

Haldane gap in the SU(3) [3 0 0] Heisenberg chain

Lukas Devos^{✉,*}, Laurens Vanderstraeten, and Frank Verstraete

Department of Physics and Astronomy, University of Ghent, Krijgslaan 281, 9000 Gent, Belgium



(Received 25 April 2022; revised 22 September 2022; accepted 26 September 2022; published 3 October 2022)

We calculate the Haldane gap of the SU(3) spin [3 0 0] Heisenberg model using variational uniform fully symmetric SU(3) matrix product states, and find that the minimal gap $\Delta/J = 0.0263$ is obtained in the [2 1 0] sector at momentum $2\pi/3$. We also discuss the symmetry protected topological order of the ground state, and determine the full dispersion relation of the elementary excitations and the correlation lengths of the system.

DOI: [10.1103/PhysRevB.106.155103](https://doi.org/10.1103/PhysRevB.106.155103)

Introduction. Tensor networks provide variational wave functions for approximating the ground states of generic quantum many-body systems in a way that is size-extensive: Local tensors serve as the building blocks for constructing global wave functions directly in the thermodynamic limit. This extensivity is also reflected in the symmetry properties, because a global symmetry is encoded as a symmetry of the local tensors that make up the state. This particular feature allows us to classify different phases of matter by characterizing the symmetry properties of these local tensors *and* gives rise to very efficient numerical algorithms by explicitly encoding the symmetry constraints in the tensors and their numerical manipulations [1].

In one dimension, matrix product states (MPSs) provide a framework for simulating the ground-state properties of quantum spin chains and electrons directly in the thermodynamic limit, and generic (non-Abelian) symmetries can be exploited in all numerical algorithms [2]. Moreover, this MPS framework can be extended to also capture the low-energy dynamics around the ground state: Interpreting the class of MPSs as a variational manifold embedded in the full many-body Hilbert space, the lowest-lying excitations are parametrized by the *tangent space* on this manifold [3,4]. Indeed, the tangent vectors around the MPS ground state have a natural interpretation as quasiparticles living on top of the strongly correlated background [5]. These states can then be used as variational ansatz states for the low-lying quasiparticle excitations [3]; they live in a specific momentum sector, which, in combination with the use of symmetries in the MPSs, allows us to target definite quantum numbers for the excited states above the ground state [6]. For isolated modes in the spectrum (see Fig. 1 for a generic example), it was proven that this local description of the excited-state wave function is essentially correct [7]. In recent years, this quasiparticle ansatz has been used to simulate the low-energy excitation spectrum of generic 1-D [8,9] and quasi 1-D [10] systems.

In this paper, we apply this formalism to simulate the low-energy features of a particular SU(3) Heisenberg chain. The numerical study of SU(N) spin chains has gained a new

impetus in the last years due to both theoretical and experimental progress. Forty years ago, Haldane made a prediction on the gapped or gapless nature of spin chains depending on which SU(2) representation is realized on each site in the lattice [12–14]. Recently, similar predictions have been made for generic SU(N) chains [15–17]. In addition, the Affleck-Kennedy-Lieb-Tasaki construction [18,19], which provided a strong motivation for Haldane’s prediction, has been extended to some SU(N) spin chains [20–24]. On the experimental side, cold atomic gasses have been used to create SU(N)-symmetric fermionic systems for values as large as $N = 10$ [25], realizing Luttinger liquids, Mott-insulating phases, and symmetry-protected topologically ordered (SPT) phases in the laboratory [26–28].

Concretely, we study the SU(3)-invariant spin [3 0 0] chain, as defined by Eq. (1), which is the “simplest” case for which a gapped spectrum has been predicted. In Ref. [29], finite-size MPS methods and intricate extrapolation techniques were used to show the presence of a small gap in this model in the [3 0 0] sector, implying a minimal gap $\Delta/J \in [0.017, 0.046]$, confirming the field-theory prediction. Here we use MPS tangent-space methods [4] to simulate the model directly in the thermodynamic limit. We determine the SPT phase of the model, extract reliable estimates for the correlation length and energy gap, and we compute the full dispersion relation. For the latter we have access to all symmetry sectors, in contrast to previous studies.

