believed that the nonlocal topological order does not exist in half-integer spin AFHCs. However, this view has never been substantiated by any serious analytic or numerical calculations. Recently a field theoretical analysis has shown [27] that end chain states appear as the lowest energy excitations in half-integer spin open chains. A numerical study [28] for $S = 3/2$ open chains has shown that quantum fluctuations do not smear out the end chain states. These results point to the existence of topological order in the ground state of gapless half-integer spin chains.

In this Letter we present a systematic study of the extended string order parameter in antiferromagnetic Heisenberg chains using analytical scaling analysis based on the bosonization theory and the VBS construction of the spin chain states, and the density matrix renormalization group (DMRG) calculations. We first show that the string order parameters in half-integer spin chains scale to zero very slowly and only beyond a certain length scale that grows quickly with increasing spin. Numerical DMRG calculations further demonstrate the behavior of the string order parameters in AFHCs and show that chains with $S = (2m - 1)/2$ and m (m = integers) share the same peak position at $\theta/\pi = 1/m$. Since this peak position reflects the topological structure of the spin chain as the fictitious gauge field in FQHE, we conjecture

 0031-9007/03/90(6)/067202(4)$20.00

that this "staircase" structure reflects a common topological feature shared by the pairs (with the same m) of integer and half-integer spin chains that are otherwise distinguished by the Haldane conjecture in their low-energy excitation behavior.

We first examine the scaling behavior of the string order parameter with the chain length. We have carried out bosonization theory calculations following the same procedure as in Ref. [29] but extending the results for spin-$1/2$ AFHC with general topological angle θ. The calculations yield the scaling behavior $O(\theta) \sim L^{-\theta^2/4\pi^2}$ (L is the chain length in terms of the number of the lattice spacing), which reproduces the $L^{-1/4}$ scaling behavior in Ref. [29] as a special case for $\theta = \pi$. Our DMRG calculations for the spin-$1/2$ chain (see below) confirm this scaling behavior. Extension to higher half-integer AFHC is achieved through the construction of the VBS and uncontracted end chain states, similar to that in the integer-spin chain case [21]. It can be shown [30] that the string order parameter of a half-integer spin ($S > 1/2$) is composed of two parts, one from an effective integer-spin part which remains finite and the other from an effective spin-1/2 chain which has the same scaling behavior obtained above and determines the overall scaling behavior of the chain. Since the topological angle $\theta = 2\pi/(2S+1)$ for half-integer spin chains (see below), the scaling function behaves like $L^{-(2S+1)^{-2}}$. This yields scaling behavior $L^{-1/4}, L^{-1/16}, L^{-1/36}, \ldots$ for $S = 1/2, 3/2, 5/2, \ldots$. Furthermore, our DMRG calculations indicate that there exists a length scale beyond which the predicted power-law decay to zero sets in. This length scale is around $L = 150$ for $S = 1/2$. Because of loss of numerical accuracy for longer chains, we are unable to determine the length scale for chains with larger spins, but it is expected to be much longer, possibly reaching macroscopic scale for larger spins. This long length scale allows the extraction of a pseudo-long-range order parameter from the slow-varying $O(\theta)$ for half-integer-spin AFHCs.

We now turn to numerical evaluation of the string order parameter to further investigate its properties. We use the infinite chain DMRG algorithm [31] and keep up to 1800 optimized states in the DMRG calculations for smaller spins ($S \leq 2$). The largest truncation error is about 10^{-6} for the largest spin (9/2) studied in this work. For a spin-S chain of length L, we calculate the extended string order parameter [20]

$$\mathcal{O}_S(\theta, L) = \frac{1}{S^2}\left\langle S_1^z \exp\left(i\theta \sum_{l=2}^{L/2} S_l^z\right) S_{L/2+1}^z \right\rangle. \qquad (1)$$

We consider even length periodic chains with the largest separation between two spins $L/2 - 1$. Results for $L = 4n$ and $L = 4n + 2$ have odd and even site parity [13,32], respectively, yielding $\mathcal{O}_S(\theta, L) = \mathcal{O}_S(2\pi - \theta, L)$ for integer-spin chains and $\mathcal{O}_S(\theta, L) = \pm\mathcal{O}_S(2\pi - \theta, L)$ for $L = 4n + 2$ and $4n$ for half-integer spin chains.

