Dequantizing the Quantum Singular Value Transform: Hardness and applications to quantum chemistry and the quantum PCP conjecture

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Theme

Where is the "boundary" between the power of classical versus quantum computers?

Guiding questions

1. Can one rigorously define such “boundaries”?
   - “Quantum advantage” frameworks (make classical look bad)
   - “Dequantization” via sampling (make classical look good)

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   - Shorter-term? This work?

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2. Can a practically "meaningful" such boundary be found?
   - Long-term: Shor's factoring algorithm
   - Shorter-term? This work?
3. What do such boundaries say about classical versus quantum physics?
   - Quantum PCP conjecture:

     "Natural" quantum systems can be "exponentially complex" even at high temperature

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4. Quantum PCP conjecture — do sampling assumptions break the conjecture?

Outline

1. The problem GLH
2. BQP-hardness of GLH within $1/\text{poly}$ precision
3. Classical tractibility of GLH within $O(1)$ precision
4. What does this say about Quantum PCP?

Recall

k-local Hamiltonian problem (LH)

- Input: k-local Hamiltonian H on n qubits, thresholds $0 \leq \alpha \leq \beta$ s.t. $|\alpha - \beta| \geq 1/\operatorname{poly}(n)$
- Promise: $\lambda_{\min}(H) \leq \alpha$ or $\lambda_{\min}(H) \geq \beta$
- Output: Decide whether $\lambda_{\min}(H) \leq \alpha$ or $\lambda_{\min}(H) \geq \beta$

History:

- [Kitaev 2002] LH is QMA-complete for $k = 5$ (QMA is Quantum Merlin-Arthur)
- Since then: Many hardness results e.g. in 2D, Heisenberg model, 1D translation-invariant, etc

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- Since then: Many hardness results e.g. in 2D, Heisenberg model, 1D translation-invariant, etc
- Variants:
  - If[1] $|\alpha - \beta| \geq \Omega(1)$?
    - ★ NP-hard by classical PCP theorem
    - ★ Quantum PCP conjecture: LH is QMA-complete

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Meanwhile on Earth

Question: What are quantum chemists *actually* doing[2]?

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- The quantum part:
  - Rigorous: Quantum Phase Estimation (QPE) [Abrams, Lloyd 1999], [ADLH 2005]
  - Heuristic: Variational approaches (VQA) (see [Cerezo *et al.*, 2021] for survey)

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GLH

Guided local Hamiltonian problem (GLH)

- Input:
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  2. Representation of guiding state $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$
- Promise:
  1. $\lambda_{\min}(H) \leq \alpha$ or $\lambda_{\min}(H) \geq \beta$
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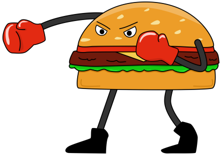
- If “representation $=$ sampling-access” $\implies$ GLH classically solvable if $\alpha, \beta, \delta \in \Theta(1)$
- If “representation $=$ semi-classical state” $\implies$ GLH BQP-hard with $|\alpha - \beta| \in \Theta(1/\text{poly})$

Punchline

- Our result: GLH with $1/\operatorname{poly}$ precision is BQP-hard
- Known: GLH with $1/\operatorname{poly}$ precision is also in BQP (i.e. can be solved efficiently quantumly)
- Thus, GLH with $1/\operatorname{poly}$ precision characterizes the power of quantum computers



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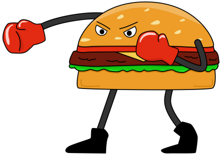

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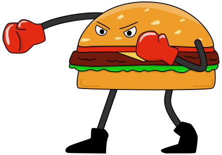

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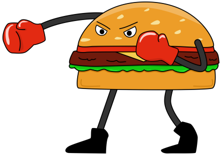

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Aside: semi-classical state $\gg$ sampling-access (given former, can simulate latter)

- Choice of representation is *not* bottleneck preventing $1/\operatorname{poly}$ precision classically

Outline

Our result, formally

Recall: Guided local Hamiltonian problem (GLH)

- Input: k-local Hamiltonian H on n qubits, $\alpha < \beta$, semi-classical $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$
- Promise: $\lambda_{\min}(H) \leq \alpha$ or $\lambda_{\min}(H) \geq \beta$, $\|\Pi_H|\psi\rangle\|_2 \geq \delta$
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Semi-classical state

Any $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$ s.t. there exists $S \subseteq \{0,1\}^n$ of size $|S| \in \text{poly}(n)$, s.t. (cf. [Grilo, Kerenidis, Sikora 2016])

$$|\psi\rangle = \frac{1}{\sqrt{|S|}} \sum_{x \in S} |x\rangle.$$

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Theorem

For any $\delta \in (0, 1/2 - 1/\text{poly}(n))$, $\exists \alpha, \beta \in [0,1]$ with $\beta - \alpha \geq 1/\text{poly}(n)$ such that GLH is BQP-hard.