Ground state. In a tensor-network representation, global symmetries are realized by local symmetric tensors which obey “pulling-through” types of equations, where the action of an arbitrary group element $g \in \text{SU}(3)$ on a single leg is realized by a representation U_g , and can be pulled through to the action on the other legs via the representation v_g , as illustrated by Eq. (3). This results in a block structure of the tensors, labeled by the irreducible representations of SU(3) that live on their legs.

The Hamiltonian for the Heisenberg model is defined as

$$\mathcal{H} = 2J \sum_{\langle ij \rangle} \mathbf{T}_i \mathbf{T}_j = 2J \begin{array}{c} \downarrow \\ \boxed{\mathbf{T}_i} \rightarrow \boxed{\mathbf{T}_j} \\ \uparrow \end{array}, \quad (1)$$

*Lukas.Devos@uGent.be

TABLE I. Extrapolated correlation length and correlation function oscillation periods.

Charge	Correlation length	Oscillation period
[3 0 0]	66(1)	0
[3 3 0]	66(1)	0
[2 1 0]	116.5(8)	$\pm 2\pi/3$
[4 2 0]	85(3)	$\pm 2\pi/3$

of the energy variance of the variational ground states. This extrapolation yields $E_0/J = -2.1763984(9)$.

We also note that both the entanglement spectrum and the transfer matrix spectrum have degenerate values in conjugate representations.

Correlation length. Spin chains whose energy spectrum has a nonvanishing gap above the ground state are characterized by exponentially decaying correlation functions with a finite correlation length ξ , while gapless models give rise to power-law behavior. As such, a finite value of ξ is a strong indicator of a finite energy gap. The correlation length of an MPS with bond dimension D can be calculated as

$$\xi_D^{-1} = -\ln |\lambda_1|, \quad (4)$$

where λ_1 is the magnitude of the second largest eigenvalue of the MPS transfer matrix (normalized to have largest eigenvalue 1). Additionally, the corresponding complex phase determines the oscillatory behavior of the correlation function. We note that this will always lead to a finite result at finite D ; thus we need to extrapolate and show that ξ_∞ remains finite. Adapting the extrapolation procedure outlined in Ref. [34], ξ^{-1} scales with the logarithm of the ratio of the second and third largest eigenvalues of the transfer matrix spectrum as

$$\xi_D^{-1} = a\delta^b + \xi_\infty^{-1}, \quad \text{where } \delta = \ln \frac{|\lambda_1|}{|\lambda_2|}. \quad (5)$$

For our purposes, it is sufficient to set $b = 1$, as a linear fit yields excellent results.

Imposing the symmetry of the local tensors again allows us to target the eigenvalues of the transfer matrix for eigenvectors with definite quantum numbers, corresponding to elementary excitations carrying those charges [35]. As such we repeat the procedure outlined above separately for several quantum numbers. The distribution of the largest magnitude eigenvalues can be seen to have distinct phases, appearing in multiples of $2\pi/3$, and the spectrum is degenerate for conjugate charges (see Fig. 2).

The resulting extrapolations, which are depicted in Fig. 3, lead to the correlation lengths shown in Table I, where we note that the dominant correlation length is $\xi = 116.5(8)$ sites in the sector [2 1 0], with an oscillation period of $\pm 2\pi/3$.

