

On preparing ground states of gapped Hamiltonians: An efficient Quantum Lovász Local Lemma

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Joint work with:

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- ▶ Understanding ground states is important, e.g., in quantum chemistry

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$H = \sum_{i=1}^m H_i$ is k -local: each term H_i acts non-trivially on k qudits (or qudits)

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$H = \sum_{i=1}^m H_i$ is frustration-free, iff $\exists |\psi\rangle$ s.t. $\langle\psi|H_i|\psi\rangle$ is minimal $\forall i \in [m]$

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E.g.: Kitaev's Toric Code

Frustration-freeness and quantum satisfiability (QSAT)

Projector description

Π_i : orthogonal projector to the subspace of excited states of H_i .

The frustration-free states of $H = \sum_{i=1}^m H_i$ and $H' = \sum_{i=1}^m \Pi_i$ are the same.

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The decision problem k-QSAT

Input: orthogonal projectors $(\Pi_i)_{i \in [m]}$, s.t. each Π_i acts on k qubits

Task: decide if $\sum_{i=1}^m \Pi_i$ is frustration-free, i.e., $\exists |\psi\rangle : |\psi\rangle \in \bigcap_{i \in [m]} \ker(\Pi_i)$

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This is a generalisation of classical satisfiability (SAT)

$$\begin{array}{ccc} \text{SAT} & \Rightarrow & \text{QSAT} \\ \underbrace{(x_1 \vee x_2 \vee x_3)}_{C_1} \wedge \underbrace{(\overline{x_1} \vee x_3 \vee \overline{x_4})}_{C_2} & \Rightarrow & \begin{array}{l} \Pi_1 := |000\rangle\langle 000|_{123} \\ \Pi_2 := |101\rangle\langle 101|_{134} \end{array} \end{array}$$

Hardness of deciding frustration-freeness

The complexity of SAT and QSAT

- ▶ 2-SAT and 2-QSAT are easy to decide (they are in P (Bravyi '06))
- ▶ 3-SAT and 3-QSAT are very hard to decide (NP-complete and QMA₁-complete (Kitaev; Gosset & Nagaj '13), respectively)

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- ▶ 3-SAT and 3-QSAT are very hard to decide (NP-complete and QMA₁-complete (Kitaev; Gosset & Nagaj '13), respectively)
- ▶ The Lovász Local Lemma (LLL) provides a sufficient condition for the satisfiability of k -SAT
- ▶ The Quantum LLL is a generalisation by Ambainis et al. for k -QSAT

The Lovász Local Lemma (LLL)

Application to k -SAT

- $\{C_i : i \in [m]\}$ are clauses of a k -SAT formula
- Each having at most d neighbours

If $p \cdot d \cdot e \leq 1$ ($p = 2^{-k}$, $e = 2.71 \dots$), then the formula is **satisfiable**.

The Lovász Local Lemma (LLL)

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Generalisation to k -QSAT

- $\{\Pi_i : i \in [m]\}$ are k -local rank- r orthogonal projectors
- Each having at most d neighbours

If $p \cdot d \cdot e \leq 1$ ($p = r \cdot 2^{-k}$, $e = 2.71 \dots$), then $\sum_{i=1}^m \Pi_i$ is **frustration-free**.

