Title: Undecidability of the spectral gap in one dimension

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Abstract: <p>The spectral gap problem consist in deciding, given a local interaction, whether the corresponding translationally invariant Hamiltonian on a lattice has a spectral gap independent of the system size or not. In the simplest case of nearest-neighbour frustration-free qubit interactions, there is a complete classification. On the other extreme, for two (or higher) dimensional models with nearest-neighbour interactions this problem can be reduced to the Halting Problem, and it is therefore undecidable.</p>

<p>There are a lot of indications that one dimensional spin chain are relatively simpler than their counterparts in higher dimensions. Nonetheless, I will present a construction of a family of nearest-neighbour, translationally invariant Hamiltonians on a spin chain, for which the spectral gap problem is undecidable.</p>

Undecidability of the spectral gap in 1D

arXiv:1810.01858

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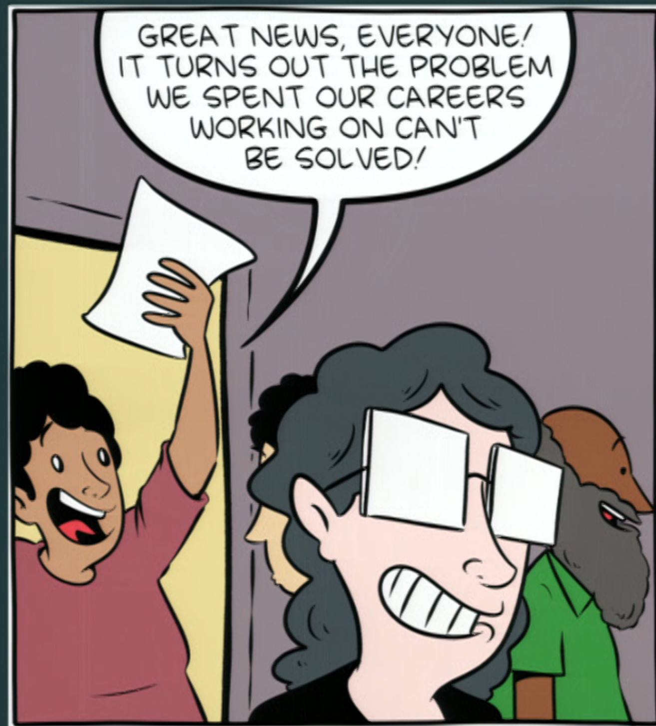
joint work with Johannes Bausch, Toby S. Cubitt, David Perez-Garcia

Perimeter Institute, October 24th 2018



Mathematicians are weird.

SMBC Comics from today!

http://smbc-comics.com/comic/problem

Spectral gap problem

A decision problem

We consider a one-dimensional spin chain of N qudits with open boundary conditions $(\mathbb{C}^d)^{\otimes N}$, coupled by translation invariant interactions:

1. $\mathbf{h}^{(1)}$ a single-site term ($d \times d$ Hermitian matrix);
2. $\mathbf{h}^{(2)}$ a nearest-neighbor term ($d^2 \times d^2$ Hermitian matrix).

The Hamiltonian $\mathbf{H}_N$ is given by

$$\mathbf{H}_N = \sum_{i=1}^{N-1} \mathbf{h}^{(2)}_{i,i+1} + \sum_{i=1}^{N} \mathbf{h}^{(1)}_i$$

Spectral gap problem

Given $\mathbf{h}^{(1)}$ and $\mathbf{h}^{(2)}$, determine if $\{\mathbf{H}_N\}_N$ is gapped or gapless.

A decision problem

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Spectral gap problem

Given $\mathbf{h}^{(1)}$ and $\mathbf{h}^{(2)}$, determine if $\{\mathbf{H}_N\}_N$ is gapped or gapless, under the promise that one of two cases holds.

gapped $\mathbf{H}_N$ has a unique ground state and $\Delta(\mathbf{H}_N) \geq \gamma > 0$;

gapless $[E_0(N), E_0(N) + c] \cap \sigma(\mathbf{H}_N)$ becomes dense for some $c > 0$.

Decidable problem

Is there an algorithm which given input $\mathbf{h}^{(1)}$ and $\mathbf{h}^{(2)}$ outputs gapped/gapless in finite time?

Hardness of the spectral gap problem

- for frustration-free $d = 2$ (qubits) models, the problem is easy (reduces to computing eigenvalues of a 2×2 matrix) [Bravyi, Gosset, 2015]

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Question:

The construction of C-PG-W does not work in 1D (more details later).

Is the spectral gap undecidable for 1D models?

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Some questions are nonetheless hard: local Hamiltonian problem (approximate ground state energy to inverse polynomial precision) is QMA-hard.

Main result

Fix a classical Universal Turing Machine (UTM).