Excitations. As outlined in the introduction, the low-lying elementary excitations can be characterized in terms of the tangent space of the ground-state manifold, which is translated into a variational ansatz commonly referred to as the quasipar-

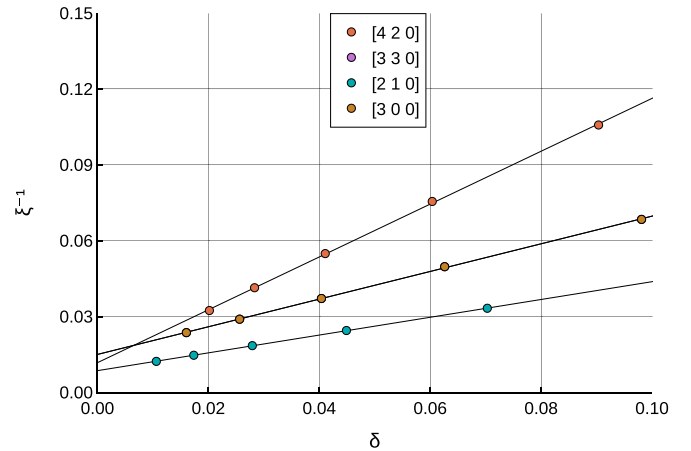


FIG. 3. Correlation length extrapolations for the ground state. The inverse correlation length ξ^{-1} is plotted against the refinement parameter δ , extrapolated to $\delta = 0$. The conjugate representations give equal results because of the degeneracy of the transfer matrix spectrum.

ticle ansatz [36],

$$|\Psi_p^\alpha(B)\rangle = \sum_n e^{ipn} \dots \rightarrow \begin{array}{c} \alpha \\ \downarrow \\ \boxed{A} \rightarrow \boxed{B} \rightarrow \boxed{A} \rightarrow \boxed{A} \rightarrow \dots \\ \uparrow \quad \uparrow \quad \uparrow \quad \uparrow \end{array} \dots \quad (6)$$

Here, α denotes the SU(3) charge of the excited state and n labels the location where we have changed a ground-state MPS tensor into a new excitation tensor B ; the latter contains all variational parameters and can be readily optimized by solving an eigenvalue problem [4]. As such this ansatz represents states with definite momentum, and through the use of symmetries can be used to effectively target isolated bands in the spectrum with definite quantum numbers [6]. The ‘‘Haldane gaps’’ are expected to be found in sectors that appear in the tensor product of two adjoint representations [29]:

$$[2 1 0] \otimes [2 1 0] \rightarrow 2 \cdot [2 1 0] \oplus [3 0 0] \oplus [3 3 0] \oplus [4 2 0]. \quad (7)$$

With a truncation error of the ground state of 10^{-4} , we compute the full dispersion relation for the elementary excitations, shown in Fig. 4, which shows that the smallest Haldane gap is situated at momentum $p = \pm 2\pi/3$ within the [2 1 0] sector. This is consistent with the results of the correlation lengths, where the maximum value is found in that same sector, with the same phase.

Further decreasing the truncation error, we are able to obtain results up to an effective bond dimension of $D = 63\,766$, and we compute that the smallest gap of the system is $\Delta/J = 0.0263$ in the aforementioned sector. In the other sectors we find values that are at least twice this value, indicating that these correspond to two-particle states.

In Ref. [29] an excitation gap of 0.040(3) was found in the [3 0 0] sector. Based on the above value and our findings that the lowest excitation in this sector is a two-particle state, we estimate a gap in this sector of $2\Delta/J \approx 0.052$, slightly outside the error bounds of the previous work. This could point to a two-particle bound state appearing in this sector, which would lead to a smaller energy gap. For these kinds of states, the