QLLL in pictures

x_1

x_2

x_3

x_4

x_5

x_6

x_7

x_8

x_9

x_{10}

x_{11}

x_{12}

x_{13}

x_{14}

x_{15}

x_{16}

QLLL in pictures

x_1

x_2

x_3

x_4

x_5

x_6

x_7

x_8

x_9

x_{10}

x_{11}

x_{12}

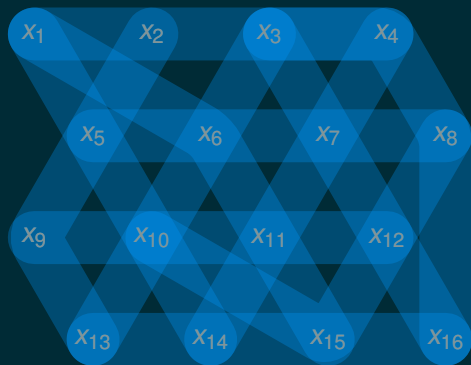
x_{13}

x_{14}

x_{15}

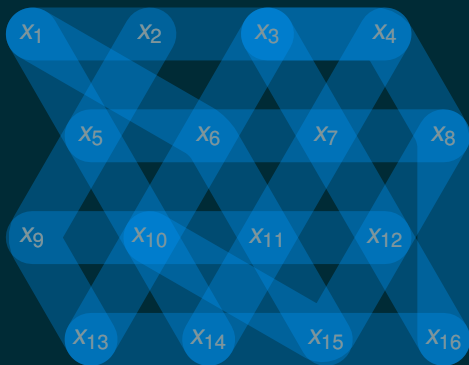
x_{16}

QLLL in pictures



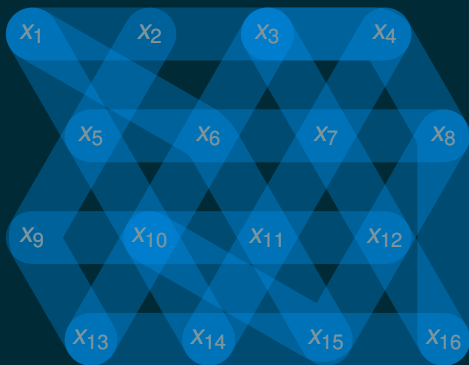
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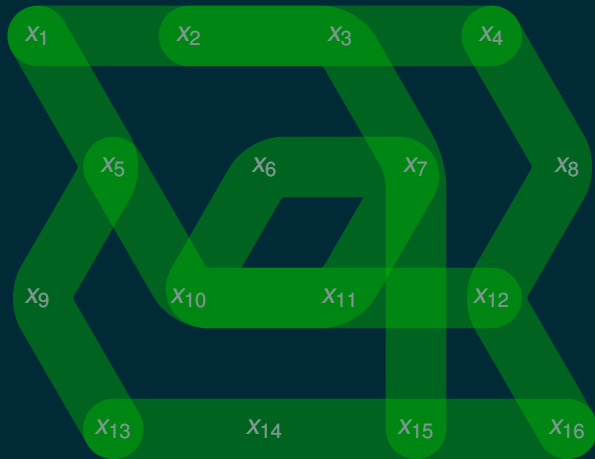


Constraints are *too interdependent*




Constraints are *too restrictive*

QLLL in pictures




The system is always frustration-free

Overview of results

		Classical	Quantum
\exists	Orig.	Lovász & Erdős ('75)	Ambainis et al. ('09)
	Best	Shearer ('85)	Sattath et al. ('16)
	Orig.	Moser & Tardos ('09)	Schwarz et al.; Arad et al. ('13) (only for commutative case)
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	Best	Kolipaka & Szegedy ('12)	This talk: Best generality + non-comm. !!!

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Finding happiness: Classical



🔧 Classical: finding a “happy” assignment

The Moser-Tardos resampling algorithm (2009)

init uniform random assignment

for all $i \in [m]$:

fix(C_i)

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check C_i

if it was “unhappy”

resample the bits of C_i

for all neighbours C_j of C_i

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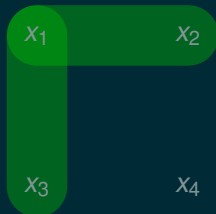
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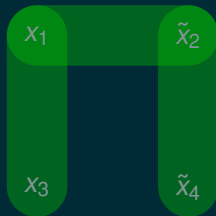
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for all neighbours C_j of C_i

fix(C_j)



⚡ Commutative quantum: finding a “happy” state

The commutative quantum resampling algorithm

init uniform random qubits

for all $i \in [m]$:

fix(Π_i)

fix(Π_i):

measure Π_i

if it was “unhappy”

resample the qubits of Π_i

for all neighbours Π_j of Π_i

fix(Π_j)

Schwarz et al.; Arad et al. (2013)

