

Spinon confinement and the Haldane gap in $SU(n)$ spin chains

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We use extensive density-matrix renormalization-group calculations to show that a classification of $SU(n)$ spin chains with regard to the existence of spinon confinement and hence a Haldane gap obtained previously for valence bond solid models applies to $SU(n)$ Heisenberg chains as well. In particular, we observe spinon confinement due to a next-nearest-neighbor interaction in the $SU(4)$ representation **10** chain.

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I. INTRODUCTION

The properties of quantum spin chains have been a vital area of research in condensed-matter physics. Starting with Bethe's solution of the spin-1/2 Heisenberg model (HM) in 1931,¹ the field quickly evolved and significantly influenced many other areas of physics. In accordance to previous findings by Andrei and Lowenstein,² Faddeev and Takhtajan³ observed in 1981 by consideration of Bethe ansatz solutions that the elementary excitations of spin chains are spinons carrying spin 1/2. From the identification of the $O(3)$ nonlinear sigma model as the low-energy field theory of antiferromagnetic $SU(2)$ spin chains, Haldane conjectured in 1983 that chains with integer spin possess a gap in the magnetic excitation spectrum, while a topological term renders half-integer spin chains gapless.⁴ This, and, in particular, the gap in the magnetic energy spectrum for integer chains, was confirmed by experiment.⁵ An elegant paradigm of the gapped spin 1 chain in terms of a valence bond solid (VBS) model was given by Affleck, Kennedy, Lieb, and Tasaki (AKLT).⁷

Haldane's classification^{4,8} applies only to $SU(2)$ spin systems. In the field of ultracold atoms and optical lattices, however, experimental realizations of $SU(n)$ spin systems may be possible in the near future. In particular, it has been proposed very recently that $SU(n)$ antiferromagnets with n up to 10 may be realized with ultracold alkaline-earth atoms without any need to fine tune any of the interaction parameters.⁹ This perspective makes a general classification of the magnetic spectra of antiferromagnetic $SU(n)$ spin chains highly desirable.

It is, however, not immediately clear how to address the question which $SU(n)$ spin chains generally possess a Haldane-type gap, as Haldane's original work cannot directly be generalized to $SU(n)$; previous attempts were limited to special cases.^{6,10} One possible route is to interpret the Haldane gap as the zero-point energy of the oscillator describing the relative motion of pairwise-confined spinons¹¹ and to employ simple paradigms to determine whether spinons in a spin chain, with spins transforming according to a given representation, are confined or not. Following this line of reasoning, two of us¹² recently formulated a variety of VBS models for $SU(n)$ spin chains and investigated which models exhibit spinon confinement and hence a Haldane gap. This led to a classification of $SU(n)$ spin chains into three categories, as reviewed below. The conjecture which motivated this work was that the "gap/no gap" classification found for the VBS models would apply to general $SU(n)$

spin chain models and, in particular, to the $SU(n)$ HMs.

In this Rapid Communication, we explicitly confirm this conjecture using extensive density-matrix renormalization-group (DMRG) calculations. In particular, we observe confinement of spinons and hence a change in the universality class triggered by a next-nearest-neighbor interaction in the simplest example of the third category: the $SU(4)$ rep. **10** model.

II. SPINON CONFINEMENT IN VBS STATES

Arovas *et al.*¹³ pointed out that the spin 1 AKLT model $H_{\text{AKLT}} = \sum_i P_2(i, i+1)$ is a good starting point to reach the Heisenberg point $H_{\text{HM}} = \sum_i \mathbf{S}_i \mathbf{S}_{i+1} = 3 \sum_i [P_2(i, i+1) + 1/3 P_1(i, i+1) - 2/3]$ perturbatively. Here $P_R(i, \dots, i+m)$ is a projector of the total spin of $m+1$ neighboring sites onto representation R of $SU(2)$. Both models show an excitation gap according to Haldane's conjecture. For the AKLT model, exact calculations¹³ showed that the static spin-spin correlations decay exponentially, being the signature of an excitation gap (see also the second line in Table I). The AKLT model contains a characteristic length scale associated with the correlation decay, which may only change quantitatively, but not qualitatively upon moving to the HM. In the following, we assume that also beyond $SU(2)$, the existence of a length scale at a VBS point persists as one moves to the Heisenberg point. This links the gap property of a VBS model with the HM for the same spin representation.

