北京大学前沿计算研究中心
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An Efficient Classical Algorithm for 1. Simulating Short Time 2D Quantum Dynamics and 2. the guided Local Hamiltonian Problem

Xiao Yuan

QTML 2024

Wu, Zhang, and Yuan, arXiv:2409.04161
Zhang, Wu, and Yuan, arXiv:2411.16163

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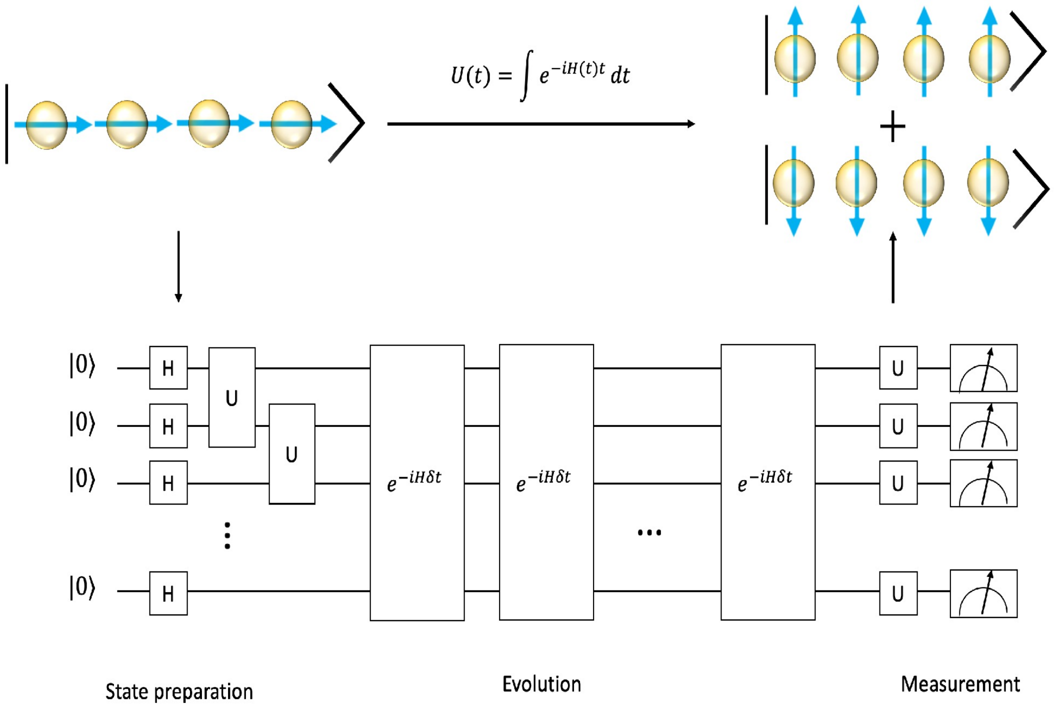
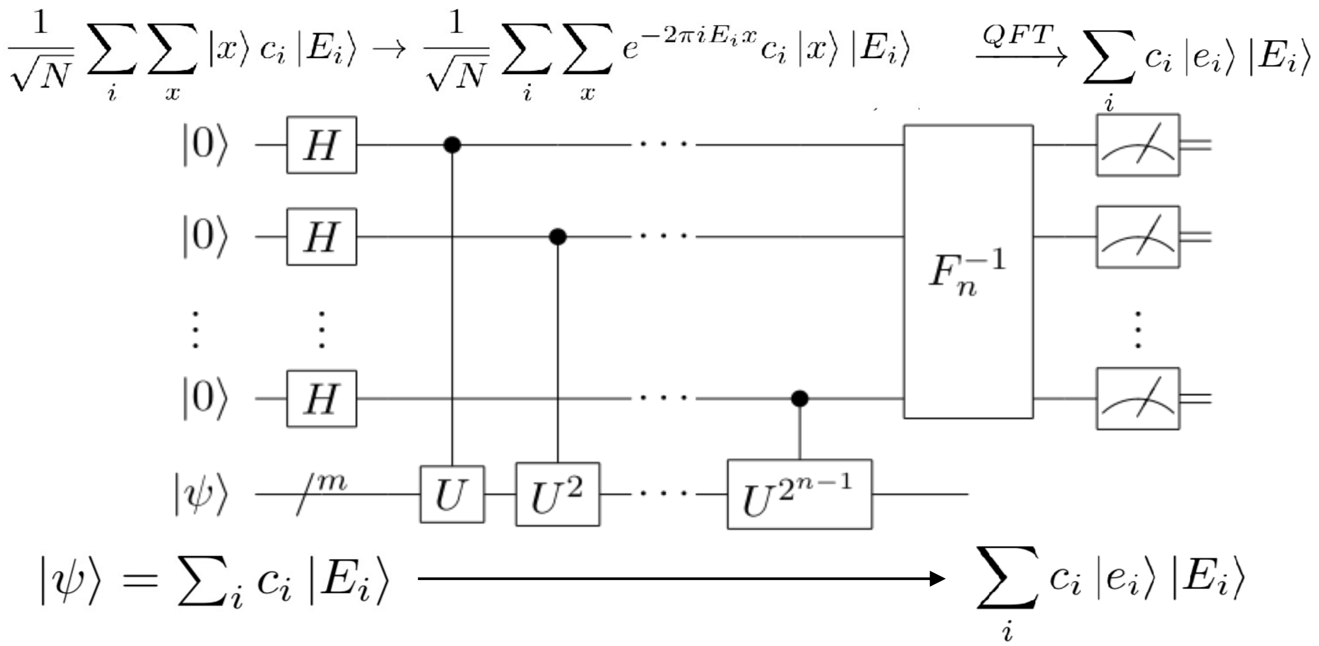
Algorithms designed for universal quantum computers

Dynamic problems: Schrodinger equation $\frac{d|\psi\rangle}{dt} = -iH|\psi\rangle$

Static problem: find the eigenstates of H



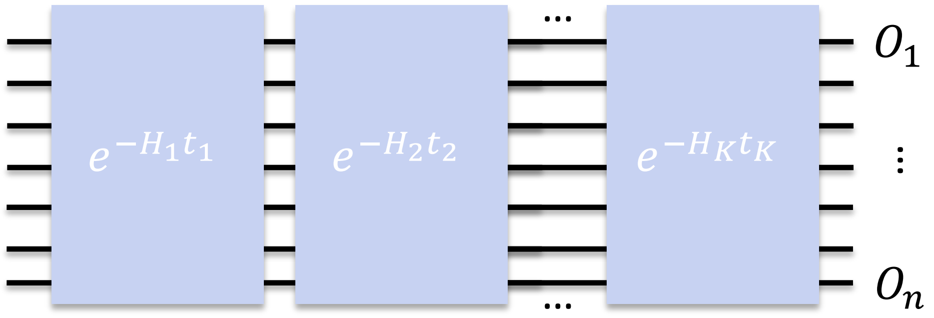


Childs, A. M., Maslov, D., Nam, Y., Ross, N. J., & Su, Y. (2018). PNAS, *115*(38), 9456-9461.

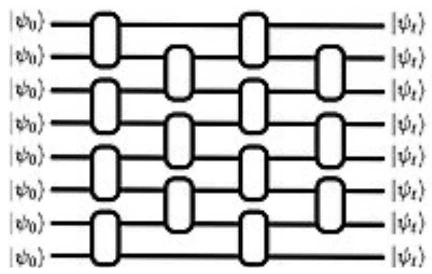
Dequantization for these quantum algorithms

Main Questions:

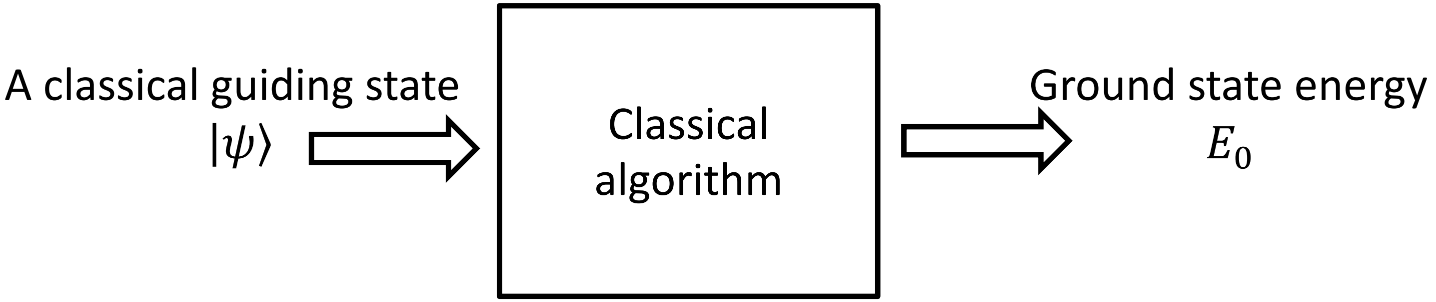
1. Classical simulation of 2D quantum system dynamics:



S Bravyi, D Gosset, R Movassagh
Nature Physics 17 (3), 337-341 (2021)



2. **Dequantization of the ground-state energy estimation (GSEE) algorithm**



Ghribian and Le Gall, STOC 2022

Dequantization of QSVT

$$|\psi_I\rangle \mapsto \frac{f(H-x)|\psi_I\rangle}{\|f(H-x)|\psi_I\rangle\|}$$

$$\|H\| \leq 1$$

1. Classical simulation of 2D quantum system dynamics

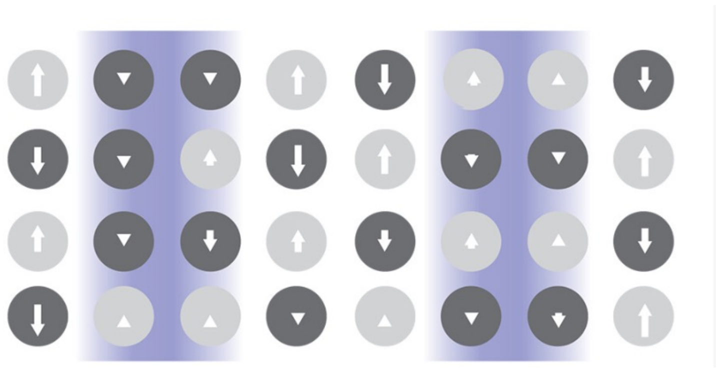
Wu, Zhang, and Yuan, arXiv:2409.04161

Understanding 2D Hamiltonian is significant

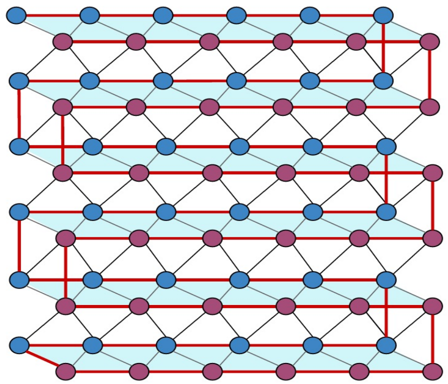
2D Hamiltonian Problems:

