Existence of a Spectral Gap in the Affleck-Kennedy-Lieb-Tasaki Model on the Hexagonal Lattice

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The $S = 1$ Affleck-Kennedy-Lieb-Tasaki (AKLT) quantum spin chain was the first rigorous example of an isotropic spin system in the Haldane phase. The conjecture that the $S = 3/2$ AKLT model on the hexagonal lattice is also in a gapped phase has remained open, despite being a fundamental problem of ongoing relevance to condensed-matter physics and quantum information theory. Here we confirm this conjecture by demonstrating the size-independent lower bound $\Delta > 0.006$ on the spectral gap of the hexagonal model with periodic boundary conditions in the thermodynamic limit. Our approach consists of two steps combining mathematical physics and high-precision computational physics. We first prove a mathematical finite-size criterion which gives an analytical, size-independent bound on the spectral gap if the gap of a particular cut-out subsystem of 36 spins exceeds a certain threshold value. Then we verify the finite-size criterion numerically by performing state-of-the-art DMRG calculations on the subsystem.

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The manifestations of antiferromagnetism in quantum spin systems depend sensitively on the underlying geometry and spin number. A subtle and famous instance of this connection was proposed by Haldane, who predicted in 1983 that the Heisenberg spin chain has a spectral gap above the ground state whenever the spin S per site is an integer [1,2]. Motivated by his considerations, Affleck, Kennedy, Lieb, and Tasaki (AKLT) introduced a new family of quantum spin systems in 1987 and proved that their one-dimensional $S = 1$ version is indeed in Haldane's eponymous quantum phase [3,4]. The influence of the seminal AKLT papers continues to this day: the valence-bond solid (VBS) aspect of the AKLT construction directly inspired the development of concepts that are by now central tenets of modern quantum physics, such as matrix product states, projected entangled pair states (PEPS), and more generally tensor network states [5–11]. Moreover, the nonlocal string order exhibited by the AKLT chain [12–14] has been developed much further into the more general concept of symmetry-protected topological order [15–18]. Finally, the AKLT ground states on some two-dimensional lattices, including the $S = 3/2$ model on the hexagonal lattice, provide rare instances of a universal resource state for measurement-based quantum computation (MBQC) [19–22].

One of the main accomplishments of the original AKLT works [3,4] is the rigorous derivation of a spectral gap above the AKLT ground state in one dimension. AKLT also investigated the $S = 3/2$ model on the hexagonal lattice and were able to demonstrate the exponential decay of the spin-spin correlations for the exact VBS ground state with periodic boundary conditions, and on the basis of this fact they conjectured that the hexagonal model also exhibits a spectral gap (see also [23]). We recall that a spectral gap implies the decay of ground state correlations, but not vice versa [24–28]. Evidence pointing to a spectral gap has been mounting [23,29–34], but, despite the paradigmatic role played by the hexagonal AKLT model, the long-standing fundamental problem to show that its spectrum is gapped has remained unresolved. The presence of a gap would have broader consequences, e.g., in supporting the widespread heuristic that PEPS arise from gapped Hamiltonians, see the recent review [35], and for the complexity and stability of the corresponding universal resource states for MBQC [19–22]. One of the main reasons why the AKLT conjecture has remained unresolved is that, while the ground states of the hexagonal AKLT model can be written down exactly, only very little is known about its excited states. More generally, the existing mathematical techniques for deriving spectral gaps in quantum spin systems of dimensions ≥ 2 are quite limited. Few examples where a spectral gap is known to exist include the product vacua with boundary states models [36–38] and, since recently, decorated variants of the AKLT models [29,34].