Theorem

There exist (explicitly constructible) $d \times d$ matrices $\mathbf{a}, \mathbf{a}', \mathbf{a}''$ and $d^2 \times d^2$ matrices $\mathbf{b}$, $\mathbf{b}'$, $\mathbf{b}''$, $\mathbf{b}''''$ for some d such that:

1. $\mathbf{a}$ *and* $\mathbf{b}$ *are diagonal with entries in* $\mathbb{Z}$;
2. $\mathbf{a}'$, $\mathbf{a}''$, $\mathbf{b}'$, $\mathbf{b}''$ *are Hermitian with enties in* $\mathbb{Q}[\sqrt{2}]$;
3. $\mathbf{b}'''$ *and* $\mathbf{b}''''$ *have entries in* $\mathbb{Q}$;
4. *For any* $n \in \mathbb{N}$ *and any rational* $0 < \beta \leq 1$ *define the interactions*

$$\mathbf{h}^{(1)}(n) = \mathbf{a} + \beta(2^{-|\phi|}\mathbf{a}' + \mathbf{a}'')$$

$$\mathbf{h}^{(2)}(n) = \mathbf{b} + \beta[2^{-|\phi|}\mathbf{b}' + \mathbf{b}'' + (e^{i\pi\phi}\mathbf{b}''' + e^{i\pi 2^{-|\phi|}}\mathbf{b}'''' + h.c.)]$$

where $\phi(n) = 0.n_1 1 n_2 1 \ldots n_{|n|-1} 1 n_{|n|}$.

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Then

a) *if the UTM halts or loops on input n, then* $\{\mathbf{H}_N(n)\}_N$ *is gapless;*

b) *if the UTM does not halt on input n, then* $\{\mathbf{H}_N(n)\}_N$ *is gapped, and* $\Delta(\mathbf{H}_N) \geq 1$.

Main result

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b) *if the UTM does not halt on input n, then* $\{\mathbf{H}_N(n)\}_N$ *is gapped, and* $\Delta(\mathbf{H}_N) \geq 1$.

Corollary

Since deciding whether the UTM will halt/loop on input n is undecidable, so is the spectral gap problem.

β can be arbitrarily small: the problem is undecidable even for small perturbations of classical Hamiltonians.

How to cook up an Hamiltonian in 54 simple steps

The ingredients

Similarly to the 2D construction, there are a few ingredients:

1. Feynmann-Kitaev's history state construction, and Gottesman-Irani's variant for Quantum Turing Machines (QTM);
2. A QTM perfoming Quantum Phase Estimation (QPE);
3. A classical Hamiltonian selecting "tape segments";
4. A gapped trivial Hamiltonian $\mathbf{H}_{\text{trivial}}$ and a gapless dense spectrum Hamiltonian $\mathbf{H}_{\text{dense}}$.

Overall idea

Read the input parameter n from $\phi(n)$ using the QPE, start the UTM on the selected tape with input n, and couple the halting/non-halting configuration to an energy switch between $\mathbf{H}_{\text{trivial}}$ and $\mathbf{H}_{\text{dense}}$ – all of this in a history state.

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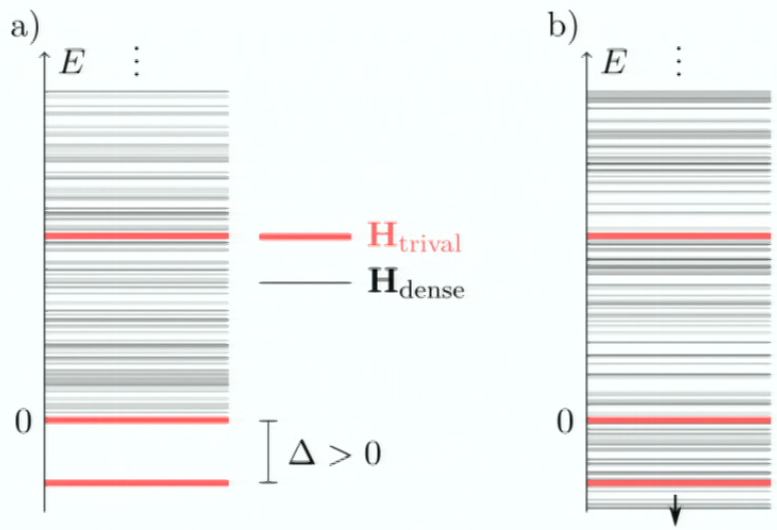
Read the input parameter n from $\phi(n)$ using the QPE, start the UTM on the selected tape with input n, and couple the halting/non-halting configuration to an energy switch between $\mathbf{H}_{\text{trivial}}$ and $\mathbf{H}_{\text{dense}}$ – all of this in a history state.