Our simplified analysis

Our key lemma

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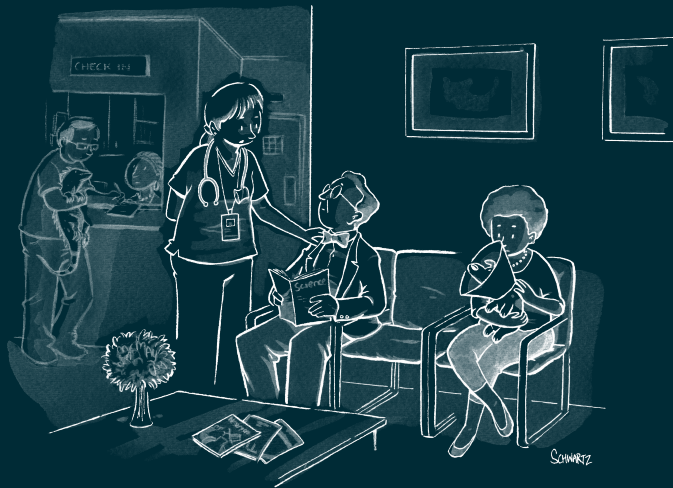
When does this algorithm terminate quickly?

► The number of length- $3m$ resample sequences is $\ll (ed)^{3m}$ (easy)

\Rightarrow The probability of seeing a length- $3m$ resample seq. $\ll (p \cdot d \cdot e)^{3m}$

If $p \cdot d \cdot e \leq 1$ then w.h.p. the alg. performs $< 3m$ resamplings

Finding happiness: Quantum



"About your cat, Mr. Schrödinger – I have good news and bad news."

Issues with non-commutativity

Becoming “unhappy” after seeing others “happy”

x_1

x_2

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x_4

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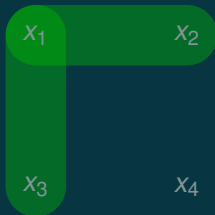
x_2

x_3

x_4

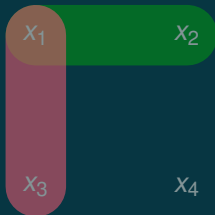
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Our key lemma

Probability of doing a specific length- ℓ resample sequence is $\leq p^\ell$

Measuring joint happiness

Perfect ground space projections of subsystems

F : set of already fixed projectors.

Define Π_F via $\ker(\Pi_F) = \bigcap_{j \in F} \ker(\Pi_j)$.

(In the commuting case $\Pi_F = \prod_{j \in F} \Pi_j$.)

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Generalised measurement procedure \mathcal{M} – for our key lemma

If $\Pi_F|\psi\rangle = 0$ (i.e. F is “happy”) and we measure it using $\mathcal{M}_{F,i}$ returning result

► “happy”, then

$$\Pi_{F \cup \{i\}} \mathcal{M}_{F,i}(|\psi\rangle) = 0$$

► “unhappy”, then

$$\Pi_i \mathcal{M}_{F,i}(|\psi\rangle) = \mathcal{M}_{F,i}(|\psi\rangle)$$

(while preserving “happiness” of non-neighbour projectors.)

Weak measurement

Weak measurement of Π_i

To weakly measure $\{\Pi_i, \text{Id} - \Pi_i\}$ use an ancilla and a Π_i -controlled rotation:

$$\Pi_i^\theta = \Pi_i \otimes R^\theta + (\text{Id} - \Pi_i) \otimes \text{Id}, \text{ where } R^\theta = \begin{pmatrix} \sqrt{1-\theta} & -\sqrt{\theta} \\ \sqrt{\theta} & \sqrt{1-\theta} \end{pmatrix}.$$

Apply Π_i^θ on $|\psi\rangle \otimes |0\rangle$ and measure the ancilla qubit (in the $|0\rangle, |1\rangle$ basis).