Theoretical perspective: quantum and anomalous Hall effects, superconductivity and magnetism

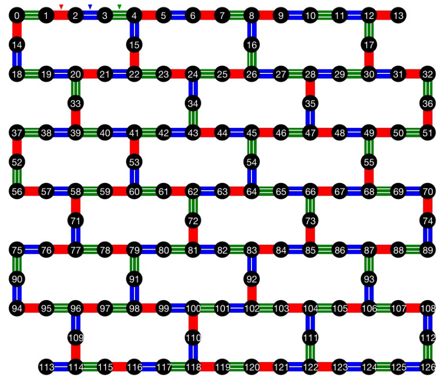
Applications: design 2D superconducting quantum computers, design functional materials such as electronics and sensors



Ground State Properties



2D Fermi-Hubbard Model

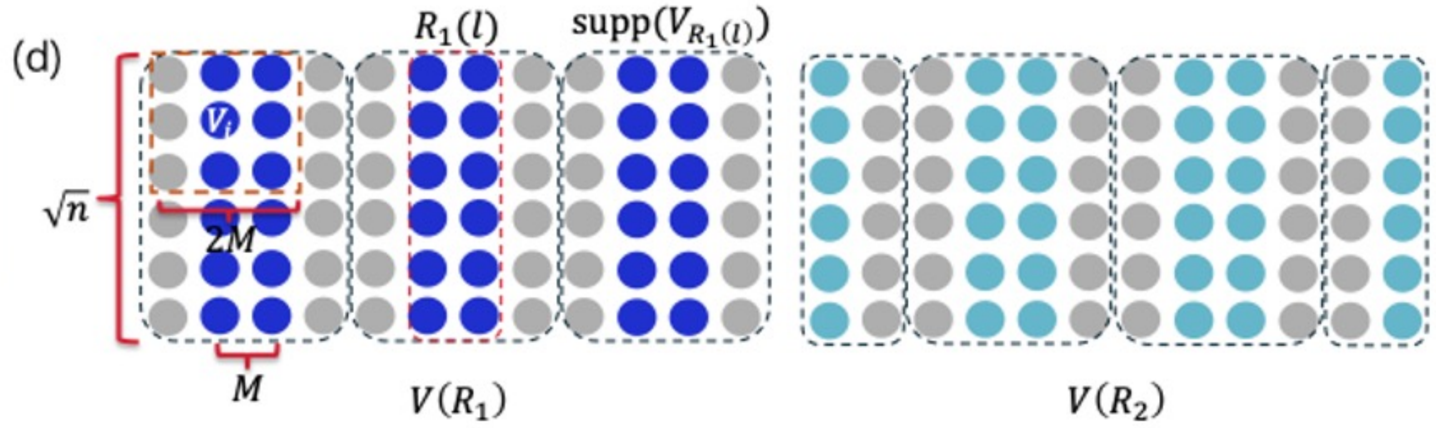


Superconducting Quantum Chip

Popular classical methods (such as MPS and PEPS) may face difficulties in tensor contraction and normalization.

Constant depth 2D quantum circuit simulation

One can efficiently calculate expectation values from constant depth 2D quantum circuits

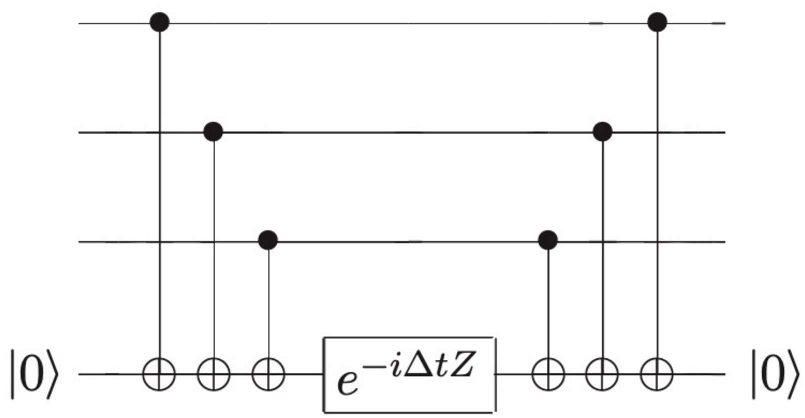


$$\hat{\mu}(t) = \sum_x \langle 0^n | V(R_1) | x \rangle \langle x | V(R_2) | 0^n \rangle = \sum_x p(x) \frac{\langle x | V(R_2) | 0^n \rangle}{\langle x | V^\dagger(R_1) | 0^n \rangle}.$$

$$p(x) = |\langle 0^n | V(R_1) | x \rangle|^2,$$

However, short (constant) time 2D dynamics may require non-constant quantum circuits

$$e^{-iZZZt} =$$

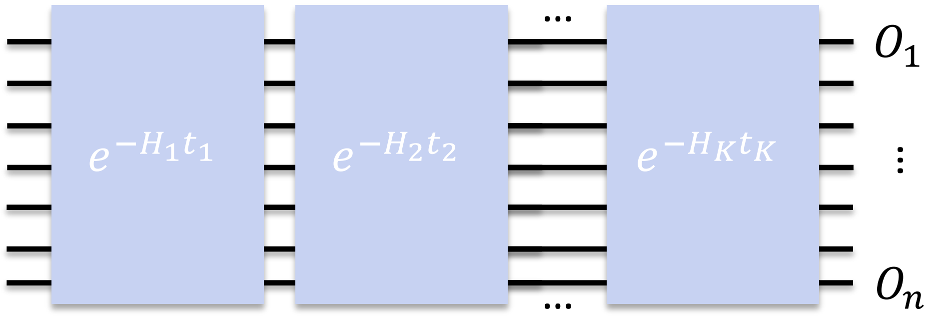


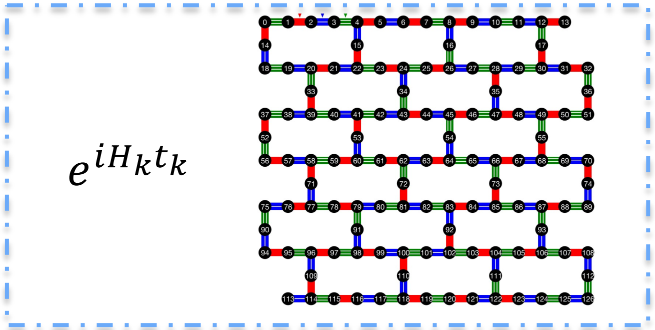
S Bravyi, D Gosset, R Movassagh, Nature Physics 17 (3), 337-341 (2021)

2D quantum system dynamics

Main Question:

Classical simulation of 2D quantum system dynamics:





Problem 1 (*K*-step Quantum Dynamics Mean Value). *Consider K local Hamiltonians $\{H^{(1)}, H^{(2)}, \cdots, H^{(K)}\}$ defined on a 2D plane, and a global observable $O = O_1 \otimes \cdots \otimes O_n$ with the operator norm $\|O_i\| \leq 1$ for $i \in [n]$. The K-step quantum mean value is defined by*

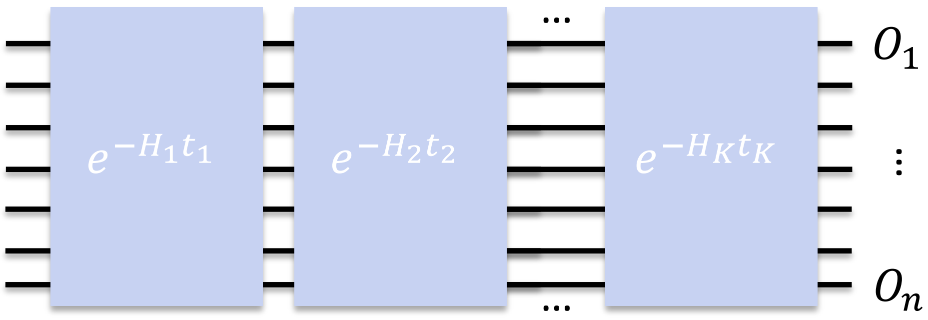
$$\mu(\vec{t}) = \langle 0^n | \left(\prod_{k=1}^{K} e^{-iH^{(k)} t_k} \right)^{\dagger} O \left(\prod_{k=1}^{K} e^{-iH^{(k)} t_k} \right) |0^n\rangle, \qquad (1)$$

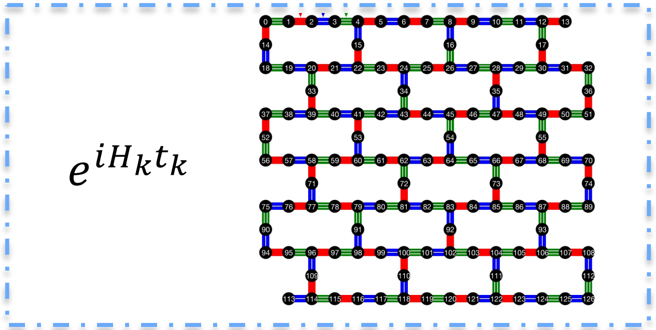
where evolution time series $\vec{t} = \{t_1, \cdots, t_K\}$ (Fig. 1. a). The target is to provide an estimation $\hat{\mu}(\vec{t})$ such that $|\mu(\vec{t}) - \hat{\mu}(\vec{t})| \leq \epsilon$.

