Improved hardness results for the guided local Hamiltonian problem

arXiv:2207.10250 (Sevag Gharibian, Ryu Hayakawa, François Le Gall, Tomoyuki Morimae)

and

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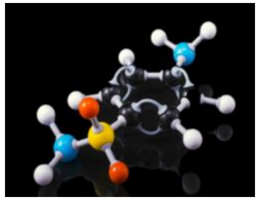
Motivation: Quantum advantage in Quantum chemistry ?

Quantum system A



"simulation"

Quantum system B

a killer app for quantum computing ?

Hermitian matrix

Ground state energy estimation (GSE, informal**):**
Given a Hamiltonian H,
compute its ground state energy $\lambda_0(H)$
up to accuracy δ

Smallest eigenvalue

The exponential quantum advantage hypothesis [LLZ+, *Nat. Comm.*'23]:

For a large set of relevant ("generic") chemistry problems, GSE may be completed exponentially more quickly (as a function of system size) on a quantum versus classical computer

But does this statement have any rigorous footing?

The local Hamiltonian problem

Definition 1

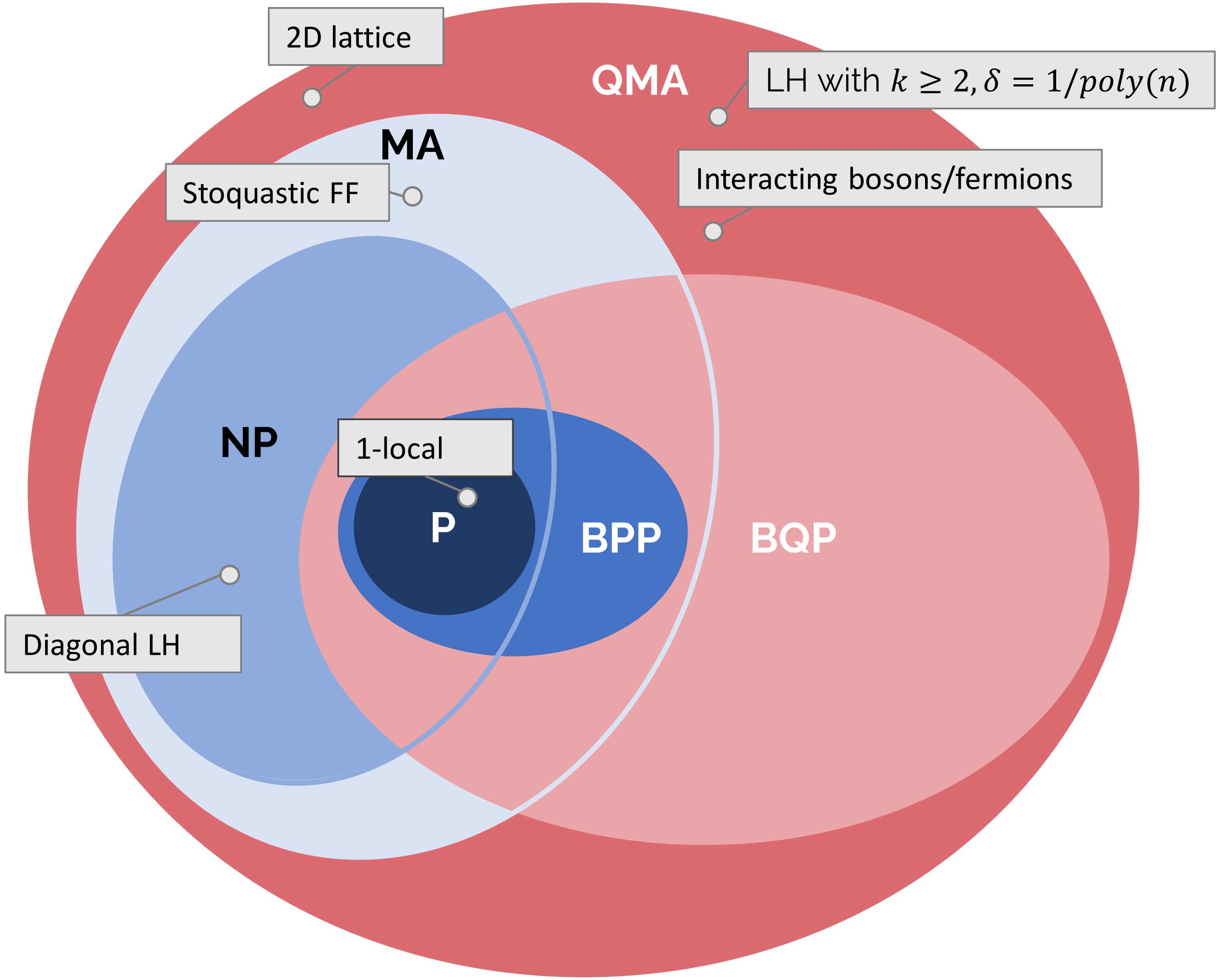
Local Hamiltonian$[k, \delta]$

Input: $H = \sum_{i=1}^{m} H_i$ on n qubits with $\|H\| \leq 1$, where each H_i acts on at most k qubits, $a, b \in \mathbb{R}$ s.t. $b - a \geq \delta > 0$.

Promise: $\lambda_0(H) \leq a$ or $\lambda_0(H) \geq b$

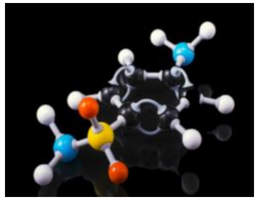
Output:
- YES if $\lambda_0(H) \leq a$
- NO if $\lambda_0(H) \geq b$

How to modify this such that it becomes a BQP-complete problem?



What is proposed in practice?

Quantum system A



“simulation”

Quantum system B

1. Ground state approximation:
A classical heuristic algorithm (e.g., Hartree-Fock) is used to obtain the description of a good guiding state $|\psi\rangle$, which is hoped to have ‘good’ fidelity with $|\psi_0\rangle$.

