Haldane Gap of the Three-Box Symmetric SU(3) Chain

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Motivated by the recent generalization of the Haldane conjecture to SU(3) chains [Lajkó *et al.*, Nucl. Phys. **B924**, 508 (2017)] according to which a Haldane gap should be present for symmetric representations if the number of boxes in the Young diagram is a multiple of three, we develop a density matrix renormalization group algorithm based on standard Young tableaus to study the model with three boxes directly in the representations of the global SU(3) symmetry. We show that there is a finite gap between the singlet and the symmetric $[3\ 0\ 0]$ sector $\Delta_{[3\ 0\ 0]}/J = 0.040 \pm 0.006$ where J is the antiferromagnetic Heisenberg coupling, and we argue on the basis of the structure of the low energy states that this is sufficient to conclude that the spectrum is gapped.

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The role played in the field of quantum magnetism by Haldane's prediction that integer spin chains have a gap while half-odd-integer spin chains do not can hardly be overemphasized [1,2]. Indeed, ever since this prediction was confirmed experimentally and numerically, the community has thought differently about antiferromagnets, and the actual value of the spin (and not simply its length as a measure of quantum fluctuations) has become a defining parameter along with the dimensionality of space, the topology of the lattice and the isotropy of the couplings [3–11]. With the progress made in ultracold fermionic experiments [12–23], the SU(N) cousins of the SU(2) Heisenberg model have become the focus of a lot of attention, and quite naturally the question of whether and how Haldane's conjecture can be generalized has been addressed by many authors [24–31]. The generalization of the Affleck-Kennedy-Lieb-Tasaki (AKLT) construction has proven to be a very useful guide in predicting which model may or may not be gapped, as well as the concept of spinon confinement [29,32–36]. More recently, Haldane's semiclassical derivation of a nonlinear sigma model with a topological term has been generalized to SU(3) chains in the symmetric representation, and the absence of topological terms in the action when the number of boxes in the Young diagram is a multiple of three is a strong indication that there should be a Haldane gap in that case without any symmetry breaking [27]. The underlying theory, the $\mathrm{SU}(3)/[\mathrm{U}(1) \times \mathrm{U}(1)]$ flag manifold nonlinear sigma model, is of interest in itself as a nontrivial generalization of the standard $\mathbb{CP}^2$ model. For instance, it has been shown using 't Hooft anomaly matching that, when the number of boxes in the Young diagram is not a multiple of three, the model is gapless in the IR and is described by a $\mathrm{SU}(3)_1$ Wess-Zumino-Witten (WZW) conformal field theory [28,37].

On the numerical front, the presence of a finite gap in the three-box symmetric SU(3) chain, the simplest possible case where the Lieb-Schultz-Mattis-Affleck theorem does not apply (or equivalently no 't Hooft anomaly is present in the flag manifold nonlinear sigma model), is not at all clear. In early density matrix renormalization group (DMRG) simulations, the saturation of the entanglement entropy has been interpreted as the evidence of a Haldane gap [35]. This conclusion has been challenged, however, by exact diagonalizations (ED) which showed that, if there is a gap, the correlation length associated with it must be much larger than that at which the entanglement saturates according to Ref. [35], suggesting that the saturation of the entanglement entropy was actually a consequence of the truncation of the Hilbert space in DMRG [38]. To actually have a chance to detect the gap, one must clearly study much longer chains, and keep far more states. This is a real challenge because it is not known *a priori* how long the chain will have to be, and how many states will have to be kept. As for SU(2) with spin S, this length scale is expected to increase exponentially with the number of boxes in the Young diagram, but since the gap has never been calculated for any irreducible representation (irrep), the prefactor is not known, and an estimate of the length is not available.

In this Letter, we have taken on this challenge, and have developed a DMRG code in the basis of standard Young tableaus (SYTs) that allows one to take advantage of the full SU(N) symmetry, and to keep the equivalent of a huge number of states without increasing too much the size of the variational space [5,6]. This has allowed us to obtain definitive numerical evidence that the spectrum is gapped, and to come up with an estimate $\Delta_{[3\ 0\ 0]}/J \simeq 0.04$ for the gap in the $[3\ 0\ 0]$ sector, where J is the antiferromagnetic coupling. Given the extremely small value of this gap,

comparable to that of SU(2) chains for spin $S = 3$ for which the correlation length $\xi \simeq 637$, it is clear *a posteriori* that there was no chance to detect it in the early attempts with standard DMRG or ED, and that it will be very challenging to look at cases with a larger number of boxes [9].