Main Result

Classical simulation of 2D quantum system dynamics:

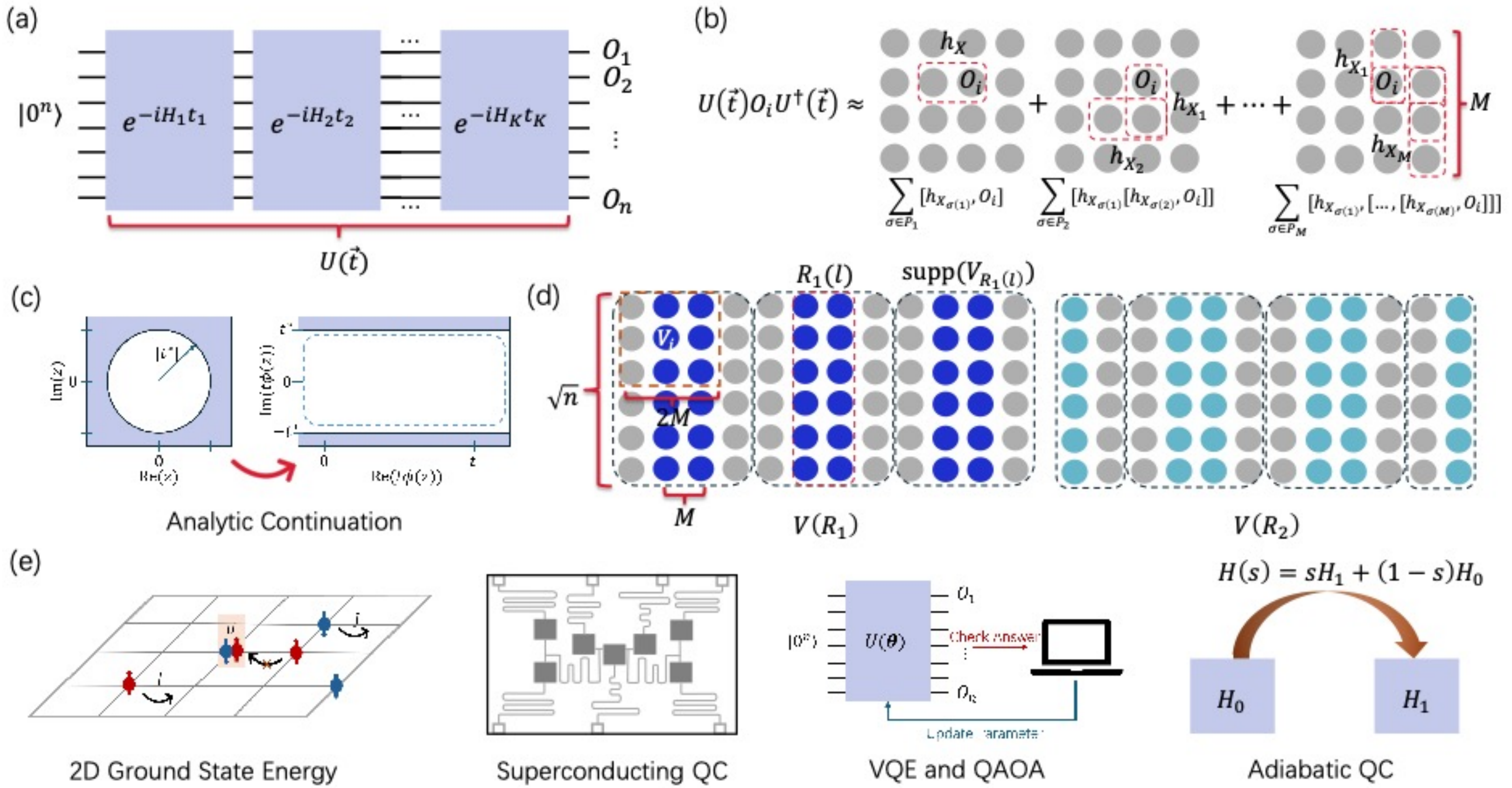
Result: *Given K Hamiltonians $\{H_1, \ldots, H_K\}$ defined on a two-dimensional Plane with n qubits, any observable $O = O_1 \otimes \cdots \otimes O_n$ with $||O_i|| \leq 1$, and time series $\{t_1, \ldots, t_K\}$ with $|t_k| \leq O(1)$, there exists a classical algorithm that outputs a ϵ-approximation to $\langle 0^n | e^{iH_1 t_1} \ldots e^{iH_K t_K} O e^{-iH_K t_K} \ldots e^{-iH_1 t_1} | 0^n \rangle$ in $n^{O(e^{Kt} \log(n/\epsilon)}$ running time, with $t = \max\{t_k\}$.*





Wu, Zhang, and Yuan, arXiv:2409.04161

Algorithm Outline



Wu, Zhang, and Yuan, arXiv:2409.04161

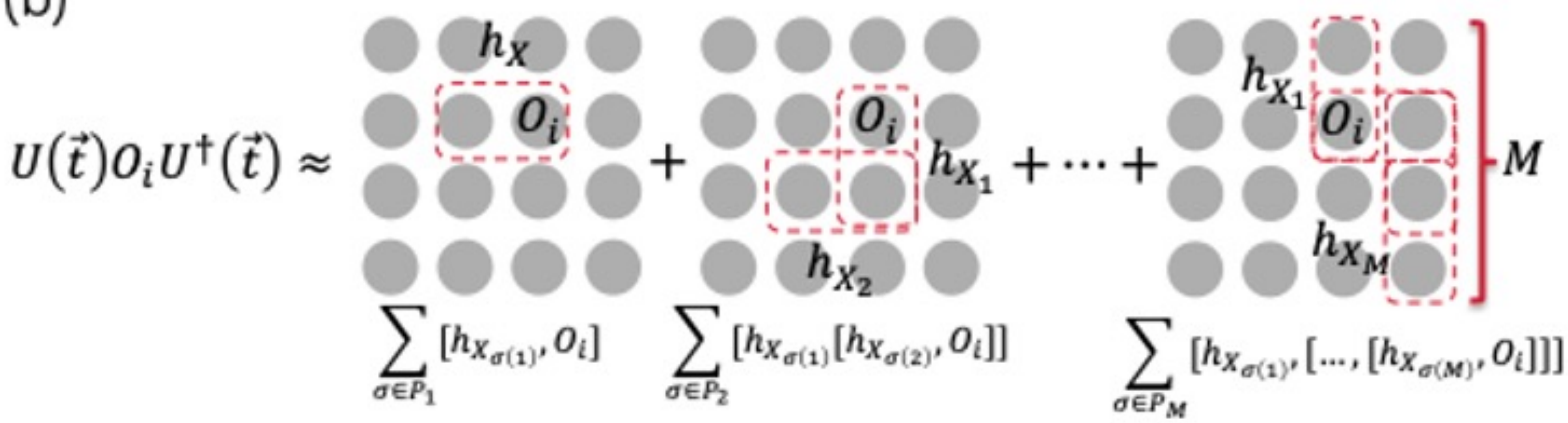
Classical simulation of 2D quantum system dynamics

Let $U = e^{-iH_K t_K} \dots e^{-iH_1 t_1}$

Observe that $\mu(\vec{t}) = \langle 0^n | U^\dagger (O_1 \otimes \cdots \otimes O_n) U | 0^n \rangle = \langle 0^n | (U^\dagger O_1 U) \dots (U^\dagger O_n U) | 0^n \rangle$

Step 1: Using the **Cluster Expansion method** to approximate $V_i = U^\dagger O_i U$ for $i \in [n]$, where V_i is limited into a $2M \times 2M$ area with $M \le O(e^{Kt} \log(n/\epsilon))$

(b)



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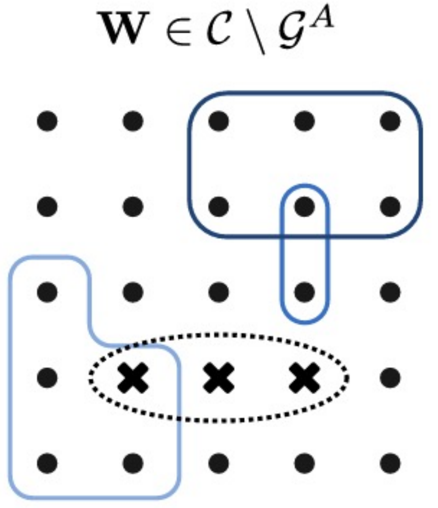
Step 1: Cluster Expansion:

Consider the Cluster Expansion:



$$e^{iHt} O_i e^{-iHt} = \sum_{m \geq 0}^{+\infty} \sum_{\boldsymbol{V} \in \mathcal{C}_m} \frac{\boldsymbol{\lambda}^{\boldsymbol{V}}}{\boldsymbol{V}!} \frac{(-it)^m}{m!} \sum_{\sigma \in \mathcal{P}_m} \left[h_{V_{\sigma(1)}}, \cdots \left[h_{V_{\sigma(m)}}, O_i \right] \right].$$

Fact 1: when the cluster $\boldsymbol{V}$ is disconnected, the commutator vanishes to 0;

Fact 2: the number of connected cluster $\boldsymbol{V}$ with size m is at most $O((e\sigma)^m)$ ($\sigma = O(1)$);

Fact 3: $\left|\left|\left[h_{V(1)}, \dots, \left[h_{V(m)}, O_i\right]\right]\right|\right| \leq 2^m ||O_i||$;

Result 1: Let the time $|t| < t^* = 1/(2e\sigma)$, then the cluster expansion of $e^{iHt} O_i e^{-iHt}$ can be truncated up to the order $M \leq O(\log(1/\epsilon(1 - 2te\sigma)))$.

Result 2: Consider more general scenarios where $U = e^{-iH_K t_K} \dots e^{-iH_1 t_1}$, the cluster expansion of $U O_i U^\dagger$ can be approximated by

$$V_i(\vec{t}) = \sum_{\substack{m_1 \geq 0 \\ \cdots \\ m_K \geq 0}}^{M} \sum_{\boldsymbol{V}_1 \cdots, \boldsymbol{V}_K \in \mathcal{G}_m^{K, O_i}} \frac{\prod_{k=1}^K (\boldsymbol{\lambda}^{\boldsymbol{V}_k} (-it_k)^{m_k})}{\prod_{k=1}^K \boldsymbol{V}_k! m_k!} \sum_{\substack{\sigma_1 \in \mathcal{P}_{m_1} \\ \cdots \\ \sigma_K \in \mathcal{P}_{m_K}}} \left[h_{V_{\sigma_1(1)}}, \cdots \left[h_{V_{\sigma_K(m_K)}}, O_i \right] \right].$$

with $O(\log(1/\epsilon(1 - 2te\sigma)^K))$ when $|\max\{t_k\}| \leq 1/(2eK\sigma)$.