History states

History state

$$\frac{1}{\sqrt{T+1}} \sum_{t=0}^{T} |t\rangle_{\text{clock}} \otimes |\phi_t\rangle$$

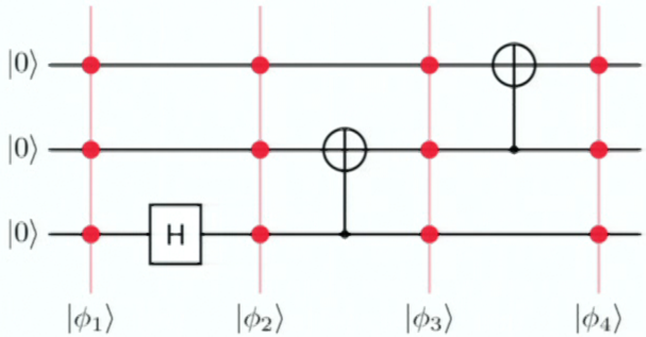
where $|\phi_t\rangle = \mathbf{U}_t \mathbf{U}_{t-1} \ldots \mathbf{U}_1 |\phi_0\rangle$.

It is the ground state of the *propagation Hamiltonian*

$$\mathbf{H}_{\text{prop}} = \sum_{t=1}^{T} (|t-1\rangle_{\text{clock}} \otimes \mathbf{1} - |t\rangle \otimes \mathbf{U}_t)(\text{h.c.})$$

$$= \sum_{t=1}^{T} (|t-1\rangle\langle t-1|_{\text{clock}} + |t\rangle\langle t|_{\text{clock}} - |t\rangle\langle t-1|_{\text{clock}} \otimes \mathbf{U}_t + \text{h.c.})$$

An example



$$
\begin{aligned}
\mathbf{H}_{\text{prop}} = &- (|0\rangle\langle 1| + |1\rangle\langle 0|) \otimes H_1 \\
&- (|1\rangle\langle 2| + |2\rangle\langle 1|) \otimes \text{CNOT}_{2,1} \\
&- (|2\rangle\langle 3| + |3\rangle\langle 2|) \otimes \text{CNOT}_{3,2} \\
&+ 4\mathbf{1} - |0\rangle\langle 0| - |3\rangle\langle 3|
\end{aligned}
$$

Quantum Turing Machines

Turing Machine

A (deterministic) Turing Machine is a triplet (Σ, Q, δ):

- Σ is a finite alphabet with a special *blank* symbol $\#$;
- Q is a finite set of state with a special *initial* q_0 and *final* $q_f \neq q_0$;
- $\delta : Q \times \Sigma \rightarrow Q \times \Sigma \times \{L, R\}$ is the transition function.

It has an infinite two-side tape initialized with $\#$.

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- $\delta : Q \times \Sigma \to \mathbb{C}^{Q \times \Sigma \times \{L,R\}}$ is the quantum transition function.

It has an infinite two-side tape initialized with $|\#\rangle$.

A history state Hamiltonian can be defined for the history of a QTM.

$|\phi_t\rangle$ encodes the state of the tape and the head position after t steps.

The propagation Hamiltonian will be translation invariant since δ does not depend on t.

Propagation Hamiltonian for QTM

Theorem ([C-PG-W 2015] using ideas from [G-I 2009])

The history state of a QTM is the groundstate of a 2-local Hamiltonian on a 1D spin chain such that

1. *it is frustration-free (g.s. energy 0)*
2. *local dimension depends only on Σ and Q*
3. *if the QTM halts and tape is not finished, the remaining time steps leave the tape unchanged*
4. *if the QTM runs out of tape the history state is truncated at that point*

Proof takes 42 pages.

Quantum Phase Estimation

Quantum Phase Estimation

Given a Universal Turing Machine M, we can construct a local Hamiltonian $\mathbf{H}_{\text{prop}}(\phi, M)$, there $\phi = 0.n_1 1 n_2 1 \ldots n_{|n-1|} 1 n_{|n|}$ whose ground state is a history state for a QTM that

1. Decodes n from ϕ using Quantum Phase Estimation [Nielsen, Chuang]
2. Execute the UTM on input n

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1. Decodes n from ϕ using Quantum Phase Estimation [Nielsen, Chuang]
   - if the tape length sufficient to contain n, the QPE will be exact;
   - using the interleaved 1s, detect incomplete expansion before the QFT step and penalize it
2. Execute the UTM on input n

The interaction terms will be of the form

$$\mathbf{b}'' + (e^{i\pi\phi}\mathbf{b}''' + e^{i\pi 2^{-|\phi|}}\mathbf{b}'''' + \text{h.c.})$$

Penalizing computation output

Checking if the head of the UTM sits next to a tape boundary, we can give different energy to the groundstate of $\mathbf{H}_{\text{prop}}(\phi, M)$ depending on whether the UTM runs out of tape.