It is easy to illustrate how the Haldane gap can be traced to spinon confinement in the AKLT state. It can be written as a product of local spin singlets consisting of two "virtual" spins 1/2 placed on adjacent sites. Projecting onto the symmetric subspace on each site gives the spin 1 representation,

$$|\Psi_{\text{AKLT}}\rangle = |\circ\text{---}\circ\text{---}\circ\text{---}\circ\text{---}\circ\text{---}\circ\text{---}\circ\rangle.$$

Here, each circle denotes a "virtual" spin 1/2 and each line a singlet bond. The dashed box illustrates exemplarily a lattice site. The AKLT Hamiltonian is just the sum over the projectors onto the subspace with total spin 2 of adjacent sites. For two neighboring sites of Ψ_{AKLT} , a spin singlet and two individual virtual spins 1/2 are present, i.e., $\mathbf{0} \otimes \frac{1}{2} \otimes \frac{1}{2} = \mathbf{0} \oplus \mathbf{1}$. The tensor decomposition of two spin 1 representations, however, additionally contains a spin 2 subspace, i.e., $\mathbf{1} \otimes \mathbf{1} = \mathbf{0} \oplus \mathbf{1} \oplus \mathbf{2}$. Hence, it follows that Ψ_{AKLT} is annihilated by H_{AKLT} , whereas all other states will be lifted to finite energy. To create a pair of spinons, one breaks a singlet bond [see Fig.

TABLE I. Classification for spin-spin correlations of certain $SU(n)$ VBS states as introduced in Ref. 12. Listed are the spin representation, the corresponding Young tableau (YT), the spin-spin correlation length ξ (Ref. 19), and the category C with respect to our conjecture. The $SU(4)$ rep. **10** VBS is the simplest model of category III. The correlations for the MG and the rep. 6 model decay abruptly and no correlation length can be defined.

Spin rep.	YT	ξ	C
$SU(2)$, $S=\frac{1}{2}$	\square		I
$SU(2)$, $S=1$	$\square\square$	$\frac{1}{\ln 3}$	II
$SU(3)$, 6	$\square\square$		I
$SU(3)$, 8	$\begin{array}{ c } \hline \square \\ \hline \square \\ \hline \end{array}$	$\frac{1}{\ln 8}$	II
$SU(4)$, 10	$\square\square$	$\frac{2}{\ln 7}$	III

1(a)]. The region between the two spinons yields an energy penalty for H_{AKLT} , or stated differently, the two spinons feel a confining potential $V(x)=F|x|$. As the Hamiltonian of the relative motion of the two spinons consists of a kinetic energy and this linear confining potential, we obtain a linear oscillator. We interpret the zero-point energy of this oscillator as the Haldane gap.

For half-integral spin chains, the corresponding VBS is the Majumdar-Ghosh (MG) model¹⁴ (see also the first line in Table I). In our terminology, both spontaneously n -merized (such as MG) and translational invariant states (such as AKLT) are VBS states. Its ground state consists of local singlet bonds placed on adjacent sites. In contrast to the AKLT model, the MG ground state is twofold degenerate and invariant only under translations by two lattice sites. As in the AKLT model, elementary excitations are created by breaking a singlet bond. The two emerging spinons can serve as domain walls interpolating between the two ground states [see Fig. 1(b)], i.e., the spinons do not feel any confining potential. Accordingly, the spin-spin correlations decay abruptly, i.e., $\langle S_i S_{i+2} \rangle = 0$, and no associated length scale, describing an exponential decay, emerges. Moving from the MG point to the isotropic HM, one passes a phase transition from the dimer phase into a critical spin liquid phase.¹⁵ The deconfined spinons of the MG model, however, remain deconfined when moving to the generic HM and give rise to the observable two-spinon continuum.¹⁶ Applied to arbitrary integer and half-integer representations, this line of argument reproduces Haldane's original conjecture for $SU(2)$ spin chains. This interpretation is consistent with earlier attempts to describe the spin 1 elementary excitation of related models as confined solitons¹⁷ or two-spinon composite particles.¹⁸