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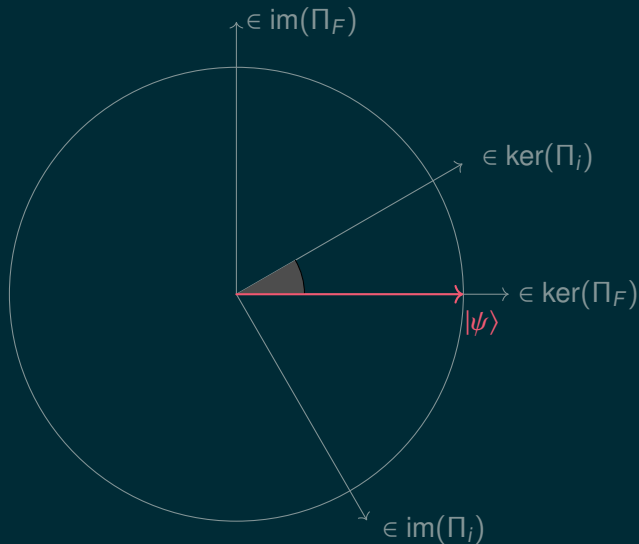
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The outcomes of a weak measurement

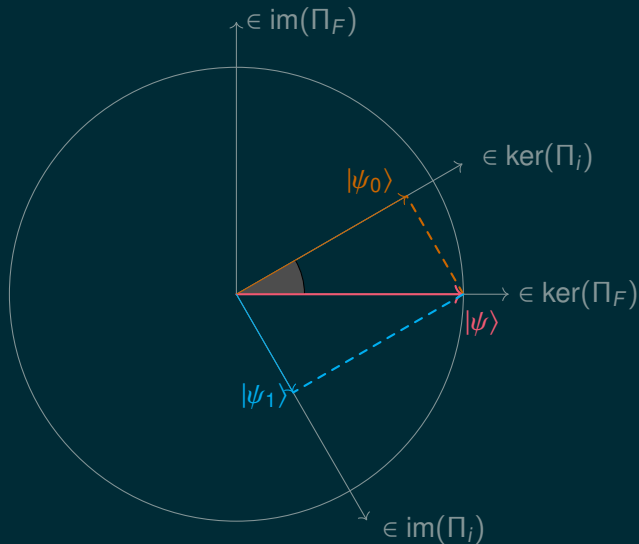
Outcome 1 : $|\psi_1^\theta\rangle = \sqrt{\theta}\Pi_i|\psi\rangle$ (unnormalised)

Outcome 0 : $|\psi_0^\theta\rangle = (\text{Id} - \Pi_i)|\psi\rangle + \sqrt{1-\theta}\Pi_i|\psi\rangle \approx |\psi\rangle - (\theta/2)\Pi_i|\psi\rangle$