For $S \leq 2$, DMRG calculations were performed for $L = 4$ to $L = 200$, followed by a scaling analysis for extrapolation (except for $S = 1/2$ where the $L^{-\theta^2/4\pi^2}$ scaling is applied directly). Numerical accuracy is good since the chain length is greater than the spin-spin correlation length ξ ($\sim e^{\pi S}$), which are 2, 6.03, 19, and 49 for $S = 1/2$, 1, 3/2, and 2, respectively [22]. For the half-integer-spin chains, the parameter ξ is a characteristic length beyond which the continuum field theory provides an effective description for the AFHCs. For higher spins, shorter chains (up to 60) were used due to the loss of accuracy for larger L, and a simple average of the results of the longest chains with even and odd site parity is used.

For extrapolation we use the scaling function [33]

$$\mathcal{O}_S(\theta, L) = O_S(\theta, L) + c\mathcal{O}_S(0, L), \qquad (2)$$

where c is a constant depending on θ only. It separates the slow-varying part $O_S(\theta, L)$ from the fast-varying high-energy contribution $\mathcal{O}_S(0, L)$. We solve the equation by evaluating the string order parameter at two different chain lengths ($L - 2$ and $L + 2$):

$$O_S(\theta, L) = \frac{\begin{vmatrix} \mathcal{O}_S(\theta, L-2) & \mathcal{O}_S(0, L-2) \\ \mathcal{O}_S(\theta, L+2) & \mathcal{O}_S(0, L+2) \end{vmatrix}}{\begin{vmatrix} 1 & \mathcal{O}_S(0, L-2) \\ 1 & \mathcal{O}_S(0, L+2) \end{vmatrix}}. \qquad (3)$$

The extrapolated value $O_S(\theta)$ is obtained by fitting $O_S(\theta, L)$ with a fourth-order polynomial in $1/L^n$. The validity of this scaling analysis is supported by our numerical fitting shown below.

Figure 1 shows the calculated extended string order parameter and the scaling behavior at selected θ for $S = 1/2$ and $S = 1$. We first examine results at several known limits and compare with previous work. Both $O_{1/2}$ and O_1 scale to zero at $\theta = 2\pi$ as expected since they reduce to the usual Néel order parameter. Also, $\mathcal{O}_{1/2}(\pi, L = 4n) = 0$ for all n since there are an odd number of

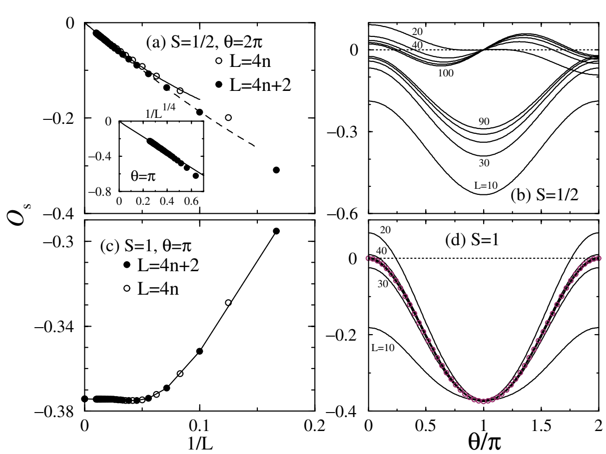

FIG. 1 (color online). Calculated $\mathcal{O}_S(\theta, L)$ and the scaling behavior of O_S at selected θ for $S = 1/2$ and $S = 1$. Open circles in (d) indicate the extrapolated results.

half-integer spins in the summation in Eq. (1). In addition, our calculated $O_S = -0.37434$ for $S = 1$ at $\theta = \pi$ (i.e., the ordinary string order parameter) is in excellent agreement with the value obtained by White and Huse [10]. Support to the use of scaling function Eq. (2) comes from the observation [see Fig. 1(c)] that when $L/2 > \xi$, or $1/L < 0.08$ for $S = 1$, $O_S(\theta, L)$ starts to converge to the extrapolated value. This behavior is also seen for $S = 3/2$ [Fig. 2(a)] and $S = 2$ [Fig. 2(c)].