Proof sketch

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Proof sketch.

Let $x \in \{0, 1\}^n$ be an input, and $U = U_m \cdots U_1$ a BQP circuit deciding x.

Goal: Map U to instance $(H, \alpha, \beta, |\psi\rangle)$ of GLH such that $\beta - \alpha \geq 1/\text{poly}(n)$ and

$$\left.\begin{array}{l} \text{if } U \text{ accepts } x \implies \lambda_{\min}(H) \leq \alpha \\ \text{if } U \text{ rejects } x \implies \lambda_{\min}(H) \geq \beta \end{array}\right\} \textbf{Both cases: } |\psi\rangle \text{ overlap} \geq \delta \text{ with ground space of } H$$

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Tool 1: Feynman-Kitaev Circuit-to-Hamiltonian construction [Kitaev 1999]

- Maps U to 5-local H satisfying left hand side above, where $H = H_{in} + H_{out} + H_{prop} + H_{stab}$.
- To design $|\psi\rangle$ (right hand side above), need to modify H further

Tool 1: Feynman-Kitaev Hamiltonian

$H = H_{\text{in}} + H_{\text{out}} + H_{\text{prop}} + H_{\text{stab}}$ encodes action of U in low-energy history state

$$|\psi_{\text{hist}}\rangle = \frac{1}{\sqrt{m+1}} \sum_{t=0}^{m} U_t \cdots U_1 |x\rangle_A |0\cdots 0\rangle_B |t\rangle_C,$$

H_{in}:	Correct ancilla initialization at time $t = 0$	$\rightarrow$	$\langle\psi_{\text{hist}}\|H_{\text{in}}\|\psi_{\text{hist}}\rangle = 0$
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Together: $|\psi\rangle := |x\rangle_A|0\rangle_B \left(\frac{1}{\sqrt{m}}\sum_{t=0}^{m}|t\rangle\right)_C \overset{\text{pre-idle}}{\approx} |\psi_{\text{hist}}\rangle \overset{\text{by }\Delta}{\approx}$ ground state of H

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H' &:= \frac{\alpha+\beta}{2} I_{ABC} \otimes |0\rangle\langle 0|_D + H_{ABC} \otimes |1\rangle\langle 1|_D, \\
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\end{aligned}
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where

- If x is YES instance (resp. NO instance), $\lambda_{\min}(H) \leq \alpha$ (resp. $\lambda_{\min}(H) \geq \beta$)
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- $\lambda_{\min}(H) \geq \beta \implies \lambda_{\min}(H')$ is in $|0\rangle\langle 0|_D$ block $\implies |\psi\rangle_{ABC}|0\rangle_D$ is good guiding state

Outline

Our result, formally

Recall: Guided local Hamiltonian problem (GLH)

- Input: sparse Hamiltonian H on n qubits, $\alpha < \beta$, samplable $|\psi\rangle \in (\mathbb{C}^2)^{\otimes n}$
- Promise: $\lambda_{\min}(H) \leq \alpha$ or $\lambda_{\min}(H) \geq \beta$, $\|\Pi_H|\psi\rangle\|_2 \geq \delta$
- Output: Decide whether $\lambda_{\min}(H) \leq \alpha$ or $\lambda_{\min}(H) \geq \beta$

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ζ-samplable state for $\zeta \in [0, 1)$

Have ζ-sampling-access to $|\psi\rangle \in \mathbb{C}^{2^n}$ if all three hold:

- (query access) For any $i \in [2^n]$, can compute $\psi_i \in \mathbb{C}$ in $\text{poly}(n)$ classical time
- (sampling access) Can sample in $\text{poly}(n)$ classical time from distribution $p\colon [2^n] \to [0, 1]$ such that

$$\forall j \in [2^n] \qquad p(j) \in \left[(1-\zeta)\frac{|\psi_j|^2}{\||\psi\rangle\|^2}, (1+\zeta)\frac{|\psi_j|^2}{\||\psi\rangle\|^2}\right]$$

- (norm approximation) Have m s.t. $|m - \||\psi\rangle\||\leq \zeta\,\||\psi\rangle\|$.

Note: When $\zeta = 0$, recover [Tang 2019]'s definition from dequantization of recommender systems

$n = \#$ of qubits

Theorem: GLH "tractable" in $O(1)$-precision setting

$\forall$ constants $\delta, \alpha, \beta \in (0, 1]$ and $k \in O(\log n)$, GLH classically solvable in $\mathrm{poly}(n)$ time with probability $1 - 2^{-n}$.

