

Quantum+HPC Utility-scale Algorithms

Hybrid quantum/classical
computing in the age of utility

Mirko Amico
IBM Quantum

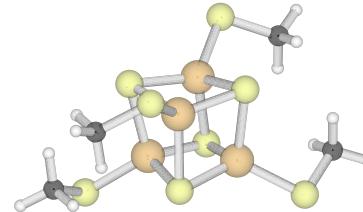
June 8th, 2025
ICS '25



Overview

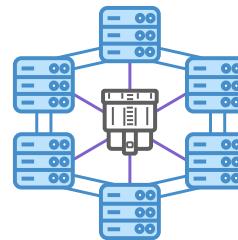
Introduction

- Variational Quantum Algorithms and their limitations

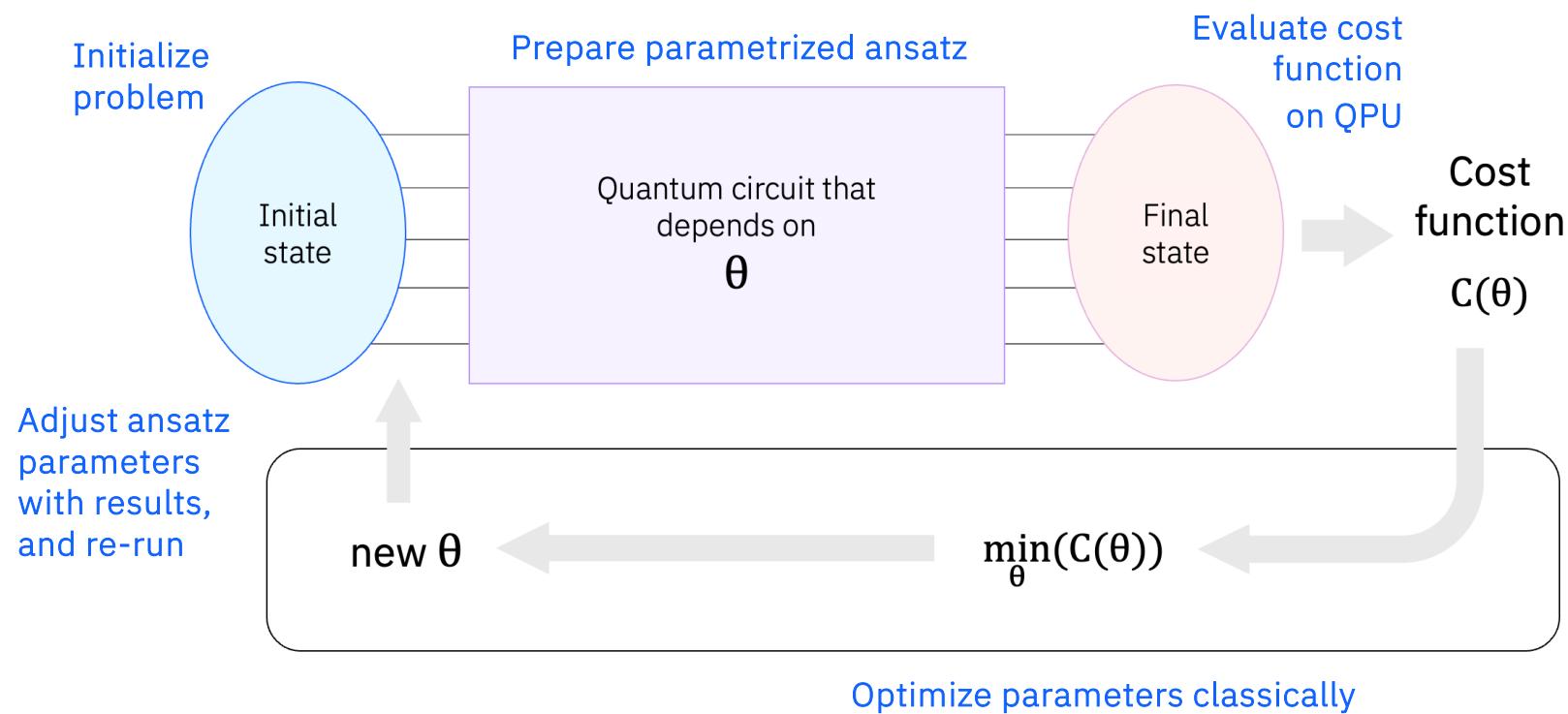


Quantum-centric Supercomputing

- Sample-based Quantum Diagonalization (**SQD**)
- Krylov Quantum Diagonalization (**KQD**)
- Sample-based Krylov Quantum Diagonalization (**SKQD**)

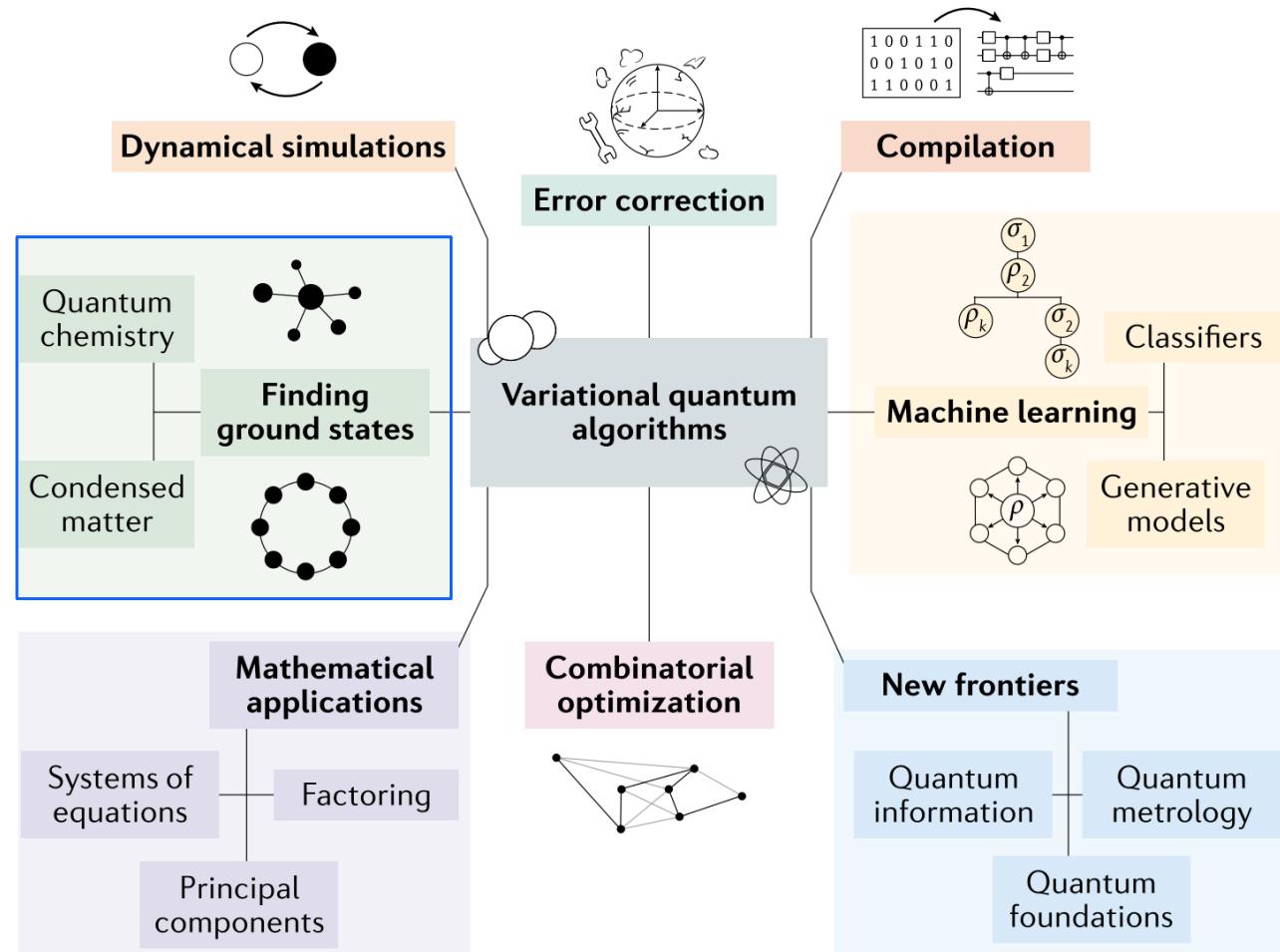


Variational quantum algorithms



Applications of variational quantum algorithms

VQE and its variants have been the main example in this category



Estimating ground state properties is relevant across disciplines

...but current classical/quantum techniques face challenges

High-Energy Physics

Understanding the fundamental nature of particles and forces

Materials

Predicting and understanding material behavior

Optimization

Discovering of optimal solutions in complex landscapes

Healthcare & Life Sciences

Understanding biochemical interactions and reactions

Current classical/quantum techniques to estimate ground state properties face challenges



Classical methods are hindered by the exponential growth of the Hilbert space with the system size and the correlations arising in entangled quantum systems.



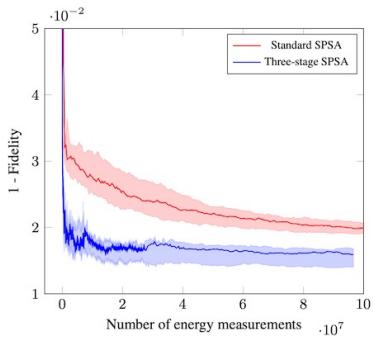
Variational quantum methods (e. g. VQE) face challenges with current devices because of trainability and the high number of measurements required in the optimization process.



Fault-tolerant quantum methods with performance guarantees (e. g. quantum phase estimation) require deep circuits that cannot be executed on pre-fault-tolerant devices.

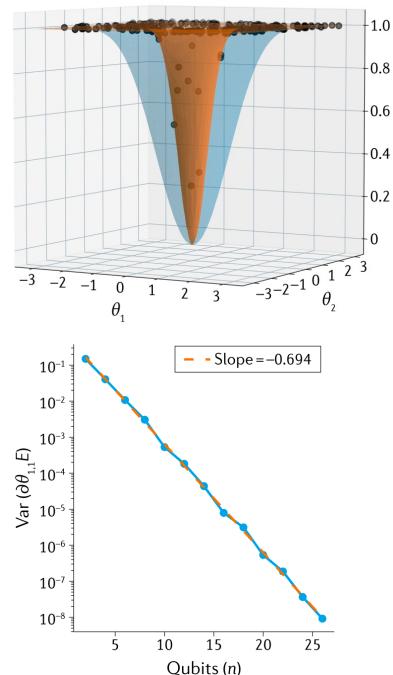
Limitations of VQE

Measurement Problem



[C Cade et al, PRB **102**, 235122 (2020)]

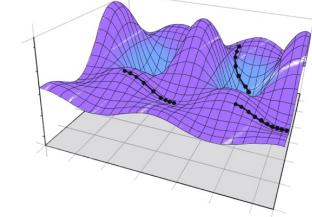
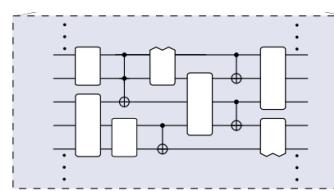
Barren Plateaus



[M Cerezo et al, Nat Rev Phys **9**, 625 (2021)]

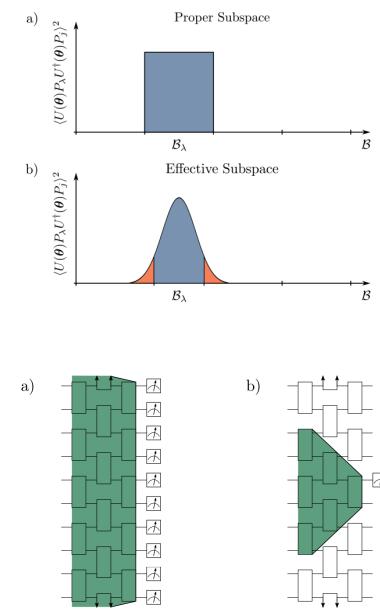
Other trainability issues

- Poor local minima
- expressivity limitations...



