Gapped and gapless phases of frustration-free spin-1/2 chains

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David Gosset

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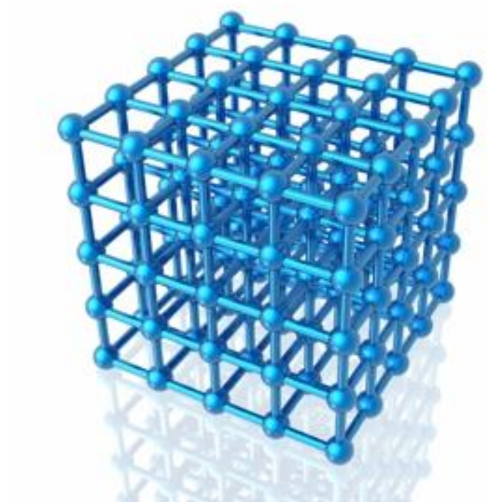
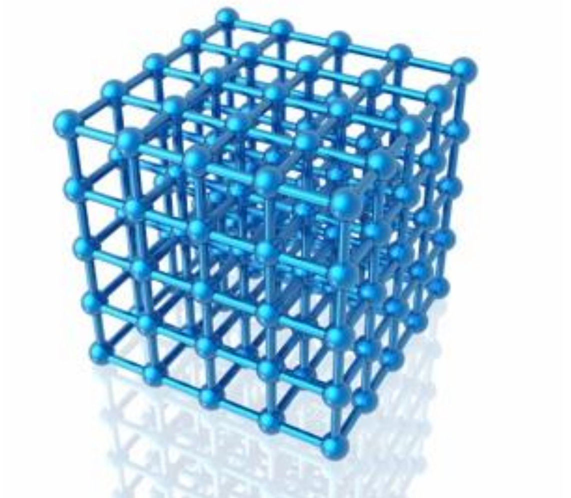


Hamiltonian H_n (system size n)

Image source: www.nist.gov



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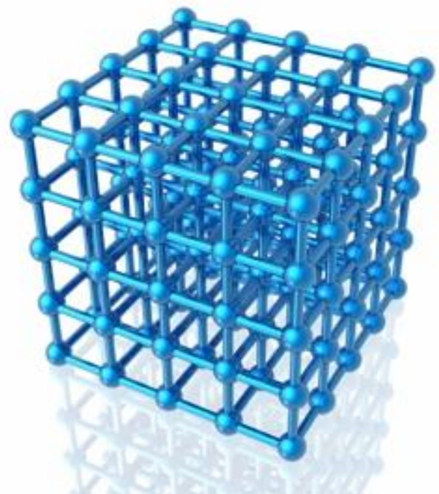

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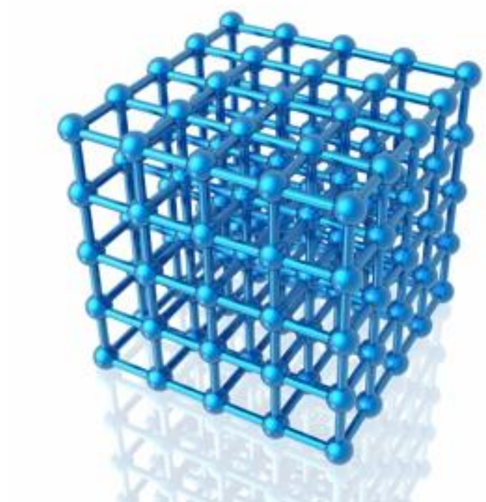

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Gapped vs. gapless has far-reaching consequences…

Image source: www.nist.gov

Gapped versus gapless in 1D

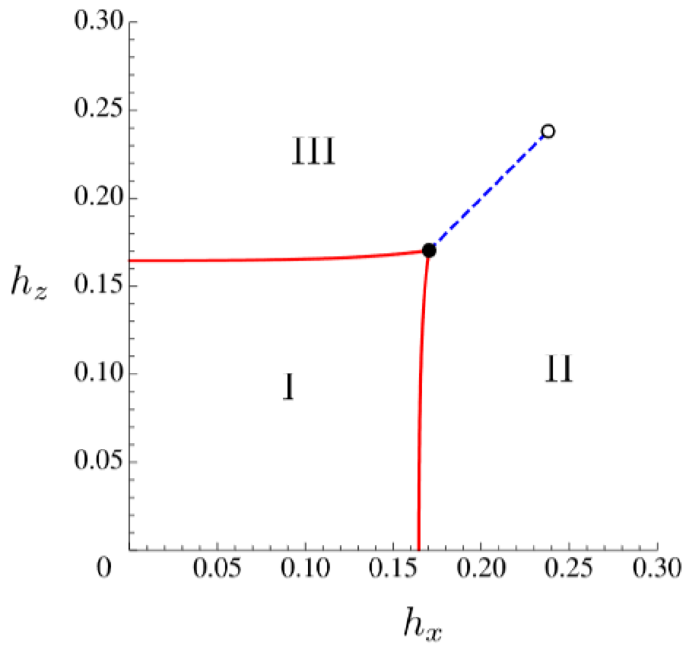
1D chain of n qudits

Hamiltonian $$H_n = \sum_{i=1}^{n-1} h_{i,i+1}$$

	Gapped	Gapless
Area law [Hastings 2007]	✓	✗
Exp. decay of correlations [Hastings, Koma 2005]	✓	✗
Efficiently compute groundstates [Landau et al 2014]	✓	✗

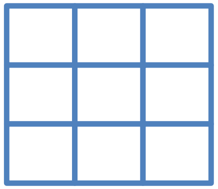
Gapped versus gapless

In quantum many-body systems at zero temperature, distinct gapped phases are separated by quantum phase transition lines where the system is gapless.



Phase diagram of the toric code, from [Vidal, Dusuel, Schmidt 2009]

Can we determine which translation-invariant systems are gapped?



Hopeless for qudits in two dimensions: the spectral gap problem is undecidable [Cubitt, Perez-Garcia, Wolf 2015]

Difficult for qudits in one dimension: A solution would resolve, e.g., the Haldane conjecture. [Haldane 1983]

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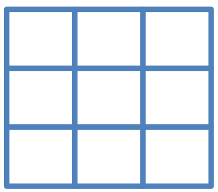

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In this work we solve this problem for all frustration-free 1D qubit systems with nearest-neighbor interactions.