Step 1: Cluster Expansion:

Using the analytical continuation method, we can extend above results to general $|max\{t_k\}| \leq O(1)$

Lemma 4 (Informal). *Given a single qubit observable O_i, then for any K-step quantum dynamics driven by $\{H^{(1)}, \cdots, H^{(K)}\}$ and corresponding constant time parameters $\{t_1, \cdots, t_K\}$, the operator $U_i(\vec{t}) = \prod_{k=1}^{K} e^{iH^{(k)}t_k} O_i \prod_{k=1}^{K} e^{-iH^{(k)}t_k}$ can be approximated by an operator $V_i(\vec{t})$ such that $\|U_i(\vec{t}) - V_i(\vec{t})\| \leq \epsilon/2L$. Here, $V_i(\vec{t})$ represents a $M = \tilde{\mathcal{O}}\left(e^{\pi teK\mathfrak{d}}\log(2L/\epsilon)\right)$-order truncated cluster expansion given by Eq. C5, $\mathfrak{d}$ represents the maximum degree of interaction graphs induced by Hamiltonians $\{H^{(1)}, \cdots, H^{(K)}\}$ and $t = \max\{t_k\}$. Meanwhile, we have*

$$\Omega(M) \leq \mathrm{supp}(V_i(\vec{t})) \leq \mathcal{O}(4M^2). \tag{D1}$$

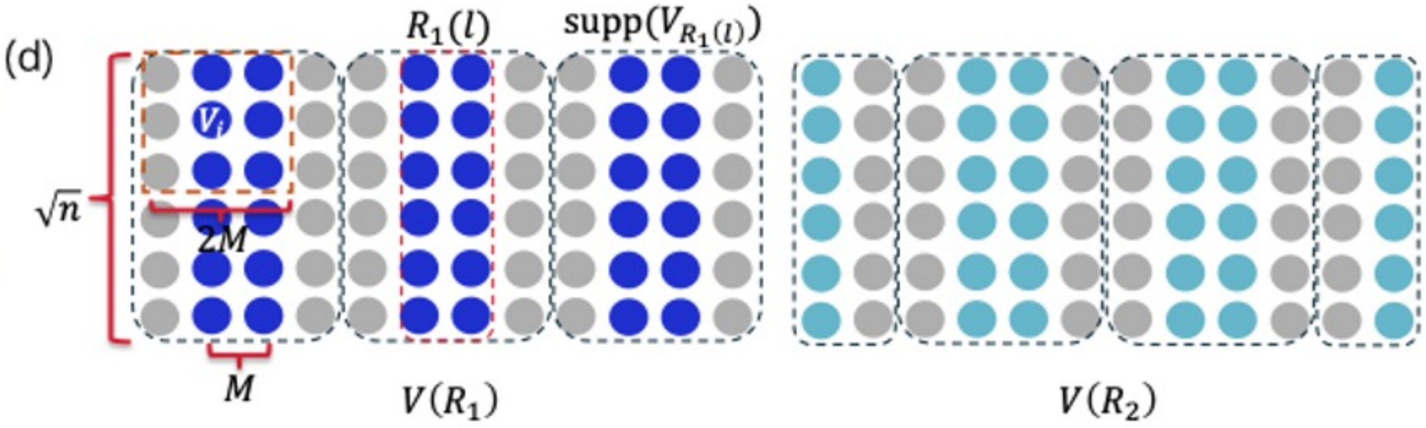
Wu, Zhang, and Yuan, arXiv:2409.04161

Step 2: local approximations:

Let $U = e^{-iH_K t_K} \dots e^{-iH_1 t_1}$

Observe that $\mu(\vec{t}) = \langle 0^n | U^\dagger (O_1 \otimes \cdots \otimes O_n) U | 0^n \rangle = \langle 0^n | (U^\dagger O_1 U) \dots (U^\dagger O_n U) | 0^n \rangle$

Step 2: Assign operators $\{V_i\}$ into two groups $V(R_1), V(R_2)$, which are easy to simulate classically



$$\hat{\mu}(t) = \sum_x \langle 0^n | V(R_1) | x \rangle \langle x | V(R_2) | 0^n \rangle = \sum_x p(x) \frac{\langle x | V(R_2) | 0^n \rangle}{\langle x | V^\dagger(R_1) | 0^n \rangle}.$$

$$p(x) = |\langle 0^n | V(R_1) | x \rangle|^2,$$

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Lemma 7. *Given the operator $V_{R_j(l)}(t)$ defined as Eq. D4, for any for $x \in \{0,1\}^n$, there exists a classical algorithm that can deterministically output $\langle x | V_{R_j(l)}(t) | 0^n \rangle$ within $C(n) \leq \mathcal{O}\left(\sqrt{n} 2^{4M^2}\right)$ running time.*

Wu, Zhang, and Yuan, arXiv:2409.04161

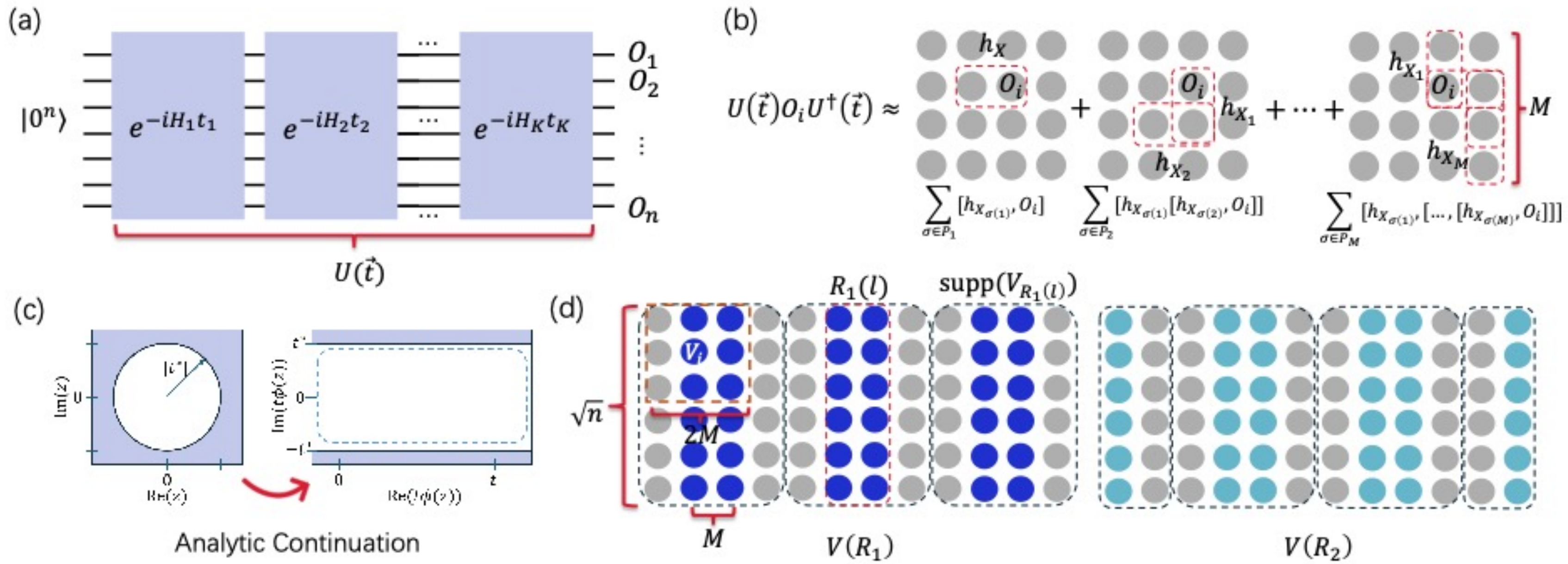
Classical simulation of 2D quantum system dynamics

Combine all together, we have

Theorem 1. *Given K Hamiltonians $\{H^{(1)}, \cdots, H^{(K)}\}$ defined on a 2D plane with n qubits, any observable $O = O_1 \otimes \cdots \otimes O_L$ with $\|O_i\| \leq 1$ and locality $L \leq n$, and a time series $\vec{t} = (t_1, \cdots, t_K)$, there exists a classical algorithm that outputs an approximation $\hat{\mu}(\vec{t})$ such that $\left|\mu(\vec{t}) - \hat{\mu}(\vec{t})\right| \leq \epsilon$ with a run time of at most*

$$\mathcal{O}\left(\frac{n}{\epsilon^2}\left(\frac{2L}{\epsilon}\right)^{e^{2\pi e K \mathfrak{d} t}\log(2L/\epsilon)}\right), \tag{2}$$

where $t = \max\{t_k\}_{k=1}^{K}$ and $\mathfrak{d}$ represents the maximum degree of the related interaction graphs.



Wu, Zhang, and Yuan, arXiv:2409.04161

A Brief Summary

Quantum Circuit	Observables	Task	Run Time
Constant depth, 2D [S. Bravyi, Nat. Phys, 2021]	Any	Mean value	Poly(n)
Constant depth, 3D [S. Bravyi, Nat. Phys, 2021]	Any	Mean value	$O(2^{n^{1/3}})$
Constant depth [S. Bravyi, STOC, 2024]	Positive semidefinite	Probability distribution	$O(n^{\log n})$
Constant depth [R. L. Mann, PRXQuantum 2024]	Close to Identity	Mean value	Poly(n)
Constant time Hamiltonian dynamics, 2D	Any	Mean value	$O(n^{\log n})$

Applications:

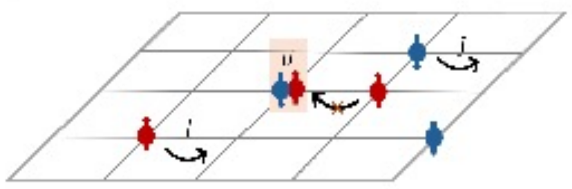
(1) 2D Guided Local Hamiltonian problem (with symmetry);

(2) Simulating shallow-depth 2D analog quantum computation;

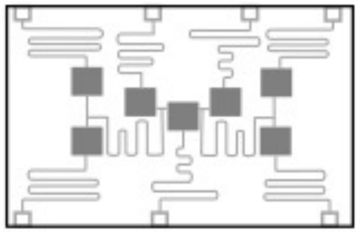
(3) Simulating 2D VQE and QAOA algorithms