III. PREVIOUS CONJECTURE

So far, we reproduced Haldane's conjecture for $SU(2)$ in terms of spinon confinement. We now review the general classification of the magnetic excitation spectra for $SU(n)$ chains motivated by the VBS states introduced previously.¹²

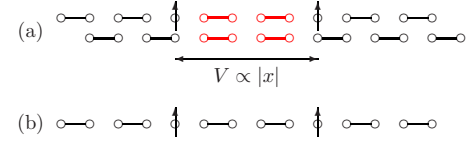


FIG. 1. (Color online) (a) Spinon confinement in the AKLT model. The potential is proportional to the distance $|x|$ between the spinons and allows an interpretation of the Haldane gap as the zero-point energy of a linear oscillator. (b) Spinons in the spin 1/2 VBS state are domain walls between the two ground states and hence free.

This classification depends only on the degree n of $SU(n)$ and the number of boxes λ in the Young tableau (YT) associated with the respective spin representation (see also Table I). (i) If λ and n have no common divisor, the model will support free spinon excitations and not exhibit a Haldane gap. (ii) If λ is divisible by n , the model will exhibit spinon confinement and hence a Haldane gap. (iii) If λ and n have a common divisor different from n , the presence of the confining potential will depend on the range of interactions. If q is the largest common divisor of λ and n , interactions ranging to the (n/q) th neighbor are required for spinon confinement.

For $SU(2)$, the classification is identical to Haldane's, as the third category becomes accessible only for $n \geq 4$. If this classification applies to the HMs as well, as we advocate here, we will find gapless spectra, unique ground states, and algebraic correlations for the first category. For the second category, we will find gapped spectra and exponentially decaying correlations, as it is possible to write the HM as VBS model plus a small perturbation (similar as for the spin 1 case¹³). For the $SU(4)$ rep. **10** chain belonging to the third category, the gapless spectrum of a nearest-neighbor HM should acquire a gap as a next-nearest-neighbor interaction term is added.

In Table I, we further list the exact values for the static spin-spin correlation length.^{19–21} We expect that Heisenberg chains for all representations without a well-defined VBS correlation length ξ (such as lines 1 and 3 in Table I) will be gapless. For representations with a well-defined correlation length ξ , we have to distinguish a “standard” gapped category II and the nontrivial category III, which we will treat separately below.

IV. VERIFICATION OF THE CONJECTURE

To verify our predictions for the $SU(n)$ HMs, we performed extensive DMRG (Refs. 22–25) studies for all $SU(n)$ representations up to the ten-dimensional representations of $SU(3)$ and $SU(4)$. Note that we use the “Abelian” quantum numbers of $SU(n)$, as the “non-Abelian version” of DMRG (Ref. 26) is not really convenient for $SU(3)$ and $SU(4)$ representations. In order to treat the large block sizes of our DMRG calculation, we use a Posix thread parallelized DMRG code.²⁷ In our list of representations, we find gapless models such as the fundamental representations of $SU(3)$ ($\lambda=1$ in YT box notation), $SU(4)$ ($\lambda=1$), and the six-dimensional representation of $SU(3)$ ($\lambda=2$). The ten-dimensional representation of $SU(3)$ ($\square\square\square, \lambda=3$) provides

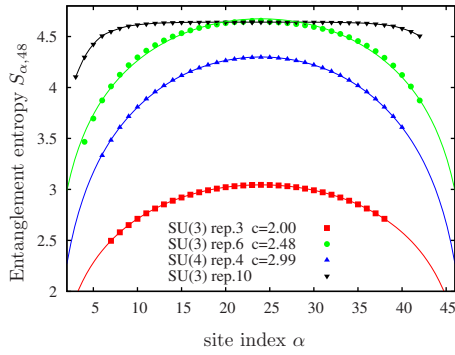


FIG. 2. (Color online) Entanglement entropy (48 sites, PBCs) for the critical $SU(n)$ Heisenberg chains with $SU(3)$ rep. **3** ($N_{\text{cut}} = 5000$ kept DMRG states), rep. **6** ($N_{\text{cut}} = 5000$), rep. **10** ($N_{\text{cut}} = 1650$), and $SU(4)$ rep. **4** ($N_{\text{cut}} = 12\,000$). Except of $SU(3)$ rep. **10**, all models are gapless and nicely follow the sinusoidal shape according to Eq. (1). The latter clearly develops a plateau structure as expected for gapped models.