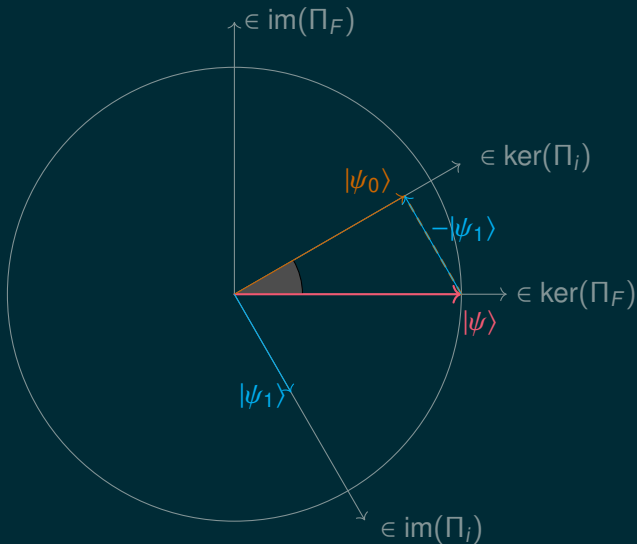
Problem with strong measurement



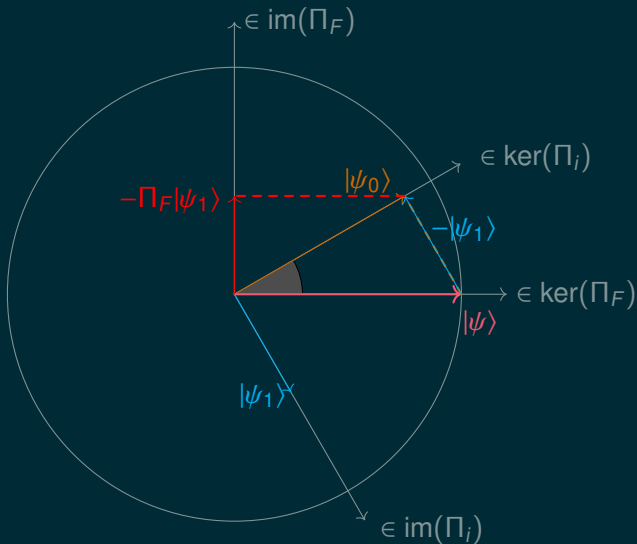
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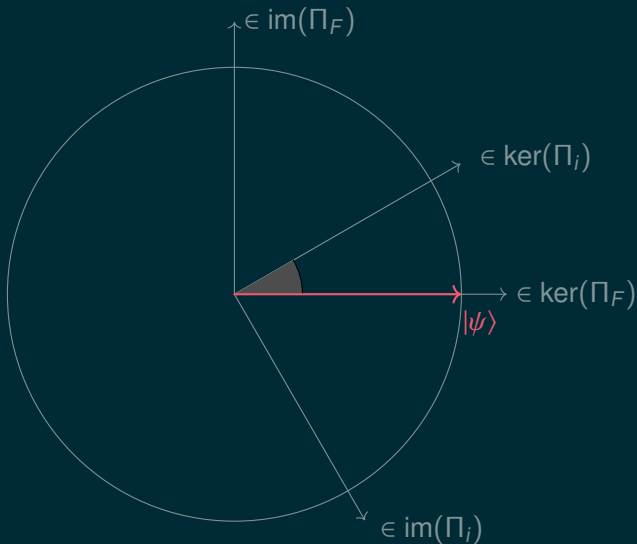
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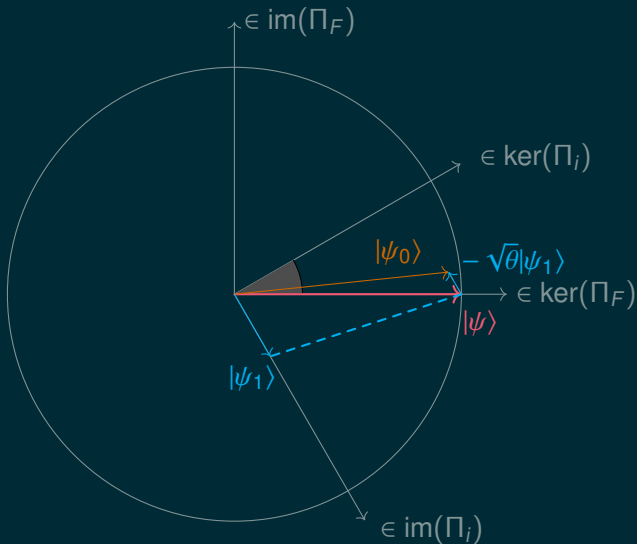
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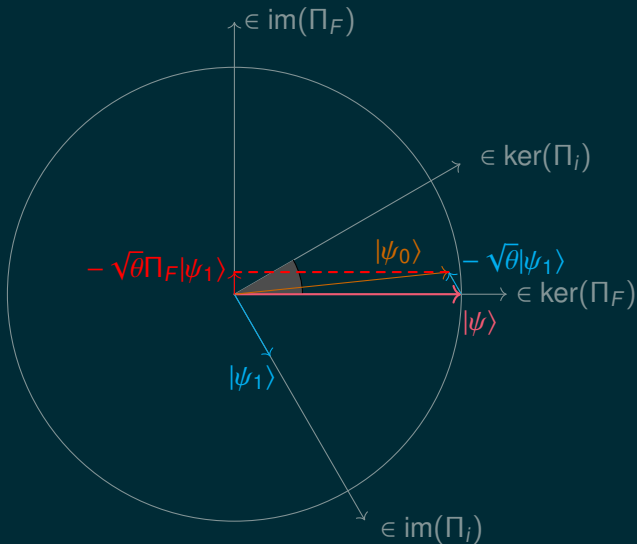
Weak measurement + quantum Zeno effect



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Implementation of \mathcal{M}

Generalised measurement $\mathcal{M}_{F,i}$

repeat T times **do**

 measure Π_i weakly **if** Π_i was detected **then return** i is “unhappy”

 measure Π_F (for quantum Zeno effect)

end repeat and return $F \cup \{i\}$ is “happy”

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We “**know in advance**” the outcome of all Π_F measurement!