The Hamiltonian of antiferromagnetic SU(N) Heisenberg chains can be written as

$$\mathcal{H} = J\sum_i \sum_{\alpha,\beta=1}^{N} \mathcal{S}_i^{\alpha\beta}\mathcal{S}_{i+1}^{\beta\alpha}, \qquad J > 0, \tag{1}$$

where the generators $\mathcal{S}^{\alpha\beta}$ satisfy the usual SU(N) commutation relations $[\mathcal{S}^{\alpha\beta}, \mathcal{S}^{\mu\nu}] = \delta^{\mu\beta}\mathcal{S}^{\alpha\nu} - \delta^{\alpha\nu}\mathcal{S}^{\mu\beta}$. For the ten-dimensional symmetric irrep of SU(3) represented by a Young diagram with three boxes in the first row, $\square\square\square \equiv [3\,0\,0]$ [39], it can be written equivalently as

$$\mathcal{H} = 2J\sum_i \mathbf{T}_i \cdot \mathbf{T}_{i+1}, \tag{2}$$

where $T_i^a, a = 1, \ldots, 8$ are ten-dimensional Hermitian traceless matrices representing the generators of $\mathfrak{su}(3)$ and are the exact analogues of the $\mathfrak{su}(2)$ spin operators S^x, S^y, and S^z (see Supplemental Material [40] for details).

To reach long enough chains, the only option is to use DMRG with open boundary conditions. In this case, edge states are expected to be present, however. This is best understood by looking at the AKLT version of the model with a biquadratic interaction [40],

$$\mathcal{H}_{\mathrm{AKLT}} = 5J\sum_i \left(\mathbf{T}_i \cdot \mathbf{T}_{i+1} + \frac{1}{5}(\mathbf{T}_i \cdot \mathbf{T}_{i+1})^2 + \frac{6}{5}\right), \tag{3}$$

for which an exact ground state can be constructed [47]. There are different ways of constructing this wave function, but the most economical one consists in writing the irrep [3 0 0] as a symmetrized product of two eight-dimensional adjoint irreps [2 1 0], and to make singlets with adjoint representations on neighboring sites, as illustrated in Fig. 1(a) [48]. This implies that there are edge states in the adjoint representation. Accordingly, the spectrum of a finite chain will have low-lying states corresponding to all the representations appearing in the product of two adjoint representations and given in Fig. 1(b). This is inconvenient for two reasons: the bulk gap does not correspond to the first excited state, and the coupling between the edge states creates long-range entanglement that makes the convergence of DMRG much more difficult. To overcome this problem, and following what has been done for SU(2) spin chains, we have added an adjoint representation at each end of the chain, with a positive coupling to ensure that it forms a singlet with the edge state [7,49–52]. The precise value of the coupling is not important and the simulations have been done with a coupling equal to J [40].

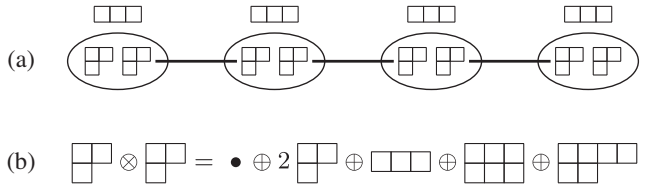

FIG. 1. (a) SU(3) AKLT state for the physical three-box symmetric irrep at each site. An ellipse denotes the projection of two adjoint representations onto the physical three-box symmetric irrep. The thick lines joining neighboring sites represent singlets made out of two adjoint irreps. (b) Decomposition of the tensor product of two adjoint representations.

The DMRG code we have developed is an extension of the code used by two of the present authors to study SU(N) chains in the fundamental representation and which builds on previous developments for exact diagonalization [38,53–55]. It is based on the formulation of the Hamiltonian in terms of permutation operators [40,56] and on the basis of SYTs. This code does not require knowing the SU(N) Clebsch-Gordan coefficients but relies on the subduction coefficients of the symmetric group [40,57]. We are currently limited to the calculation of the subduction coefficients when the outer multiplicity is one [55]. Technically this means that we cannot diagonalize the Hamiltonian in sectors characterized by certain SU(N) symmetry, such as the adjoint representation [2 1 0], to which the first excited state belongs according to ED on small chains [40]. We can, however, diagonalize the Hamiltonian in the singlet sector, which is the irrep of the ground state whatever the number of sites thanks to the adjoint edge irreps, and also in the symmetric irrep [3 0 0] [58].