2. Ground state energy approximation:
Quantum phase estimation is used on $|\psi\rangle$ to estimate $\lambda_0(H)$.

Quantum advantage in ground state energy approximation?

The *guided* local Hamiltonian problem (GLH)

Definition 2

Guided local Hamiltonian$[k, \delta, \zeta]$

Input: $H = \sum_{i=1}^{m} H_i$ on n qubits, where each H_i acts on at most k qubits, $\|H\| \leq 1$, parameters $a, b \in \mathbb{R}$ s.t. $b - a \geq \delta > 0$, and a description of semi-classical quantum state $u \in \mathbb{C}^{2^n}$.

Promises: $\lambda_0(H) \leq a$ or $\lambda_0(H) \geq b$ and $\|\Pi_0 u\|^2 \geq \zeta$

(Π_0: projection into the space spanned by the ground states)

Output:

- YES if $\lambda_0(H) \leq a$
- NO if $\lambda_0(H) \geq b$

* semi-classical: efficient classical description (+ classically samplable)

SUSTech-Nagoya 2022

[GL'22]: BQP-completeness results for GLH in the precision setting $\delta = \Theta(1/poly(n))$ when

- H has locality $k \geq 6$
- The fidelity is $\zeta \in \left(\frac{1}{poly(n)}, \frac{1}{2} - \frac{1}{poly(n)}\right)$

Differs from the QMA-setting

What if it is larger?

These Hamiltonians are not physical (and hence not "generic")!

[GL'22]: The problem is in BPP when the desired precision is $\delta = \Omega(1)$ (under sampling assumptions)

This work

Definition 2

Guided local Hamiltonian$[k, \delta, \zeta]$

Input: $H = \sum_{i=1}^{m} H_i$ on n qubits, where each H_i acts on at most k qubits, $\|H\| \leq 1$, parameters $a, b \in \mathbb{R}$ s.t. $b - a \geq \delta > 0$, and a description of semi-classical quantum state $u \in \mathbb{C}^{2^n}$.