(4) Simulating 2D short time Adiabatic Evolution

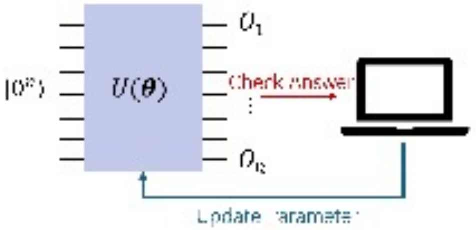
(e)



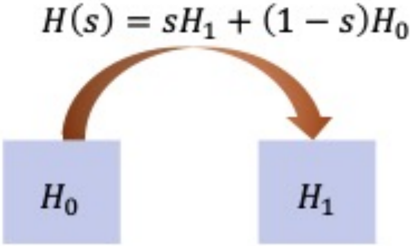
2D Ground State Energy



Superconducting QC



VQE and QAOA



Adiabatic QC

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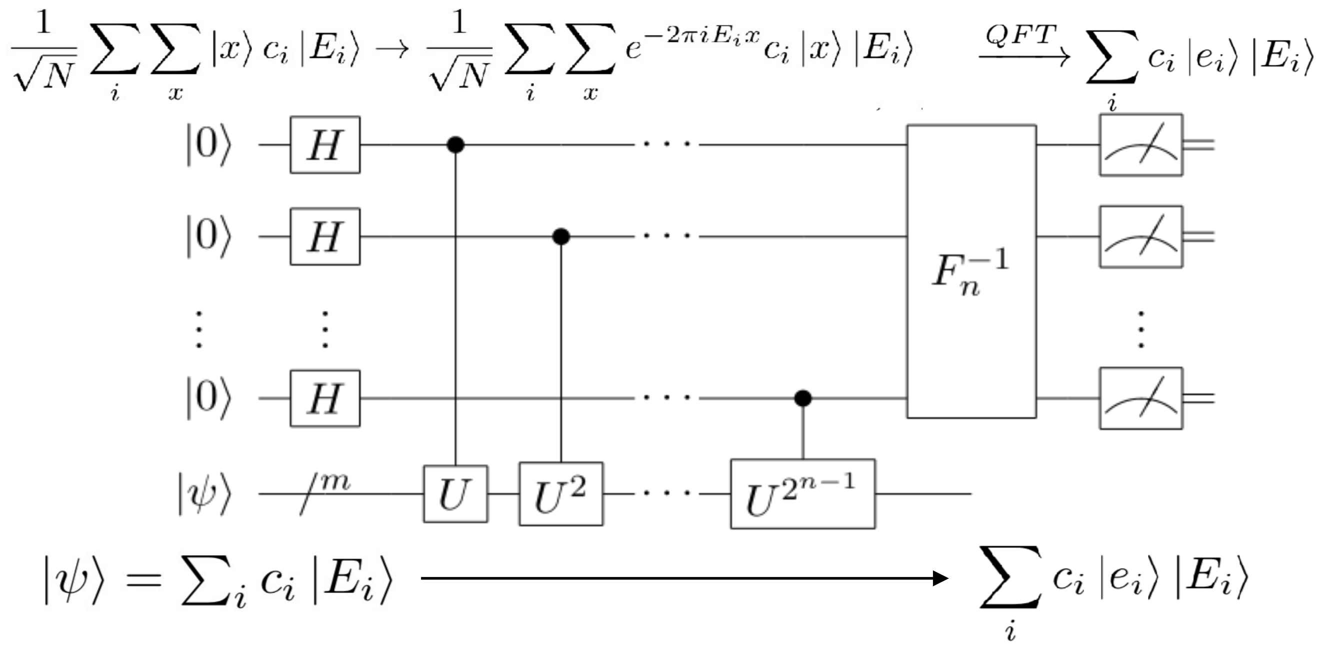
Applications 1: 2D Guided Local Hamiltonian Problem

Definition 2 (Guided local Hamiltonian problem)**.** *Input: a k-local Hamiltonian $\hat{H}$ acting on n qubits such that $\|\hat{H}\| \leq 1$ query-access to an initial state (density matrix) ρ_I*
Promise: $\|\Pi_0 \rho_I\| \geq \gamma$
Output: an estimate E_0' such that $|E_0' - E_0| \leq \epsilon$

The GLH is proved to be BQP-hard[1], meaning efficiently solvable.



[1] Gharibian, Le Gall STOC (2023)

Applications 1: 2D Guided Local Hamiltonian Problem

First define the spectrum function of the initial state as follows[1]

$$P(x) := \sum_{j=0}^{N-1} p_j \delta(x - E_j),$$

where $p_i = |c_i|^2$. Then, define the convolution function

$$\begin{aligned} C(x) &:= (f * P)(x) \\ &= (P * f)(x) = \sum_{j=0}^{N-1} p_j \int_{-\infty}^{\infty} \delta(\tau - E_j) f(x - \tau) d\tau = \sum_{j=0}^{N-1} p_j \cdot f(x - E_j). \end{aligned}$$

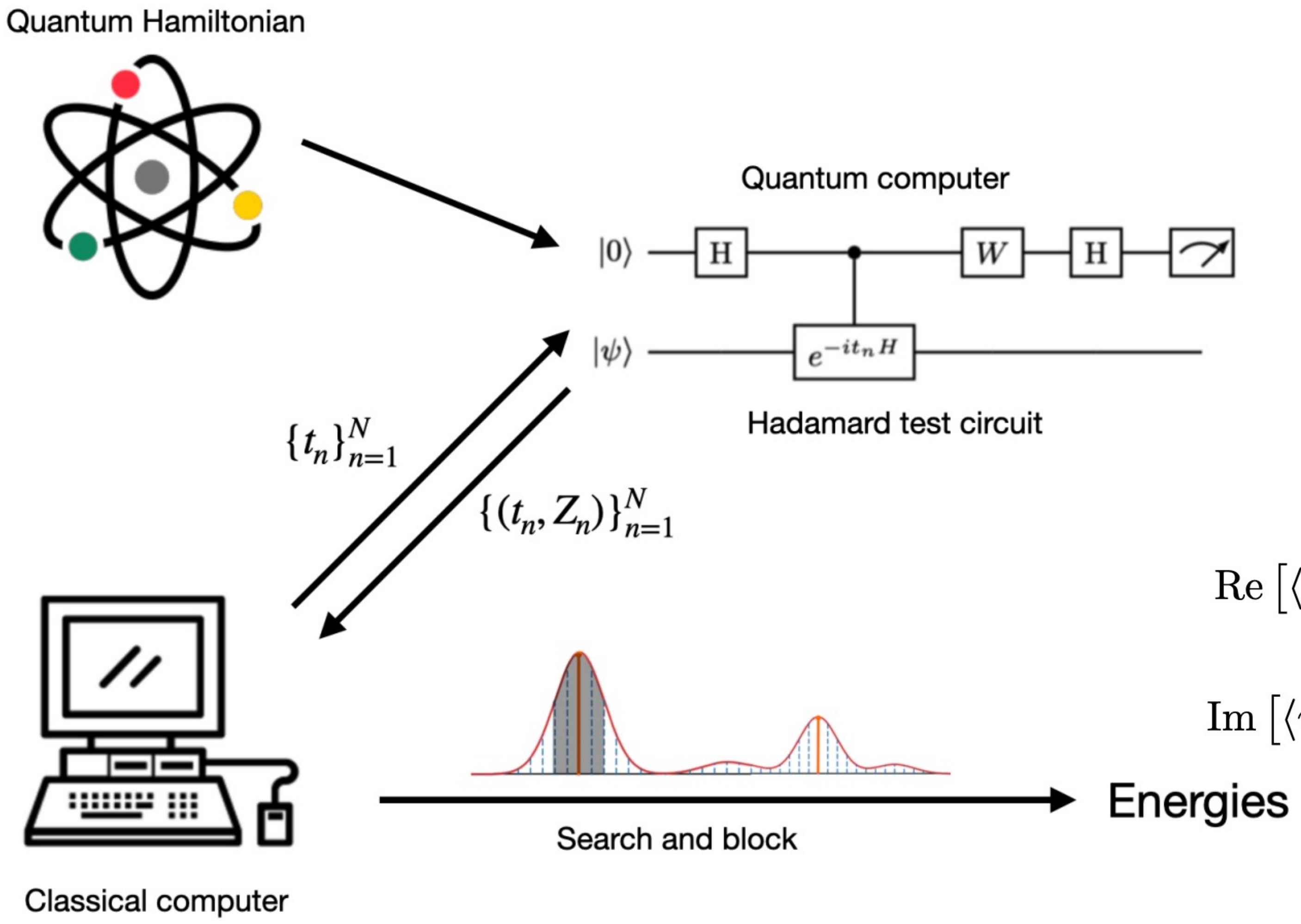
The function can be estimated in a probabilistic way:

$$C(x) = \int_{-\infty}^{\infty} \hat{f}(t) e^{2\pi i x t} \operatorname{Tr}\left(\rho e^{-2\pi i H t}\right) \mathrm{d}t,$$

$\hat{f}(t)$ is the Fourier transformation of $f(x)$.

[1] Tong, Lin PRX Quantum (2022).

Applications 1: 2D Guided Local Hamiltonian Problem



Key to dequantization: ability to approximate $\mathrm{Tr}\left(\rho e^{-2\pi i H t}\right)$

Ancilla-free Hadamard test:
Using symmetry

$$e^{-iHt}|\Omega\rangle = |\Omega\rangle.$$

$$e^{-iHt}|\psi_1\rangle = \frac{1}{\sqrt{2}}\left(|\Omega\rangle + e^{-iHt}|\psi_c\rangle\right).$$

Then,

$$\mathrm{Re}\left[\langle\psi_c|e^{-iHt}|\psi_c\rangle\right] = \langle\psi_1|e^{iHt}\left(|\Omega\rangle\langle\psi_c| + |\psi_c\rangle\langle\Omega|\right)e^{-iHt}|\psi_1\rangle,$$

$$\mathrm{Im}\left[\langle\psi_c|e^{-iHt}|\psi_c\rangle\right] = i\langle\psi_1|e^{iHt}\left(|\psi_c\rangle\langle\Omega| - |\Omega\rangle\langle\psi_c|\right)e^{-iHt}|\psi_1\rangle.$$

The Loschmidt echo is transformed into a quantum mean value problem

Courtesy: Ding et al., 2024

Wu, Zhang, and Yuan, arXiv:2409.04161

Applications 1: 2D Guided Local Hamiltonian Problem

Corollary 2. *Given a 2D geometrical local Hamiltonian H that satisfies certain symmetry, and a corresponding classical initial state $|\psi_c\rangle$ with R configurations which has p_0 overlap to the ground state. There exists a classical algorithm that can output δ-approximation to the ground state energy with the run time of*

$$\mathcal{O}\left((2Rn)^{e^{f(p_0,\delta)}\log(2Rn)+\mathcal{O}(1)}\right), \tag{7}$$

where $f(p_0,\delta) \le \mathcal{O}(\delta^{-1}\log(\delta^{-1}p_0^{-1}))$.