Frustration-free spin-1/2 chains

n-qubit Hamiltonian: $$H_n = \sum_{i=1}^{n-1} h_{i,i+1}$$

We consider all cases in which the Hamiltonian is frustration-free.

This means that any ground state $|\psi\rangle$ has minimal energy for each term $h_{i,i+1}$.

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In each case we determine gapped/gapless.

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There are less interesting "exceptional" cases: If h is rank 2 or 3 there are only a handful of cases where the Hamiltonian is frustration-free.

There is an interesting "generic" case: If h is rank 1 the Hamiltonian is always frustration-free. In the rest of this talk we specialize to this case.

1. **Hamiltonian (rank-1 case) and its ground space**
2. Our result and examples
3. Proof sketch
4. Open questions

The Hamiltonian

Hilbert space: $(\mathbb{C}^2)^{\otimes n}$ (n qubits)

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- We are unable to construct an orthonormal basis for the ground space.
- The ground space dimension is $n+1$ for almost all $|\psi\rangle$.

Ground space: warm-up special case

Consider the special case

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \qquad\qquad H_n(\psi) = \sum_{i=1}^{n-1} |\psi\rangle\langle\psi|_{i,i+1}$$

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$$|\widehat{w}\rangle = \sum_{z\in\{0,1\}^n, |z|=w} |z\rangle \qquad\qquad w = 0, \dots, n$$

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E.g., for $n = 3$: $|000\rangle, \quad |100\rangle + |010\rangle + |001\rangle, \quad |110\rangle + |101\rangle + |011\rangle, \quad |111\rangle$

Ground space: general case for entangled $|\psi\rangle$

Define

$$T_\psi = \begin{pmatrix} \langle\psi|0,1\rangle & \langle\psi|1,1\rangle \\ -\langle\psi|0,0\rangle & -\langle\psi|1,0\rangle \end{pmatrix}$$

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Lemma [follows from Bravyi 2006]
If $|\psi\rangle$ is entangled, the zero energy ground space of $H_n(\psi)$ is the image of the n-qubit symmetric subspace under the linear map

$$1 \otimes T_\psi \otimes T_\psi^2 \otimes T_\psi^3 \otimes \cdots \otimes T_\psi^{n-1}$$

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For large $\boldsymbol{n}$, this linear map behaves very differently if both eigenvalues of $\boldsymbol{T_\psi}$ have the same magnitude.

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- **Case 1: Both eigenvalues of $\boldsymbol{T_\psi}$ are zero. Equivalently, $|\boldsymbol{\psi}\rangle = |\boldsymbol{v} \otimes \boldsymbol{v}\rangle$.** $H_n(\psi)$ is diagonal in $\{|v\rangle, |v^\perp\rangle\}$ basis. The ground space dimension is $> n + 1$.

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- **Case 2: $\boldsymbol{T_\psi}$ has exactly one zero eigenvalue. Equivalently, $|\boldsymbol{\psi}\rangle = |\boldsymbol{v} \otimes \boldsymbol{w}\rangle$.**
  Ground space spanned by $n + 1$ orthonormal product states. E.g., for $n = 4$:

$$\begin{array}{l}
|w^\perp \; w^\perp \; w^\perp \; w^\perp\rangle \\
|w \; w^\perp \; w^\perp \; w^\perp\rangle \\
|v^\perp \; w \; w^\perp \; w^\perp\rangle \\
|v^\perp \; v^\perp \; w \; w^\perp\rangle \\
|v^\perp \; v^\perp \; v^\perp \; w\rangle
\end{array}$$

So…the matrix T_ψ can be used to construct the ground space of $H_n(\psi)$. The eigenvalues of T_ψ are related to qualitative features of the ground space.

Are these eigenvalues related to the spectral gap?

1. Hamiltonian (rank-1 case) and its ground space
2. **Our result and examples**
3. Proof sketch
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Main result

$$H_n(\psi) = \sum_{i=1}^{n-1} |\psi\rangle\langle\psi|_{i,i+1}$$

We prove that the system is gapless if and only if the eigenvalues of T_ψ have equal non-zero absolute value.

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Subsequently improved to $\frac{6}{n(n+1)}$ [G., Mozgunov 2015].

Example 1

Consider the special case

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$

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Gapless

We can also deduce gaplessness using our theorem:

$$T_\psi = \begin{pmatrix} \langle\psi|0,1\rangle & \langle\psi|1,1\rangle \\ -\langle\psi|0,0\rangle & -\langle\psi|1,0\rangle \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Eigenvalues have same non-zero absolute value

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Eigenvalues have distinct absolute values whenever $q \neq 1$

In examples 1-2 there is a symmetry which enables an exact computation of the spectral gap. This is not true in general…

Example 3

Consider a two parameter family of states:

$$|\psi\rangle = \sqrt{1-p}\,|0 \otimes \theta\rangle + \sqrt{p}\,|1 \otimes \theta^{\perp}\rangle$$

$$|\theta\rangle = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}$$

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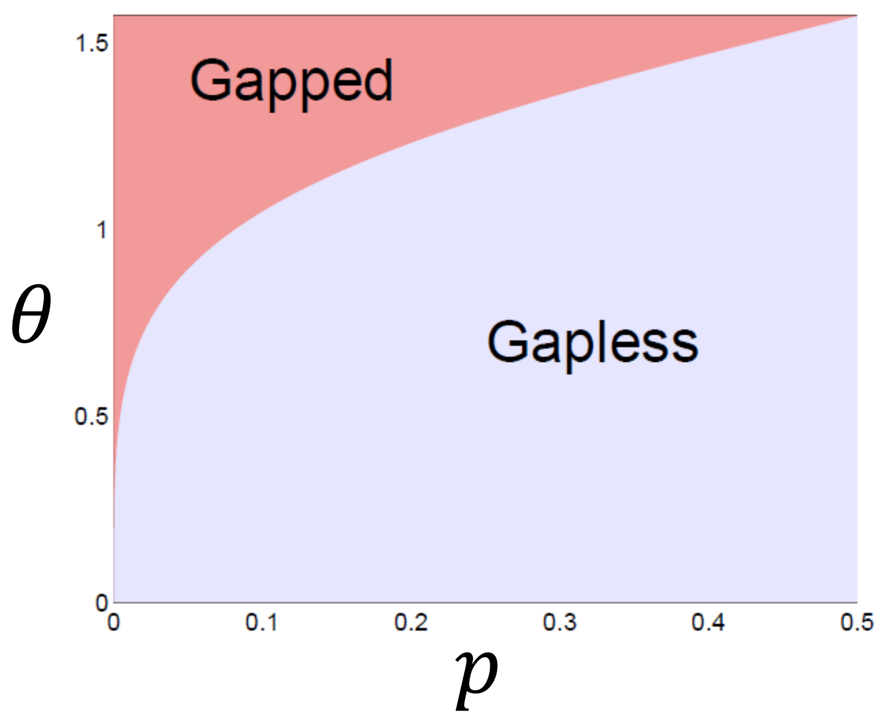