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Gap of $\mathbf{H}_{\text{prop}}$

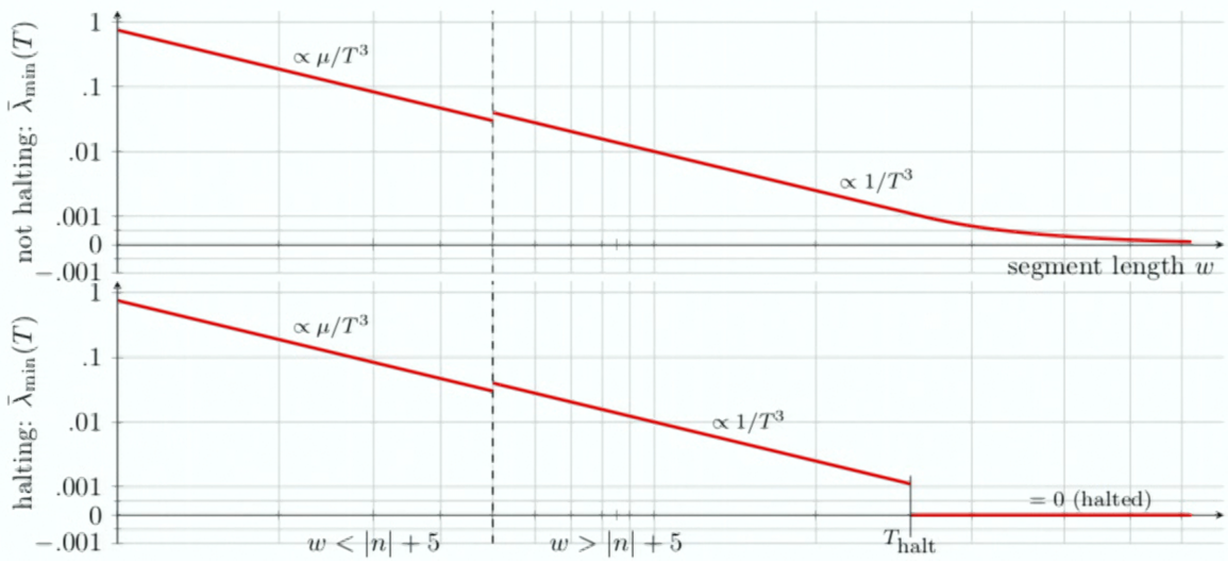
The gap of the propagation Hamiltonian is $\Omega(T^{-3})$.

Recent works have improved this to roughly T^{-2}
[Bausch, Crosson 2018] [Caha, Landau, Nagaj 2018],
but it cannot be smaller than $O(T^{-1})$
[González-Guillén, Cubitt arXiv:1810.06528]

Energy penalty for running out of tape tends to 0 in the length of the tape.

We cannot apriori estimate T (it is undecidable!).

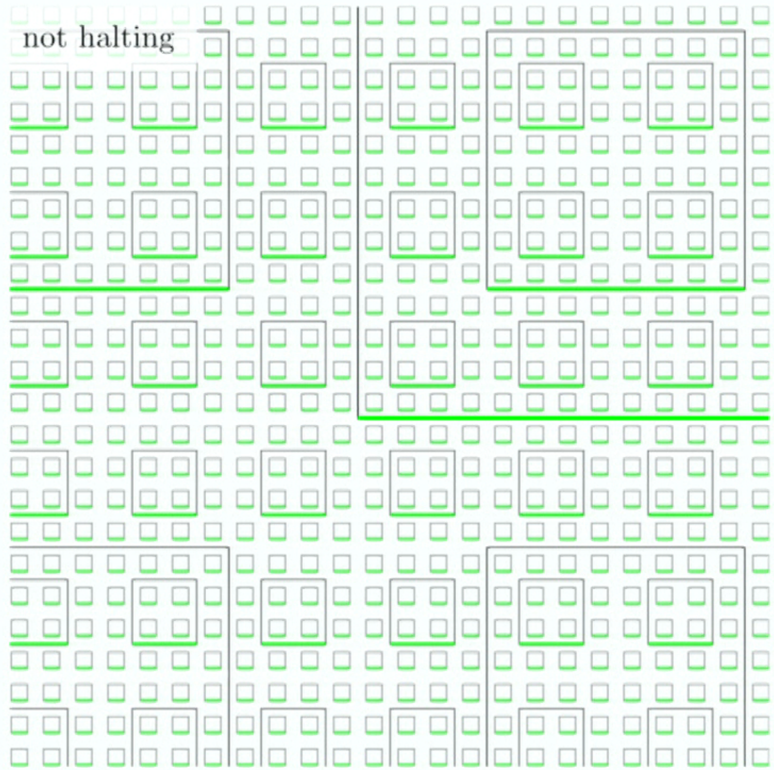
Computation penalty



Spanning multiple instances

The 2D solution

- Construct a quasi-periodic tiling known as Robinson Tiling;
- It has finite density of squares of any given size;
- Run one instance of the QTM on each lower edge;
- If the QTM runs forever: no penalty