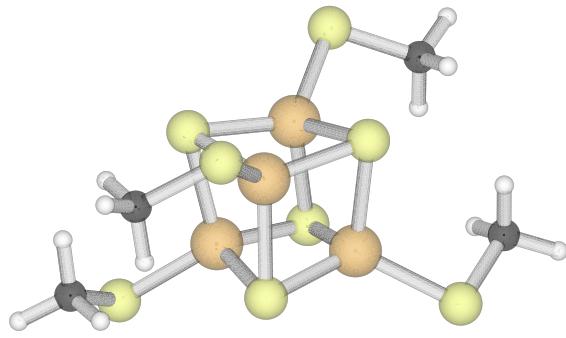
[Zimborás, Zoltán, et al. arXiv:2501.05694]

Classically Simulable



[M Cerezo et al, arXiv:2312.09121]

The cost for the accurate prediction of nature



Goal: Compute ground-state energies by solving the Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$ in the Born Oppenheimer approximation with given precision.

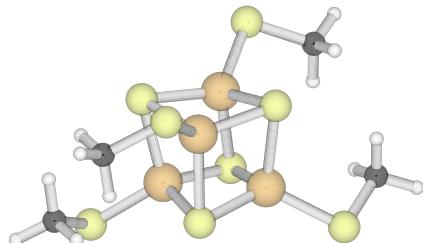
- Fix atom nucleus
- Choose atomic basis set
- Solve Hartree Fock
- Write electron integrals in terms of the basis of molecular orbitals
- Map fermions to qubits.

$$\hat{H} = \sum_{pr\sigma} h_{pr} \hat{a}_{p\sigma}^\dagger \hat{a}_{r\sigma} + \sum_{\substack{prqs \\ \sigma\tau}} \frac{(pr|qs)}{2} \hat{a}_{p\sigma}^\dagger \hat{a}_{q\tau}^\dagger \hat{a}_{s\tau} \hat{a}_{r\sigma}$$

What if we leverage classical computers to obtain the expectation values of H ?

Fe₄S₄ on **72** qubits (TZP-DKH basis set): **6.7M** Pauli operators to get to the precision required for chemical accuracy (milliHartree) the runtime blows up.

Quantum-centric supercomputing: a new computational framework



Fe₄S₄ on **72** qubits (TZP-DKH basis set): **6.7M** Pauli operators

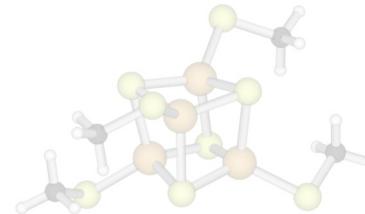
Pre-fault tolerant	VQE estimation at 10µs/circuit ~3M years
Quantum-centric supercomputing	Subspace estimation at 10µs/circuit ~2 hours
Fault-tolerant	Phase estimation qubits: 4.53M 13 days runtime *

QCSC enables complex use cases such as quantum chemistry **before fault-tolerance**

Overview

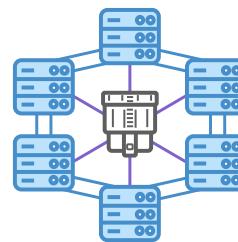
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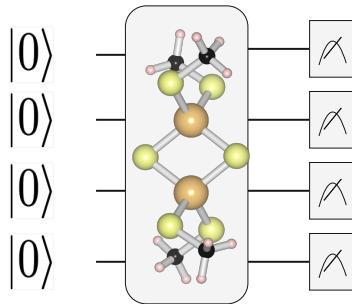


Quantum-centric Supercomputing

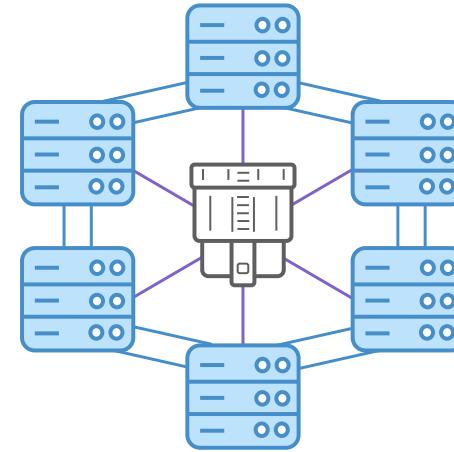
- Sample-based Quantum Diagonalization (SQD)
 - Krylov Quantum Diagonalization (KQD)
- Sample-based Krylov Quantum Diagonalization (SKQD)



Chemistry on quantum-centric supercomputing



+



Sample from quantum circuits that
accurately prepare the quantum
probability distribution of a set of states

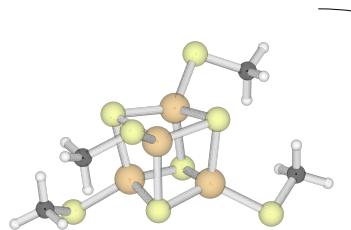
Use massive classical computing to
process individual quantum samples
and obtain an expectation value

Quantum-centric Supercomputing

- Sample-based Quantum Diagonalization (**SQD**) May 2024

Chemistry Beyond Exact Solutions on a Quantum-Centric Supercomputer

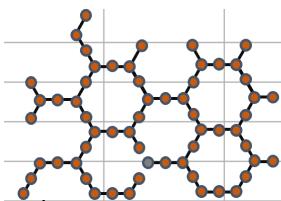
Javier Robledo-Moreno,^{1,*} Mario Motta,^{1,†} Holger Haas,¹ Ali Javadi-Abhari,¹ Petar Jurcevic,¹ William Kirby,² Simon Martiel,³ Kunal Sharma,¹ Sandeep Sharma,⁴ Tomonori Shirakawa,^{5,6,7} Iskandar Sitedikov,¹ Rong-Yang Sun,^{5,6,7} Kevin J. Sung,¹ Maika Takita,¹ Minh C. Tran,² Seiji Yunoki,^{5,6,7,8} and Antonio Mezzacapo^{1,‡}



- Krylov Quantum Diagonalization (**KQD**) July 2024

Diagonalization of large many-body Hamiltonians on a quantum processor

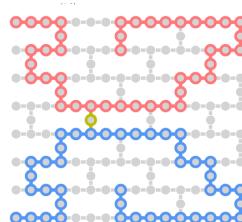
Nobuyuki Yoshioka*,^{1,†} Mirko Amico*,^{2,‡} William Kirby*,^{3,§} Petar Jurcevic,² Arkopal Dutt,³ Bryce Fuller,² Shelly Garion,⁴ Holger Haas,² Ikko Hamamura**,⁵ Alexander Ivrii,⁴ Ritajit Majumdar,⁶ Zlatko Minev,² Mario Motta,² Bibek Pokharel,⁷ Pedro Rivero,² Kunal Sharma,² Christopher J. Wood,² Ali Javadi-Abhari,² and Antonio Mezzacapo²



- Sample-based Krylov Quantum Diagonalization (**SKQD**) January 2025

Sample-based Krylov Quantum Diagonalization

Jeffery Yu,^{1,2,3,*} Javier Robledo Moreno,^{1,†} Joseph Iosue,^{1,2,3} Luke Bertels,⁴ Daniel Claudio,⁴ Bryce Fuller,¹ Peter Groszkowski,⁵ Travis S Humble,⁶ Petar Jurcevic,¹ William Kirby,⁷ Thomas A. Maier,⁸ Mario Motta,¹ Bibek Pokharel,¹ Alireza Seif,¹ Amir Shehata,⁶ Kevin J. Sung,¹ Minh C. Tran,¹ Vinay Tripathi,¹ Antonio Mezzacapo,^{1,‡} and Kunal Sharma^{1,§}



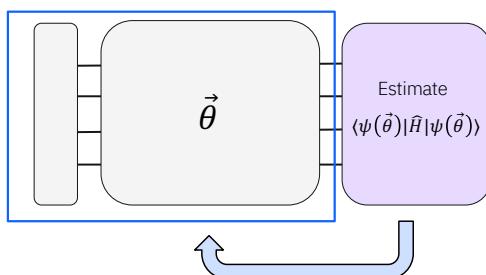
Subspace
methods

Two main approaches to solve the ground state problem: variational and subspaces-based

Variational principle

1. Define a parametrized ansatz that prepares $|\psi(\vec{\theta})\rangle$
2. Evaluate its energy $E(\vec{\theta}) = \langle\psi(\vec{\theta})|\hat{H}|\psi(\vec{\theta})\rangle$
3. Optimize parameters $\vec{\theta}$ to minimize the energy estimate
4. By definition: $E(\vec{\theta}) \geq E_g$ (variational principle)

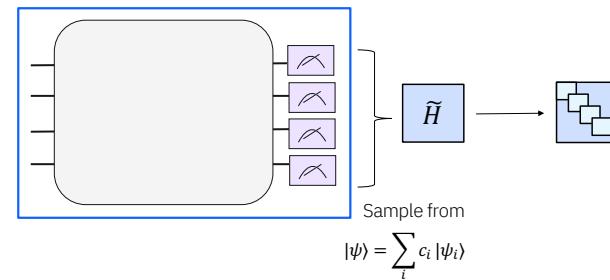
Minimizing the energy gets you closer to the ground state



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Subspace methods

1. Prepare a quantum state and express it as a linear combination of basis states $|\psi\rangle = \sum_i c_i |\psi_i\rangle$
2. Sample from the set of basis states $|\psi_i\rangle$
3. Project the Hamiltonian \hat{H} in the subspace spanned by $|\psi_i\rangle$ to obtain an effective Hamiltonian \tilde{H}
4. Find spectrum of \tilde{H} by solving the corresponding eigenvalue problem $\tilde{H} \vec{c} = \tilde{E} \vec{c}$
5. Estimate the ground state, by looking for c_i that minimize \tilde{E}



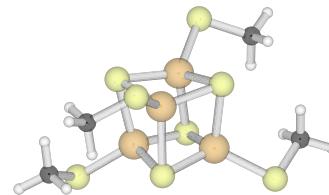
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Quantum-centric Supercomputing

- Sample-based Quantum Diagonalization (**SQD**) May 2024

Chemistry Beyond Exact Solutions on a Quantum-Centric Supercomputer

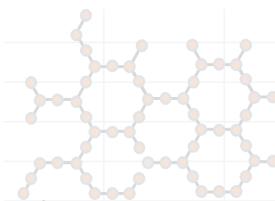
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- Krylov Quantum Diagonalization (**KQD**) October 2024

Diagonalization of large many-body Hamiltonians on a quantum processor

Nobuyuki Yoshioka^{*1,†} Mirko Amico^{*2,‡} William Kirby^{*3,§} Petar Jurcevic,² Arkopal Dutt,³ Bryce Fuller,² Shelly Garion,⁴ Holger Haas,² Ikko Hamamura^{**5}, Alexander Ivrii,⁴ Ritajit Majumdar,⁶ Zlatko Minev,² Mario Motta,² Bibek Pokharel,⁷ Pedro Rivero,² Kunal Sharma,² Christopher J. Wood,² Ali Javadi-Abhari,² and Antonio Mezzacapo²



- Sample-based Krylov Quantum Diagonalization (**SKQD**) January 2025

Sample-based Krylov Quantum Diagonalization

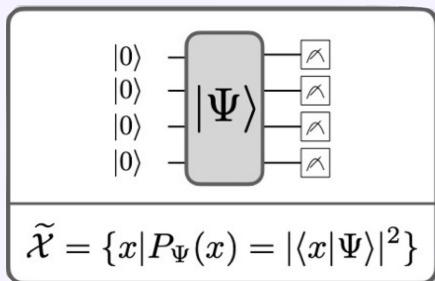
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Sample-based Quantum Diagonalization (SQD)

