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

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Joint work with:
Or Sattath
Hebrew University and MIT
Ground states and frustration

- Understanding ground states is important, e.g., in quantum chemistry
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- Local Hamiltonians can describe various many-body quantum systems
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**k-local Hamiltonians**

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

\[ H = \sum_{i=1}^{m} H_i \] 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

\( \Pi_i \): 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.
Frustration-freeness and quantum satisfiability (QSAT)

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The decision problem k-QSAT

Input: orthogonal projectors $(\Pi_i)_{i \in [m]}$, s.t. each $\Pi_i$ acts on $k$ qubits
Task: decide if $\sum_{i=1}^{m} \Pi_i$ is frustration-free, i.e., $\exists \ket{\psi}: \ket{\psi} \in \bigcap_{i\in[m]} \ker(\Pi_i)$
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This is a generalisation of classical satisfiability (SAT)

$$\text{SAT} \quad \Rightarrow \quad \text{QSAT}$$

$$\left( (x_1 \lor x_2 \lor x_3) \land (\overline{x_1} \lor x_3 \lor \overline{x_4}) \right) \quad \Rightarrow \quad \Pi_1 := |000\rangle\langle 000|_{123}$$

$$\Pi_2 := |101\rangle\langle 101|_{134}$$
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 QMA$_1$-complete (Kitaev; Gosset & Nagaj ’13), respectively)
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- 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 $p \cdot d \cdot e \leq 1$ ($p = 2^{-k}$, $e = 2.71\ldots$), 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 $p \cdot d \cdot e \leq 1$ ($p = r \cdot 2^{-k}$, $e = 2.71 \ldots$), then $\sum_{i=1}^{m} \Pi_i$ is frustration-free.
QLLL in pictures

\[ x_1 \quad x_2 \quad x_3 \quad x_4 \]
\[ x_5 \quad x_6 \quad x_7 \quad x_8 \]
\[ x_9 \quad x_{10} \quad x_{11} \quad x_{12} \]
\[ x_{13} \quad x_{14} \quad x_{15} \quad x_{16} \]
QLLL in pictures

<table>
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<tr>
<th>x_1</th>
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Constraints are too interdependent
Constraints are *too interdependent*
Constraints are *too interdependent*.

Constraints are *too restrictive*.
The system is always frustration-free
Overview of results

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No constructive version was known for non-commuting projectors
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No constructive version was known for non-commuting projectors.
Finding happiness: Classical
The Moser-Tardos resampling algorithm (2009)

**init** uniform random assignment

for all $i \in [m]$ :

fix($C_i$)

**fix($C_i$):**

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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Classical: finding a “happy” assignment

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  - **resample** the bits of $C_i$
  - **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($\Pi_i$)

fix($\Pi_i$):
  measure $\Pi_i$
  if it was “unhappy"
    resample the qubits of $\Pi_i$
    for all neighbours $\Pi_j$ of $\Pi_i$
      fix($\Pi_j$)

Schwarz et al.; Arad et al. (2013)
Our simplified analysis

Our key lemma

Probability of doing a specific length-$\ell$ resample sequence is $\leq p^{\ell} \ (p = r/2^k)$
Our simplified analysis

Our key lemma

Probability of doing a specific length-$\ell$ resample sequence is $\leq p^\ell$ ($p = r/2^k$)

When does this algorithm terminate quickly?

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

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

If $p \cdot d \cdot e \leq 1$ then w.h.p. the alg. performs < 3$m$ resamplings
“About your cat, Mr. Schrödinger – I have good news and bad news.”
Issues with non-commutativity

Becoming “unhappy” after seeing others “happy”

\[
\begin{align*}
X_1 & \quad X_2 \\
X_3 & \quad X_4
\end{align*}
\]
Issues with non-commutativity

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\[ x_1 \quad x_2 \]
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Non-commutative quantum: finding a “happy” state

The quantum resampling algorithm

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for all \( i \in [m] \):
  \( \text{fix}(\Pi_i) \)

\( \text{fix}(\Pi_i) \):
  measure \( \Pi_i \)
  if it was “unhappy”
    resample the qubits of \( \Pi_i \)
    for all neighbours \( \Pi_j \) of \( \Pi_i \)
    \( \text{fix}(\Pi_j) \)

Our key lemma

Probability of doing a specific length-\( \ell \) resample sequence is \( \leq p^{\ell} \)
Measuring joint happiness

Perfect ground space projections of subsystems

\( F : \) set of already fixed projectors.

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

Generalised measurement procedure \( M \) – for our key lemma

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

- “happy”, then

\[ \Pi_{F \cup \{i\}} M_{F,i}(|\psi\rangle) = 0 \]

- “unhappy”, then

\[ \Pi_i M_{F,i}(|\psi\rangle) = M_{F,i}(|\psi\rangle) \]
(while preserving “happiness” of non-neighbour projectors.)
Weak measurement

Weak measurement of $\Pi_i$

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

$$\Pi_i^\theta = \Pi_i \otimes R^\theta + (\text{Id} - \Pi_i) \otimes \text{Id}$$

where

$$R^\theta = \begin{pmatrix} \sqrt{1 - \theta} & -\sqrt{\theta} \\ \sqrt{\theta} & \sqrt{1 - \theta} \end{pmatrix}.$$