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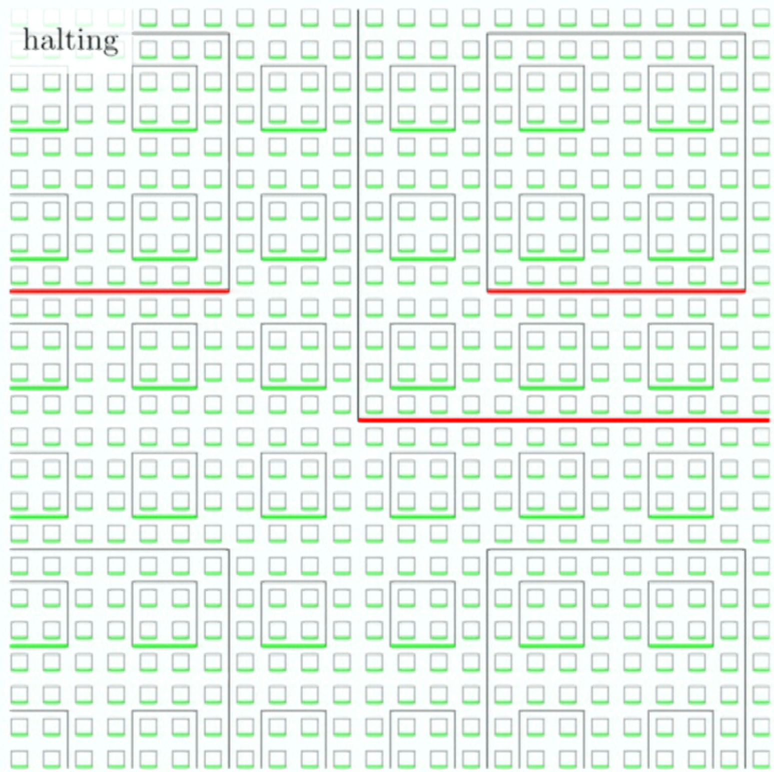

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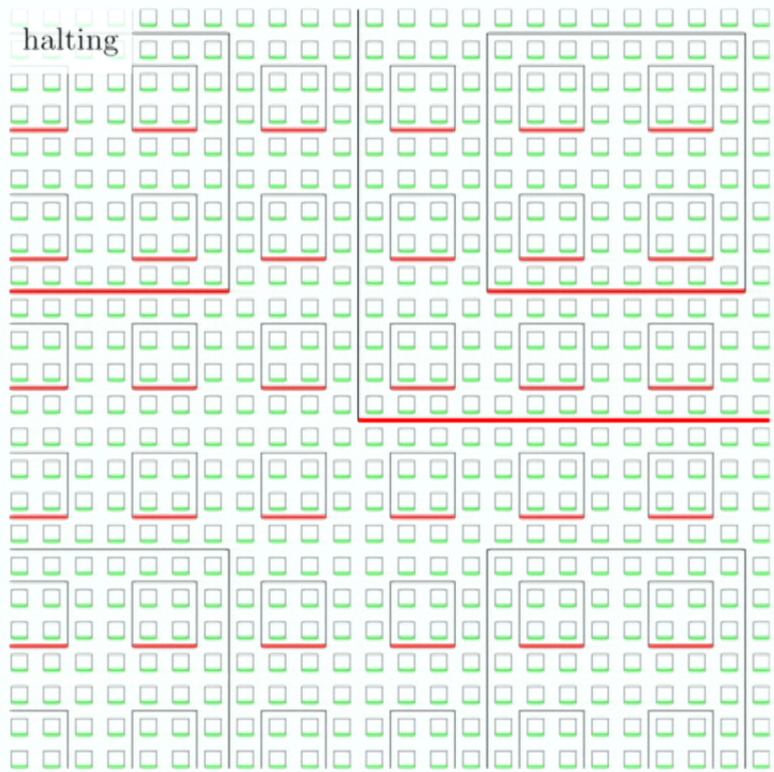


13/25

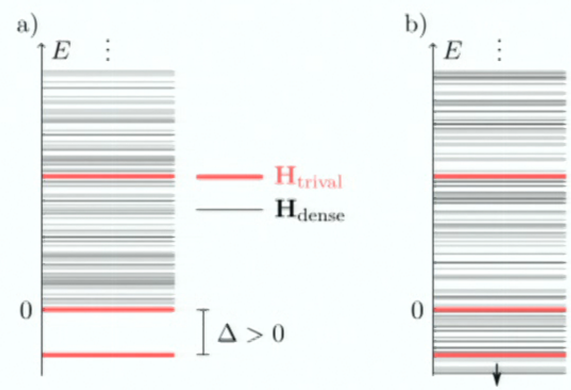
Quasi-periodic tiling

1. If the QTM does not halt $\rightarrow$ no penalty
2. If it halts, every instance above a certain tape length will get a (small but fixed) penalty.