Promises: $\lambda_0(H) \leq a$ or $\lambda_0(H) \geq b$ and $\|\Pi_0 u\|^2 \geq \zeta$

(Π_0: projection into the space spanned by the ground states)

Output:

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- NO if $\lambda_0(H) \geq b$

* semi-classical: efficient classical description (+ classically samplable)

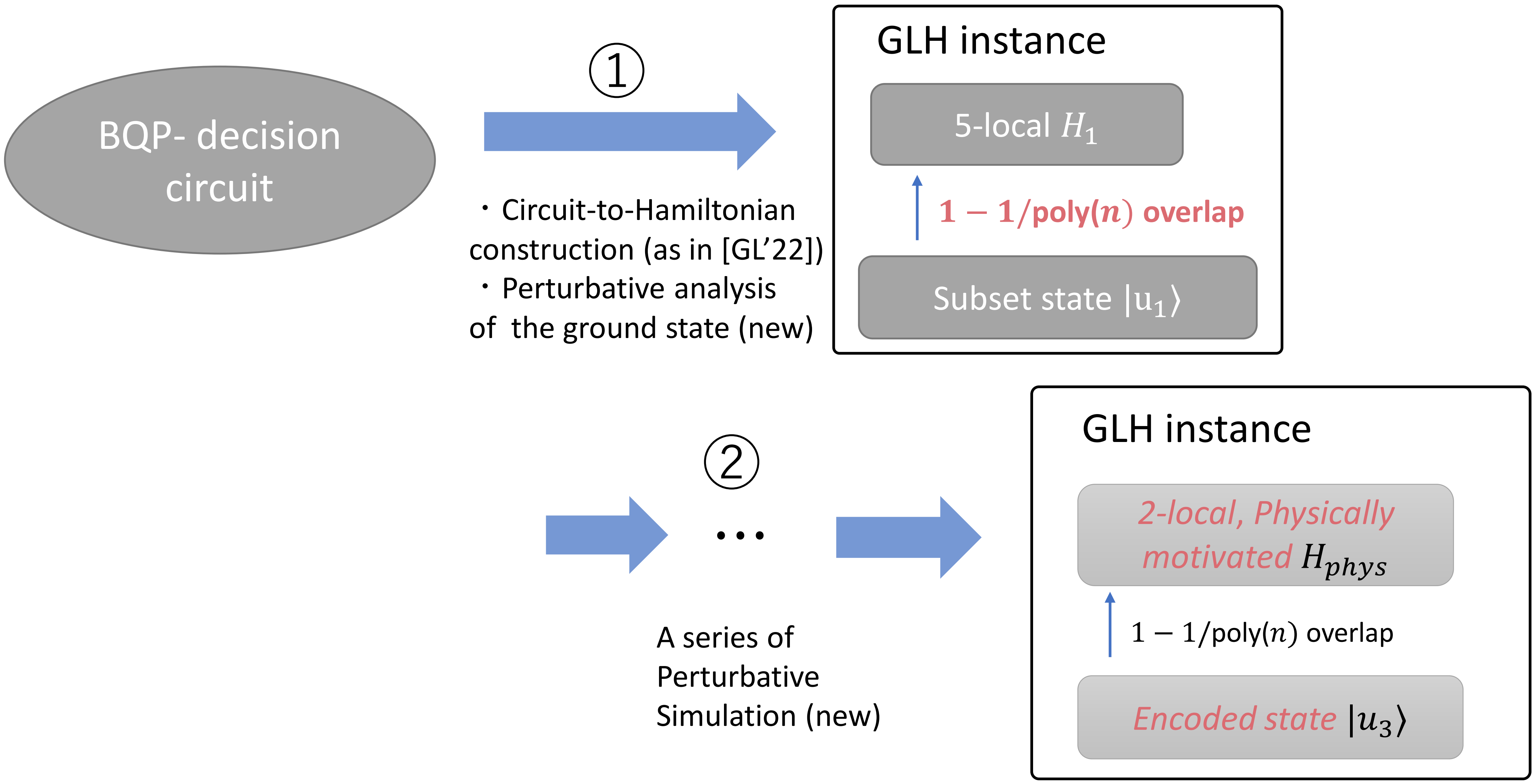
BQP-completeness results for GLH in the precision setting $\delta = \Theta(1/poly(n))$ when

