Title: Spectral gaps without frustration

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Abstract: In quantum spin systems, the existence of a spectral gap above the ground state has strong implications for the low-energy physics. We survey recent results establishing spectral gaps in various frustration-free spin systems by verifying finite-size criteria. The talk is based on collaborations with Abdul-Rahman, Lucia, Mozgunov, Nachtergaele, Sandvik, Yang, Young, and Wang.

Spectral gaps without frustration

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based on various joint works with:
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Quantum spin systems

Quantum spin systems are many-body models defined on a graph.

Hilbert space: Let Λ_N be a finite subset of an infinite lattice Λ (e.g., a box of sidelength N in $\mathbb{Z}^D$). We place a qudit, equivalently a spin $S = \frac{d-1}{2}$, at each site so the total Hilbert space is

$$\mathcal{H}_N = \bigotimes_{j \in \Lambda_N} \mathbb{C}^d.$$

Hamiltonian: Fix a local interaction, that is, a Hermitian operator $h : \mathbb{C}^d \otimes \mathbb{C}^d \to \mathbb{C}^d \otimes \mathbb{C}^d$, and embed it into the operators on $\mathcal{H}_N$ by defining

$$h_{i,j} = h \otimes \mathrm{id}_{\Lambda_N \setminus \{i,j\}}, \qquad \forall i \sim j \text{ in } \Lambda_N.$$

The Hamiltonian H_N is the sum of local interactions

$$\boxed{H_N = \sum_{\substack{i,j \in \Lambda_N: \\ i \sim j}} h_{i,j}}$$

The spectral gap and why we care

Spectrum: $\mathrm{spec}\, H_N = \{E_0(N) < E_1(N) < E_2(N) < \ldots\}$
(This is defined with possible degeneracy.)

Spectral gap: $\boxed{\gamma_N = E_1(N) - E_0(N) > 0}$

Remark: There are many gaps in the spectrum. γ_N is the one most relevant for condensed-matter (low-energy) physics.

Basic dichotomy in the thermodynamic limit $N \to \infty$:

(1) *Gapped.* $\limsup \gamma_N = c > 0$.

(2) *Gapless.* $\limsup \gamma_N = 0$.

Importance of the spectral gap: Ground states of gapped Hamiltonians satisfy strong complexity bounds especially in 1D (exponential decay of correlations; bounded entanglement entropy; approximable in polynomial time)
Also: Closing of the gap as a system parameter is varied indicates a quantum phase transition.

The frustration-free assumption

Given that it is so consequential, it is unsurprising that showing the existence of a spectral gap is difficult in general.

Conjecture: (Haldane 1983) The antiferromagnetic Heisenberg chain is gapped for any integer spin S. — *Completely open!*

Simplifying assumption: H_N is frustration-free (FF), i.e.,

$$h \geq 0 \text{ and } \boxed{\ker H_N \neq \{0\}}.$$

So $E_0(N) = 0$ for FF Hamiltonians.

Why does this help? For FF Hamiltonians the energy minimization problem is local. Excitations are sum of local energy costs $\langle \psi, h_{i,j}\psi \rangle \geq 0$ with no possible cancellations.

Remark: Upper bounds on γ_N obtainable from variational principle

$$\gamma_N = \min_{\psi \perp g.s.} \langle \psi, H_N \psi \rangle.$$

Two examples of frustration-free spin systems

(1) Heisenberg ferromagnet

- Local interaction

$$h_{i,j} = S^2 \mathrm{Id} - \vec{S}_i \cdot \vec{S}_j$$

- Gapless with gap closing like N^{-2} as $N \to \infty$ (spin wave excitations with quadratic dispersion).

(2) AKLT (Affleck-Kennedy-Lieb-Tasaki) models

- On a degree-z graph, place a spin-$z/2$ at each vertex and set

$$h_{i,j} = P_{\text{total spin(i,j)}=z}$$

- AKLT models are isotropic antiferromagnets with exact VBS ground states (MPS in 1D; PEPS in 2D)
- Rigorously proved to be gapped in 1D (AKLT 1987)
- **AKLT Conjecture (1987):** The AKLT model on the hexagonal lattice is gapped.

A method: Finite-size criteria

Methods for establishing spectral gaps in FF systems:

- Finite-size criteria (Knabe; Fannes-Nachtergaele-Werner)
- Martingale method (Lu-Yau; Nachtergaele and coworkers)
- Markov chain methods for stoquastic Hamiltonians (Bravyi, Terhal, and others)

Starting point of finite-size criteria: By the spectral theorem, for a FF Hamiltonian H_N, the gap bound $\gamma_N \geq c$ is equivalent to the operator inequality

$$H_N^2 \geq cH_N.$$

The LHS can be computed as (assume $h^2 = h$ for simplicity):

$$H_N^2 = H_N + \sum_{\text{edges } e \neq e'} \{h_e, h_{e'}\}$$

and for edges that don't share a vertex $\{h_e, h_{e'}\} \geq 0$. So the main task is to bound $\{h_e, h_{e'}\}$ when e and e' do share a vertex.

Finite-size criteria à la Knabe

Define the 1D-Hamiltonians

$$H_N = \sum_{i=1}^{N-1} h_{i,i+1}, \qquad H_N^{per} = H_N + h_{N,1}$$

(an open and periodic chain) and let γ_N, respectively γ_N^{per}, be their spectral gaps. Assume that local interactions h are projections, without loss of generality.

Theorem (Knabe '88)

Let H_N be FF and $3 \leq n \leq N/2$. Then $\boxed{\gamma_N^{per} \geq \gamma_n - \frac{1}{n-1}}$

Corollary (useful for applications)

If there exists any finite size n such that γ_n exceeds the gap threshold $\frac{1}{n-1}$, then H_N^{per} is gapped.