$\Rightarrow \Pi_F$ can be simulated by meas. $\sim \frac{|F|}{\gamma}$ times a randomly chosen $(\Pi_j)_{j \in F}$

Runtime

The uniform gap

For $H = \sum_{i \in [m]} \Pi_i$ we define the uniform gap of H as

$$\gamma(H) := \min_{F \subseteq [m]} \text{gap} \left(\sum_{i \in F} \Pi_i \right).$$

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The overall runtime of the quantum algorithm using \mathcal{M}

$$\text{total number of measurements} = \tilde{O} \left(\frac{m^3 \cdot d}{\gamma^2} \cdot \log^2 \left(\frac{1}{\delta} \right) \right)$$

- ▶ m : number of projectors
- ▶ d : maximum number of neighbours of a projector
- ▶ γ : uniform gap
- ▶ δ : maximum trace distance of the output from a density operator supported on the ground space

Without a promise on the gap

What can we do without knowing the size of the gap?

For any input $(\Pi_i)_{i \in [m]}$ satisfying the Lovász (or Shearer) condition and $\epsilon \in \mathbb{R}_+$ we can do one of the following:

- Prepare a quantum state supported on energy eigenstates with energy below ϵ .

Or Conclude that the uniform gap is below ϵ .

Preparing low-energy quantum states

Let Π_S^δ denote the projection to the subspace of energy eigenstates with energy at least δ , with respect to $H_S = \sum_{i \in S} \Pi_i$.

Generalising the two main properties to low energy subspaces

Suppose $|\psi\rangle$ is such that $\Pi_S^\delta |\psi\rangle = 0$. We need a quantum channel $\mathcal{M}_{S,i}$ with two possible (probabilistic) outcomes:

- ▶ “happy”: $\Pi_{S \cup \{i\}}^{\delta+\varepsilon} \mathcal{M}_{S,i}(|\psi\rangle) = 0$
- ▶ “unhappy”: $\left(\Pi_{S \setminus \Gamma(i)}^{\delta+\varepsilon} \leq \Pi_S^\delta \otimes (\text{Id} - \Pi_i) \right) \mathcal{M}_{S,i}(|\psi\rangle) = 0.$

Main issue

$\Pi_{S \setminus \Gamma(i)}^{\delta+\varepsilon} \leq \Pi_S^\delta$ does not always hold! (Only if $\delta = 0$.)

Simulation results for the non-commuting case

- ▶ Various topologies tested up to 21 qubits, including cycles, grids, octahedron, dodecahedron
- ▶ Poor performance even for cycles? 2-SAT easy even classically!

Output of the LIQUi|> simulation, on C_{10}

```
0:0000.0/Classical upper bound on the expected number of resamplings : 45.0
0:0003.0/Projectors constructed
0:0003.3/Singular values found: 1022, smallest: 0.039998
0:0003.3/Hamiltonian constructed
0:0003.7/Kernel Gate constructed
0:0003.7/Run quantum test on a fixed random projector set
0:0017.2/Average resamplings in 100 simulation runs:
 0: M: 0    R: 0    E: 2.6074 P: 0.0010
 1: M: 22.1 R: 4.0 E: 0.4994 P: 0.0204
 2: M: 14.4 R: 1.5 E: 0.1820 P: 0.0364
 3: M: 12.2 R: 0.7 E: 0.1082 P: 0.0413
 4: M: 12.3 R: 0.8 E: 0.1177 P: 0.0516
 5: M: 11.3 R: 0.4 E: 0.0774 P: 0.0514
10: M: 10.6 R: 0.2 E: 0.0406 P: 0.0701
15: M: 10.7 R: 0.2 E: 0.0370 P: 0.0740
20: M: 10.6 R: 0.2 E: 0.0264 P: 0.0716
```