In this Letter, we confirm the AKLT conjecture by demonstrating a lower bound, $\Delta > 0.006$, on the spectral gap of the hexagonal model. More precisely, we consider a sequence of AKLT models where the hexagonal lattice is

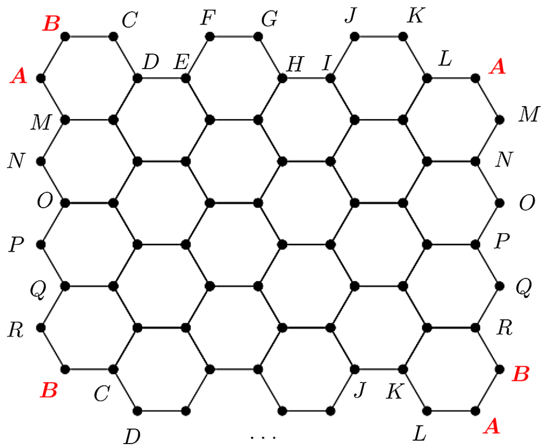

FIG. 1. The patch Λ_{m_1,m_2} with parameters $m_1 = 6$ and $m_2 = 4$. (m_1 and m_2 are the width and height of Λ_{m_1,m_2} in units of hexagonal cells, respectively.) Periodic boundary conditions are imposed by identifying the boundary vertices which are assigned the same letter. Note that the letters A and B appear three times in total.

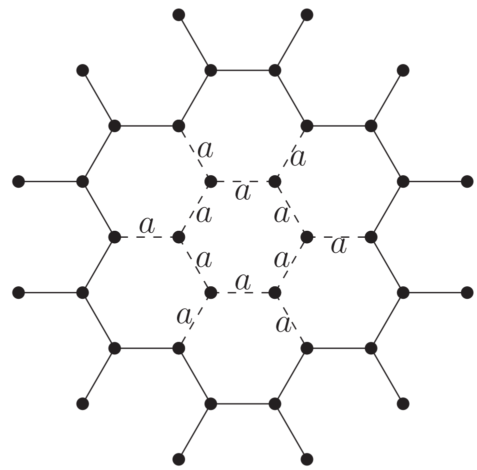

FIG. 2. The fixed-size patch $\mathcal{F}$ whose spectral gap we compute numerically. It is equipped with open boundary conditions, in contrast to $\Lambda_{m_1,m2}$. The weights w_e in Eq. (5) are assigned as follows: dashed edges are weighted by $w_e = a \geq 1$ as indicated, while all other edges are unweighted (i.e., $w_e = 1$).

wrapped on an $m_1 \times m_2$ torus and show that their spectral gaps are all bounded from below by 0.006 for arbitrarily large system-size parameters m_1 and m_2; see Fig. 1 for the definition of the periodic boundary conditions on a 6×4 torus. Methodologically, our approach consists of two steps. Step 1 comes from mathematical physics and step 2 is based on state-of-the-art computational physics. In step 1, we prove a mathematical finite-size criterion which is tailor-made for the problem at hand. In a nutshell, the finite-size criterion says that if the spectral gap of the 36-site cluster displayed in Fig. 2 exceeds an explicit numerical threshold, then the AKLT model has a spectral gap for all system sizes m_1, m_2. To prove the criterion, we follow the combinatorial approach pioneered by Knabe [32], strengthened by using interaction weights as in Refs. [39,40]. In step 2, we combine the rigorous analytical insight from step 1 by numerically verifying the finite-size criterion via a high-precision density-matrix renormalization group (DMRG) calculation (see also Ref. [33] for a one-dimensional analog studied with Lanczos diagonalization). We present tests of the correctness of our implementation of the well-established DMRG method in the Supplemental Material [41]. Since it is not possible to establish a rigorous precise estimate of any remaining convergence errors, our result may not be considered a rigorous mathematical proof as a matter of principle. However, in practice, the computed gap exceeds the threshold by such a wide margin that it can be regarded as a conclusive demonstration.