- $k \geq 2$ — improvement, optimal
- $\zeta \in \left(\frac{1}{poly(n)}, 1 - \frac{1}{poly(n)}\right)$ — improvement, optimal
- H is physically motivated — New
  - XY Hamiltonian on 2D lattice
  - Antiferromagnetic XY Hamiltonian
  - Heisenberg Hamiltonian on 2D lattice
  - Antiferromagnetic Heisenberg Hamiltonian

$$H_{XY} = \sum_{\langle i,j \rangle \in E} J_{i,j}(XX + YY)_{i,j} \qquad H_{heis} = \sum_{\langle i,j \rangle \in E} J_{i,j}(XX + YY + ZZ)_{i,j}$$

Quantum advantage (assuming BPP≠BQP) for GLH for physically motivated Hamiltonians

Proof overview



Proof sketch ①: Encoding the BQP decision problem into GLH

SAME as [GL'22]

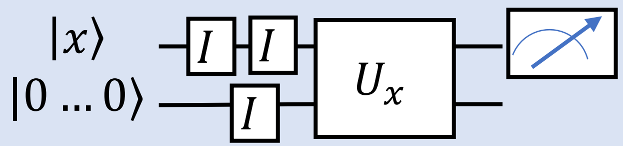
U_x: Quantum circuit that decides x

↓ Pre-idling

$\tilde{U}_x$

↓ Circuit-to-Hamiltonian construction

$$H_1 = \Delta \left(H_{in} + H_{prop} + H_{stab}\right) + H_{out}$$



Yes: $p_1 \geq \alpha = 1 - 2^{-n}$
No: $p_1 \leq \beta = 2^{-n}$

- The *unique* ground state is

$$|\psi_{\text{hist}}\rangle := \frac{1}{\sqrt{M+1}} \sum_{t=0}^{M} \tilde{U}_t \tilde{U}_{t-1} \cdots \tilde{U}_1 |x, 0\rangle \otimes |t\rangle$$