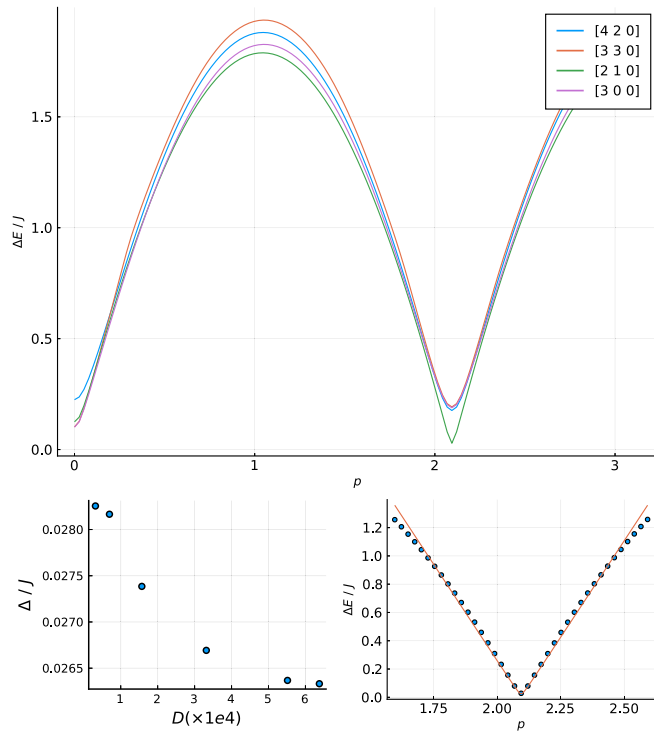


FIG. 4. Top: Dispersion relation of the elementary excitations of different charges. Bottom left: Value of the smallest Haldane gap, in the sector $[2\ 1\ 0]$, for different bond dimensions D . Bottom right: Calculated dispersion relation around the minimum, along with the theoretical prediction for Lorentz-invariant gapped systems from Eq. (8).

quasiparticle ansatz is less well suited, which could explain the difference in results. We have attempted to improve on our results by using a string ansatz for broader excitations, as

described in Ref. [37], but a systematic growing of the string ansatz proved computationally unfeasible for this model.

As a consistency check, we verify the prediction that the low-energy behavior in this system can be described by an effective field theory, yielding a dispersion relation of the form

$$E(p) = \sqrt{\Delta^2 + v^2(p - p_{\min})^2}, \quad (8)$$

where v denotes the characteristic velocity in the system. Exploiting Lorentz invariance, we can relate this velocity to the correlation length and the gap as $v = \xi \Delta$ [35,38]. This prediction can then be compared to the obtained dispersion relation around the minimum, and supplies proof of the validity of our results, as it ties together the correlation length and excited states, which have been calculated independently (Fig. 4).

Conclusions. In this work we have confirmed the theoretical predictions of a Haldane gap in the SU(3) spin $[3\ 0\ 0]$ chain using tensor-network methods directly in the thermodynamic limit, where the local tensors obey the symmetry of the system. In agreement with the numerical results using finite-size scaling methods presented in Ref. [29], we find that the ground state has an energy density of $E_0/J = -2.1763984(9)$ and we argue that it belongs to the trivial SPT phase. The ground state of this system is shown to have a maximal correlation length of $\xi = 116.5(8)$ in the sector $[2\ 1\ 0]$ with a phase of $\pm 2\pi/3$. The dispersion relation of the elementary excitations is shown to reach its minimum value of $\Delta/J = 0.0263$ in the same sector at momentum $p = 2\pi/3$.

Acknowledgments. We would like to thank B. Vanhecke, S. Gozel, and F. Mila for inspiring discussions. This work has received funding from the European Research Council (ERC) under the European Unions Horizon 2020 research and innovation programme (Grant Agreement No 647905 (QUTE)), and from Research Foundation Flanders (FWO) via Grant FWO20/PDS/115.