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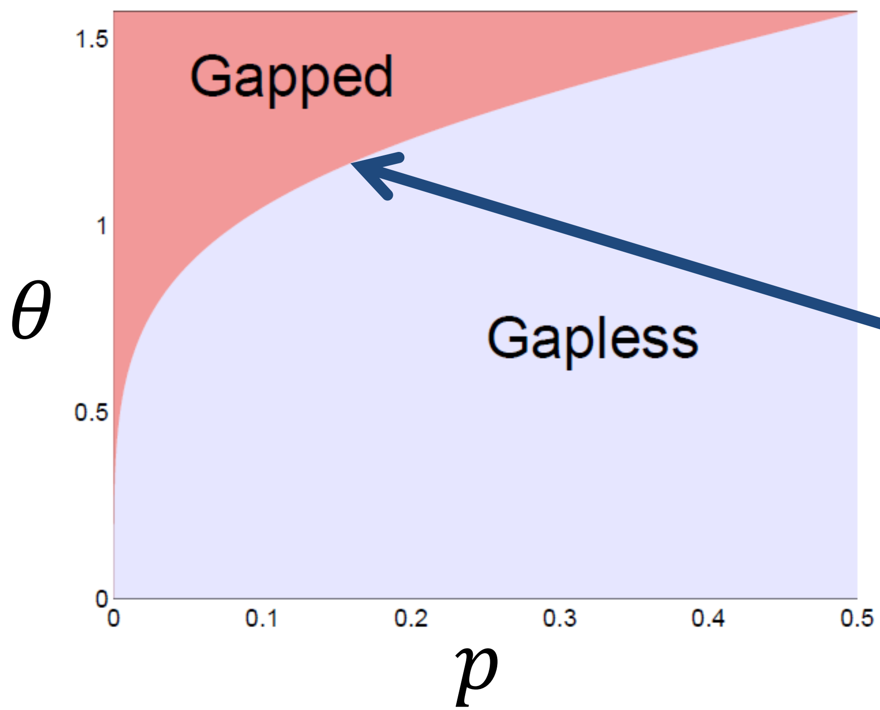

Phase boundary:

$$\sin^2(\theta) = \frac{4}{2 + \left(p(1-p)\right)^{-\frac{1}{2}}}$$

1. Hamiltonian (rank-1 case) and its ground space

2. Our result and examples

3. **Proof sketch**

4. Open questions

Aside: Continued fractions

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… …

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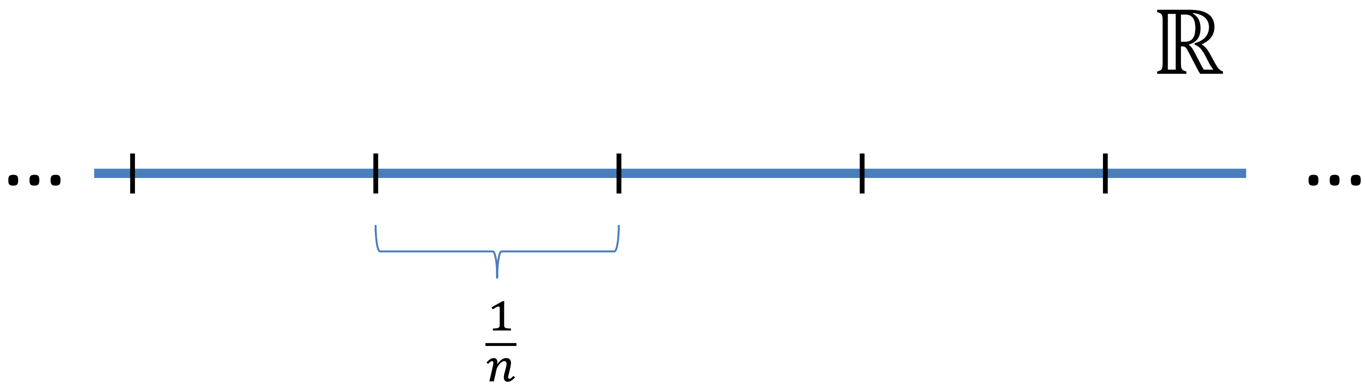
Each positive integer n defines a grid. Grid marks are the rational numbers with denominator n.



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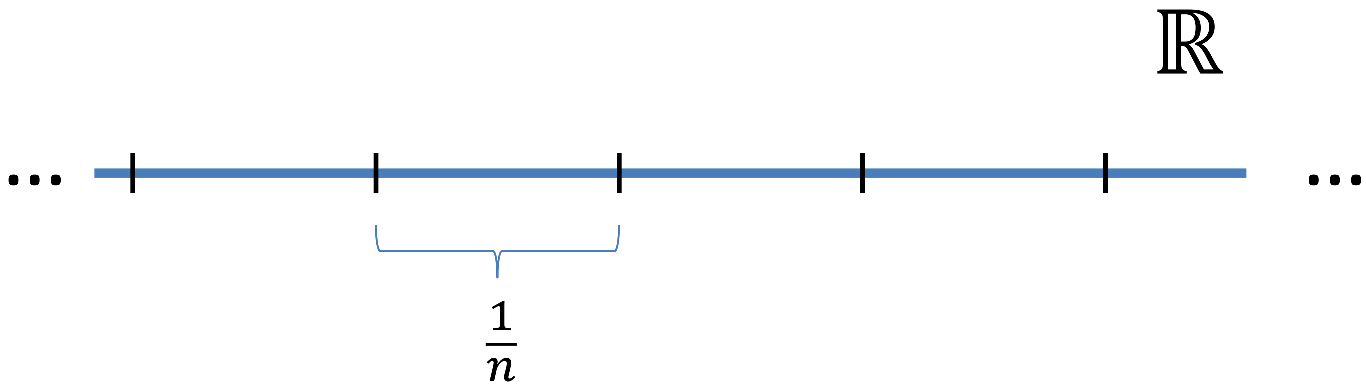