TABLE I. Comparisons of our results with related previous studies on solving the GLH problem, focusing on accuracy, input constraints, and computational time complexity.

Algorithm	Method	Accuracy	Constraints	Complexity
Refs [24, 25]	—	$\varepsilon = \frac{1}{\mathrm{poly}(n)}$	k-local, $\lVert H\rVert \le 1$, $\gamma \in (\frac{1}{\mathrm{poly}(n)}, 1-\frac{1}{\mathrm{poly}(n)})$	BQP-complete
Ref [23]	Dequantized QSVT	$\varepsilon = \mathcal{O}(1)$	s-sparse, $\lVert H\rVert \le 1$	$\mathcal{O}\left(\gamma^{-4}(\lvert S\rvert\, 2^s+1)^{(2+4/\varepsilon)\log(1/\gamma)}\right)$
Ref [26]	Dequantized QSVT	$\varepsilon\lVert H\rVert = \mathcal{O}(\lVert H\rVert)$	k-local	$(\mathcal{O}(1))^{\log(1/\gamma)/\varepsilon}$
Ref [29]	Dequantized 2D Dynamics	$\varepsilon = \mathcal{O}(1)$	k-local, 2D Symmetry	$\mathcal{O}\left(n^{e^{\log(1/\gamma)/\varepsilon}\log n}\right)$

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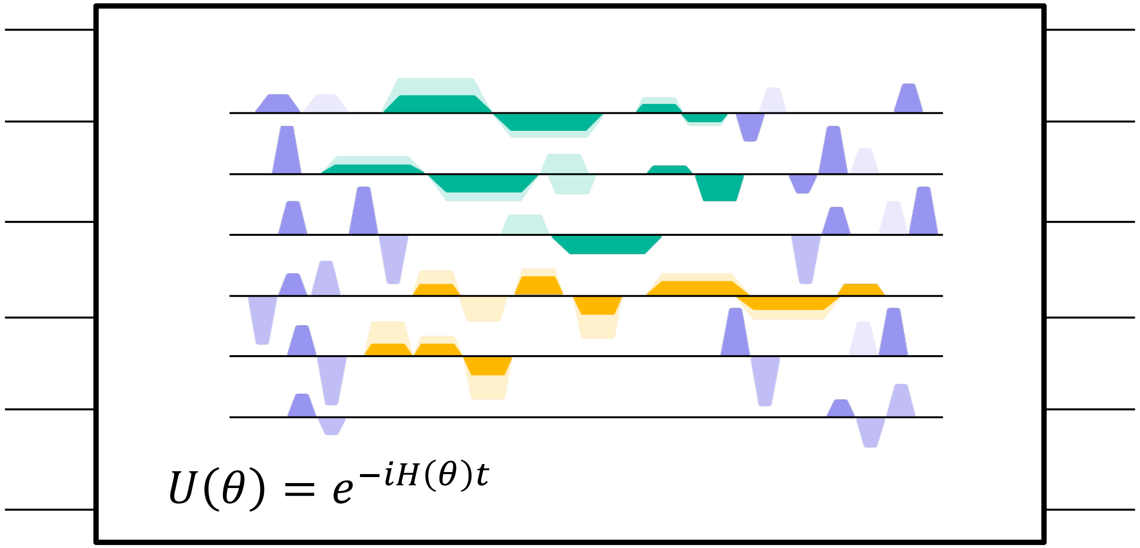
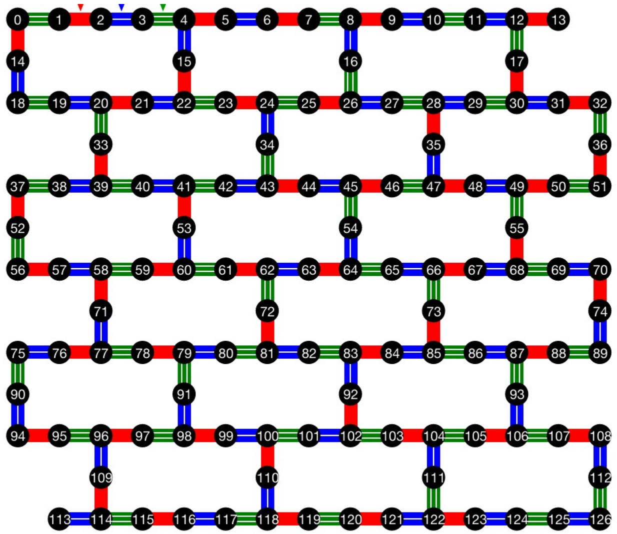
Applications 2: Simulate Analog 2D QC

Corollary 3 (Simulate Superconducting Quantum Computation). *Consider a* $\sqrt{n} \times \sqrt{n}$ *lattice graph* $G = (V, E)$*, where vertex set* V *represents the qubit array and* E *represents the qubit connection set. The analog superconducting quantum computation can achieve* e^{-iHt} *in each layer, with* $H = \sum_{(i,j)\in E} h_{i,j}$*, operator norm* $\|h_{i,j}\| \leq 1$ *and* $t \leq \mathcal{O}(1)$*. Any* $K \leq \mathcal{O}(\log\log n)$*-layer analog superconducting quantum computation can be simulated by a classical algorithm with a quasi-polynomial running time in terms of the system size* n*.*

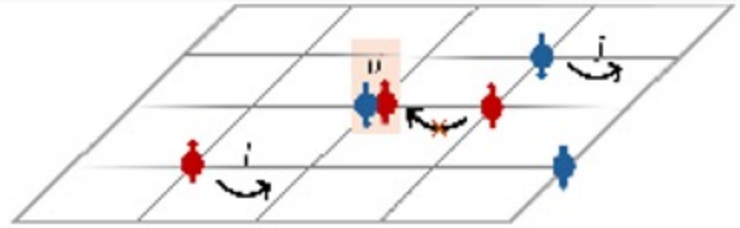




Wu, Zhang, and Yuan, arXiv:2409.04161

Applications 3: Simulate 2D VQE Algorithm

Corollary 4 (Dequantization Quantum Variational Algorithm). *Given a 2D Fermi-Hubbard model defined on a $(n_a \times n_b)$-sized lattice, a p-depth Hamiltonian Variational ansatz with parameters $\{t_v^{(j)}, t_h^{(j)}, t_o^{(j)}\}_{j=1}^{p} \in [-\pi, \pi]^{3p}$ and a slater determinant initial state, a ϵ-approximation to the VQE energy function can be simulated by a classical algorithm with a run time $\mathcal{O}\left(\frac{4n_a n_b}{\epsilon^2}\left(\frac{2L}{\epsilon}\right)^{e^{4\pi^2 ep\eth}\log(2L/\epsilon)}\right)$, where the constant $\eth$ represents the maximum degree of the interaction graph induced by 2D Fermi-Hubbard model and the locality $L \leq 8$.*



2D Fermi-Hubbard model

$$H_{FH} = -\tau \sum_{(i,j)\in E, \sigma\in\{\uparrow,\downarrow\}} (a_{i\sigma}^\dagger a_{j\sigma} + a_{j\sigma}^\dagger a_{i\sigma}) + U \sum_{i\in V} n_{i\uparrow} n_{i\downarrow},$$

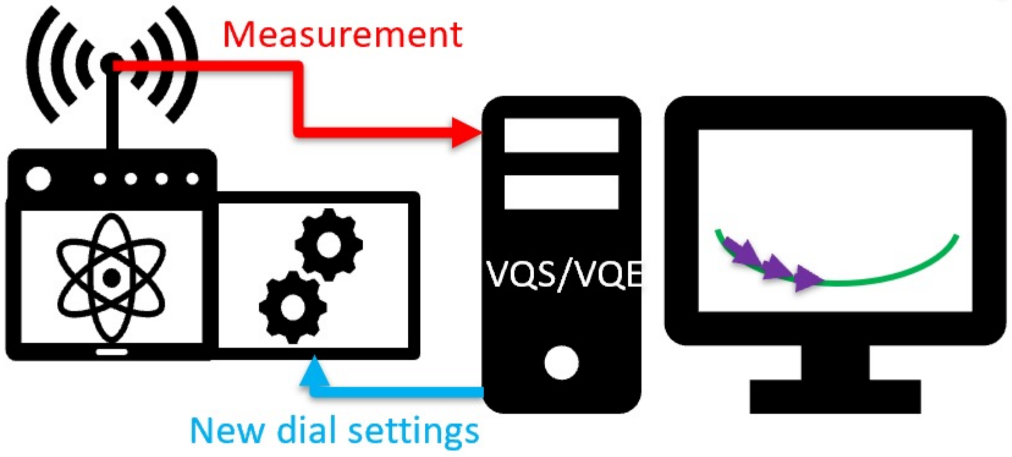
$$a_{k+1}^\dagger a_k + a_k^\dagger a_{k+1} \mapsto \frac{1}{2} Y_k^{\rightarrow}\left(Z_k^{\downarrow} Z_{k+1}^{\uparrow} - Z_k^{\uparrow} Z_k^{\leftarrow} Z_{k+1}^{\rightarrow} Z_{k+1}^{\downarrow}\right),$$

$$a_j^\dagger a_k + a_k^\dagger a_j \mapsto \frac{1}{2}\left(Z_k^{\leftarrow} Z_k^{\rightarrow} Z_k^{\uparrow} Z_j^{\leftarrow} Z_j^{\rightarrow} Z_j^{\downarrow} - I\right)$$

$$n_{i\uparrow} n_{i\downarrow} \mapsto \frac{1}{4}\left(I - Z_k^{\leftarrow} Z_k^{\uparrow} Z_k^{\rightarrow} Z_k^{\downarrow}\right)\left(I - Z_{k'}^{\leftarrow} Z_{k'}^{\uparrow} Z_{k'}^{\rightarrow} Z_{k'}^{\downarrow}\right)$$

Super-Fast Encoding

$$E(\vec{t}) = \langle\phi| \prod_{j=1}^{p} e^{iH_v t_v^{(j)}} e^{iH_h t_h^{(j)}} e^{iH_o t_o^{(j)}} H_{FH} \prod_{j=1}^{p} e^{-iH_v t_v^{(j)}} e^{-iH_h t_h^{(j)}} e^{-iH_o t_o^{(j)}} |\phi\rangle$$



Wu, Zhang, and Yuan, arXiv:2409.04161

Application 4: Simulating short-time adiabatic dynamics

Given a one-parameter family of Hamiltonians

$$H(t) := (1-t)H_0 + tH_1 \text{ for } t \in [0,1]$$

The family of Hamiltonian describes a smooth adiabatic path such that a constant gap is promised.
The adiabatic evolution is given by $U(t) = \mathcal{T}e^{-i\int_0^t H(s)\mathrm{d}s}$,

where $\mathcal{T}$ is the time-ordering operator.