Quasi-periodic tiling

1. If the QTM does not halt → no penalty
2. If it halts, every instance above a certain tape length will get a (small but fixed) penalty. They will accumulate and push the dense spectrum up, which will reveal the gap of the trivial Hamiltonian.

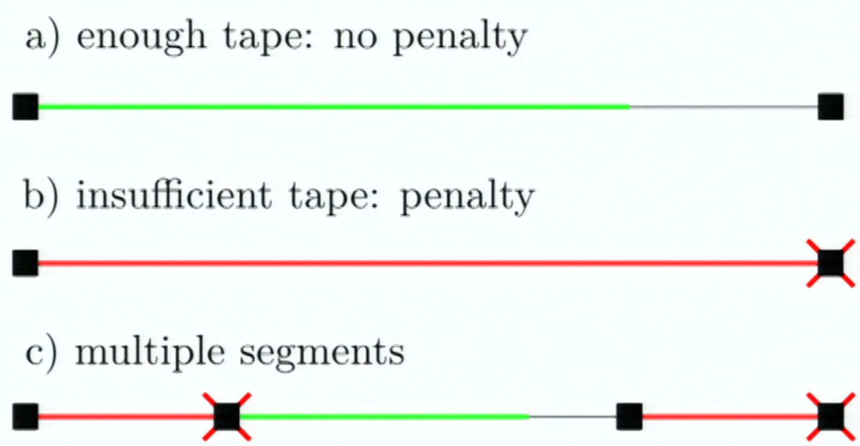
Halting → gapped (a)
Non halting → gapless (b);



Only works in 2D

There are no quasi-periodic tilings in 1D!

The 1D marker Hamiltonian



We divide the spin chain into tape segments delimited by a special marker.

On each tape segment we will start one instance of the QTM. We will penalize the QTM for running out of tape (unlike in 2D!).

We will give a bonus to each tape segment which decreases with the length of the segment, and which is always smaller than the QTM penalty.

Competing bonus and penalty

If the UTM with input n:

does not halt/loop:

- each tape segment will be exhausted, getting a penalty $\sim 1/T^3$
- each tape segment of length ℓ gets a bonus of $-\exp(\text{poly}(\ell))$

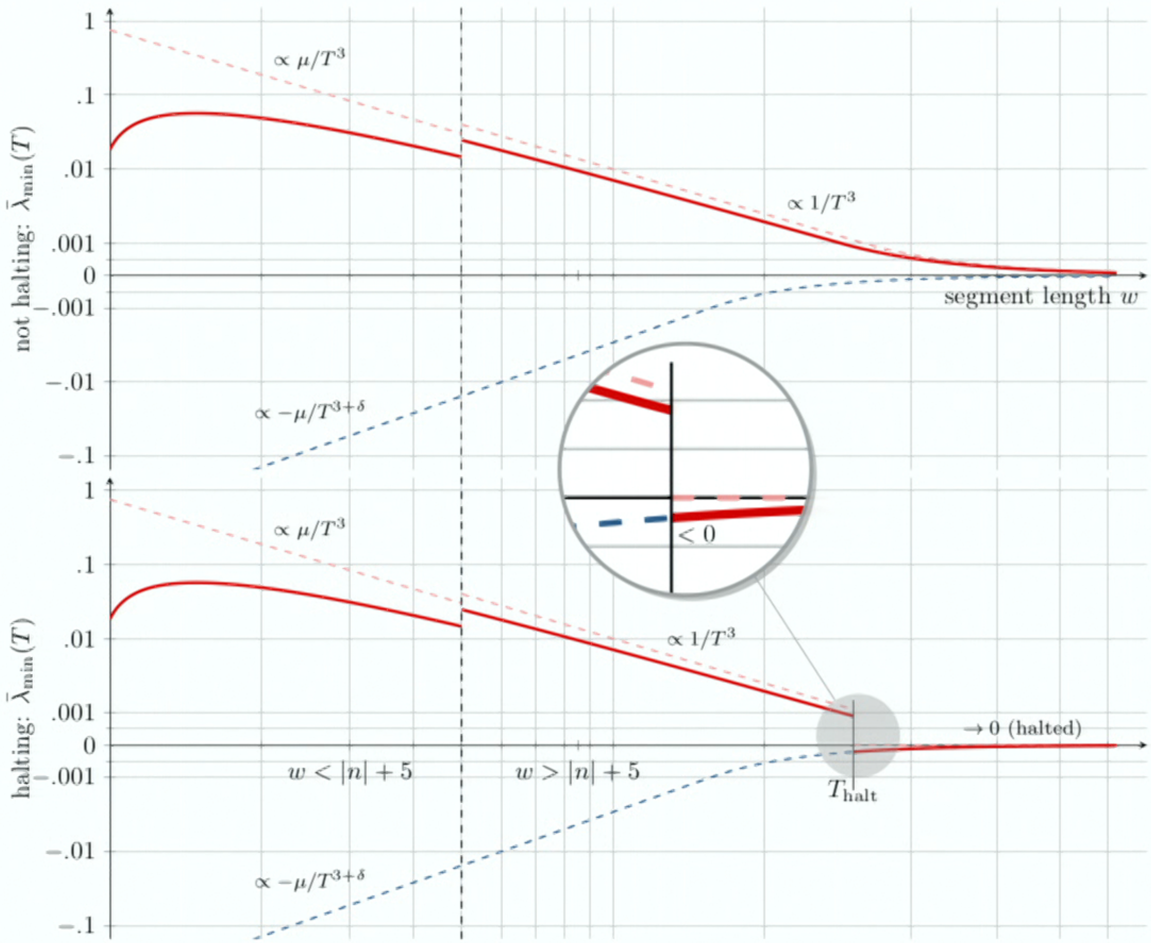
The most energetically favourable configuration is to have a single tape segment.