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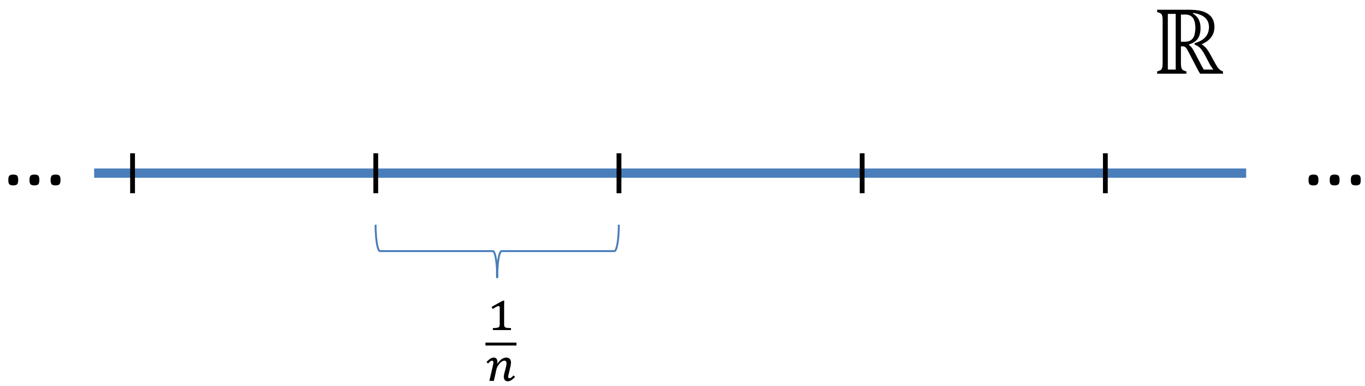

Obvious: any number is approximated by nearest grid point to within $\frac{1}{n}$.

Less obvious (continued fractions): For any irrational α there is a subsequence $\{n_j\}$ such that α is always within $\frac{1}{n_j^2}$ of the nearest grid point.

How do we prove the first part of the theorem?

Theorem:
Suppose the eigenvalues of T_ψ have equal non-zero absolute value. Then the spectral gap of $H_n(\psi)$ is at most $1/(n-1)$. Otherwise the spectral gap is lower bounded by a positive constant independent of n, which depends only on the state ψ .

Periodic vs. open boundary conditions

Open boundary conditions

$$H_n(\psi) = \sum_{i=1}^{n-1} |\psi\rangle\langle\psi|_{i,i+1} \qquad \mathrm{gap}(\psi, n)$$

Periodic boundary conditions

$$H_n^p(\psi) = H_n(\psi) + |\psi\rangle\langle\psi|_{n,1} \qquad \mathrm{gap}^p(\psi, n)$$

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The spectral gaps are related:

Lemma (Knabe 88):
For all $m \geq n > 2$:

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If $\mathrm{gap}^{\mathrm{p}}(\psi, m_j) \to 0$ we are done, since then $\mathrm{gap}(\psi, n) \leq {}^{1}/_{n-1}$.

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To finish proof, show that the periodic chain is gapless if the eigenvalues of $\boldsymbol{T_\psi}$ have equal nonzero magnitude.

Gaplessness of the periodic chain

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The lemma implies

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Imagine fixing n and plotting curves where this function is zero. To visualize this we'll now specialize to a two-parameter family of states…

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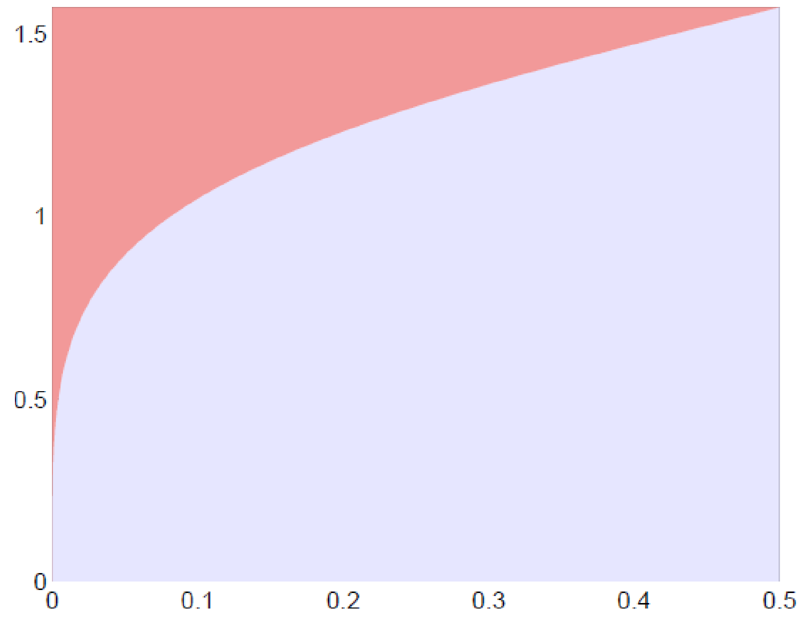