The adiabatic theorem guarantees that for a slow enough evolution, a state initialized to the ground state of H_0 will persists as the ground state of the instantaneous eigenstate.

Our goal is to estimate the properties of the observable O of the ground state of H_1 to accuracy ϵ:

$$|\langle O\rangle' - \langle O\rangle| \leq \epsilon.$$

We assume that the ground state of H_0 is a product state.

Wu, Zhang, and Yuan, arXiv:2409.04161

Application 4: Simulating short-time adiabatic dynamics

Theorem 3 (Time-dependent cluster expansion). *Given* $O(t) = \mathcal{T}e^{i\int_0^t H(s)\mathrm{d}s} O \mathcal{T}e^{-i\int_0^t H(s)\mathrm{d}s}$, *its cluster expansion is*

$$O(t) = \lim_{M\to\infty} \sum_{m=0}^{+\infty} \frac{(-it)^m}{m!M^m} \sum_{\boldsymbol{V}\in\mathcal{C}_m, V=(X_1,\cdots,X_m)} \frac{\tilde{\boldsymbol{\lambda}}^{\boldsymbol{V}}}{\boldsymbol{V}!} \Bigg(\mathcal{T}\Bigg[\sum_{n_m,\cdots,n_1=0}^{M-1} \sum_{\sigma\in\mathcal{P}_m} \Big[h_{X_{\sigma(m)}} f(n_m, t, X_{\sigma(m)}), \cdots, \Big[h_{X_{\sigma(1)}} f(n_1, t, X_{\sigma(1)}), O\Big], \cdots\Big]\Bigg]\Bigg)_{z=(0,\cdots,0)}, \tag{13}$$

where $\tilde{\lambda}_X(t) = \lambda_X(t) + t\lambda'_X(t)$ *with* $\lambda'_X(t) = \frac{\mathrm{d}\lambda_X(t)}{\mathrm{d}t}$, $\tilde{\boldsymbol{\lambda}}^{\boldsymbol{V}} = \prod_{X\in S} \tilde{\lambda}_X^{\mu_{\boldsymbol{V}}(X)}$, $\boldsymbol{V}! = \prod_{X\in S} \mu_{\boldsymbol{V}}(X)!$, $f(n_m, t, X) := \frac{\partial Z_X(n_m)}{\partial Z_X(t)}$ *and* $Z_X(t) = -it\lambda_X(t)$.

Wu, Zhang, and Yuan, arXiv:2409.04161

Application 4: Simulating short-time adiabatic dynamics

Theorem 4. *Given a family of Hamiltonians* $H(t) := (1-t)H_0 + tH_1$ *for* $t \in [0,1]$ *with* $\mathfrak{d}$ *the maximal degree of the interaction graph, and an observable* O*, let* $U(t) = \mathcal{T} e^{-i\int_0^t H(s)\mathrm{d}s}$ *be the Hamiltonian evolution operator of the family of Hamiltonians with evolution time* t*. Then, for any* $t < t^* = \frac{1}{2\sqrt{e\mathfrak{d}}}$*, there exists an algorithm with the run time*

$$\mathrm{poly}\left(\left(\frac{\|O\|}{\epsilon} t^2 e^{t^2}\right)^{\frac{\log\left(\frac{\epsilon}{\|O\|}(t/t^*-1)\right)}{\log(t^*/t)}}\right) \tag{29}$$

that outputs an estimation $\langle O \rangle'$ *to* $\langle O \rangle := \langle \psi | U^\dagger(t) O U(t) | \psi \rangle$ *for some product state* $|\psi\rangle$ *within* ϵ *accuracy:*

$$|\langle O \rangle' - \langle O \rangle| \leq \epsilon. \tag{30}$$

Wu, Zhang, and Yuan, arXiv:2409.04161

2. Dequantization of the GSEE algorithm

Zhang, Wu, and Yuan, arXiv:2411.16163

Applications 1: 2D Guided Local Hamiltonian Problem

The ground-state energy estimation problem is perennial and fundamental problem for both physics and computer science studies.

Definition 1 (Local Hamiltonian problem). *Given as input a k-local Hamiltonian $\hat{H}$ acting on n qudits, specified as a collection of constraints $\left\{\hat{H}_i\right\}_{i=1}^{r} \subseteq \mathcal{H}\left(\mathbb{C}^d\right)^{\otimes k}$ where $k, d \in \Theta(1)$, and threshold parameters $a, b \in \mathbb{R}$, such that $0 \leq a < b$ and $(b-a) \geq 1$, decide, with respect to the complexity measure $\langle H\rangle + \langle a\rangle + \langle b\rangle$:*

1. *If $\lambda_{\min}(\hat{H}) \leq a$, output YES.*
2. *If $\lambda_{\min}(\hat{H}) \geq b$, output NO.*

Yet, the problem is proved to be QMA-complete[1], meaning inefficiency for quantum computing.

Definition 2 (Guided local Hamiltonian problem). *Input: a k-local Hamiltonian $\hat{H}$ acting on n qubits such that $\|\hat{H}\| \leq 1$ query-access to an initial state (density matrix) ρ_I*
Promise: $\|\Pi_0 \rho_I\| \geq \gamma$
Output: an estimate E_0' such that $|E_0' - E_0| \leq \epsilon$

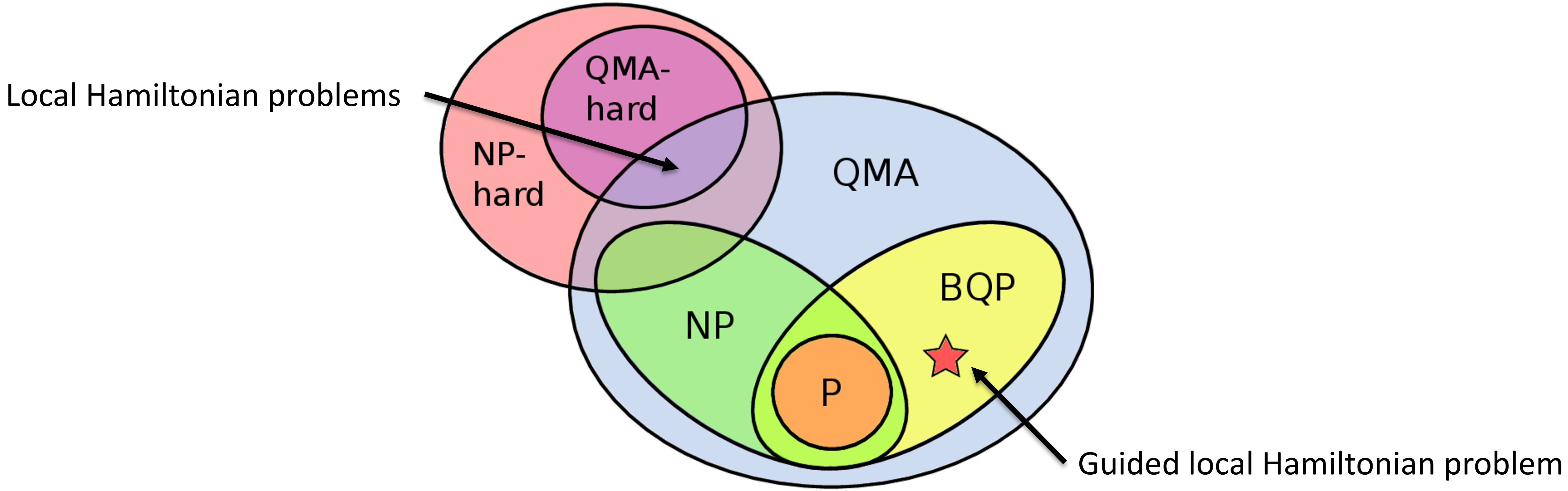
The GLH is proved to be BQP-hard[2], meaning efficiently solvable.

[1] Kiteav et al., (2002) [2]Gharibian, Le Gall STOC (2023)

Dequantization of the GSEE algorithm

The local Hamiltonian problem corresponds to the ground-state problem

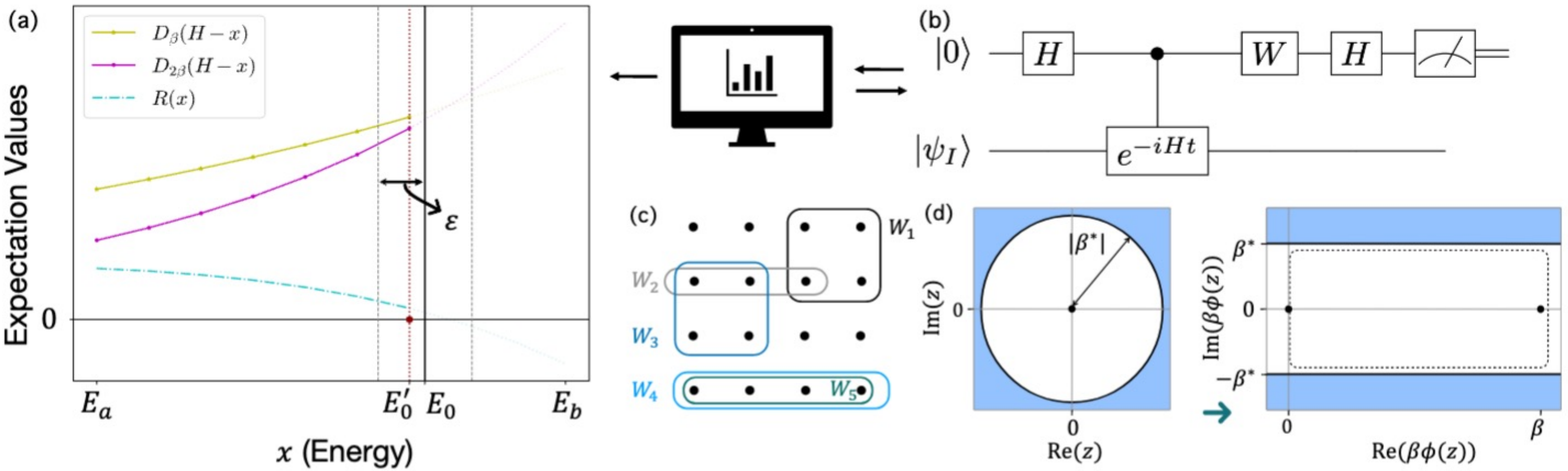
The guided local Hamiltonian problem corresponds to the ground-state problem with a nontrivial guiding state