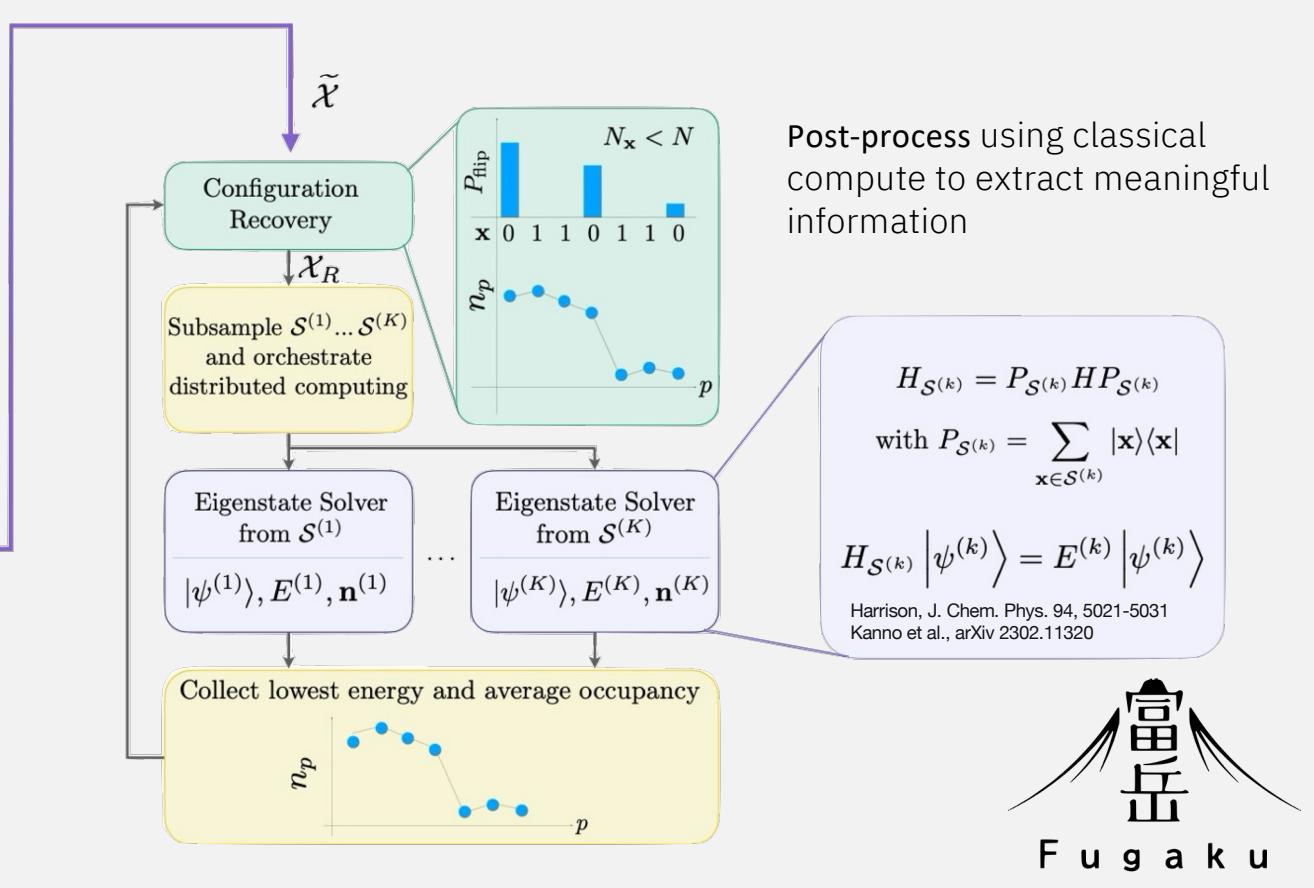
Execute using Qiskit
Runtime Primitives. Quantum compute generates samples from prepared quantum state

Sampler()



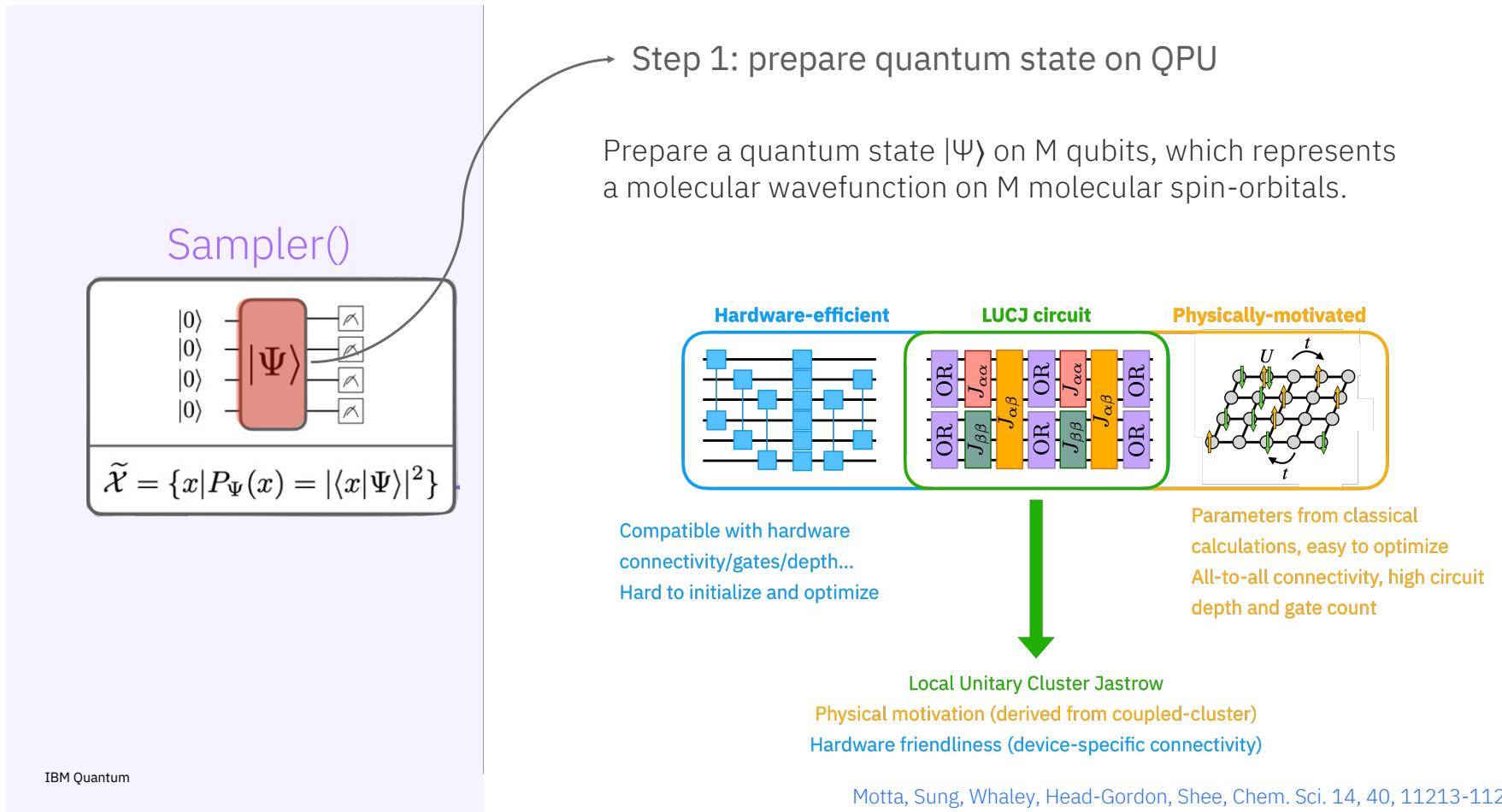
IBM Quantum

Efficient data transfer from QPU to HPC.



<https://arxiv.org/abs/2405.05068>

Sample-based Quantum Diagonalization (SQD)



Sample-based Quantum Diagonalization (SQD)

Step 1: prepare quantum state on QPU

Unitary coupled-cluster singles and doubles (UCCSD)

$|\Psi\rangle = e^{T-T^+} |\Phi_0\rangle$

$$T = \sum_{ai} t_i^a \hat{c}_a^\dagger \hat{c}_i + \sum_{abij} t_{ij}^{ab} \hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_j \hat{c}_i$$

Jastrow form of the UCCSD:

$$T - T^+ \simeq \sum_{\mu} e^{-K_{\mu}} e^{iJ_{\mu}} e^{K_{\mu}}$$

$$K_{\mu} = \sum_{pr,\sigma} K_{pr}^{\mu} \hat{c}_{p\sigma}^\dagger \hat{c}_{r\sigma}$$

$$J_{\mu} = \sum_{pr,\sigma\tau} J_{pr}^{\sigma\tau} \hat{n}_{p\sigma} \hat{n}_{r\tau}$$

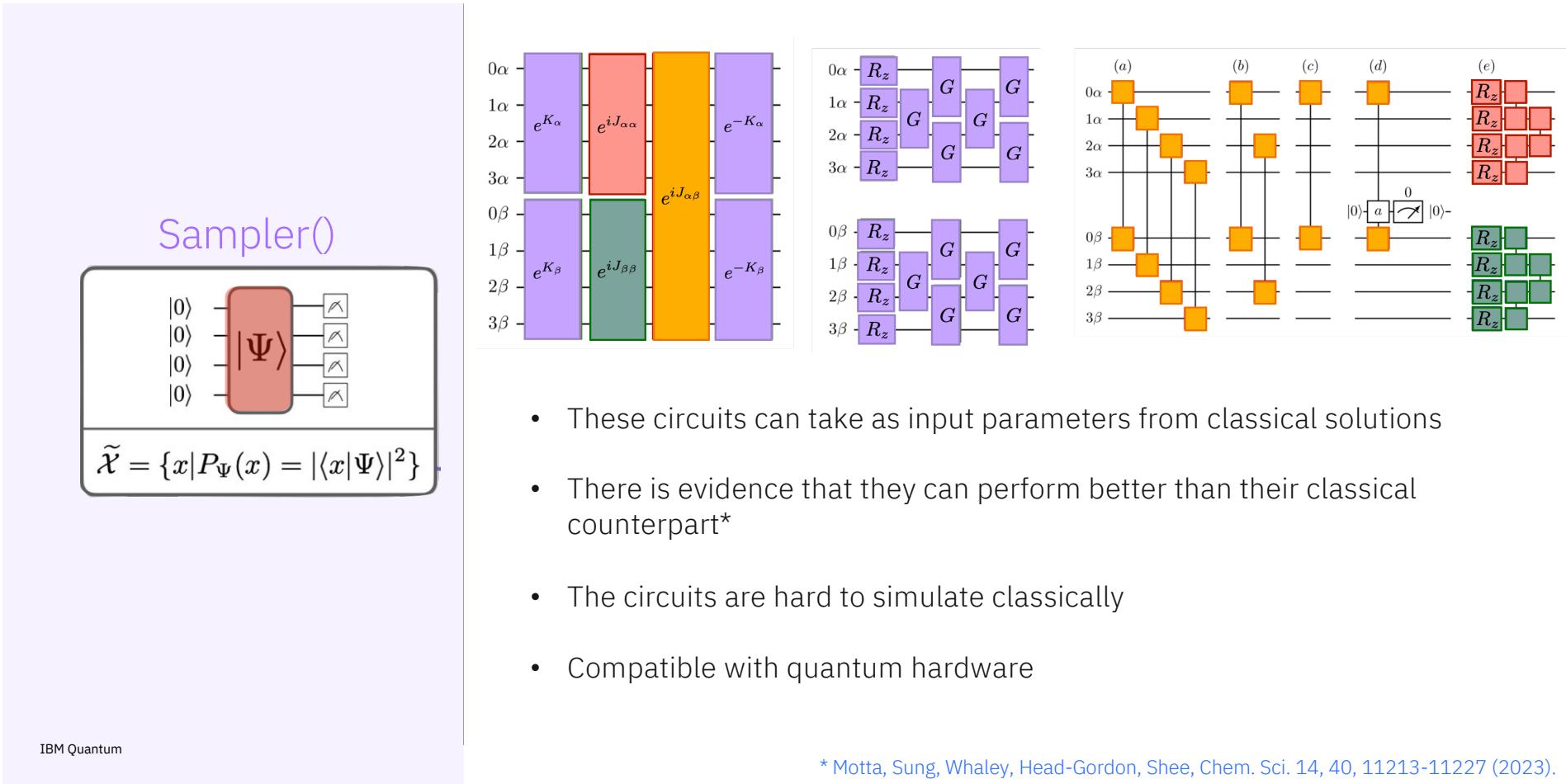
Local Unitary Cluster
Jastrow ansatz (LUCJ)