One challenge in the numerical part of the argument is that the relevant open-boundary system (Fig. 2), whose gap we need to compute, has a massive ground state degeneracy due to the 12 "dangling" effective boundary $S = 1$ spins which arise in the AKLT construction when only one out of the three nearest-neighbor couplings is active. This results in a 3^{12}-fold ground state degeneracy. To reduce the number of levels which have to be converged, we use a variant of DMRG with full SU(2) symmetry and calculate the ground state and several excited states over all sectors of total spin. Crucially, in the process of successively orthogonalizing the calculations to previously converged states, we have used the AKLT construction to exactly project out the full degenerate subspace. Without this preliminary step, which we discuss further below and describe in more detail in [41], it would currently not be possible to converge the excited states in all total spin (J) sectors and conclusively identify the smallest gap of the system. We find that the lowest gap originates from the $J = 13$ sector and that it exceeds the analytical gap threshold well beyond any conceivable remaining DMRG truncation errors.

Our main result is a size-independent lower bound on the spectral gap of the AKLT Hamiltonian on finite patches of the hexagonal lattice $\mathbb{H}$ with periodic boundary conditions, which we call Λ_{m_1,m_2}. The key point is that the lower bound on the gap is independent of the size parameters m_1 and m_2 of these patches and thus extends to the thermodynamic limit.

For m_1 and m_2 two positive integers, the finite patch Λ_{m_1,m_2} is defined by wrapping the hexagonal lattice on an $m_1 \times m_2$ torus. We invite the reader to view Fig. 1 for a specific example of how the periodic boundary conditions are realized. Since the hexagonal lattice has valence 3, one takes each site to host an $S = 3/2$ spin and considers the Hilbert space

$$\mathcal{H}_{m_1,m_2} = \bigotimes_{j \in \Lambda_{m_1,m_2}} \mathbb{C}^4. \tag{1}$$

On $\mathcal{H}_{m_1,m_2}$, the AKLT Hamiltonian is defined by

$$H^{\mathrm{AKLT}}_{m_1,m_2} = \sum_{\substack{j,k\in\Lambda_{m_1,m_2}: \\ j\sim k}} P^{(3)}_{j,k}, \tag{2}$$

where $P^{(3)}_{j,k}$ denotes the projection onto total spin 3 across the bond connecting vertices j and k. By convention, the neighboring relation $\sim$ includes the periodic boundary conditions inherent to Λ_{m_1,m_2}.

As a sum of projections, the Hamiltonian $H^{\mathrm{AKLT}}_{m_1,m_2}$ is automatically a positive semidefinite operator. The valence-bond construction of AKLT [3,4] yields a ground state which is a nonzero element of $\ker H^{\mathrm{AKLT}}_{m_1,m_2}$, making this Hamiltonian frustration-free. Its spectral gap $\gamma^{\mathrm{AKLT}}_{m_1,m_2}$ is the smallest strictly positive eigenvalue, that is,

$$\gamma^{\mathrm{AKLT}}_{m_1,m_2} = \inf\ \mathrm{spec}(H^{\mathrm{AKLT}}_{m_1,m_2})\backslash\{0\}. \tag{3}$$

We can now state our main result, which provides a lower bound on the spectral gap $\gamma^{\mathrm{AKLT}}_{m_1,m_2}$ that is independent of the system size parameters m_1 and m_2.

Main result.—Let m_1, $m_2 \geq 12$. Then, it holds that

$$\gamma^{\mathrm{AKLT}}_{m_1,m_2} \geq 0.00646. \tag{4}$$

A few remarks about this result are in order: (i) We work with periodic boundary conditions for convenience and the results imply a bulk gap in the thermodynamic limit under these boundary conditions. Moreover, it was proved in Ref. [23] that the infinite-volume ground state is unique. (ii) This main result is not a rigorous mathematical theorem because it relies on numerical input from the DMRG algorithm. While the DMRG algorithm becomes exact for large bond dimension and the computations are sufficiently precise and well-tested to firmly establish (4) beyond doubt, we do not claim to have a mathematical proof of sufficiently tight error estimates. (iii) From previous numerical investigations, see e.g., [31], it is believed that the true spectral gap of the hexagonal model is ≈0.1, but the results depend on extrapolations in the system size that assume an asymptotic scaling regime has been reached.