- $1/poly(n)$ gap

$1 - 1/poly(n)$ overlap for long idling

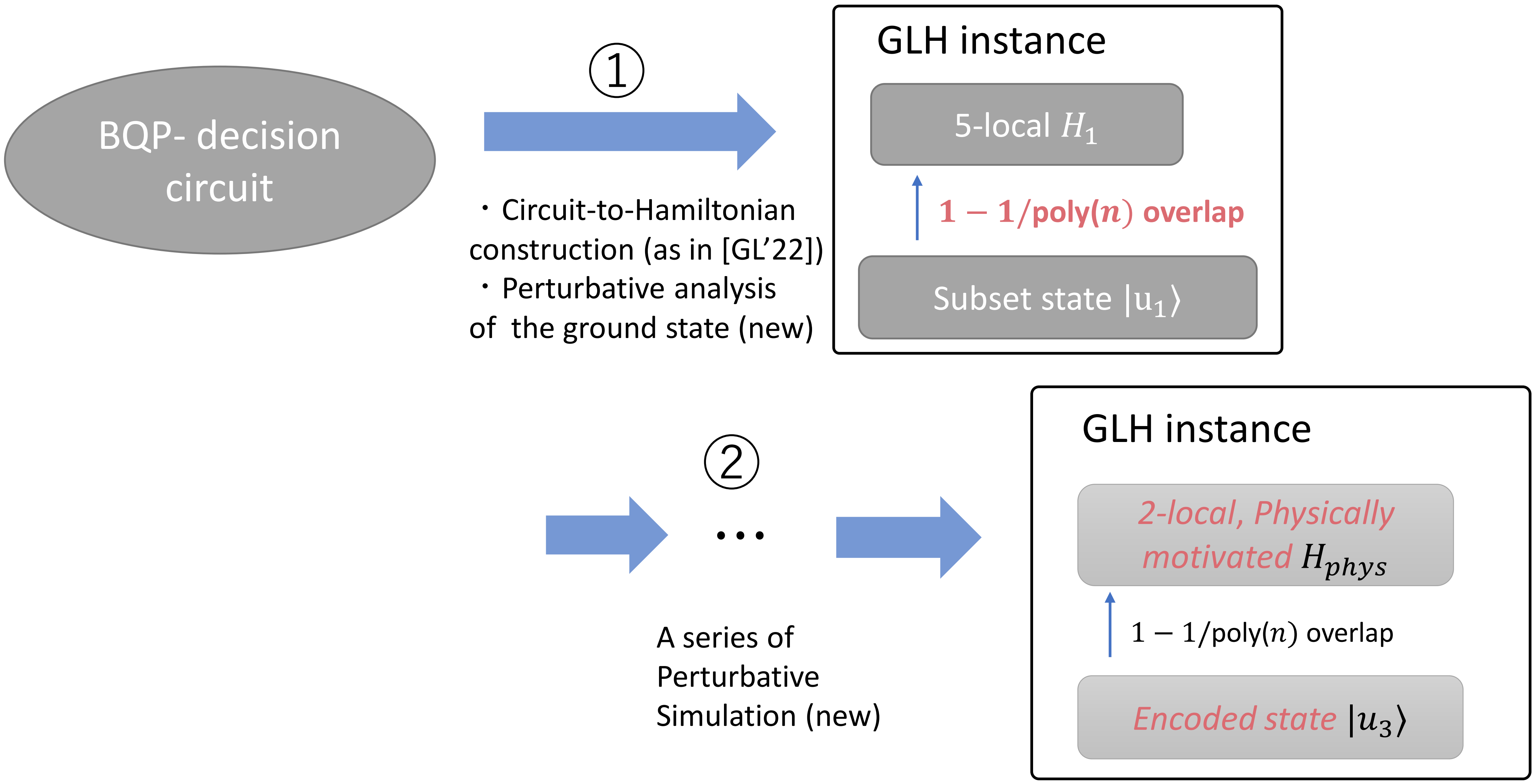
$$|u\rangle_1 := \frac{1}{\sqrt{N}} \sum_{t=1}^{N} |x\rangle_A \otimes |0\ldots0\rangle_B \otimes |t\rangle_C$$

Take large enough Δ, and apply long enough idling

Our contribution: better analysis by perturbation theory (e.g., Schrieffer-Wolf transformation)

- $1 - 1/poly(n)$ overlap between $|\psi_{hist}\rangle$ and the ground state of H_1 (instead of 1/2-1/ $poly(n)$ in the analysis from [GL'22])
- The ground state energies in the YES/NO cases have $1/poly(n)$ gap