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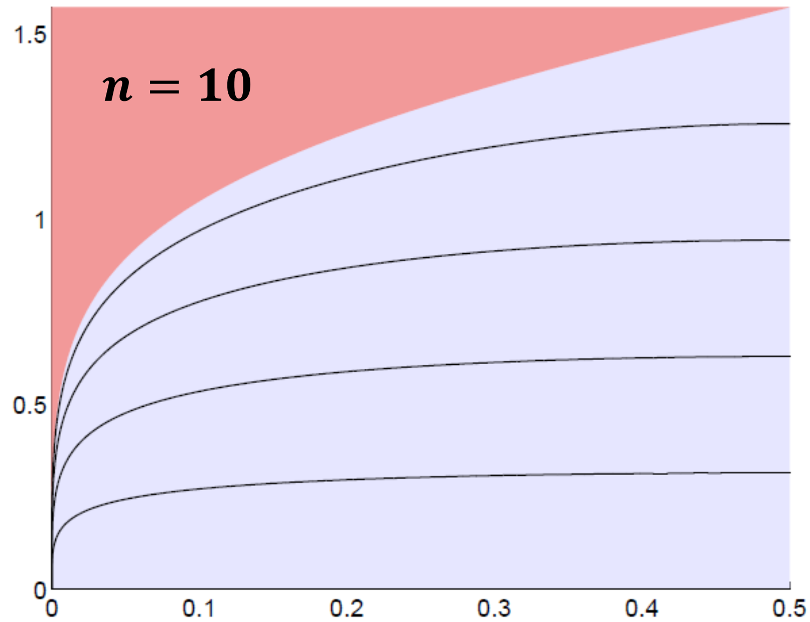

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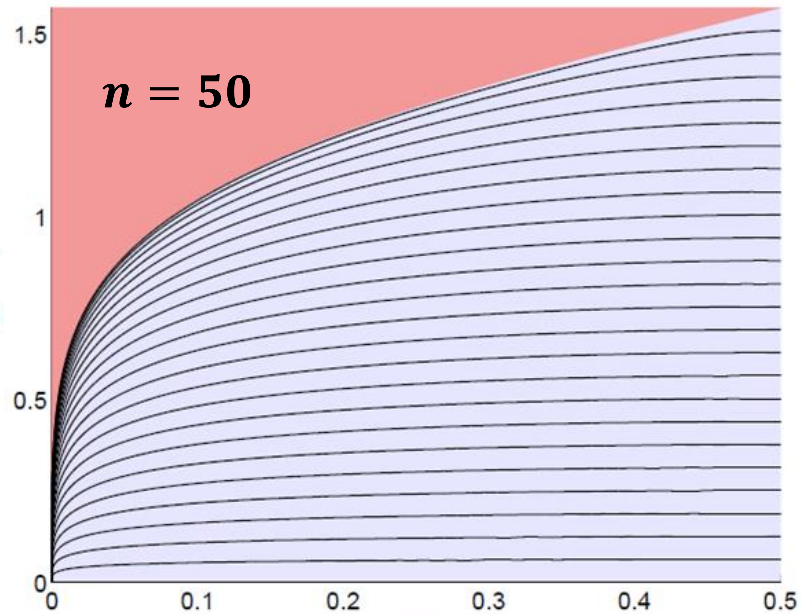

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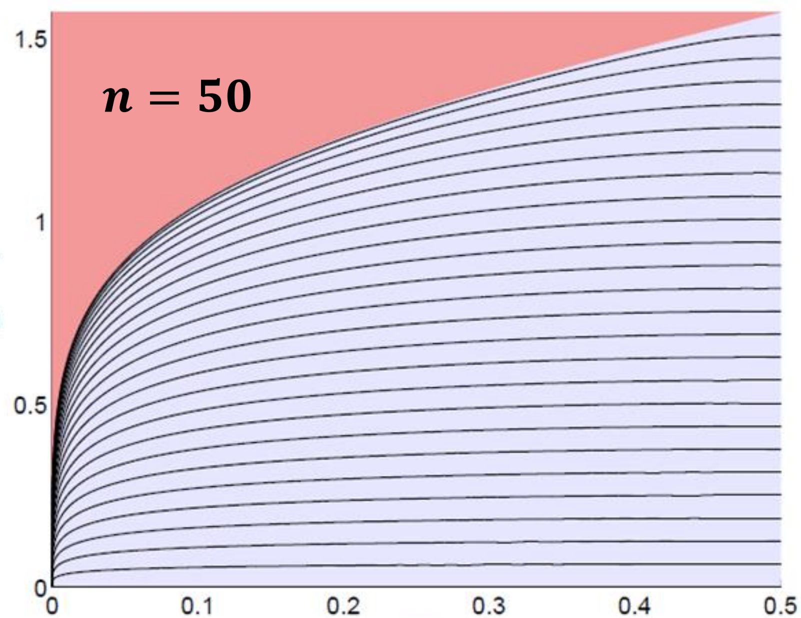

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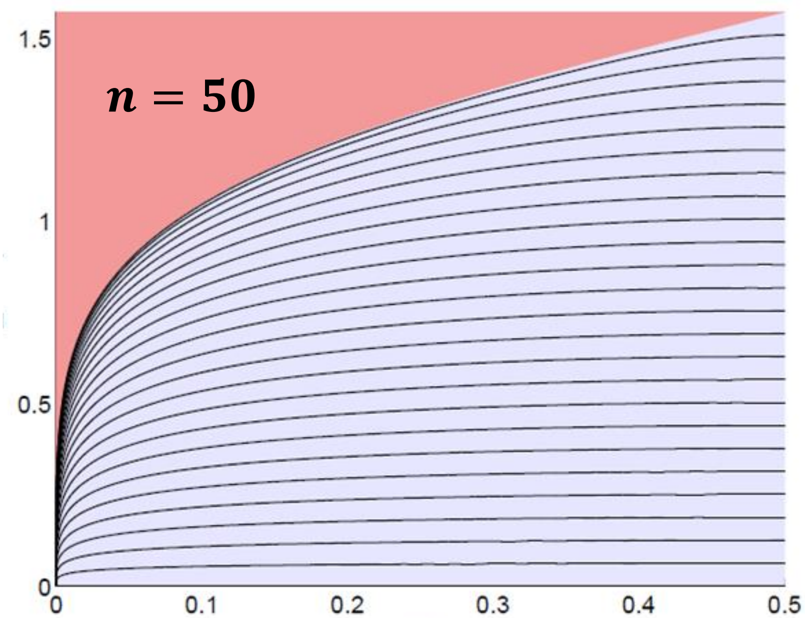