The finite-size criterion.—We now discuss the main mathematical tool, which is a finite-size criterion for deriving a spectral gap. In a nutshell, it says that if the spectral gap of the system $\mathcal{F}$ depicted in Fig. 2 exceeds some explicit numerical threshold, then we also obtain a lower bound on the spectral gap $\gamma^{\mathrm{AKLT}}_{m_1,m_2}$ that is independent of the size parameters m_1, m_2 as desired. The intuition behind the finite-size criterion is that, thanks to the frustration-freeness of the AKLT Hamiltonian, the problem of finding the lowest possible excitation energy (gap) is a local question. Hence, it is enough to know that local patches of the whole system are "sufficiently gapped" in a way that the criterion makes precise. For related finite-size criteria that ours here is inspired by, see Refs. [32,33,39,40,44–46]. The idea behind the finite-size criterion is to construct $H^{\mathrm{AKLT}}_{m_1,m_2}$ from translated copies of an appropriate finite-size Hamiltonian, which we call $H_{\mathcal{F}}$. For the criterion to work in practice, the patch has to be sufficiently large because the criterion depends on the cluster size and shape, and even if there is a gap in the thermodynamic limit the finite-size criterion may not be satisfied on a small cluster. Our criterion is based on the following Hamiltonian $H_{\mathcal{F}}$ defined on the 36-site patch $\mathcal{F}$ shown in Fig. 2, with open boundary conditions.

The patch lives on the local Hilbert space $\mathcal{H}_{\mathcal{F}} = \bigotimes_{j\in\mathcal{F}} \mathbb{C}^4$. We write $\mathcal{E}_{\mathcal{F}}$ for the set of edges $e = (j,k)$ with $j,k\in\mathcal{F}$, i.e., we equip $\mathcal{F}$ with open boundary conditions (in contrast to Λ_{m_1,m_2}). Let $a \geq 1$ be a parameter. We define the finite-size Hamiltonian by

$$H_{\mathcal{F}} = \sum_{e\in\mathcal{E}_{\mathcal{F}}} w_e P^{(3)}_e, \tag{5}$$

where $P^{(3)}_e$ is the projection onto total spin 3 for the pair of vertices j, k that form the end points of the edge e. The weights w_e are defined as follows:

$$w_e = \begin{cases} a, & \text{if the edge } e \text{ is labeled by } a \text{ in Fig. 2}, \\ 1, & \text{otherwise.} \end{cases} \tag{6}$$

The valence-bond ground state construction of AKLT [3,4] still applies to $H_{\mathcal{F}}$ and proves that it is frustration-free. Its spectral gap is $\gamma_{\mathcal{F}}(a) = \inf\ \mathrm{spec}(H_{\mathcal{F}})\backslash\{0\}$.

Theorem.—(The finite-size criterion) Let m_1, $m_2 \geq 12$ be integers and let $a \geq 1$. Then we have the gap bound

$$\gamma^{\mathrm{AKLT}}_{m_1,m_2} \geq \frac{10+4a}{3a^2+2a+7}\left(\gamma_{\mathcal{F}}(a) - \frac{a^2-2a+3}{10+4a}\right). \tag{7}$$

The general way of applying this theorem is as follows: if for some parameter value $a \geq 1$, one finds that the finite-size gap $\gamma_{\mathcal{F}}(a)$ exceeds the threshold $\{[a^2-2a+3]/[10+4a]\}$, then (7) provides a lower bound on $\gamma^{\mathrm{AKLT}}_{m_1,m_2}$ that is independent of m_1, m_2 (subject to m_1, $m_2 \geq 12$ of course). The proof of the finite-size criterion is deferred to the Supplemental Material [41].