$|\Psi\rangle \simeq \prod_{\mu} e^{-K_{\mu}} e^{iJ_{\mu}} e^{K_{\mu}} |\Phi_0\rangle$

IBMQ Quantum

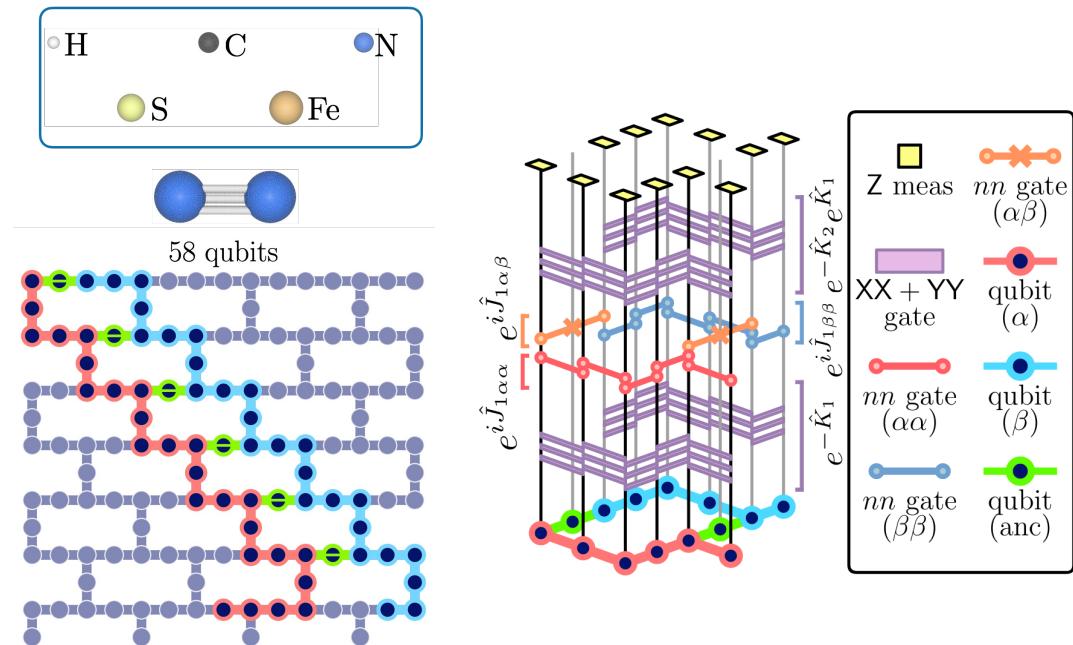
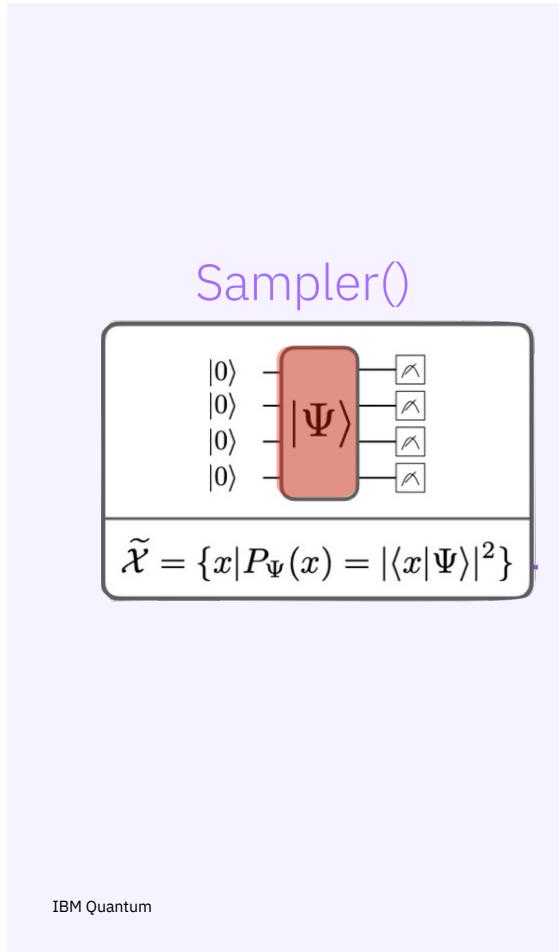
Motta, Sung, Whaley, Head-Gordon, Shee, Chem. Sci. 14, 40, 11213-11227 (2023).

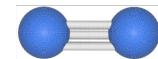
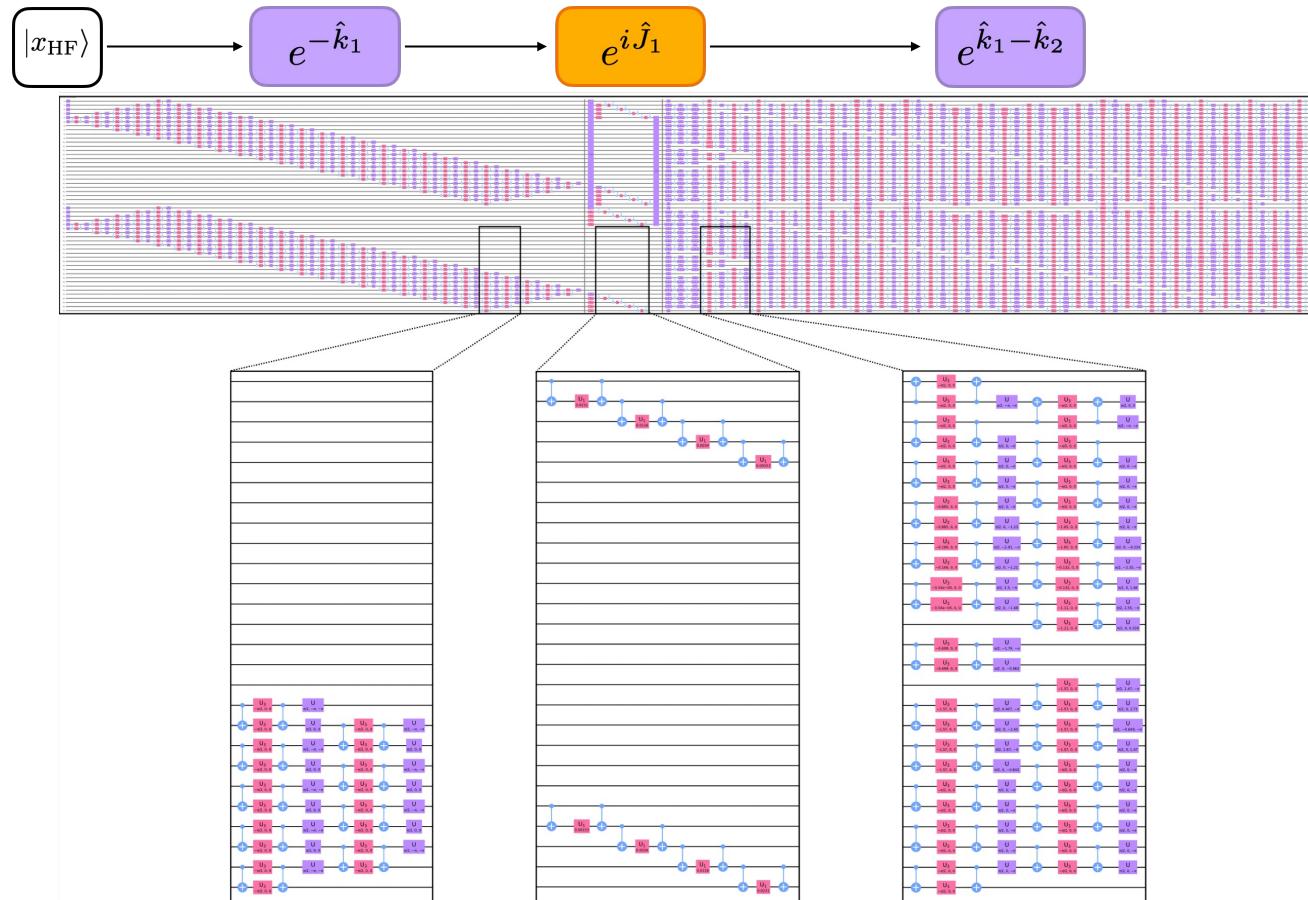
Sample-based Quantum Diagonalization (SQD)



Sample-based Quantum Diagonalization (SQD)