an example for a gapped model. As the local basis dimension can become very large, we are not always able to extrapolate to the thermodynamic limit and read off the gap from there. Instead, we use the entanglement entropy $S_{\alpha} = -\text{Tr}[\rho_{\alpha} \log \rho_{\alpha}]$, where ρ_{α} is the reduced density matrix in which all the degrees of freedom on sites $i > \alpha$ are traced out. This way, there is no need to extrapolate. In particular, for critical spin models associated with conformal field theories (CFTs), the entanglement entropy is given by²⁸

$$S_{\alpha,L} = \frac{c}{3} \log \left[\left(\frac{L}{\pi} \right) \sin \left(\frac{\pi \alpha}{L} \right) \right] + c_1, \quad (1)$$

where L is the chain length, c_1 a nonuniversal constant, and c is the central charge of the associated CFT. In case of Heisenberg-like $SU(n)$ spin chains, the CFT is a Wess-Zumino-Witten model with topological coupling k [$SU(n)_k$ WZW] with central charge $c = k(n^2 - 1)/(k + n)$. We use periodic boundary conditions (PBCs) rather than hard wall boundary conditions in our DMRG calculations, as the latter shows even/odd oscillation triggered by the boundaries. These would render the interpretation of our results for the category III models below ambivalent.

If the models exhibit a gap in the excitation spectrum, the entanglement entropy does not have the sinusoidal shape but saturates after a few sites. If the models have dimerized (or trimerized, tetramerized, etc.) ground states, this manifests itself in the entanglement entropy by oscillations of the entropy with an oscillation period of two sites (or three, four, etc.), reflecting that the ordered states get pinned by numerical noise. The numerical results are shown in Fig. 2. For the nearest-neighbor $SU(n)$ HMs with fundamental representation ($\lambda = 1$), we find the sinusoidal shape (1) with fitting parameter $c = n - 1$ for $n = 2, 3, 4$.²⁹ For the $SU(3)$ representation **6** HM, we find a critical model with a central charge larger than $c = 2$, with the difference due to marginal operator perturbations. For larger chain lengths, the associated inverse logarithmic corrections disappear and the central charge approaches $c = 2$, as expected. The situation is hence compa-

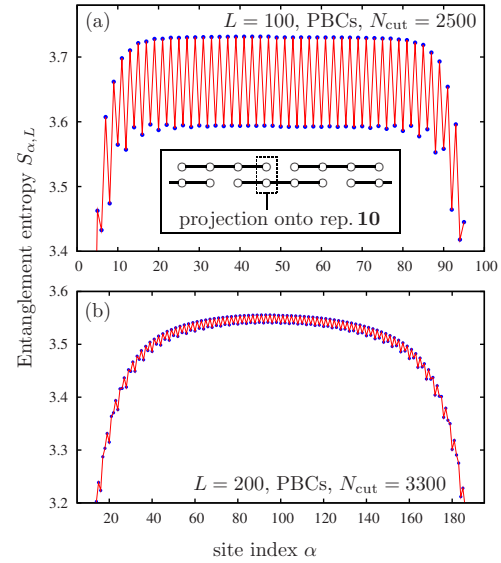


FIG. 3. (Color online) Entanglement entropy of the $SU(4)$ rep. **10** HM with next-nearest-neighbor interactions for (a) $J_2 = 0.5J_1$ and (b) $J_2 = 0.15J_1$, as discussed in the text. The inset in (a) illustrates the $SU(4)$ rep. **10** VBS state, where each circle denotes a fundamental $SU(4)$ representation and the horizontal line denotes anti-symmetric coupling. Four connected circles hence represent an $SU(4)$ singlet.

able to the spin 3/2 HM.³⁰ This implies that the $SU(3)$ representation **6** HM belongs to the $SU(3)_1$ WZW universality class. For the ten-dimensional representation of $SU(3)$ ($\lambda = 3$), we find that the entanglement entropy saturates after a few sites. This indicates a gap (see Fig. 2).