- [1] J. I. Cirac, D. Pérez-García, N. Schuch, and F. Verstraete, Matrix product states and projected entangled pair states: Concepts, symmetries, theorems, *Rev. Mod. Phys.* **93**, 045003 (2021).
- [2] I. P. McCulloch and M. Gulácsi, The non-Abelian density matrix renormalization group algorithm, *Europhys. Lett.* **57**, 852 (2002).
- [3] J. Haegeman, T. J. Osborne, and F. Verstraete, Post-matrix product state methods: To tangent space and beyond, *Phys. Rev. B* **88**, 075133 (2013).
- [4] L. Vanderstraeten, J. Haegeman, and F. Verstraete, Tangent-space methods for uniform matrix product states, *SciPost Phys. Lect. Notes* **7** (2019).
- [5] L. Vanderstraeten, F. Verstraete, and J. Haegeman, Scattering particles in quantum spin chains, *Phys. Rev. B* **92**, 125136 (2015).
- [6] V. Zauner-Stauber, L. Vanderstraeten, J. Haegeman, I. P. McCulloch, and F. Verstraete, Topological nature of spinons and holons: Elementary excitations from matrix product states with conserved symmetries, *Phys. Rev. B* **97**, 235155 (2018).
- [7] J. Haegeman, S. Michalakis, B. Nachtergaele, T. J. Osborne, N. Schuch, and F. Verstraete, Elementary Excitations in Gapped Quantum Spin Systems, *Phys. Rev. Lett.* **111**, 080401 (2013).
- [8] A. K. Bera, B. Lake, F. H. L. Essler, L. Vanderstraeten, C. Hubig, U. Schollwöck, A. T. M. N. Islam, A. Schneidewind, and D. L. Quintero-Castro, Spinon confinement in a quasi-one-dimensional anisotropic Heisenberg magnet, *Phys. Rev. B* **96**, 054423 (2017).
- [9] L. Vanderstraeten, M. Van Damme, H. P. Büchler, and F. Verstraete, Quasiparticles in Quantum Spin Chains with Long-Range Interactions, *Phys. Rev. Lett.* **121**, 090603 (2018).
- [10] M. Van Damme, R. Vanhove, J. Haegeman, F. Verstraete, and L. Vanderstraeten, Efficient matrix product state methods for extracting spectral information on rings and cylinders, *Phys. Rev. B* **104**, 115142 (2021).
- [11] L. Vanderstraeten, *Tensor Network States and Effective Particles for Low-Dimensional Quantum Spin Systems*, Springer Theses (Springer International Publishing, Cham, 2017).
- [12] F. Haldane, Continuum dynamics of the 1-D Heisenberg antiferromagnet: Identification with the O(3) nonlinear sigma model, *Phys. Lett. A* **93**, 464 (1983).
- [13] F. D. M. Haldane, Nonlinear Field Theory of Large-Spin Heisenberg Antiferromagnets: Semiclassically Quantized Solitons of the One-Dimensional Easy-Axis Néel State, *Phys. Rev. Lett.* **50**, 1153 (1983).