- Compatible with quantum hardware

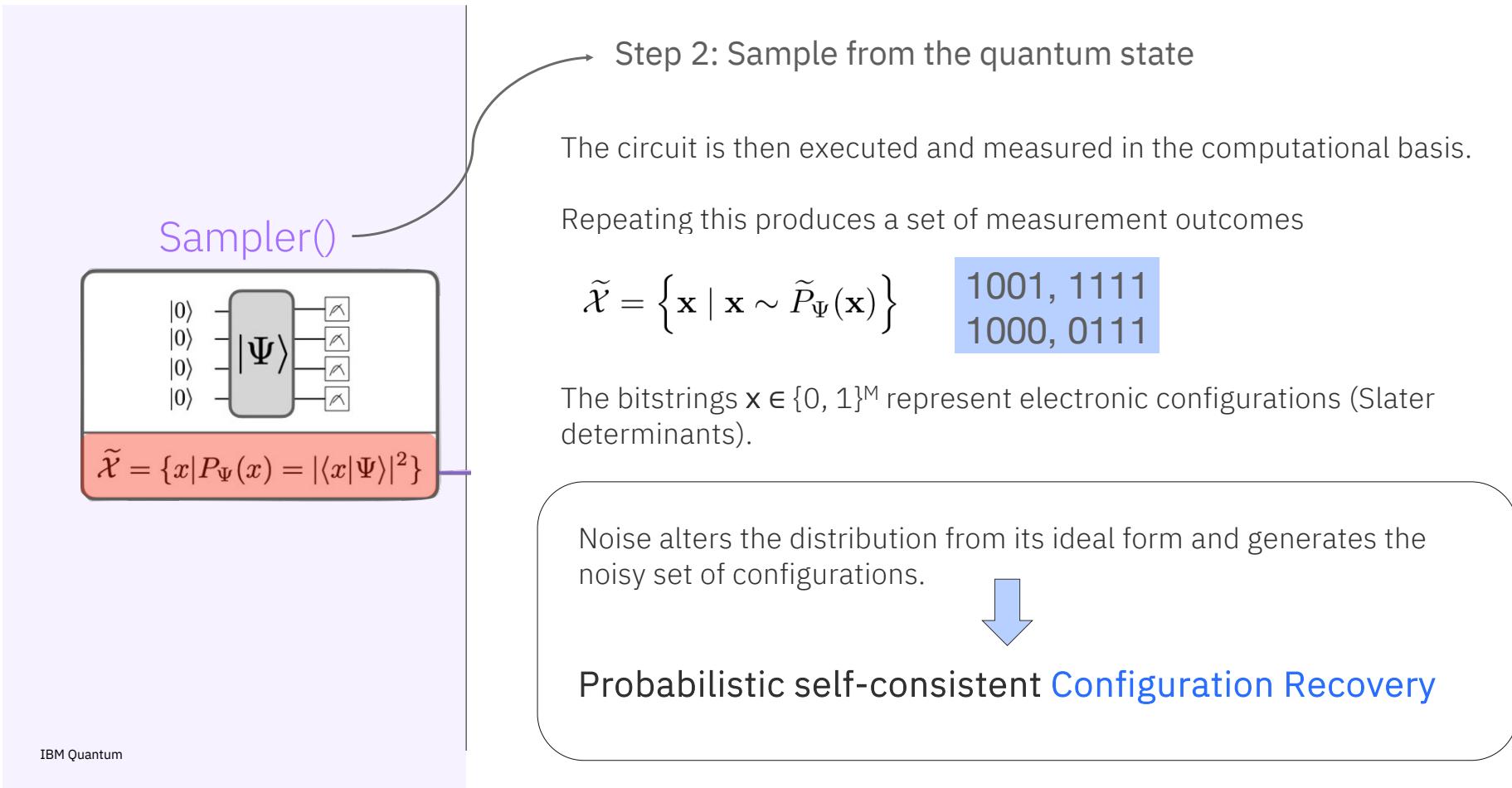




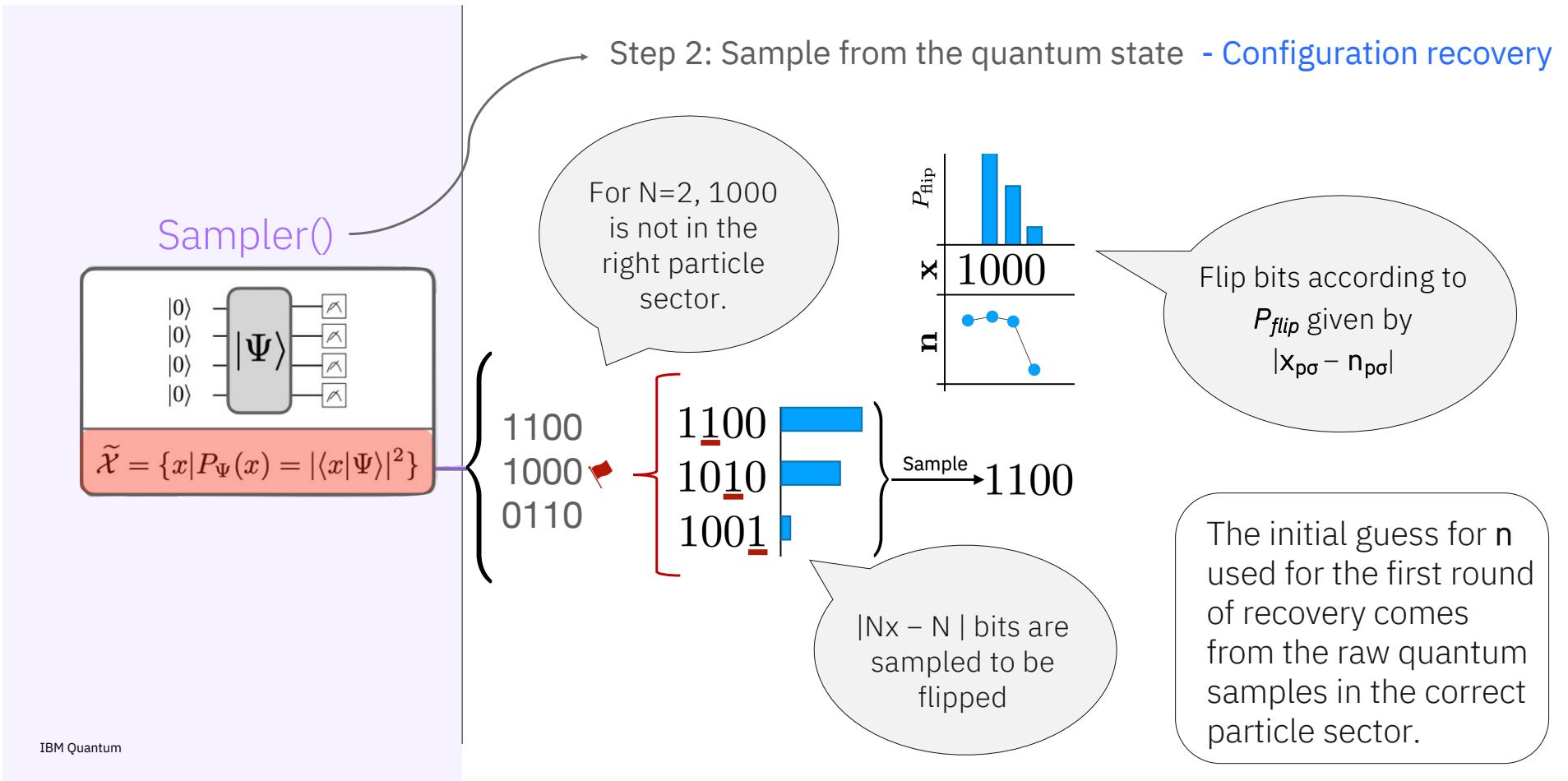
N_2

Qubits	CNOT layers	Number of CNOTS
52	108	~ 1760

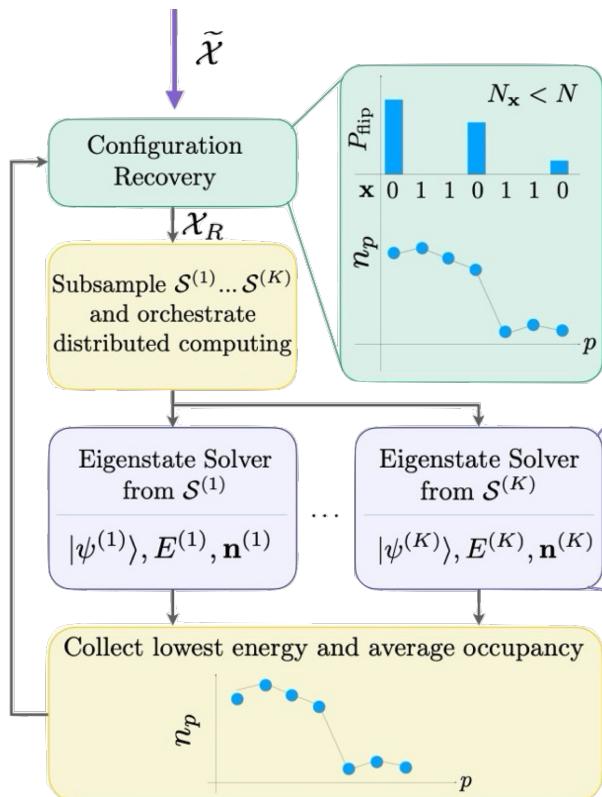
Sample-based Quantum Diagonalization (SQD)



Sample-based Quantum Diagonalization (SQD)



Sample-based Quantum Diagonalization (SQD)



Step 3: Classical post-processing using an HPC

$$H_{S^{(k)}} = P_{S^{(k)}} H P_{S^{(k)}}$$

with $P_{S^{(k)}} = \sum_{\mathbf{x} \in S^{(k)}} |\mathbf{x}\rangle\langle\mathbf{x}|$

$$H_{S^{(k)}} |\psi^{(k)}\rangle = E^{(k)} |\psi^{(k)}\rangle$$

The final energy is the average minimum energy obtained.

Create K batches of d configurations $S(1), \dots, S(K)$.

* Using corrected samples with repetition according to the empirical frequencies.

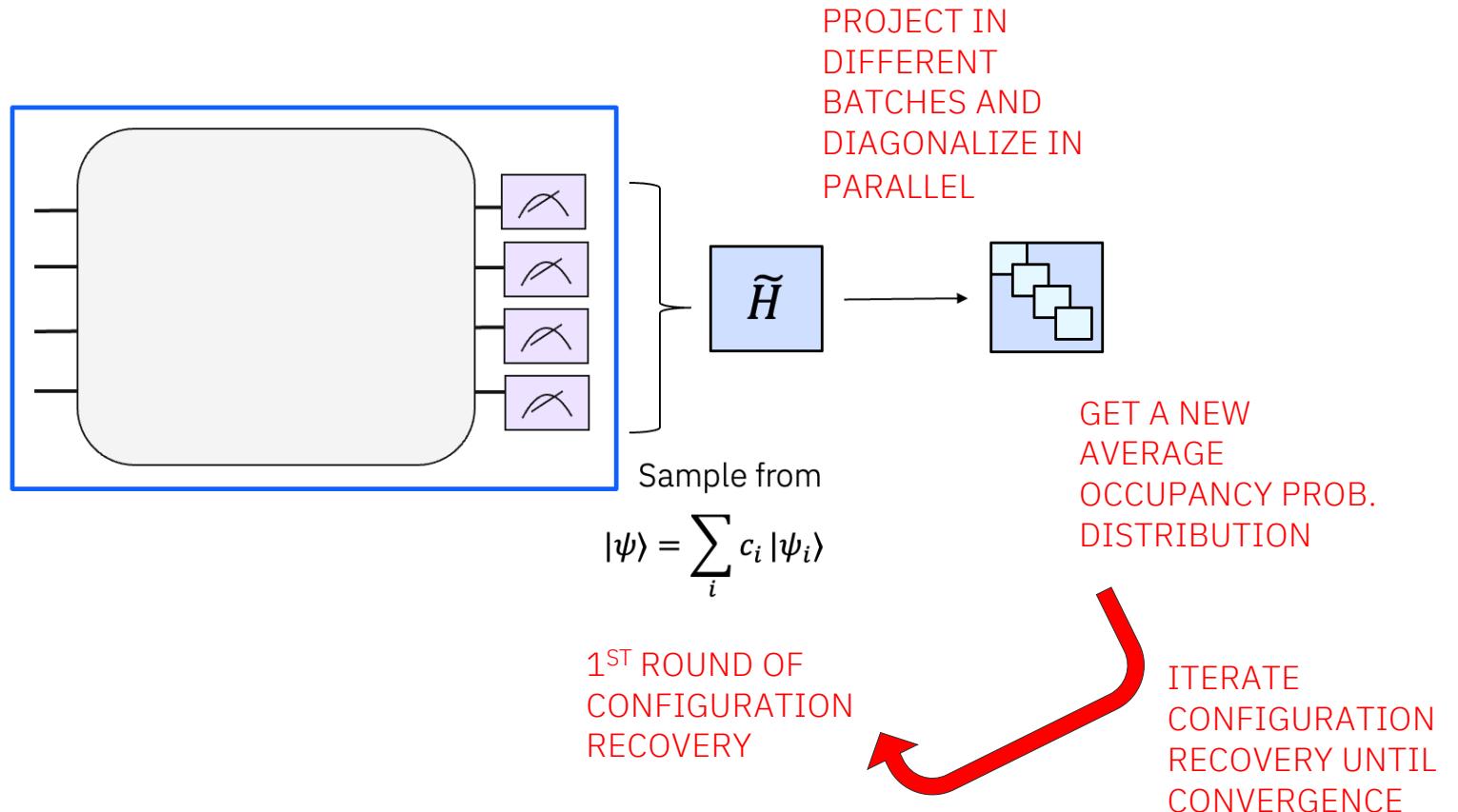
Project and diagonalize the Hamiltonian over each $S(k)$, using iterative Davidson method on multiple classical nodes.

Resulting ground states are used to obtain a new occupancy

$$n_{p\sigma} = \frac{1}{K} \sum_{1 \leq k \leq K} \langle \psi^{(k)} | \hat{n}_{p\sigma} | \psi^{(k)} \rangle$$

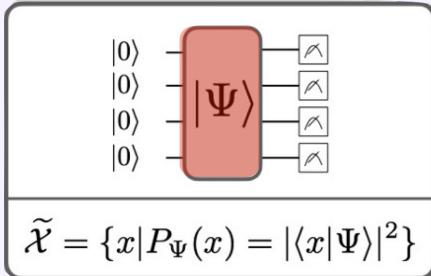
and configuration recovery loop is repeated until convergence.