halts/loops:

- tape segments sufficiently large get no penalty
- each tape segment of length ℓ gets a bonus of $-\exp(\text{poly}(\ell))$

The most energetically favourable configuration is to have cut the spin chain into tape segment exactly of the minimal length required for halting.

Computation penalty + tape length bonus



17/25

The 1D Marker Hamiltonian

Building the Marker Hamiltonian

Tape segments are delimited by a special state $|\blacksquare\rangle$.

The decaying attractive interaction can be easily implemented with long range terms $f(|j-i|)\,|\blacksquare\rangle\langle\blacksquare|_i \otimes |\blacksquare\rangle\langle\blacksquare|_j$. Can we make it 2-local?

18/25

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The decaying attractive interaction can be easily implemented with long range terms $f(|j-i|)\,|\blacksquare\rangle\langle\blacksquare|_i \otimes |\blacksquare\rangle\langle\blacksquare|_j$. Can we make it 2-local?

Idea: use a counter! With special symbols $|\blacksquare\rangle$, $|\triangleright\rangle$, $|\blacktriangleright\rangle$, we want to select subspaces with a definite signature $\mathrm{sig}(|\phi_1\rangle \ldots |\phi_N\rangle) = (\langle\blacksquare|\phi_1\rangle, \ldots, \langle\blacksquare|\phi_N\rangle)$ which between segments marked by $|\blacksquare\rangle$ are of the form

$$|\blacksquare \triangleright\triangleright\triangleright \ldots \triangleright\triangleright \blacksquare\rangle + |\blacksquare \blacktriangleright\triangleright\triangleright \ldots \triangleright\triangleright \blacksquare\rangle + |\blacksquare \blacktriangleright\blacktriangleright\triangleright \ldots \triangleright\triangleright \blacksquare\rangle$$
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18/25

Marker interactions

These subspaces are groundstates of

$$\mathbf{h}_1 = |\blacktriangleright\rangle\langle\blacktriangleright| \otimes (|\triangleright\triangleright\rangle - |\blacktriangleright\triangleright\rangle)(\langle\triangleright\triangleright| - \langle\blacktriangleright\triangleright|)$$
$$\mathbf{h}_2 = (|\blacktriangleright\triangleright\rangle - |\blacktriangleright\blacktriangleright\rangle)(\langle\blacktriangleright\triangleright| - \langle\blacktriangleright\blacktriangleright|) \otimes |\blacksquare\rangle\langle\blacksquare|$$

plus the penalty terms

$$2\,|\blacksquare\blacksquare\rangle\langle\blacksquare\blacksquare| + 2\,|\triangleright\blacktriangleright\rangle\langle\triangleright\blacktriangleright| + 2\,|\blacksquare\,\triangleright\rangle\langle\blacksquare\,\triangleright|$$

This gives a 3-local Hamiltonian, positive, and block-diagonal w.r.t. states with identical signature.

Tape segments

We can get rid of segments which are not terminated by $|\blacksquare\rangle$ using a boundary trick [Gottesman-Irani]:

$$-4\sum_{i=1}^{N}|\blacksquare\rangle\langle\blacksquare|_i + 2\sum_{i=1}^{N-1}|\blacksquare\rangle\langle\blacksquare|_i \otimes |*\rangle\langle *|_{i+1} + |*\rangle\langle *|_i \otimes |\blacksquare\rangle\langle\blacksquare|_{i+1}$$

where $*$ is any of the possible symbols.