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$$\Uparrow$$

Theorem (informal)

The sparse “Guided Singular Value Estimation” problem is efficiently solvable to $O(1)$ precision.

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choose constant-degree polynomial P in QSVT to “process” singular values

$\rightarrow$ possible in $O(1)$-precision setting

Theorem (informal)

The sparse Quantum Singular Value Transform (QSVT) can be “dequantized” for $O(1)$ precision.

Dequantizing the QSVT

Singular Value Transform (SVT)

Input: (1) query-access to s-sparse matrix $A \in \mathbb{C}^{M \times N}$ with $\|A\| \leq 1$
(2) query-access to $u \in \mathbb{C}^N$ s.t. $\|u\| \leq 1$
(3) ζ-samplable $v \in \mathbb{C}^N$ s.t. $\|v\| \leq 1$
(4) even polynomial $P \in \mathbb{R}[x]$ of degree d (even $\implies$ for all $x \in \mathbb{R}$, $P(x) = P(-x)$)

Output: estimate $\hat{z} \in \mathbb{C}$ s.t. $|\hat{z} - v^\dagger P(\sqrt{A^\dagger A})u| \leq \epsilon$

Lemma: Dequantizing SVT

$\forall \epsilon \in (0, 1]$ and $\zeta \leq \epsilon/8$, SVT solvable classically with probability $1 - 1/\operatorname{poly}(N)$ in $O^*((s^{2d+1})/\epsilon^2)$ time.

Proof sketch for dequantizing SVT

SVT(s, ϵ, ζ) (singular value transform)

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Proof sketch.

Idea (à la [Tang 2019]): Compute r random entries of $\langle v, P(\sqrt{A^\dagger A})u\rangle$, take arithmetic mean:

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Correctness: High probability bound obtained via Chebyshev's inequality

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Choosing the polynomial

Suppose we wish to decide if A has a singular value in range $[a, b]$.

Then, roughly:

1. Modify polynomial construction of [Low, Chuang, 2017] to compute $O(1)$-degree polynomial P s.t.

$$\begin{aligned} \forall x \in [a, b] \quad &\Longrightarrow \quad P(x) \approx 1 \\ \forall x \notin [a, b] \quad &\Longrightarrow \quad P(x) \approx 0. \end{aligned}$$

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2. Apply classical SVT algorithm to estimate $u^\dagger P(\sqrt{A^\dagger A})u$.

Outline

1. The problem GLH
2. BQP-hardness of GLH within $1/\text{poly}$ precision
3. Classical tractibility of GLH within $O(1)$ precision
4. What does this say about Quantum PCP?

Quantum PCP conjecture

Recall: k-local Hamiltonian problem (LH)

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This work: Theorem

LH with $b - a \geq \Omega(1)$, and promise there *exists* ζ-samplable guiding state $|\psi\rangle$ with constant overlap with ground space, is in Merlin-Arthur (MA).

A new NLTS-inspired conjecture

NLTS conjecture [Freedman, Hastings 2014]

$\exists$ family of $O(1)$-local n-qubit Hamiltonians $\{H_n\}_{n\in\mathbb{N}}$, and constant $\epsilon > 0$ s.t. for any family of states $\{|\varphi_n\rangle\}_{n\in\mathbb{N}}$ generated by constant-depth quantum circuits, we have for any sufficiently large n:

$$\langle\varphi_n|H_n|\varphi_n\rangle > \lambda_{\min}(H_n) + \epsilon.$$

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This work: NLSS conjecture

$\exists$ family of $O(1)$-local n-qubit Hamiltonians $\{H_n\}_{n\in\mathbb{N}}$, and constant $\epsilon > 0$ s.t. for any family of states $\{|\varphi_n\rangle\}_{n\in\mathbb{N}}$ allowing perfect-sampling-access (i.e. $\zeta = 0$), we have for any sufficiently large n:

$$\langle\varphi_n|H_n|\varphi_n\rangle > \lambda_{\min}(H_n) + \epsilon.$$


THANK YOU

Shameless self-promotion

S. Gharibian, D. Rudolph. Quantum space, ground space traversal, and how to embed multi-prover interactive proofs into unentanglement.

- Finally posted today: arXiv:2206.05243 (same work as presented at QIP 2022)
- Theme: What can one "achieve" with exponentially long quantum proofs?
  - Quantum space complexity + no-go for "quantum Savitch's theorem"
  - Compressing exp-length proofs into poly-size QMA(2)/unentangled proof systems
  - Fooling quantum error-correcting codes with exp-length error processes