Sample-based Quantum Diagonalization (SQD)

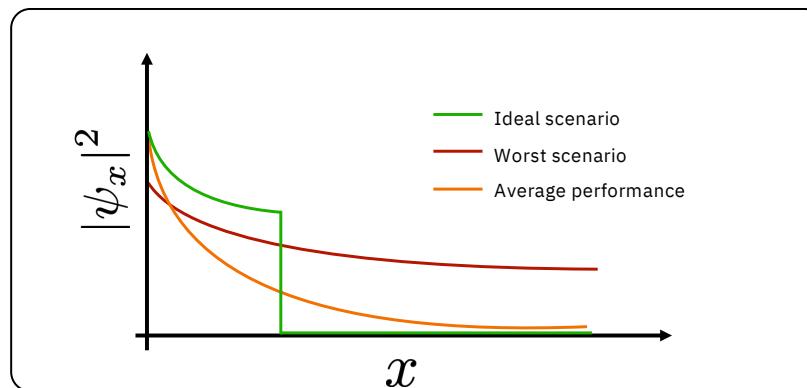


Sample-based Quantum Diagonalization (SQD)

Sampler()



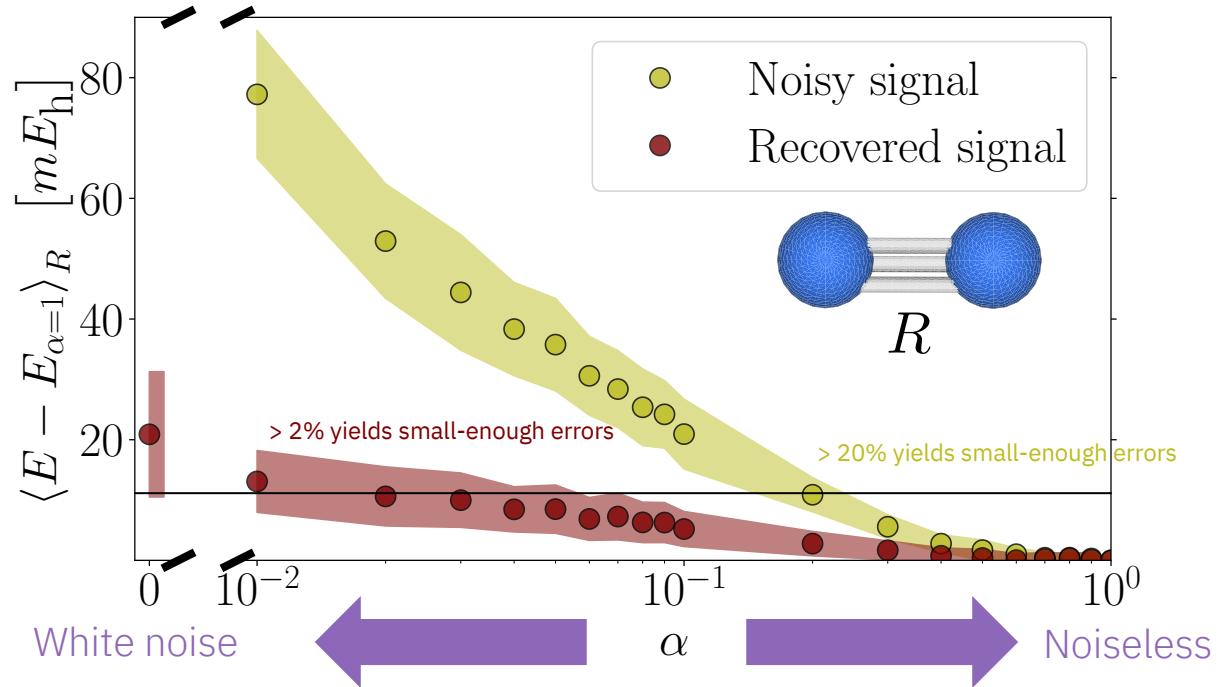
How do we make sure that the quantum state we prepare spans the right set of determinants?



Wavefunction should be concentrated
(shared assumption with classical SCI)

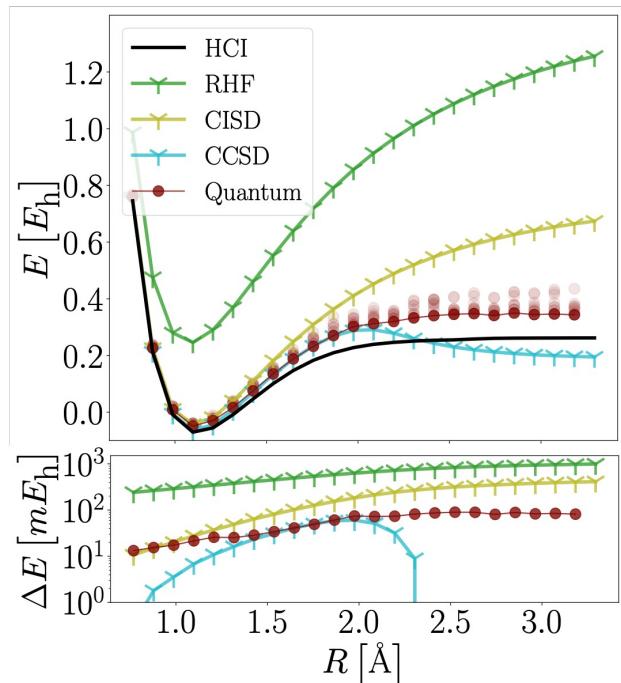
The goal of the quantum circuit is not to exactly approximate the **probability distribution underlying the ground state**, but to sample from its support – or a subset of it - to give the lowest energy possible.

SQD results: Signal retrieval using configuration recovery



$$P_{\text{noisy}}(x) = \alpha \cdot P_{\text{noiseless}}(x) + (1 - \alpha) \cdot \frac{1}{2M}$$

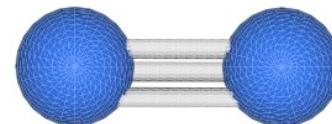
SQD results: Bond breaking on large basis sets



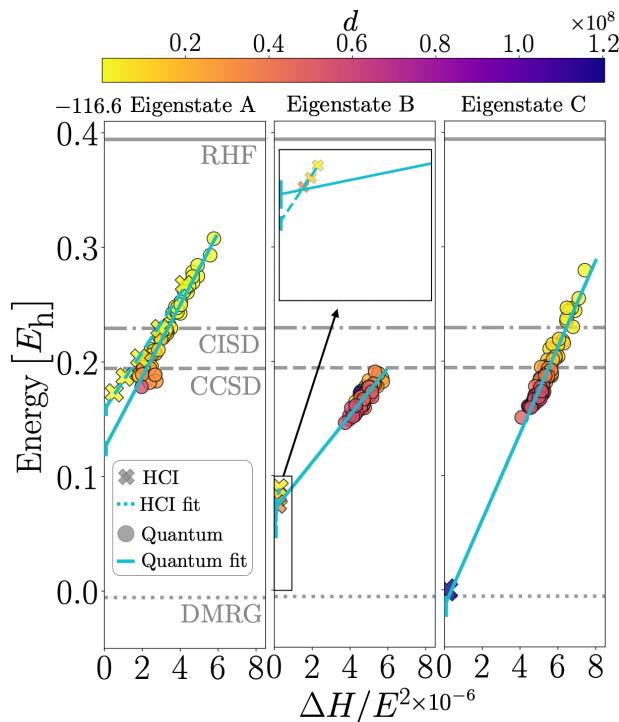
58 qubits
5204 quantum gates
1792 two-qubit gates

The breaking of the N_2 bond is a recognized test of the accuracy for electronic structure methods against static electronic correlation

Quantum data can qualitatively capture multi-reference ground states on molecular systems of 52 spin-orbitals



SQD results: precision many-body physics



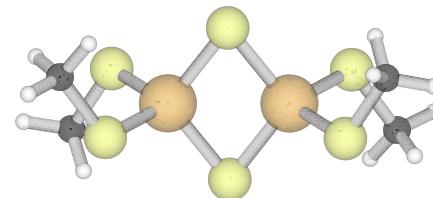
45 qubits
3170 quantum gates
1100 two-qubit gates

IBM Quantum

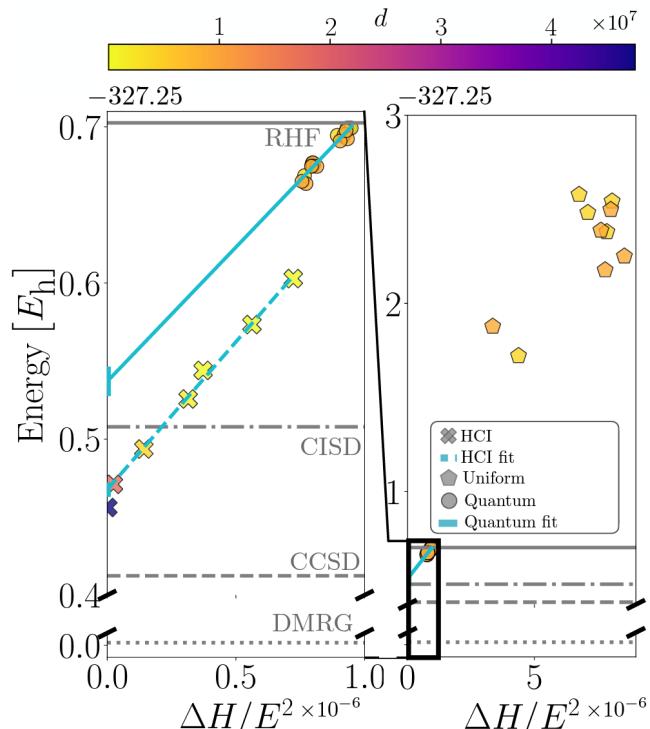
No false positives: the energies produced are upper bounds, and lower energies are certifiably better

A linear arrangement of points in the energy-variance plane signals that we are sampling an eigenstate

Linear extrapolations of the quantum data confirms that we have found three eigenstates of Fe_2S_2



SQD results: Pushing hardware capabilities

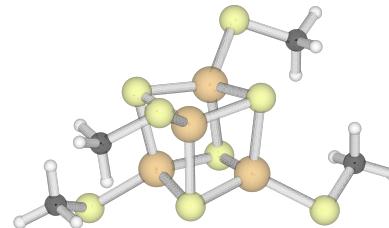


77 qubits
10570 quantum gates
3590 two-qubit gates

IBM Quantum

The largest quantum circuit for molecular simulations: active space Fe_4S_4

Pre-fault-tolerant quantum data on a circuit of 10k gates can provide a useful signal for chemistry



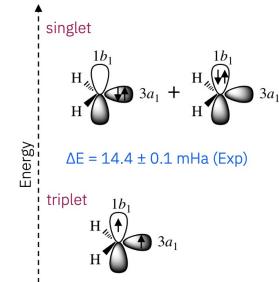
Sample-based Quantum Diagonalization (SQD)

- Quantum-centric supercomputing enables realistic use cases beyond problems tailored to the device connectivity.
- Chemistry is a first: classical processes large classical data, quantum executes a few large quantum circuits.
- Processing of quantum data at the sample level: no false positive solutions and certifiable advantage.
- SQD is guaranteed to succeed on a noiseless signal if GS has a polynomial size support and the wavefunction prepared on QPU has a support similar to that of the ground state.
- There is value in trying the approach with different input circuits because any solution can be certified and ranked by quality.
- The approximate solutions can be stored in classical memory, which permits further classical processing.