The inset of Fig. 1(a) shows the scaling behavior of the extended string order parameter for $S = 1/2$. The agreement between the DMRG data and the result of the bosonization theory calculation is excellent. The calculated $\mathcal{O}_S$ for finite chain lengths show very slow convergence [see Fig. 1(b); for clarity, only the results up to $L = 100$ are plotted], consistent with the scaling analysis. These results suggest that the $S = 1/2$ AFHC has "marginal" topological order in the sense that it decays extremely slowly and remains finite for $L \gg \xi$.

One striking feature in Figs. 1(b) and 1(d) is that the peak positions for $S = 1/2$ and $S = 1$ are both located at π. This pattern of O_S with $S = (2m - 1)/2$ and $S = m$ (m = integers) sharing the same peak position (at $\theta/\pi = 1/m$) extends to higher spin cases (see Table I). The significance of the peak in O_S for integer-spin chains has been discussed in both the VBS [21] and AFHC [34,35] pictures. The topological angle θ corresponding to the peak in O_S plays a role similar to the fictitious gauge field in FQHE and $O_S(\theta = \pi/S)$ reflects the fundamental features of the ground-state wave function of the quantum spin system. Our results show that half-integer spin AFHCs share the same topological feature.

Calculated extended string order parameters for $S = 3/2$ and $S = 2$ are shown in Fig. 2. For $S = 3/2$, the peak position is located near $\theta = \pi/2$, the same as in the $S = 2$ case, rather than at $\theta = \pi/S = 2\pi/3$. It is clear that O_S is finite in both cases. $O_S = 0$ at $\theta = 0$ (2π), where it reduces to the usual Néel order parameter. For $S = 3/2$, $\mathcal{O}_S(\pi, L = 4n) = 0$ for all n as in the $S = 1/2$ case. For $S = 2$, $O_S = 0$ at $\theta = \pi$. This is understood in the VBS picture as the result of the Z_2 symmetry which leads to vanishing string order in integer-spin chains with even S [21]. It is noticed that in the $S = 3/2$ case the peak values for chains with even and odd site parities scale to slightly different values while they share the same peak position. This behavior is observed in all half-integer spin AFHCs studied in this work. A possible source for this difference is the site parity effect that manifests itself in the gapless half-integer AFHCs where quantum fluctuations are stronger than in integer AFHCs. The most pronounced effect is seen near $\theta = \pi$. However, for half-integer spin chains with $S \geq 3/2$ the peak positions occur increasingly away from this point, yielding insignificant differences in the values of O_S.

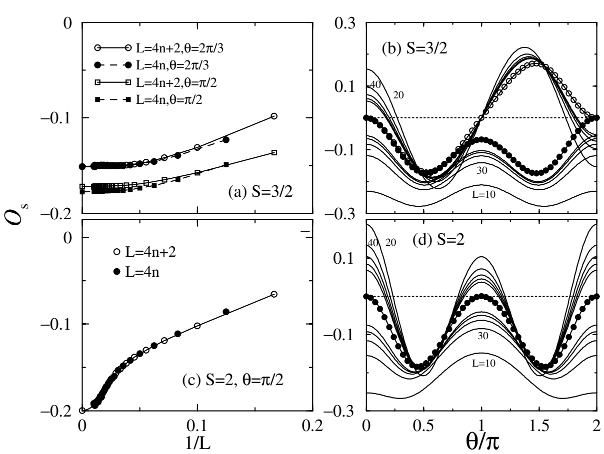

FIG. 2. Calculated $\mathcal{O}_S(\theta, L)$ and the scaling behavior of O_S at selected θ for $S = 3/2$ and $S = 2$. Circles in (b) and (d) indicate the extrapolated results [filled and open circles in (b) are for chains with even and odd site parities, respectively].

We have calculated the extended string order parameter O_S (the peak value) and the corresponding topological angle (peak position) for AFHCs with spins up to $S = 9/2$. The results for all spins are summarized in Table I. Results for integer-spin VBS models [21] are also listed for comparison. It is seen that O_S is always smaller in AFHCs than in the corresponding VBS models. This is the consequence of the stronger fluctuation in AFHCs [35]. It is also noticed that within the same pair of integer-spin and half-integer-spin chains (i.e., $S = 3/2$ and 2, 5/2 and 3, etc.), O_S is always smaller in the half-integer-spin chains, reflecting the stronger quantum fluctuation in chains with gapless excitation spectra.