Proof overview

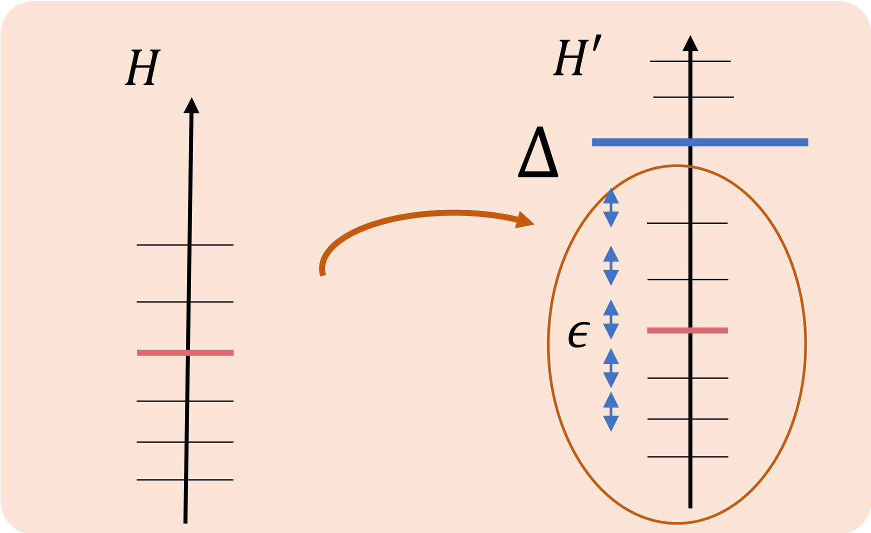


Proof sketch ② : Reduction to 2-local physically motivated Hamiltonians

Apply a chain of *Perturbative simulation*

$$H \longrightarrow H_{sparse} \longrightarrow H_{sparse,2-local} \longrightarrow \cdots \longrightarrow H_{Phys}$$

- Preserve the *energy spectrum* of the original Hamiltonian
- Preserve the *semi-classical property* of the original guiding state



This is possible because the target families of Hamiltonians are strongly universal [ZA21].

They can simulate any $O(1)$-local n-qubit Hamiltonian efficiently up to polynomially large Δ, ϵ^{-1}

Only local encodings that preserve the semi-classical property appear!

$$\left(\otimes_i V_i\right)\left(|u_1\rangle \otimes |0\rangle \otimes |1\rangle \otimes |1\rangle \otimes |+_y\rangle \otimes \cdots \otimes |+_y\rangle\right)$$

Subspace encoding *Subset state* *mediator qubits*

Summary

- Previous result [GL, STOC22] has shown the BQP-completeness (classical intractability) of the guided local Hamiltonian problem. However, the locality and the approximation parameter were not optimal. Also, it was not known if the BQP-hardness persists for physically motivated Hamiltonians

- We have shown the BQP-completeness of estimating the ground state energy of physically motivated Hamiltonians in the guided setting while improving the locality (6→2) and the approximation parameter $\left(\frac{1}{2} - \frac{1}{poly(n)} \rightarrow 1 - \frac{1}{poly(n)}\right)$.

Future directions

- Average-case classical hardness of guided local Hamiltonian problem?

Related to the quantum PCP conjecture

- The promise gap can be improved to $\Theta(1/n)$?

  (instead of $1/poly(n)$)

Quantum PCP Conjecture

no guiding vector!

LH(k,a,b) "Local Hamiltonian problem" (for $a < b$)

input: a k-local Hamiltonian H acting on n qubits such that $\|H\| \leq 1$
promise: either $\lambda_0(H) \leq a$ or $\lambda_0(H) \geq b$ holds
goal: decide which of $\lambda_0(H) \leq a$ or $\lambda_0(H) \geq b$ holds

known: [Kitaev et al. 02,06]

There exist $a,b \in [-1,1]$ with $b-a = 1/\mathrm{poly}(n)$ such that LH(2,a,b) is QMA-hard.

Currently: $\Theta(1/n^3)$
(similar in this work)
Can it be improved (say, to $\Theta(1/n)$)?

Quantum generalization of the class NP

"there exist local Hamiltonians for which estimating the ground energy with inverse-polynomial precision is very hard"

Quantum PCP conjecture:

There exist $k=O(1)$ and $a,b \in [-1,1]$ with $b-a = \Omega(1)$ such that LH(k,a,b) is QMA-hard.

"there exist local Hamiltonians for which estimating the ground energy even with constant precision is very hard"

any quantum circuit that prepares the state has at least log depth

Recent breakthrough (solution of the NLTS conjecture by Anshu, Breuckmann and Nirkhe):

There exist local Hamiltonians for which any state that estimates the ground energy with small-enough constant precision is non-trivial.