V. CATEGORY III MODELS

We have further performed extensive calculations for the HM of the ten-dimensional representation of $SU(4)$ ($\lambda = 2$) with nearest- and next-nearest-neighbor interactions. This is the simplest example belonging to the third category. Let us first look at the corresponding VBS state shown in the inset of Fig. 3(a). The state is twofold degenerate and invariant under translations by two lattice spacings. Its parent Hamiltonian involves three-site interactions.¹² The correlations decay exponentially with length ξ (see Table I).

For nearest-neighbor interactions, we find that the model is gapless and critical as required by the Affleck-Lieb theorem.⁶ The fitted central charge is larger than 3 in accordance with the $SU(4)_1$ WZW universality class in the presence of logarithmic corrections. Following our categorization, applying a next-nearest-neighbor interaction should force the system in a gapped phase with confined spinons. As a first test, we approximate the Hamiltonian of the VBS state within the J_1 - J_2 model $H_{\text{VBS}} \approx \sum_i \mathbf{S}_i \mathbf{S}_{i+1} + 1/2 \sum_i \mathbf{S}_i \mathbf{S}_{i+2}$. The corresponding entanglement entropy is shown in Fig. 3(a). It shows a strongly oscillating behavior, indicating dimerization, as expected from the analogy with the VBS state shown in the inset. The conjecture that the HMs behave as the associated VBS models thus is confirmed for this type of models. It still remains to be shown, however, that this gap is not

TABLE II. Critical couplings (Refs. 15, 31, and 32) of J_1 - J_2 models of different $SU(n)$ representations are shown. For representations belonging to the category II with Haldane gap, no phase transition occurs. All other $SU(n)$ models tend to n -merize (i.e., dimerize for $n=2$, etc.) (Refs. 30 and 32). We further conjecture that the critical couplings $(J_2/J_1)_c$ increase when n and/or λ is increased. Consequently, the $SU(4)$ rep. **10** chain is expected to tetramerize for a critical coupling, which is larger than $(J_2/J_1)_c \approx 0.5$. For the $SU(3)$ rep. **6** and the $SU(4)$ rep. **4** model, only preliminary results are available, as indicated by the asterisks.

$SU(n)$	\square	$\square\square$	$\square\square\square$
$n=2$	0.2411	cat. II	0.33
$n=3$	0.45	$\geq 0.5^*$	cat. II
$n=4$	$\approx 0.5^*$?	

due to a tetramerized phase as expected for a frustrated $SU(4)$ model driven by J_2 . To rule this out, we have collected the critical couplings of all relevant $SU(n)J_1$ - J_2 models in Table II. From there, one would expect that a transition into a tetramerized phase for $SU(4)$ rep. **10** would only occur for some critical coupling $(J_2/J_1)_c > 0.5$. By contrast, we find a dimer phase rather than a tetramer phase and for couplings smaller than the expected critical coupling. In our DMRG calculations, we observe the existence of the dimer phase for a value as small as $J_2 \approx 0.15J_1$ [see Fig. 3(b)]. The oscillation amplitude of the dimerization becomes weaker but is still present. Our data cannot be understood in the context of frustrated HMs but are fully consistent with our conjecture of

spinon confinement triggered by a next-nearest-neighbor interaction.

Physically, the opening of a gap can be understood as follows. As we apply a next-nearest-neighbor coupling J_2 , pairs of neighboring sites effectively cluster into new sites, and pairs of spins transforming under the original representation form new representations on the new sites. The state hence dimerizes on the original lattice, while it remains invariant under translations of the new lattice. The original representations implied that spinons were deconfined and no gap occurred. Spinons in the effective model with spins transforming under the new representations, however, are confined and the spectrum is gapped. The next-nearest-neighbor coupling J_2 in our category III model here hence produces an effect similar to the effect produced by a coupling of two spin 1/2 chains into a spin ladder.

VI. CONCLUSION

We have shown that a classification of $SU(n)$ spin chains with regard to the existence of a Haldane gap obtained previously for VBS models applies to $SU(n)$ Heisenberg chains as well. The results provide evidence in favor of our hypothesis that this gap can be interpreted as the zero-point energy of an oscillator describing the relative motion of confined spinons.

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