Furthermore, the calculated peak positions converge to the same value for the even and odd parity chains in all the cases and the values for integer-spin AFHCs are in excellent agreement with those obtained in a matrix product formalism for the integer-spin VBS models [21]. These numerical results strongly suggest that AFHCs with $S = (2m - 1)/2$ and $S = m$ (m = integers) share the same topological angle $\theta/\pi = 1/m$, leading to the conjecture

TABLE I. Calculated peak values and positions of the extended string order parameter for AFHCs with spin up to 9/2. Results for integer-spin VBS models (Ref. [21]) are listed for comparison. Notice that use of different phase conventions causes the difference of a negative sign in the peak value.

	Peak Value O_S		Peak Position (θ/π)	
S	AFHC	VBS	AFHC	VBS
1/2	0		1.0	
1	−0.374 34(1)	0.444	1.0	1.0
3/2	−0.175(5)		0.51(1)	
2	−0.1955(5)	0.250	0.46(1)	0.5
5/2	−0.17(1)		0.375(5)	
3	−0.18(3)	0.218	0.325(5)	0.35
7/2	−0.16(3)		0.27(2)	
4	−0.20(3)	0.205	0.26(1)	0.27
9/2	−0.17(3)		0.23(2)	
5		0.195		0.22

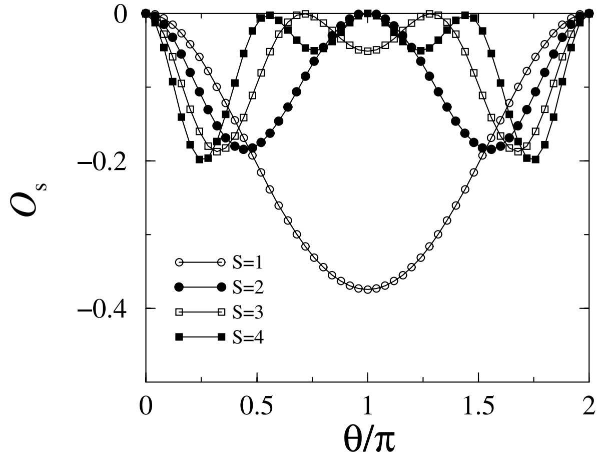

FIG. 3. Calculated O_S for integer spin chains.

that there is a common underlying topological feature shared by integer and half-integer spin chains. This raises the possibility to supplement the Haldane conjecture and classify quantum spin chain ground states by certain hidden order parameters as proposed for the fractional quantum Hall effect. It is interesting to note that a previous work on frustrated spin chains [36] showed that as the frustration becomes strong free end spins disappear suddenly for *both* integer and half-integer spin chains, suggesting a common feature shared by the two systems.

The calculated extended string order parameters for integer-spin AFHCs with spins up to $S = 4$ are shown in Fig. 3. The alternation between vanishing and finite values at $\theta = \pi$ for even and odd integer-spin chains previously observed in VBS models [21] is clearly seen here in AFHCs. These results reinforce the notion that VBS and AFHC chains share the same qualitative topological features.

In summary, we have shown that nonlocal topological string order exists on macroscopic scale in half-integer-spin AFHCs with the only exception of $S = 1/2$. Numerical evidence suggests a common topological feature shared by pairs of integer and half-integer AFHCs that may serve to further classify quantum spin chains. Although the extended string order in half-integer-spin chains is only pseudo long ranged, there are physical consequences such as end chain states that survive even in the limit of infinite chain length. It also indicates the existence (and possible breaking) of certain hidden symmetries in AFHCs as observed in VBS models. Details on the nature of the topological order in AFHCs with general spin and the underlying symmetry remain important open questions for future studies.

Finally, it is important to note [11,37] that string order exists not just in Haldane phases but also in *XY* and large-*D* phases where the VBS construction and the successive phase transitions predicted [20] in the VBS picture become questionable. The link between the string order, the VBS construction, and the gapped Haldane phases for integer-spin chains remains to be explored further.

We are grateful to M. Oshikawa, K. Totsuka, and especially Tai-Kai Ng for stimulating discussions. This work was supported in part by the Department of Energy at UNLV and by the Chinese Natural Science Foundation.

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