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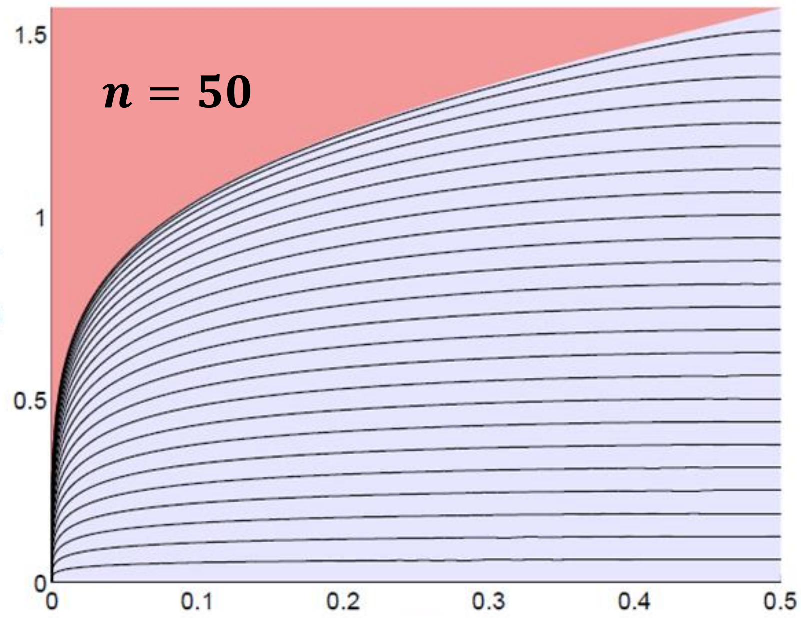

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So…if a point $|\psi_{blue}\rangle$ in the blue region is close enough to a point $|\phi_{black}\rangle$ on a black curve then $gap^p(\psi_{blue}, n)$ must be small. **How close does it need to be?**

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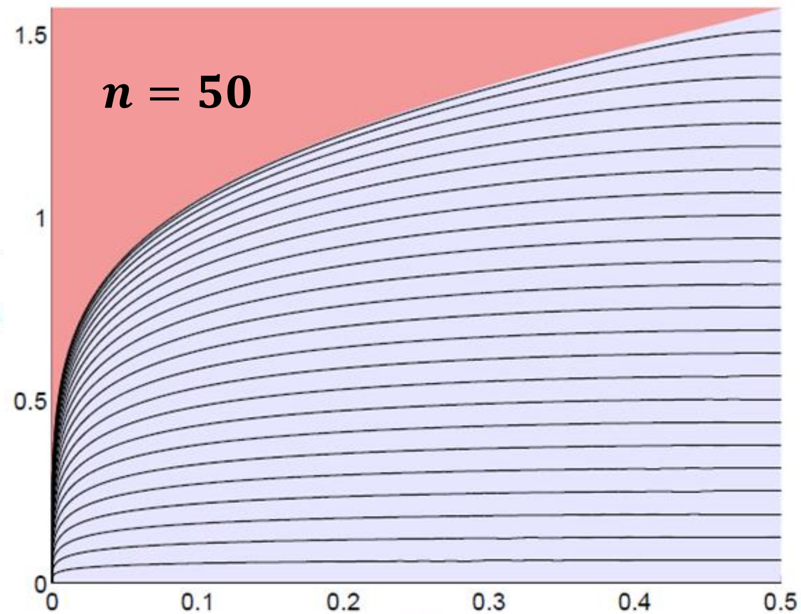

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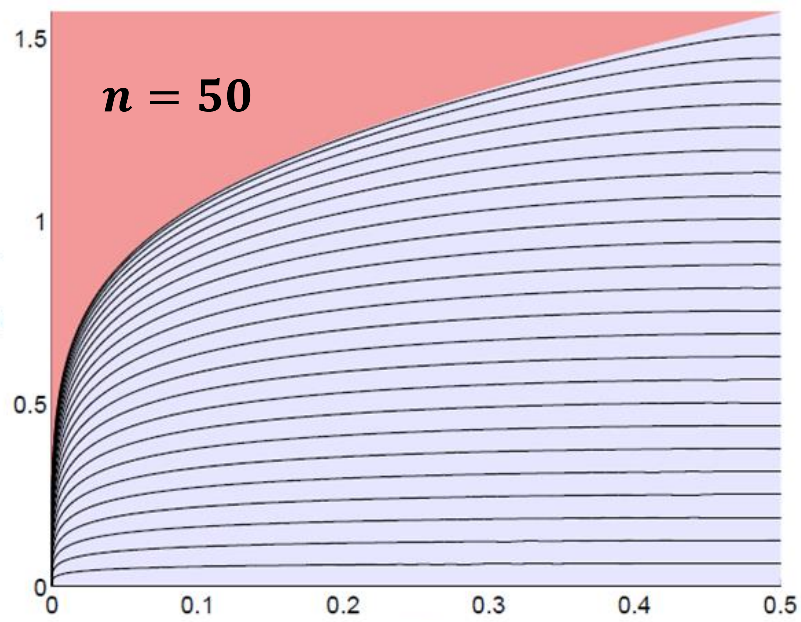

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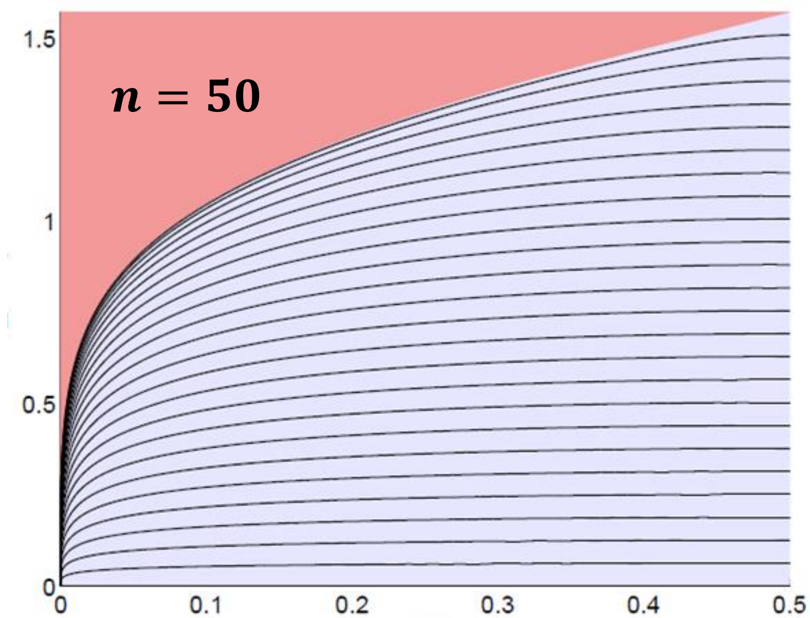

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Weyl's inequality for perturbed eigenvalues

Bad news: although the black curves become dense, they are not close enough together to ensure $2n \| |\psi_{blue}\rangle - |\phi_{black}\rangle \| \to 0$ as $n \to \infty$.