This forces g.s. to start and end with $|\blacksquare\rangle$, and lowers their energy to -4.

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The Hamiltonian is block diagonal in the "good" signature subspaces $\mathbf{H} = \oplus_s \mathbf{H}_s$ where each $\mathbf{H}_s$ is a sum of path graph Laplacians Δ_w (one for each of of the tape segments).

Energy bonus

We are finally ready to add the energy bonus which decays as the length of the segment.

We push up the energy of the boundaries (again) with $\frac{1}{2}\sum_{i=1}^{N} |\blacksquare\rangle\langle\blacksquare|_i$

We give a bonus to $|w\rangle = \underbrace{|\blacktriangleright \ldots \blacktriangleright\rangle}_{w}$ with $-\sum_{i=1}^{N-1} |\blacktriangleright\rangle\langle\blacktriangleright|_i \otimes |\blacksquare\rangle\langle\blacksquare|_{i+1}$.

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This has the effect of transforming Δ_w into $\Delta_w - |w\rangle\langle w|$.

$$\Delta_5 = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}$$

21/25

Energy bonus decay

Lemma: $\sigma(\Delta'_w) \subset (-\frac{1}{2} - \frac{1}{2^w}, -\frac{1}{2} - \frac{1}{4^w}) \cup [0, \infty)$ and it has gap $\geq \frac{1}{2}$.

Theorem

The minimal eigenvalue λ of $\mathbf{H}'_s$ satisfies

$$-\sum_i 2^{-w_i} \leq \lambda \leq -\sum_i 2^{-w_i}$$

where $(w_i)_i$ are the lengths of the segments in s. Moreover $\mathbf{H}'_s$ has gap $\geq \frac{1}{2}$.

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2-local Hamiltonian

We can replace the unitary counter with a 2-local counter (i.e. using a Quantum Thue System [Bausch, Cubitt, Ozols 2017]).

Using local dimension $d > 5$, we can achieve decay

$$-\sum_i 2^{-(d-5)^{w_i}} \leq \lambda \leq -\sum_i 2^{-(d-5)^{w_i}}$$

Marker + Propagation Hamiltonian

The groundstate energy of $\mathbf{H}_{\mathrm{QTM}} = \mathbf{H}_{\mathrm{prop}}(\phi(n), M) + \mathbf{H}_{\mathrm{comp}} + \mathbf{H}_{\mathrm{marker}}$ is

- tending to 0 if M does not halt on input n
- diverging to $-\infty$ if it does halt

Using $\mathbf{H}_{\mathrm{trivial}}$ with trivial spectrum and g.s. energy -1 and $\mathbf{H}_{\mathrm{dense}}$ with dense spectrum $[0, \infty)$ we construct:

$$\mathbf{H} = (\mathbf{H}_{\mathrm{QTM}} + \mathbf{H}_{\mathrm{dense}}) \oplus 0 + 0 \oplus \mathbf{H}_{\mathrm{trivial}} + \mathbf{H}_{\mathrm{switch}}$$

where $\mathbf{H}_{\mathrm{switch}}$ ensures that the groundstate is either an eigenstate of $\mathbf{H}_{\mathrm{trivial}}$ or of $\mathbf{H}_{\mathrm{QTM}} + \mathbf{H}_{\mathrm{dense}}$.

Marker + Propagation Hamiltonian

The groundstate energy of $\mathbf{H}_{\mathrm{QTM}} = \mathbf{H}_{\mathrm{prop}}(\phi(n), M) + \mathbf{H}_{\mathrm{comp}} + \mathbf{H}_{\mathrm{marker}}$ is

- tending to 0 if M does not halt on input n
- diverging to $-\infty$ if it does halt

Using $\mathbf{H}_{\mathrm{trivial}}$ with trivial spectrum and g.s. energy -1 and $\mathbf{H}_{\mathrm{dense}}$ with dense spectrum $[0, \infty)$ we construct:

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Low-energy spectrum

Halting $\rightarrow$ dense. Not halting $\rightarrow$ trivial.

Summary

- Combining a QTM history Hamiltonian and a 1D marker Hamiltonian, we obtain a Hamiltonian whose g.s. energy depends on the halting/non-halting of a UTM with input n
- This can be used to switch between $\mathbf{H}_{\text{dense}}$ and $\mathbf{H}_{\text{trivial}}$
- The transition is the opposite of the 2D construction
  - Before halting (because of insufficient tape **or** because UTM will never halt): trivial gapped groundstate
  - After halting (at an uncomputable system size): gapless groundstate
- Finite size analysis will not be conclusive

24/25

Open questions

- no attempt to optimize local dimension, which is huge (and unphysical) but independent of input n
- qubits are decidable: is there a threshold?
- periodic boundary conditions?
  Our construction can be extended to periodic chains of length coprime with a fixed prime P.

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Thank you for your attention!