- [14] I. Affleck, Quantum spin chains and the Haldane gap, *J. Phys.: Condens. Matter* **1**, 3047 (1989).
- [15] M. Lajkó, K. Wamer, F. Mila, and I. Affleck, Generalization of the Haldane conjecture to SU(3) chains, *Nucl. Phys. B* **924**, 508 (2017).
- [16] K. Wamer, M. Lajkó, F. Mila, and I. Affleck, Generalization of the Haldane conjecture to SU(n) chains, *Nucl. Phys. B* **952**, 114932 (2020).
- [17] I. Affleck, D. Bykov, and K. Wamer, Flag manifold sigma models: Spin chains and integrable theories, *Phys. Rep.* **953**, 1 (2022).
- [18] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Rigorous Results on Valence-Bond Ground States in Antiferromagnets, *Phys. Rev. Lett.* **59**, 799 (1987).
- [19] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Valence bond ground states in isotropic quantum antiferromagnets, *Commun. Math. Phys.* **115**, 477 (1988).
- [20] M. Greiter, S. Rachel, and D. Schuricht, Exact results for SU(3) spin chains: Trimer states, valence bond solids, and their parent Hamiltonians, *Phys. Rev. B* **75**, 060401(R) (2007).
- [21] S. Rachel, R. Thomale, M. Führinger, P. Schmitteckert, and M. Greiter, Spinon confinement and the Haldane gap in SU(n) spin chains, *Phys. Rev. B* **80**, 180420(R) (2009).
- [22] T. Morimoto, H. Ueda, T. Momoi, and A. Furusaki, \mathbb{Z}_3 symmetry-protected topological phases in the SU(3) AKLT model, *Phys. Rev. B* **90**, 235111 (2014).
- [23] K. Wamer, F. H. Kim, M. Lajkó, F. Mila, and I. Affleck, Self-conjugate representation SU(3) chains, *Phys. Rev. B* **100**, 115114 (2019).
- [24] S. Gozel, D. Poilblanc, I. Affleck, and F. Mila, Novel families of SU(n) AKLT states with arbitrary self-conjugate edge states, *Nucl. Phys. B* **945**, 114663 (2019).
- [25] A. V. Gorshkov, M. Hermele, V. Gurarie, C. Xu, P. S. Julienne, J. Ye, P. Zoller, E. Demler, M. D. Lukin, and A. M. Rey, Two-orbital SU(n) magnetism with ultracold alkaline-earth atoms, *Nat. Phys.* **6**, 289 (2010).
- [26] S. Capponi, P. Lecheminant, and K. Totsuka, Phases of one-dimensional SU(n) cold atomic fermi gases from molecular Luttinger liquids to topological phases, *Ann. Phys.* **367**, 50 (2016).
- [27] C. Hofrichter, L. Riegger, F. Scazza, M. Höfer, D. R. Fernandes, I. Bloch, and S. Fölling, Direct probing of the Mott crossover in the SU(n) Fermi-Hubbard model, *Phys. Rev. X* **6**, 021030 (2016).
- [28] S. Capponi, P. Fromholz, P. Lecheminant, and K. Totsuka, Symmetry-protected topological phases in a two-leg SU(n) spin ladder with unequal spins, *Phys. Rev. B* **101**, 195121 (2020).
- [29] S. Gozel, P. Nataf, and F. Mila, Haldane Gap of the Three-Box Symmetric SU(3) Chain, *Phys. Rev. Lett.* **125**, 057202 (2020).
- [30] N. D. Mermin and H. Wagner, Absence of Ferromagnetism or Antiferromagnetism in One- or Two-Dimensional Isotropic Heisenberg Models, *Phys. Rev. Lett.* **17**, 1133 (1966).
- [31] D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac, Matrix Product State Representations, *Quantum Inf. Comput.* **7**, 401 (2007).
- [32] K. Duivendoorn and T. Quella, Topological phases of spin chains, *Phys. Rev. B* **87**, 125145 (2013).
- [33] M. Hauru, M. V. Damme, and J. Haegeman, Riemannian optimization of isometric tensor networks, *SciPost Phys.* **10**, 040 (2021).
- [34] M. M. Rams, P. Czarnik, and L. Cincio, Precise Extrapolation of the Correlation Function Asymptotics in Uniform Tensor Network States with Application to the Bose-Hubbard and XXZ Models, *Phys. Rev. X* **8**, 041033 (2018).
- [35] V. Zauner, D. Draxler, L. Vanderstraeten, M. Degroote, J. Haegeman, M. M. Rams, V. Stojevic, N. Schuch, and F. Verstraete, Transfer matrices and excitations with matrix product states, *New J. Phys.* **17**, 053002 (2015).
- [36] J. Haegeman, B. Pirvu, D. J. Weir, J. I. Cirac, T. J. Osborne, H. Verschelde, and F. Verstraete, Variational matrix product ansatz for dispersion relations, *Phys. Rev. B* **85**, 100408(R) (2012).
- [37] L. Vanderstraeten, E. Wybo, N. Chepiga, F. Verstraete, and F. Mila, Spinon confinement and deconfinement in spin-1 chains, *Phys. Rev. B* **101**, 115138 (2020).
- [38] E. S. Sørensen and I. Affleck, Equal-time correlations in Haldane-gap antiferromagnets, *Phys. Rev. B* **49**, 15771 (1994).