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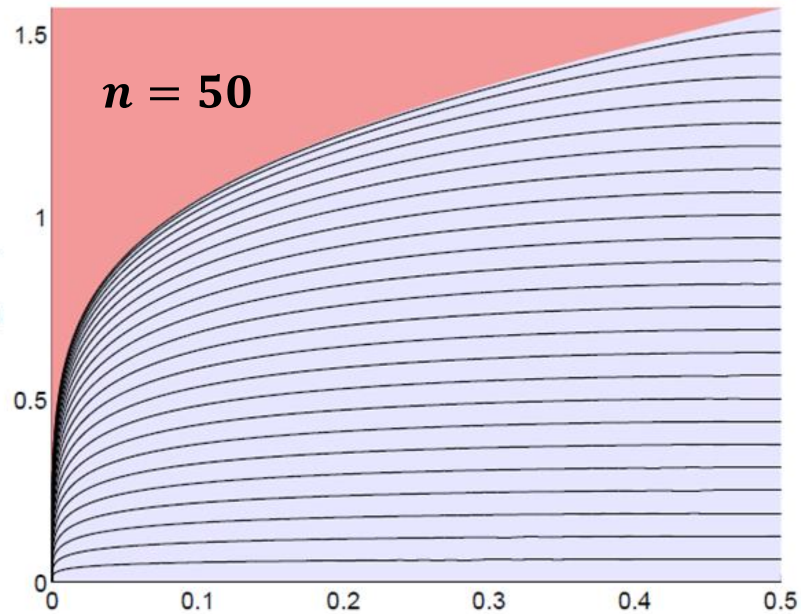

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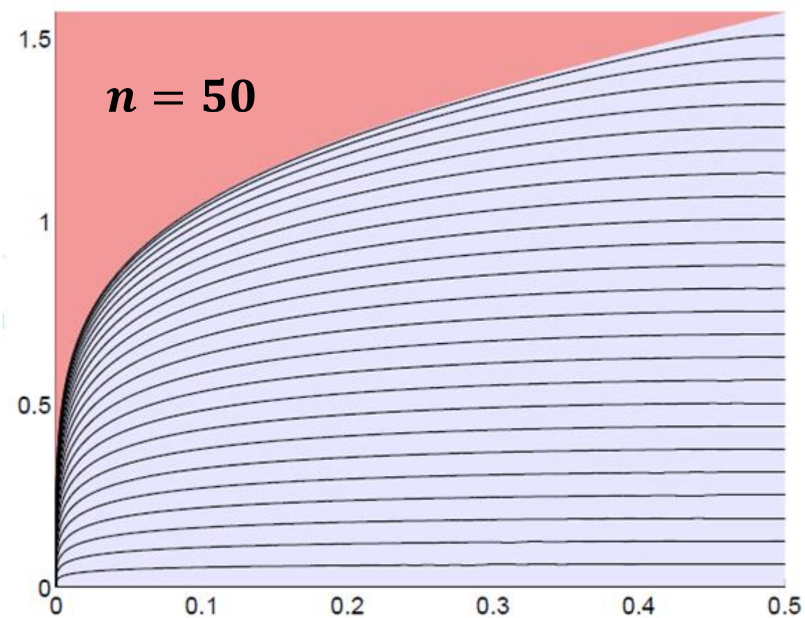

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Good news: Using continued fractions and the functional form of the curves one can show that there is a subsequence $\{n_j\}$ (depending on $|\psi_{\mathrm{blue}}\rangle$) such that

$$\| |\psi_{\mathrm{blue}}\rangle - |\phi_{\mathrm{black}}\rangle \| = O(1/n_j^2) \Rightarrow \mathrm{gap}^p(\psi_{\mathrm{blue}}, n_j) = O({}^1/_{n_j}).$$

This technique has to be modified slightly to handle the states corresponding to points which lie directly on one of the black curves.

In our paper we give a general proof which handles arbitrary states $|\psi\rangle$ (not just the two-parameter family discussed above) using this proof strategy.

How do we prove the second part of the theorem?

Theorem:
Suppose the eigenvalues of T_ψ have equal non-zero absolute value. Then the spectral gap of $H_n(\psi)$ is at most $1/(n-1)$. Otherwise the spectral gap is lower bounded by a positive constant independent of n, which depends only on the state ψ .

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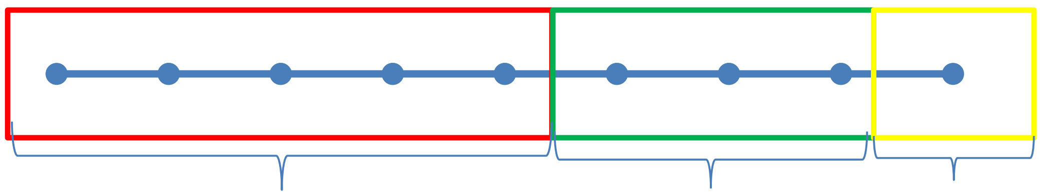
If both eigenvalues of T_ψ are zero then $|\psi\rangle = |v \otimes v\rangle$ and the terms in the Hamiltonian commute with one another (therefore spectral gap is an integer ≥ 1).