Further demonstrations of SQD

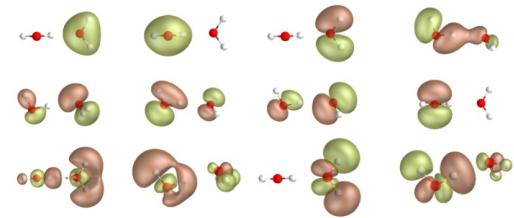
Quantum-Centric Study of Methylenes Singlet and Triplet States

Ieva Liepuoniute*,¹ Kirstin D. Doney,² Javier Robledo Moreno,³ Joshua A. Job,² Will S. Friend,² Gavin O. Jones¹



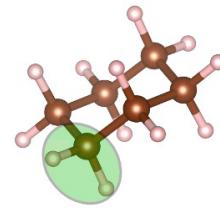
Towards quantum-centric simulations of extended molecules: sample-based quantum diagonalization enhanced with density matrix embedding theory

Akhil Shajan,^{1,2} Danil Kaliakin,¹ Abhishek Mitra,¹ Javier Robledo Moreno,³ Zhen Li,¹ Mario Motta,³ Caleb Johnson,³ Abdullah Ash Saki,³ Susanta Das,¹ Iskandar Situdikov,³ Antonio Mezzacapo,³ and Kenneth M. Merz Jr.^{1,2,*}



Accurate quantum-centric simulations of supramolecular interactions

Danil Kaliakin,¹ Akhil Shajan,^{1,2} Javier Robledo Moreno,³ Zhen Li,¹ Abhishek Mitra,¹ Mario Motta,³ Caleb Johnson,³ Abdullah Ash Saki,³ Susanta Das,¹ Iskandar Situdikov,³ Antonio Mezzacapo,³ and Kenneth M. Merz Jr.^{1,2,*}



Quantum-centric Supercomputing

- Sample-based Quantum Diagonalization (**SQD**) May 2024

Chemistry Beyond Exact Solutions on a Quantum-Centric Supercomputer

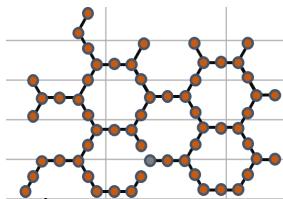
Javier Robledo-Moreno,^{1,*} Mario Motta,^{1,†} Holger Haas,¹ Ali Javadi-Abhari,¹ Petar Jurcevic,¹ William Kirby,² Simon Martiel,³ Kunal Sharma,¹ Sandeep Sharma,⁴ Tomonori Shirakawa,^{5,6,7} Iskandar Siddikov,¹ Rong-Yang Sun,^{5,6,7} Kevin J. Sung,¹ Maika Takita,¹ Minh C. Tran,² Seiji Yunoki,^{5,6,7,8} and Antonio Mezzacapo^{1,‡}



- Krylov Quantum Diagonalization (**KQD**) July 2024

Diagonalization of large many-body Hamiltonians on a quantum processor

Nobuyuki Yoshioka*,^{1,†} Mirko Amico*,^{2,‡} William Kirby*,^{3,§} Petar Jurcevic,² Arkopal Dutt,³ Bryce Fuller,² Shelly Garion,⁴ Holger Haas,² Ikko Hamamura**,⁵ Alexander Ivrii,⁴ Ritajit Majumdar,⁶ Zlatko Minev,² Mario Motta,² Bibek Pokharel,⁷ Pedro Rivero,² Kunal Sharma,² Christopher J. Wood,² Ali Javadi-Abhari,² and Antonio Mezzacapo²



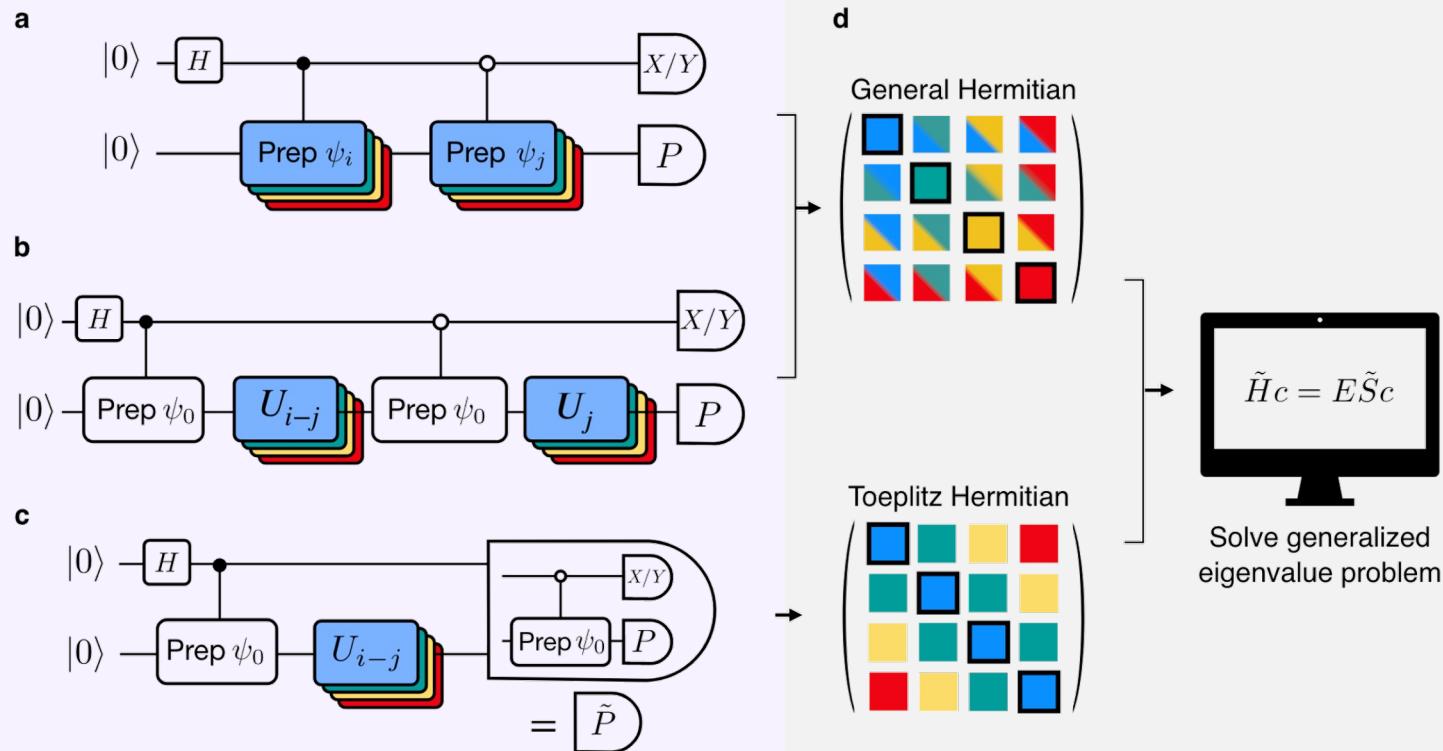
- Sample-based Krylov Quantum Diagonalization (**SKQD**) January 2025

Sample-based Krylov Quantum Diagonalization

Jeffery Yu,^{1,2,3,*} Javier Robledo Moreno,^{1,†} Joseph Iosue,^{1,2,3} Luke Bertels,⁴ Daniel Claudino,⁴ Bryce Fuller,¹ Peter Groszkowski,⁵ Travis S Humble,⁶ Petar Jurcevic,¹ William Kirby,⁷ Thomas A. Maier,⁸ Mario Motta,¹ Bibek Pokharel,¹ Alireza Seif,¹ Amir Shehata,⁶ Kevin J. Sung,¹ Minh C. Tran,¹ Vinay Tripathi,¹ Antonio Mezzacapo,^{1,‡} and Kunal Sharma^{1,§}



Krylov Quantum Diagonalization (KQD)



<https://arxiv.org/abs/2407.14431>

Krylov Quantum Diagonalization (KQD)

Main idea: Project the Hamiltonian into a Krylov space spanned by various time evolutions of an initial reference state.

Inspired in the [classical Lanczos algorithm](#).

Step 1. Build an orthonormalized subspace iteratively from the Hamiltonian H and reference state $|\psi_0\rangle$.

Initialize: $|q_0\rangle = |\psi_0\rangle$

At each step: $|w'_j\rangle = H^j|q_j\rangle$ + orthonormalize

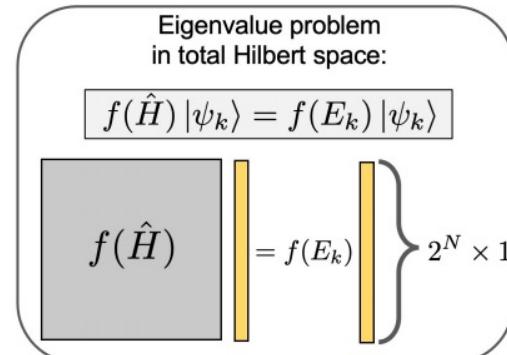
Step 2. Project the Hamiltonian onto the subspace.

Projection matrix: $Q = (|q_1\rangle|q_2\rangle \dots |q_k\rangle)$

$$\tilde{H} = Q^*HQ$$

The ground state energy is then estimated by diagonalizing \tilde{H} .

Classical methods run into memory issues when trying to store the wavefunction of large strongly correlated quantum systems.



Phys. Rev. A **105**, 022417

Krylov Quantum Diagonalization (KQD)

Main idea: Project the Hamiltonian into a Krylov space spanned by various time evolutions of an initial reference state.

In the quantum Krylov algorithm is implemented on a quantum circuit by replacing H with U . $H \rightarrow U = e^{-iHt}$

$$K_r^U = \{|\psi_0\rangle, U|\psi_0\rangle, U^2|\psi_0\rangle, U^3|\psi_0\rangle, \dots, U^{r-1}|\psi_0\rangle\}$$

Non-orthogonal subspace!

The projected Hamiltonian \tilde{H} and the matrices of overlaps are obtained through calculating expectation values (for example via Hadamard test)

$$\tilde{H}_{jl} = \langle \psi_j | H | \psi_l \rangle = \langle \psi_0 | U^{j+} H U^l | \psi_0 \rangle$$

$$\tilde{S}_{jl} = \langle \psi_j | \psi_l \rangle$$

solve generalized eigenvalue problem

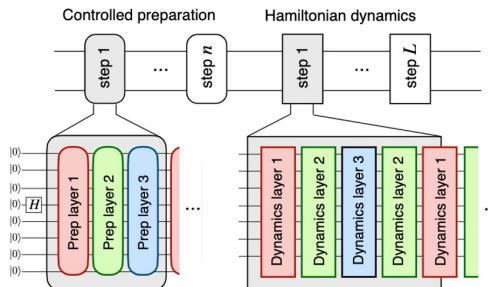
$$\tilde{H}\vec{c} = E\tilde{S}\vec{c}$$

Memory limitations are addressed but non-orthonormalized subspace can lead to numerical instabilities!

Krylov Quantum Diagonalization (KQD)

Using $U = e^{-iHt}$ has two advantages:

- **Trotter circuits** allow for short enough depth to be implemented on existing quantum devices.



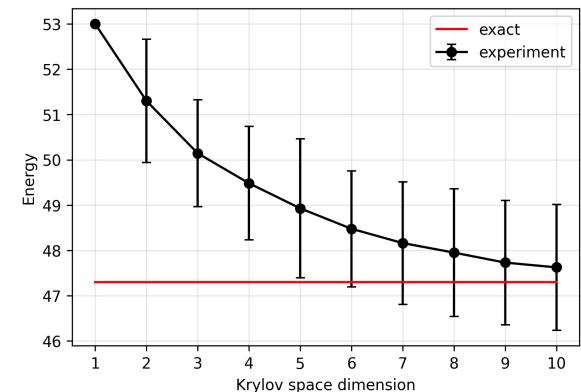
Better suited for spin models
rather than quantum
chemistry Hamiltonians.