In our DMRG algorithm, the parameter which mainly controls the accuracy is m, the total number of SYTs kept at each step. Each SYT represents a class of wave functions living in the Hilbert space of the half-chain, with the same properties under the action of permutations, but with different SU(N) weights, so that the color degrees of freedom are factorized out by the use of SYTs [40,53,55]. The complexity of our algorithm is then dictated by the diagonalization of the superblock Hamiltonian of dimension m^2. In this work we take m to be as large as $m = 16\,000$: the discarded weight is then less than 10^{-7} in the singlet sector and less than 10^{-5} in the [3 0 0] sector [40]. This gives an accuracy equivalent to the one obtained with over 860 000 states in a code which does not keep track of the SU(N) symmetry. Our main results are summarized in Fig. 2.

Two strategies have been used to extract information about the gap. The first one follows closely the paper of Schollwöck *et al.* about the spin-2 chain [50]. For a given number of sites, the energies in each sector are extrapolated as a function of the discarded weight [40]. The resulting gap curve remains linear for the largest system sizes, which shows that the size beyond which this curve should bend if

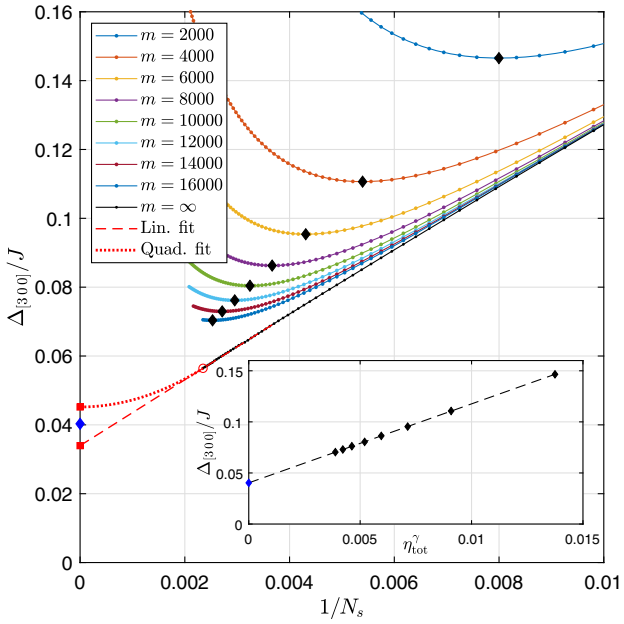

FIG. 2. Gap from the singlet sector to the symmetric [3 0 0] sector versus inverse chain length for different values of the number m of states kept. The inset shows a power-law fit with exponent $\gamma = 0.47$ of the minimum of each finite-m curve, denoted by a black diamond in the main plot, as a function of the total discarded weight $\eta_{\rm tot}$, which is dominated by the discarded weight in the [3 0 0] sector [40]. The extrapolated value, shown with a blue diamond, falls approximately in the middle between our lower and upper bounds of the gap, denoted by red squares.

there is a gap has not been reached yet. However, and most importantly, this linear curve extrapolates to a finite value. If the system was critical, this curve should extrapolate to zero. In fact, as noted by Schollwöck *et al.*, the extrapolated value is a lower bound of the gap. Qualitatively, this is the most important result of the present Letter: the spectrum of the three-box symmetric SU(3) chain is gapped. To get an upper bound, the curvature is assumed to develop for systems immediately larger than the largest system for which we could extrapolate the finite-m results, and we plot a parabola tangent to the gap curve for the largest system size with zero slope in the limit of $1/N_s \to 0$. The intersection of this parabola with the vertical axis is the upper bound. This analysis leads to the estimate $\Delta_{[3\,0\,0]}/J \in [0.034, 0.046]$.

The other strategy is inspired by the investigation of the Haldane gap in spin-1 and spin-2 chains by Tatsuaki [52]: for a fixed m, the gap goes through a minimum as a function of the size. The value at the minimum is an estimate for the gap for a given m, and this estimate can be extrapolated as a function of the discarded weight, see inset of Fig. 2. The results for SU(3) appear to follow very accurately a power law with exponent $\gamma = 0.47$, and the extrapolated value $\Delta_{[3\,0\,0]}/J \simeq 0.040$ is in good agreement with the above bounds.