In the following we consider the case where eigenvalues have distinct magnitudes…

Nachtergaele's condition ("martingale method")

Partition n qubits into three regions A, B, C



$|A| = n - r - 1$ $\quad$ $|B| = r$ $\quad$ $|C| = 1$

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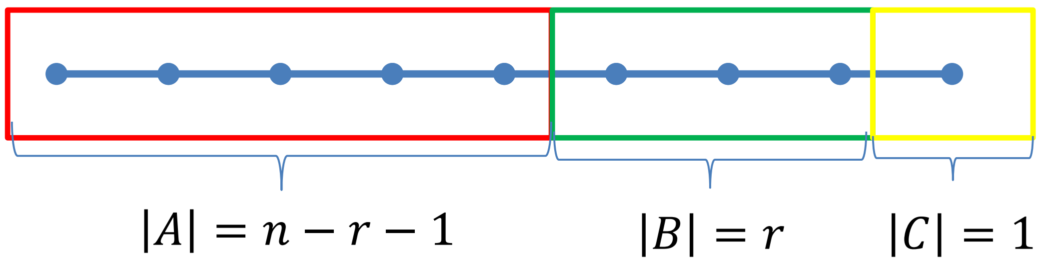

Define

G_{ABC} =projector onto groundspace of the full chain
G_{AB} = proj. onto groundspace of AB (acts trivially on C)
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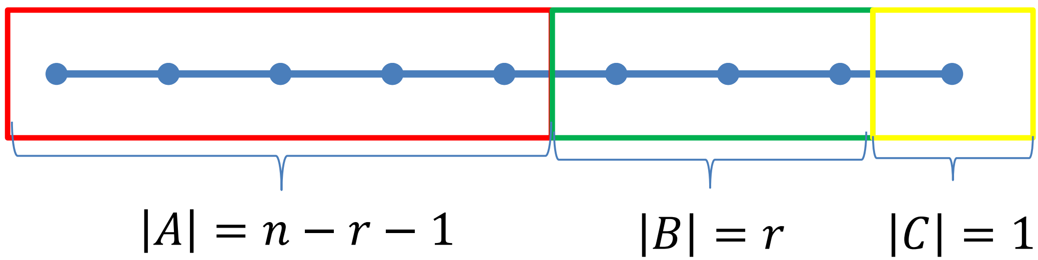

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Theorem [special case of Nachtergaele 1996]

Suppose there exists an integer $r \geq 1$ and a positive number $\epsilon < \frac{1}{\sqrt{r+1}}$ such that for all sufficiently large n we have

$$\|G_{ABC} - G_{AB}G_{BC}\| \leq \epsilon.$$

Then $H_n(\psi)$ is gapped.

Satisfying Nachtergaele's condition

Let λ be the ratio of the eigenvalues of T_ψ and let c be the inner product between the eigenvectors.

$$1 < |\lambda| \leq \infty \quad \text{and} \quad |c| < 1$$

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For any partition of n qubits into consecutive regions ABC with $|B| = r$ we have

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Applying Nachtergaele's theorem establishes that $H_n(\psi)$ is gapped when the eigenvalues of T_ψ have distinct magnitudes.

Proving this bound is the main technical work of our paper. The challenge is that we do not have explicit expressions for G_{AB}, G_{BC} or G_{ABC}…

Monotonicity under the partial trace

The key ingredient in the proof is a new operator inequality for the ground space projector:

$$\underbrace{\mathrm{Tr}_n(G_n)}_{\text{Partial trace of ground space projector with respect to last qubit in the chain}} \geq \underbrace{G_{n-1}}_{\text{Ground space projector for the chain with } n-1 \text{ spins}}$$

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Aside: It is an open question how general this monotonicity is. Our proof applies to all 1D qubit chains composed of rank-1 projectors (translation invariance not required).

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This inequality implies that certain expectation values $\boldsymbol{f_n = \mathrm{Tr}_{[1,\ldots,n]}(QG_n)}$ form non-decreasing sequences.

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Using monotonicity under the partial trace we establish other inequalities involving the ground space projector. Let $|\alpha\rangle, |\beta\rangle$ be the eigenvectors of T_{ψ}.

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We prove that $\tau(i,j,n)$ decays exponentially in $j - i$, and that $\tau(n)$ approaches a finite limit as $n \to \infty$.

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Region Exclusion Identities

We prove 3 identities which involve excluding a region from some partition of the chain. E.g., for any partition ABC with $|B| = r$:

$$\left\|(G_{ABC} - G_{AB} \otimes I_C) I_A \otimes |\beta\rangle\langle\beta|^{\otimes|BC|}\right\|^2 \leq O(|c|^r) + O(r|\lambda|^{-r})$$

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We show that the claimed bound on $\|G_{ABC} - G_{AB}G_{BC}\|$ follows from the region exclusion identities.

1. Hamiltonian (rank-1 case) and its ground space
2. Our result and examples
3. Proof sketch
4. **Open questions**

Open questions

There is an infinite family of 1D frustration-free models, of which ours is the simplest case:

Hilbert space: $\left(\mathbb{C}^d\right)^{\otimes n}$ (n qudits)

Hamiltonian: Let Π be a two-qudit projector of rank r

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Can we generalize our results to the qudit models with $\boldsymbol{d > 2}$?

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- Is it possible to certify that a frustrated 1D chain is gapped in the thermodynamic limit using data from finite-size numerics?

Extra slides

Exceptional cases

$$H_n = \sum_{i=1}^{n-1} h_{i,i+1}$$

h is a two-qubit projector with rank 2 or 3.

Rank 3 case: If h is a rank-3 projector and H_n is frustration-free then

$$h = I - |\theta \otimes \theta\rangle\langle\theta \otimes \theta|$$

So H_n is a sum of commuting projectors and has spectral gap 1.

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Theorem (rank-2 case)
Suppose h is a rank-2 projector which cannot be written as $1 \otimes P$ or $P \otimes 1$. Then exactly one of the following holds for the null space G_4 of the 4-spin chain:

1. $G_4 = span\{|\theta\theta\theta\theta\rangle\}$
2. $G_4 = span\{|\theta\theta\theta\theta\rangle, |\phi\phi\phi\phi\rangle\}$
3. $G_4 = span\{|\theta\phi\theta\phi\rangle, |\phi\theta\phi\theta\rangle\}$
4. $G_4 = span\{|\theta\theta\theta\theta\rangle, |\theta^\perp\theta\theta\theta\rangle + z|\theta\theta^\perp\theta\theta\rangle + z^2|\theta\theta\theta^\perp\theta\rangle + z^3|\theta\theta\theta\theta^\perp\rangle\}$
5. G_4 is empty.

In cases 1,2,3,4 the system is frustration-free and in case 5 it is frustrated. The system is gapless in case 4 iff $|z| = 1$ and gapped in all other cases.