We now follow this procedure to show the spectral gap bound (4). As explained in detail further below, by a numerical DMRG calculation we obtain the following explicit lower bound on the finite-size gap $\gamma_{\mathcal{F}}(a)$ with $a = 1.4$,

$$\gamma_{\mathcal{F}}(1.4) > 0.145. \tag{8}$$

This value exceeds the gap threshold $\{[a^2-2a+3]/[10+4a]\} \approx 0.138$ and thus verifies the finite-size criterion. The exact numerical bound on $\gamma^{\mathrm{AKLT}}_{m_1,m_2}$ can be computed by noting that $\{[a^2-2a+3]/[10+4a]\} < 0.1385$ and $\{[10+4a]/[3a^2+2a+7]\} > 0.994$, which together with (8) can be applied to (7) to show

$$\gamma_{m_1,m_2}^{\mathrm{AKLT}} \geq 0.994\left(0.145 - \frac{a^2 - 2a + 3}{10 + 4a}\right) \geq 0.00646.$$

This establishes the main result, the spectral gap bound (4).

DMRG calculations.—We next discuss our implementation of the DMRG algorithm and results for the gap of the open boundary 36-site cluster $\mathcal{F}$ shown in Fig. 2. Additional details, including detailed convergence tests, are relegated to the Supplemental Material [41].

The ground states of the cluster $\mathcal{F}$ can be understood as follows: each physical $S = 3/2$ spin is made out of three auxiliary $S = 1/2$ spins, each of which will pair with another auxiliary $S = 1/2$ from a neighboring site, forming a singlet and dropping out. This construction ensures that any pair of neighboring physical $S = 3/2$ spins can never fuse into a total spin-3 state, and the AKLT ground state condition is therefore fulfilled. However, on the open boundary sites, two auxiliary $S = 1/2$ spins per site are left over, and these are only allowed to fuse into an $S = 1$ state due to the symmetric constraint. Therefore, there are 12 boundary $S = 1$ degrees of freedom that can form any total spin $0 \leq J \leq 12$, spanning a degenerate ground state manifold of dimension 3^{12}. The lowest excitation above the ground states, which can be interpreted as swapping a bulk singlet with a triplet that further fuses with the boundary total angular momentum, can in principle form any angular momentum $0 \leq J \leq 13$. In order to conclusively determine the smallest nonzero gap among all possible total-spin sectors, one has to find the lowest excitation in every sector $J \in \{0, 1, \ldots, 13\}$. For even higher J sectors, the lowest excitation requires breaking more than one singlet and therefore costs significantly more energy. For completeness, we also computed the gaps in all other sectors where $J > 13$.

An SU(2) symmetric DMRG algorithm is used to automatically generate the degenerate ground state manifold in all sectors of total spin $J \in \{0, 1, \ldots, 12\}$ and compute the lowest excited state therein by projecting out the complete ground state manifold exactly. Two of us previously used such an orthogonalization procedure for successively converging excited states of a different model [47], but here the simple form of the degenerate AKLT ground-state manifold enables us to eliminate it directly. Let L denote the maximum-spin multiplet formed by the unpaired boundary $S = 1$ spins in the ground state manifold. For the 36-site cluster in Fig. 2, we have $L = 12$. The ground state manifold contains the following number of states with total spin J: 4213 ($J = 0$), 11298 ($J = 1$), 15026 ($J = 2$), 14938 ($J = 3$), 12078 ($J = 4$), 8162 ($J = 5$), 4642 ($J = 6$), 2211 ($J = 7$), 869 ($J = 8$), 274 ($J = 9$), 66 ($J = 10$), 11 ($J = 11$), and 1 ($J = 12$). Accordingly, the lowest excitation for each J is computed by projecting out that many degenerate ground states, which make the excited state computationally challenging. For sectors with total spin $J > L$, which are devoid of ground states, the lowest excitation can be computed more straightforwardly without projecting out any states. Upon computing the lowest excitation gaps for all $J \leq L + 1$ sectors of the 36-site cluster at $a = 1.4$, we found that the smallest one originates from the $J = L + 1 = 13$ sector; in Fig. 3, we show results for $J = 11$, 12, and 13. The $J = 13$ gap obtained by extrapolating to vanishing DMRG discarded weight ϵ is $\Delta(13) = 0.14599$. The lowest gaps within all other J sectors remain well above $\Delta(13)$ and there is no doubt (but also no rigorous proof) that the smallest gap exceeds the relevant threshold 0.138. In the Supplemental Material [41], the convergence of the gaps with ϵ is illustrated in Fig. S8 for all $0 \leq J \leq 16$.

