

Title: Spectral gaps without frustration

Speakers: Marius Lemm

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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

Marius Lemm (Harvard)

*based on various joint works with:  
Houssam Abdul-Rahman, Angelo Lucia, Jenia Mozgunov,  
Bruno Nachtergaele, Anders W. Sandvik, Amanda Young, and  
Ling Wang*

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## Quantum spin systems

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

**Hilbert space:** Let  $\Lambda_N$  be a finite subset of an infinite lattice  $\Lambda$  (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  $h : \mathbb{C}^d \otimes \mathbb{C}^d \rightarrow \mathbb{C}^d \otimes \mathbb{C}^d$ , and embed it into the operators on  $\mathcal{H}_N$  by defining

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

The **Hamiltonian**  $H_N$  is the sum of local interactions

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



## The spectral gap and why we care

**Spectrum:**  $\text{spec } H_N = \{E_0(N) < E_1(N) < E_2(N) < \dots\}$   
(This is defined with possible degeneracy.)

**Spectral gap:**  $\gamma_N = E_1(N) - E_0(N) > 0$

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

**Basic dichotomy** in the thermodynamic limit  $N \rightarrow \infty$ :

- (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  $\gamma_N$  obtainable from variational principle

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



## Two examples of frustration-free spin systems

### (1) Heisenberg ferromagnet

- Local interaction

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

- **Gapless** with gap closing like  $N^{-2}$  as  $N \rightarrow \infty$  (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

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

(an open and periodic chain) and let  $\gamma_N$ , respectively  $\gamma_N^{per}$ , 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  $\gamma_N^{per} \geq \gamma_n - \frac{1}{n-1}$

Corollary (useful for applications)

*If there exists any finite size  $n$  such that  $\gamma_n$  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.

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

## 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  $\gamma_n$ , 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:

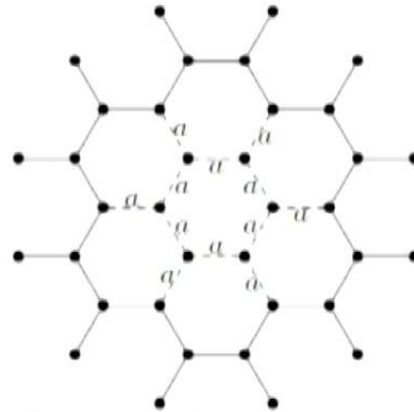
- **PVBS models** at arbitrary species number and dimension, in a perturbative regime (with Nachtergaele)
- AKLT model on **decorated** hexagonal lattices, for decoration number  $\geq 3$  (with Abdul-Rahman, Lucia, Nachtergaele and Young); extended to other decorated lattices (including square) by Pomata-Wei.
- **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)

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



$\gamma_{\mathcal{F}}(a)$  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  $\gamma_N^{AKLT}$  (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  $\text{ran } h$ .)

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

### Theorem

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

**Remarks:** For qubits this 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).