Note that since the discarded weight stops increasing for a given m for sufficiently long chains, one can also extract the ground state energy per site in the thermodynamic limit by extrapolating the saturated energy per added bond with respect to the saturated discarded weight [7]. We obtain $\epsilon/J = -2.176\,397\,3(2)$ [40].

As a further check of the existence of a finite gap in the Heisenberg chain, we have studied the evolution of the gap between the AKLT point, Eq. (3), and the Heisenberg point Eq. (2). At the AKLT point the correlation length is given by $\xi = 1/\ln 5 \simeq 0.62$ [48]. It is very short, and accordingly the gap is expected to be quite large. Indeed using the same analysis as in Fig. 2 we extract the AKLT gap, $\Delta_{[3\,0\,0]}/J \in [0.970\,705, 0.970\,719]$ using no more than $m = 2000$ states [40]. Away from the AKLT point the gap decreases smoothly to the value we found at the Heisenberg point, as shown in Fig. 3.

In view of the conflicting results between the early DMRG results [35] and the ED results on systems up to 12 sites [38], we have investigated the entanglement entropy, and we have extracted the central charge using the Calabrese-Cardy formula [59]. For systems as large as 300 sites, the entanglement entropy still has a significant curvature for m large enough, as can be seen in Fig. 4, and the finite size estimate of the central charge is not negligible, but it is clearly below the value $c = 2$ for the WZW $\mathrm{SU}(3)_1$ universality class, the only alternative to a gapped spectrum [60]. Moreover, the results are consistent with a vanishing value in the thermodynamic limit, as expected for a gapped system.

So there is ample evidence that there is a gap in the [3 0 0] sector of the three-box symmetric SU(3) chain. Let us now discuss the implications of this result for the low-energy spectrum of the model. This discussion relies on two propositions: (i) There are five branches of bulk elementary excitations belonging to four irreps, including [3 0 0]; (ii) The presence of a finite gap in any of these irreps, and in particular [3 0 0], implies that there is also one in all other irreps, and hence the spectrum is gapped.

(i) The presence of five branches of bulk elementary excitations is best understood by looking at the ground state

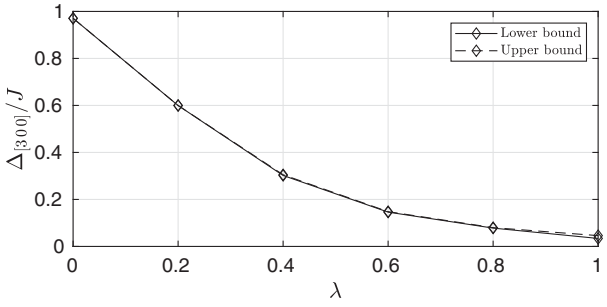

FIG. 3. Gap from the singlet sector to the symmetric [3 0 0] sector of the interpolation Hamiltonian $\mathcal{H}_\lambda = (1-\lambda)\mathcal{H}_{\rm AKLT} + \lambda\mathcal{H}, \lambda \in [0, 1]$.

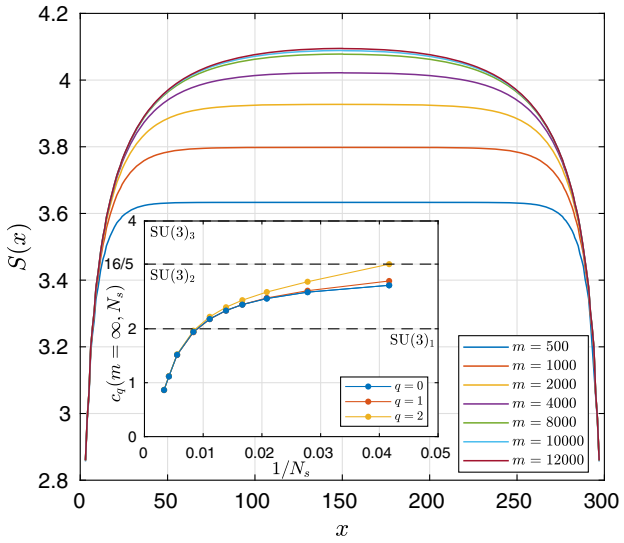

FIG. 4. Entanglement entropy of the ground state for a chain with $N_s = 300$ sites. Over 839 000 states would be needed to reproduce the curve $m = 12\,000$ with a code which does not have the SU(3) symmetry. The inset shows the scaling of the extrapolated central charge in the middle of the chain for different values of the chain length, and comparison with the central charges for the $\mathrm{SU}(3)_k$ WZW conformal field theory with $k = 1$, 2, 3. There are three sets of data $c_q(m = \infty, N_s), q = 0, 1, 2$ because of the oscillation of the entanglement entropy along the chain for $x = q$ mod 3 where x is the position of the cut.

of the AKLT model, which has singlets on every bond and which is pictured in Fig. 1(a). To create a bulk excitation one needs to break one singlet, liberating an adjoint irrep on each side of the broken singlet. These adjoint representations can then recombine according to Fig. 1(b) to form five excited states belonging to the [2 1 0] (two states), [3 0 0], [3 3 0], and [4 2 0] irreps [61].