Conclusions.—We have verified the AKLT conjecture from 1987 that the hexagonal AKLT model has a spectral gap above the ground state. This confirms that the original Hamiltonian with a PEPS ground state is gapped, a question emphasized, e.g., in the recent collection of open problems [35]. More generally, the existence of a spectral gap is an immensely consequential property in any quantum many-body system. First, a spectral gap implies the exponential decay of ground state correlations (but not vice versa) [24–28] and is expected to imply other complexity bounds on the ground state such as the area law for the entanglement entropy. Second, the existence of a spectral gap is a crucial assumption in the classification of topological quantum phases and the many-body adiabatic theorem [48–53]. We also mention that the existence of a spectral gap is perturbatively stable [50,54–57]. While our result confirms the long-standing AKLT conjecture, we hope that it inspires future work on the spectral gap of this timeless model. In particular, we believe that it would be useful to have a purely analytical derivation of a spectral gap, because the argument here relies on numerical computations without suitable rigorous error bounds and because a purely analytical argument will presumably be accompanied by an improved understanding of the model's low-energy excitations.

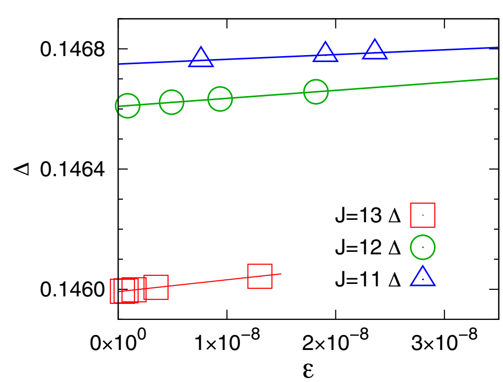

FIG. 3. Gaps in the sectors $J = 11$, 12, and 13 graphed versus the DMRG discarded weight ϵ. The discarded weight decreases with increasing number of SU(2) states used, and we used up to $D = 2400$ for $J = 11$, 12, and $D = 1200$ for $J = 13$. Line fits are used for $\epsilon \to 0$ extrapolation.

Let us briefly discuss the wider scope of the approach we use here. The mathematical physics step is the derivation of a finite-size criterion in the general spirit of Knabe's combinatorial criteria [32] with weights as in Refs. [39,40]. The computational physics step consists of verifying the finite-size criterion by a high-precision DMRG implementation. Our approach of numerically verifying a combinatorial finite-size criterion is in principle applicable to any frustration-free spin system. Concerning the AKLT models, for example, the square lattice is a natural next candidate to consider [31,34,58], as well as SU(n)-symmetric variants [59–61]. The cubic lattice is another interesting case which also displays novel phase-transition phenomena [62].

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Note added.—After our preprint appeared, Pomata and Wei [63] demonstrated the existence of a spectral gap in AKLT models on various two-dimensional degree-3 lattices including the hexagonal lattice. Their argument is different, but it also combines analytics (inspired by [29,34]) with numerics.

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[41] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.124.177204 for details of the proof of the finite-size criterion, implementation of the SU(2) DMRG algorithm for the AKLT model, and convergence properties of the gaps, which includes Refs. [42,43].

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Correction: During the production process, an incorrect connector label was inserted in Ref. [63] and has been fixed.