[1]Ghribian and Le Gall, STOC 2022; Zhang, Wu, and Yuan, arXiv: XXX

Dequantization of the GSEE algorithm

Consider local Hamiltonians and dequantization of the partition function (exponential function of H)



Zhang, Wu, and Yuan, arXiv:2411.16163

Dequantization of the GSEE algorithm

Theorem 2. *Suppose an R-configurational semi-classical guiding state $|\psi_c\rangle$ is given, and the condition in Eq. 4 holds. Then, there exists a classical algorithm to solve the GSEE problem with a runtime of*

$$\frac{R^2\,|S|}{\varepsilon}\text{poly}\left[\left(\frac{|S|}{\gamma^2\beta\varepsilon[1-\beta/\beta^*]}\right)^{\log(\beta^*/\beta)}\right], \tag{8}$$

where $\beta = \Delta^{-1}\ln(\gamma^{-2}\varepsilon^{-1})$ and $\beta^* = (2e^2\mathfrak{d}(\mathfrak{d}+1))^{-1}$. The algorithm is efficient when $\beta < \beta^*$, which corresponds to the accuracy limit:

$$\varepsilon > \varepsilon^* = 2e^2\mathfrak{d}(\mathfrak{d}+1). \tag{9}$$

Theorem 3. *Let the semi-classical guided state $|\psi_c\rangle = U\,|0^n\rangle$ that is prepared by a constant-depth quantum circuit U and $\gamma = 1/\sqrt{2}$. Suppose H representing a k-local Hamiltonian defined on a $\mathcal{O}(1)$-dimensional lattice. Let the similarity-transformed Hamiltonian $H' = U^\dagger H U$ and the maximum degree of its corresponding interaction graph be denoted as $\mathfrak{d}'$. Then, if the condition in Eq. (4) holds, there exists a classical algorithm that solves the GSEE problem with a run time*

$$\left[\frac{e^{2\pi\beta/\beta^*}}{\beta\varepsilon^2}\text{poly}(|S|)\right]^{e^{2\pi\beta/\beta^*}}, \tag{11}$$

where $\beta = \Delta^{-1}\ln(\gamma^{-2}\varepsilon^{-1})$, and $\beta^* = (2e^2\mathfrak{d}'(\mathfrak{d}'+1))^{-1}$.

Zhang, Wu, and Yuan, arXiv:2411.16163

Dequantization of the GSEE algorithm

TABLE I. Comparisons of our results with related previous studies on solving the GLH problem, focusing on accuracy, input constraints, and computational time complexity.

Algorithm	Method	Accuracy	Constraints	Complexity
Refs [24, 25]	—	$\varepsilon = \frac{1}{\text{poly}(n)}$	k-local, $\|H\| \leq 1$, $\gamma \in (\frac{1}{\text{poly}(n)}, 1 - \frac{1}{\text{poly}(n)})$	BQP-complete
Ref [23]	Dequantized QSVT	$\varepsilon = \mathcal{O}(1)$	s-sparse, $\|H\| \leq 1$	$\mathcal{O}\left(\gamma^{-4}(\|S\| 2^s + 1)^{(2+4/\varepsilon)\log(1/\gamma)}\right)$
Ref [26]	Dequantized QSVT	$\varepsilon\|H\| = \mathcal{O}(\|H\|)$	k-local	$(\mathcal{O}(1))^{\log(1/\gamma)/\varepsilon}$
Ref [29]	Dequantized 2D Dynamics	$\varepsilon = \mathcal{O}(1)$	k-local, 2D Symmetry	$\mathcal{O}\left(n^{e^{\log(1/\gamma)/\varepsilon}\log n}\right)$
Theorem 2	Dequantized RQITE	$\varepsilon > \varepsilon^* = \Omega(1)$	k-local	$\varepsilon^{-1}\text{poly}\left[(\|S\|\Delta^2\gamma^{-2}\varepsilon^{-1})^{\log(\Delta/(2\varepsilon^*\log(\gamma^{-2}\varepsilon^{-1})))}\right]$
Corollary 1	Dequantized RQITE	$\varepsilon > \varepsilon^*/\|H\|$	k-local, $\tilde{H} = H/\|H\|$	-
Theorem 3	Dequantized RQITE	$\varepsilon = \mathcal{O}(1)$	k-local, $\gamma > 1/\sqrt{2}$, $\mathcal{O}(1)$-dimension	$\mathcal{O}\left((\Delta\varepsilon^{-2}\text{poly}(\|S\|))^{e^{\log(1/(\gamma\varepsilon^2))/\Delta}}\right)$
Corollary 2	Dequantized RQITE	$\varepsilon = \mathcal{O}(1/\|H\|)$	k-local, $\gamma > 1/\sqrt{2}$, $\tilde{H} = H/\|H\|$, $\mathcal{O}(1)$-dimension	-

Zhang, Wu, and Yuan, arXiv:2411.16163

Can we achieve quantum advantage with near-term hardware?

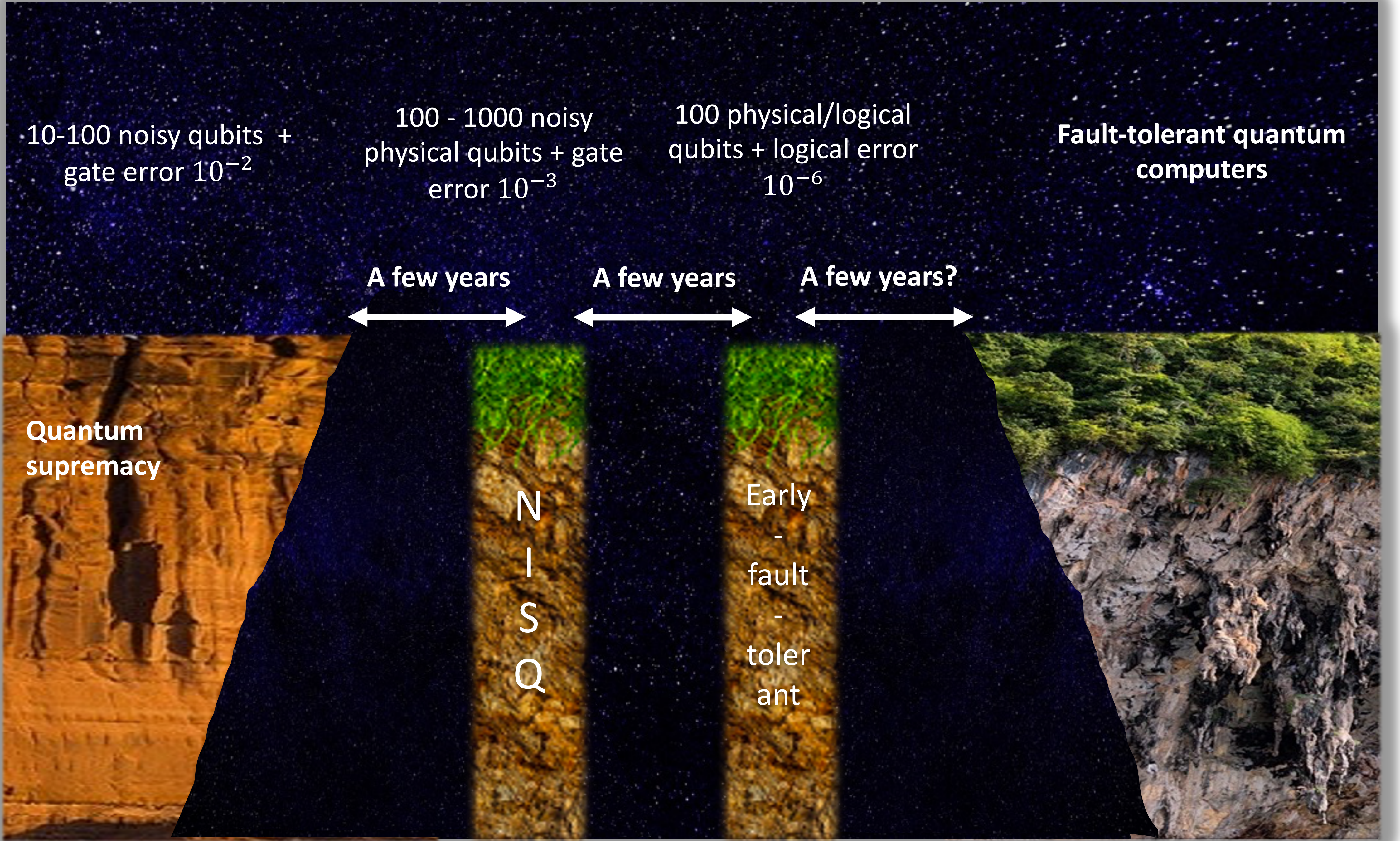
Classically Easy:

- 2D superconducting system with a constant time
- Noisy quantum circuits with constant noise
- Ground state estimation for constant gap 2D Hamiltonian with constant accuracy

We may achieve quantum advantage with near-term hardware

Classically hard:

- 2D superconducting system with time ~ qubit number
- Quantum system with all-to-all connection
- Noisy quantum circuits with noise rate ~ 1/gate number
- Ground state estimation for (polynomially) small gap 2D Hamiltonian with high accuracy


10-100 noisy qubits + gate error 10^{-2}
100 - 1000 noisy physical qubits + gate error 10^{-3}
100 physical/logical qubits + logical error 10^{-6}
Fault-tolerant quantum computers
A few years
A few years
A few years?
Quantum supremacy
N I S Q
Early - fault - toler ant

北京大学前沿计算研究中心
Center on Frontiers of Computing Studies, Peking University

Thanks!