Beyond Knabe I

Knabe's gap bound

$$\gamma_N^{per} \geq \gamma_n - \frac{1}{n-1}$$

Corollary

If H_N is gapped, then H_N^{per} is gapped.

Caveats about last corollary: (1) The converse is false — edge modes can spoil an existing bulk gap. (2) This does *not* follow from $H_N^{per} \geq H_N$ because $\ker H_N^{per} \neq \ker H_N$ in general.

Improvements of Knabe's bound have focused on three aspects.

- Generalization to higher dimensions
- Extension to other boundary conditions (especially open b.c. are of interest)
- Improved threshold scaling (compared to the $\frac{1}{n}$ above)

Results by Gosset-Mozgunov (2016); Kastoryano-Lucia (2017); L-Mozgunov (2018); L (2019); Anshu (2019)

Beyond Knabe II

Theorem (L-Mozgunov)

Let $N > 2n$. Then

$$\gamma_N \geq \frac{1}{2^8\sqrt{6n}}\left(\min_{n/2\leq\ell\leq n}\gamma_\ell - \frac{2\sqrt{6}}{n^{3/2}}\right).$$

Corollary

2D FF spin systems with open b.c. cannot have $\frac{C_1}{N} \leq \gamma_N \leq \frac{C_2}{n}$.
Interpretation: 2D FF systems cannot host edge modes with linear dispersion $\epsilon(k) = v|k|$, i.e., no CFT gap scaling.

The best improvement of Knabe's bound was recently obtained via the detectability lemma.

Theorem (Anshu)

For FF Hamiltonians on $\mathbb{Z}^D$, there exist constants $C_D, C'_D > 0$ s.t.

$$\gamma_N \geq C_D\left(\gamma_n - C'_D\frac{1}{n^2}\right)$$

Recent applications to concrete models

In applications, a finite-size criterion is verified in one of two ways:

(a) By explicitly computing the finite-size gap γ_n, possibly with computer assistance.

(b) By introducing an appropriate large parameter that monotonically affects the finite-size gap.

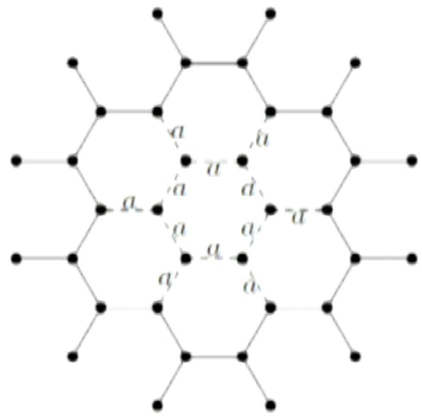
Concrete models where this yields a spectral gap:

- PVBS models at arbitrary species number and dimension, in a perturbative regime (with Nachtergaele)
- AKLT model on decorated hexagonal lattices, for decoration number ≥ 3 (with Abdul-Rahman, Lucia, Nachtergaele and Young); extended to other decorated lattices (including square) by Pomata-Wei.
- AKLT model on the hexagonal lattice (with Sandvik and Wang). This confirms the AKLT conjecture from 1987 by a computer-assisted argument. Independently achieved by Pomata-Wei by verifying a different finite-size criterion with a computer.

The AKLT conjecture

Theorem (Finite-size criterion for hexagonal AKLT model)

$$\gamma_N^{AKLT} \geq \frac{10+4a}{3a^2+2a+7}\left(\gamma_{\mathcal{F}}(a) - \frac{a^2-2a+3}{10+4a}\right), \qquad \forall a \geq 1, \forall N \geq 30.$$



$\gamma_{\mathcal{F}}(a)$ is the gap of the relevant finite-size system $H_{\mathcal{F}}$, equipped with open boundary conditions. Dashed edges are weighted by $a \geq 1$.

By DMRG, the gap $\gamma_{\mathcal{F}}(1.4) > 0.145$ which exceeds the relevant threshold $\frac{a^2-2a+3}{10+4a} = 0.138$ when $a = 1.4$. This yields the lower bound $\gamma^{AKLT} > 0.006$ on the gap of the AKLT model on the infinite hexagonal lattice γ_N^{AKLT} (though we do not claim to have rigorous bounds on the numerical errors).

A probabilistic theorem about gaps

In 2017, Movassagh showed that i.i.d. random Hamiltonians are gapless with probability 1 in any dimension. But what about random translation-invariant Hamiltonians?

A random translation-invariant Hamiltonian: Take h to be a random local projection of fixed rank r. (E.g., let U be a $d^2 \times d^2$ Haar-random unitary and use its first r columns as span of $\operatorname{ran} h$.)

$$H_N^{per,1D} = \sum_{j=1}^{N} h_{j,j+1}.$$

Theorem

Let $r \leq d-1$. Then $H_N^{per,1D}$ is gapped with positive probability.

Remarks: For qubits this was follows from prior work of Bravyi-Gosset. The argument works similarly for all trees, but not for higher $\mathbb{Z}^D$.

Work in preparation: extension to rank $d \leq r \leq d^2/4$ and more.

Summary

Main message: The existence of a spectral gap above the ground state has far-reaching mathematical and physical consequences. Finite-size criteria are a coarse, but sometimes effective method for deriving spectral gaps, at least for frustration-free Hamiltonians.

Open problems:

- AKLT models on other lattices, especially the square lattice where there is not even consensus whether a spectral gap is expected.
- Understanding the typical gaps of random translation-invariant Hamiltonians in higher dimensions.
- Exploring the connection between entanglement of the local interactions and the existence of a spectral gap.
- Leaving the frustration-free class (Haldane conjecture).