(ii) The presence of a gap in a sector α implies that there is also a gap in another sector β if, by combining two or more β excitations, one can construct a state that belongs to the α sector. Now, the symmetric irrep [3 0 0] appears in the product of two adjoint irreps, as well as in that of two [3 3 0] or two [4 2 0] irreps. Thus, the presence of a gap in the [3 0 0] sector implies that there is a gap in all other sectors of elementary excitations, in agreement with additional results we have obtained for the [3 3 0] irrep [40], hence that the spectrum is gapped. This discussion implies that there are actually four Haldane gaps Δ_α corresponding to the four irreps $\alpha = [2\ 1\ 0], [3\ 0\ 0], [3\ 3\ 0], [4\ 2\ 0]$, and that they must satisfy $\Delta_{[2\ 1\ 0]}, \Delta_{[3\ 3\ 0]}, \Delta_{[4\ 2\ 0]} \geq \Delta_{[3\ 0\ 0]}/2$. Note that any of the irreps of the elementary excitations can be obtained by combining two or more excitations of the other irreps, leading to other inequalities, and the presence of a gap in any of these irreps is a necessary and sufficient condition for a gapped spectrum.

We can actually prove that these inequalities are strict in the case of the AKLT model in Eq. (3) because the lowest excitation in the sector [3 0 0] is not a composite one. Indeed, if it were, the bond energy on a finite chain should show a double peak structure, as observed in the spin-2 sector of the spin-1 chain [40,62], and it does not, as clearly demonstrated by DMRG results on a 60-site chain [40].

To summarize, using finite-chain DMRG simulations with full SU(N) symmetry, we have obtained clear numerical evidence that the spectrum of the three-box symmetric SU(3) chain is gapped, in agreement with field theory arguments, and we have estimated the gap in the [3 0 0] sector to be $\Delta_{[3\ 0\ 0]}/J = 0.040 \pm 0.006$. The smallest gap is at least half this gap, hence bounded from below by $0.017J$ (half the lower bound of $\Delta_{[3\ 0\ 0]}$), and at most $0.046J$ (the upper bound of $\Delta_{[3\ 0\ 0]}$). These bounds point to a very large correlation length of a few hundred sites.

Finally, let us comment on the possible experimental implementation of this model. Fermions with an SU(3) degree of freedom can be obtained with ^{87}Sr or ^{173}Yb atoms after selecting three out of the ten respectively six nuclear states [16,63,64], and protocols are well documented to implement irreps with up to two columns [15]. Building on Hund's rule that allows one to realize large spins with spin-1/2 electrons, a possible route to implement a symmetric irrep with three boxes could be to create a Mott insulating phase by loading three fermions in different orbitals of the same anharmonic trap since the contact interactions between the fermions is expected to lead to a ground state which is antisymmetric in orbital degrees of freedom and symmetric in color SU(3) space [65].

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[39] We denote an irrep α of SU(3) by three integers $[\alpha_1\,\alpha_2\,\alpha_3]$ corresponding to the lengths of the rows in the corresponding Young diagram. It will indeed sometimes be useful to keep track of the columns with three boxes.
[40] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.125.057202 for (i) the derivation of the Heisenberg and AKLT Hamiltonians in terms of permutation operators; (ii) details on the DMRG algorithm and the calculation of the reduced matrix elements of the interaction using the subduction coefficients; (iii) explanations on the extrapolation procedure; (iv) a study of the effect of the edge coupling; (v) the analysis of the entanglement entropy and the calculation of the central charge; (vi) the calculation of the gap in the [3 3 0] sector; (vii) extensive results at the AKLT point, in particular the calculation of the gap in the [3 0 0], [3 3 0], and [6 0 0] sectors, as well as the calculation of the bond energy along the chain in these sectors; (viii) benchmark results on the SU(2) spin-1 chain. The Supplemental Material includes Refs. [41–46].
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