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

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

\[ \psi \rangle \]

\[ \in \text{im}(\Pi_F) \]

\[ \in \text{ker}(\Pi_i) \]

\[ \in \text{im}(\Pi_i) \]

\[ \in \text{ker}(\Pi_F) \]
Problem with strong measurement

\[ \psi \in \ker(\Pi_F) \in \text{im}(\Pi_F) \]

\[ \psi_0 \in \ker(\Pi_i) \in \text{im}(\Pi_i) \]

\[ \psi_1 \]
Problem with strong measurement

\[ \psi \in \ker(\Pi_F) \]
\[ \psi \in \text{im}(\Pi_i) \]
\[ \psi_0 \]
\[ \psi_0 \in \ker(\Pi_i) \]
\[ \psi_1 \]
\[ \psi_1 \in \ker(\Pi_F) \]
\[ \psi \in \text{im}(\Pi_i) \]

\[ \psi_1 \]
\[ \psi \]
Problem with strong measurement

\[|\psi_1\rangle - |\psi_1\rangle = -\Pi_F|\psi_1\rangle \in \ker(\Pi_F) \notin \text{im}(\Pi_F) \notin \ker(\Pi_i) \notin \text{im}(\Pi_i) \ni |\psi_0\rangle \ni |\psi_0\rangle \]
Weak measurement + quantum Zeno effect

\[ \in \text{im}(\Pi_F) \]

\[ \in \text{ker}(\Pi_i) \]

\[ |\psi\rangle \]

\[ \in \text{im}(\Pi_i) \]
Weak measurement + quantum Zeno effect

\[ |\psi_0\rangle \hspace{1cm} - \sqrt{\theta} |\psi_1\rangle \hspace{1cm} |\psi\rangle \]

\[ \in \text{im}(\Pi_F) \]

\[ \in \ker(\Pi_i) \]

\[ \in \text{im}(\Pi_i) \]
Weak measurement + quantum Zeno effect

\[ |\psi_0\rangle - \sqrt{\theta} \Pi_F |\psi_1\rangle \]

\[ \in \ker(\Pi_i) \]

\[ \in \im(\Pi_F) \]

\[ \in \im(\Pi_i) \]

\[ |\psi_1\rangle - \sqrt{\theta} \Pi_F |\psi_1\rangle \]

\[ \in \ker(\Pi_F) \]
Implementation of $\mathcal{M}$

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

```
repeat $T$ times do
    measure $\Pi_i$ weakly
    if $\Pi_i$ was detected then return $i$ is "unhappy"
    measure $\Pi_F$ (for quantum Zeno effect)
end repeat and return $F \cup \{i\}$ is "happy"
```
Implementation of $M$

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- If $|\psi\rangle$ was “happy" w.r.t. $F \cup \{i\}$, then $M$ always returns $F \cup \{i\}$ is “happy"
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▶ If $|\psi\rangle$ was “happy" w.r.t. $F \cup \{i\}$, then $M$ always returns $F \cup \{i\}$ is “happy"

Let $\gamma$ be the energy gap (smallest non-zero. energy) of $H_{F \cup \{i\}} = \Pi_i + \sum_{j \in F} \Pi_j$.

▶ If $|\psi\rangle$ was “unhappy" w.r.t. $F \cup \{i\}$: $T \approx \frac{1}{\theta \gamma}$ suffices to find it “unhappy"
Implementation of $\mathcal{M}$

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\text{end repeat and return } F \cup \{i\} \text{ is “happy”}
\end{align*}
\]

- If $|\psi\rangle$ was “happy” w.r.t. $F \cup \{i\}$, then $\mathcal{M}$ always returns $F \cup \{i\}$ is “happy”

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- If $|\psi\rangle$ was “unhappy” w.r.t. $F \cup \{i\}$: $T \approx \frac{1}{\theta \gamma}$ suffices to find it “unhappy”

We “know in advance” the outcome of all $\Pi_F$ 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

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

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The overall runtime of the quantum algorithm using $M$

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

- $m$: number of projectors
- $d$: maximum number of neighbours of a projector
- $\gamma$: uniform gap
- $\delta$: maximum trace distance of the output from a density operator supported on the ground space
Discussion

Benefits of the algorithm

- The algorithm *only* uses local (weak and strong) measurements
Discussion

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- The algorithm **only** uses local (weak and strong) *measurements*
- Can prepare the ground state of a **50 qubit system using 51 qubits!**
Discussion

Benefits of the algorithm

- The algorithm only uses local (weak and strong) measurements
- Can prepare the ground state of a 50 qubit system using 51 qubits!
- Due to quantum Zeno effect it probably does not need error correction

Open questions

- Is there a variant which can prepare low-energy states without gap promise?
- Physically motivated examples? (quantum chemistry, spin systems, ...)
- Getting speed ups for some interesting classical problem?
- Can this result be used for showing quantum supremacy?
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 \(\epsilon\).

Or Conclude that the uniform gap is below \(\epsilon\).
Preparing low-energy quantum states

Let $\Pi^\delta_S$ denote the projection to the subspace of energy eigenstates with energy at least $\delta$, 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 $\Pi^\delta_S |\psi\rangle = 0$. We need a quantum channel $M_{S,i}$ with two possible (probabilistic) outcomes:

- "happy": $\Pi^\delta_{S \cup \{i\}} M_{S,i}(|\psi\rangle) = 0$
- "unhappy": $\left( \Pi^\delta_{S \setminus \Gamma(i)} \leq \Pi^\delta_S \otimes (\text{Id} - \Pi_i) \right) M_{S,i}(|\psi\rangle) = 0$.

Main issue

$\Pi^\delta_{S \setminus \Gamma(i)} \leq \Pi^\delta_S$ 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/Hamiltoninan 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
```