- Even in the presence of noise, the error due to projection exponentially decreases with the Krylov dimension, just as in classical Krylov algorithms.

The accuracy of the method can be bounded theoretically

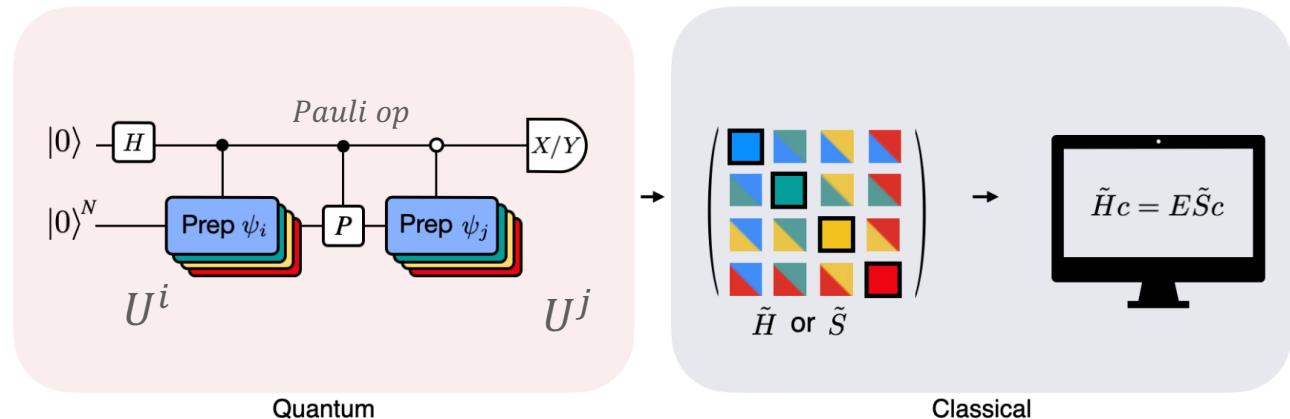
error of projecting
into the subspace
(overlap GS - initial state)

Algorithmic (trotter),
statistical (sampling),
hardware errors



Krylov Quantum Diagonalization (KQD)

Simplest implementation uses Hadamard test to calculate (\tilde{H}, \tilde{S})



$$\text{Yields } \langle X \rangle_a = \text{Re}[\langle \psi_0 | (U^j)^\dagger P U^k | \psi_0 \rangle], \quad \langle Y \rangle_a = \text{Im}[\langle \psi_0 | (U^j)^\dagger P U^k | \psi_0 \rangle]$$

No advanced error mitigation

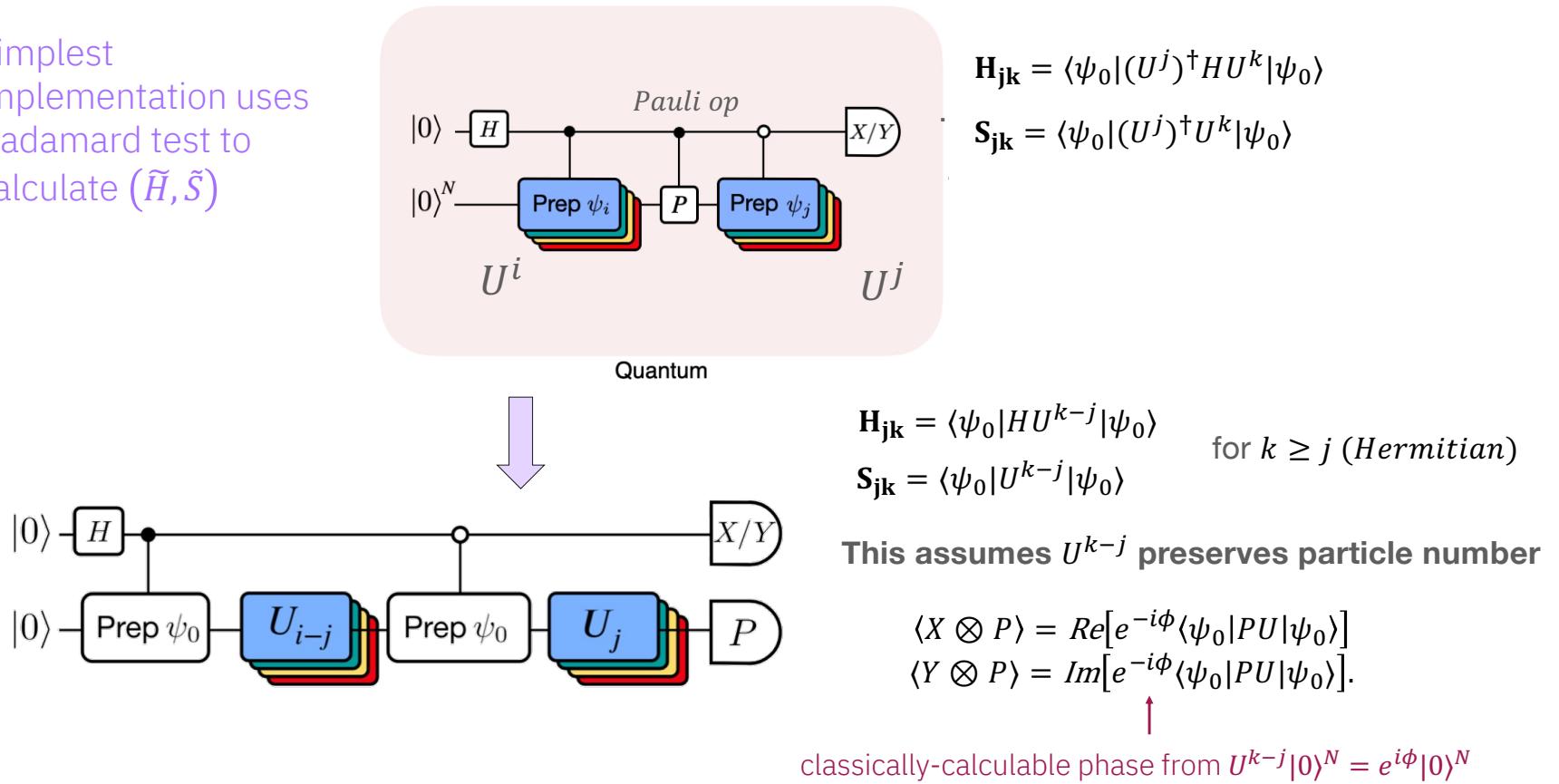
Circuits for the Hadamard test don't have the required structure for error mitigation.

Deep circuits

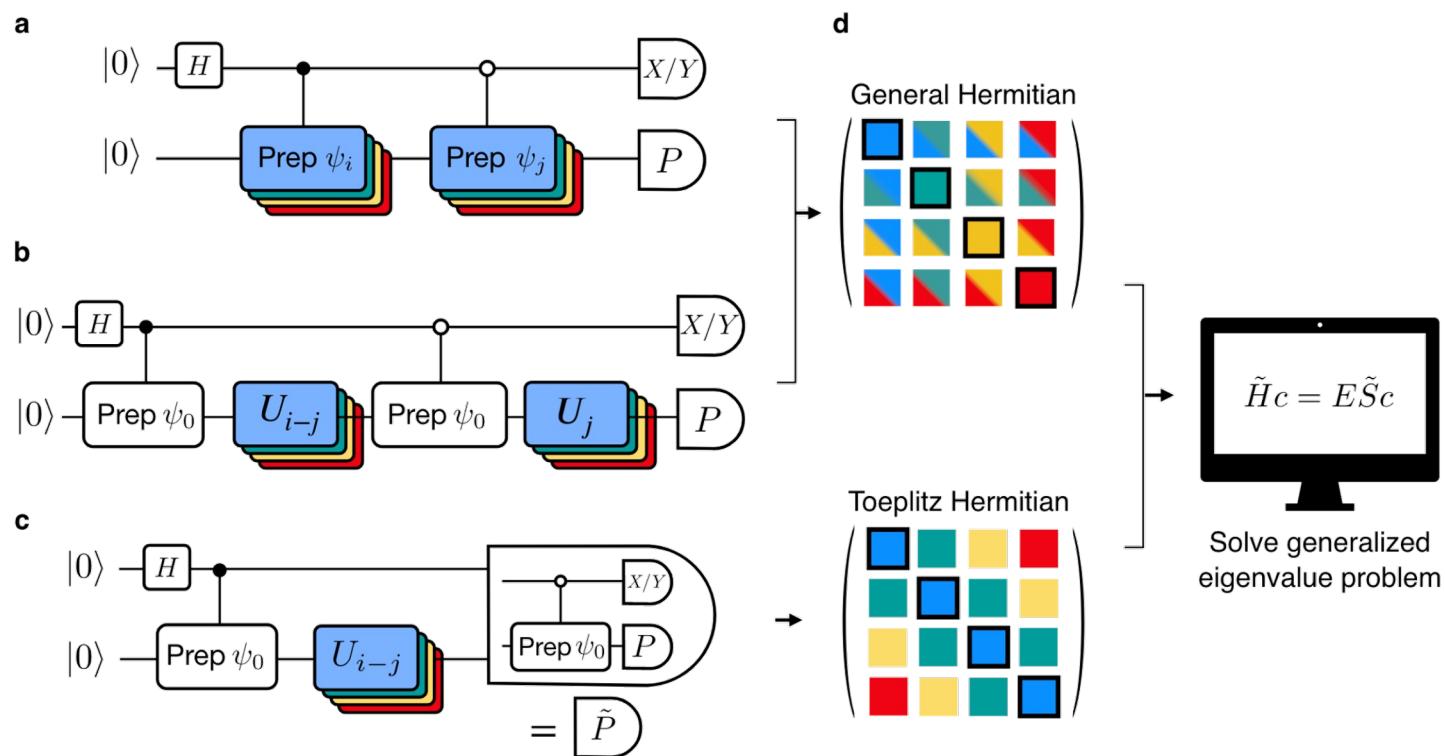
Hadamard test produces deep circuits -> propose alternatives to avoid controlled unitaries.

Krylov Quantum Diagonalization (KQD)

Simplest implementation uses Hadamard test to calculate (\tilde{H}, \tilde{S})

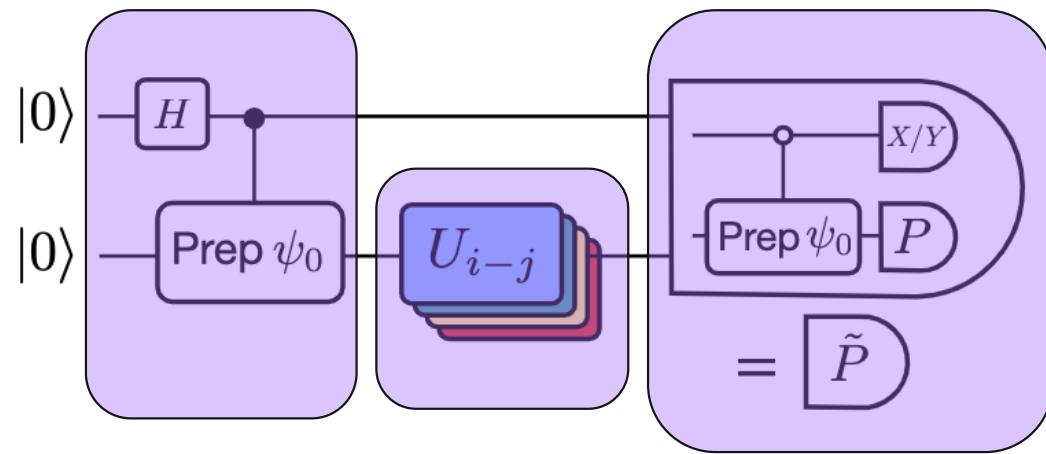


Krylov Quantum Diagonalization (KQD)



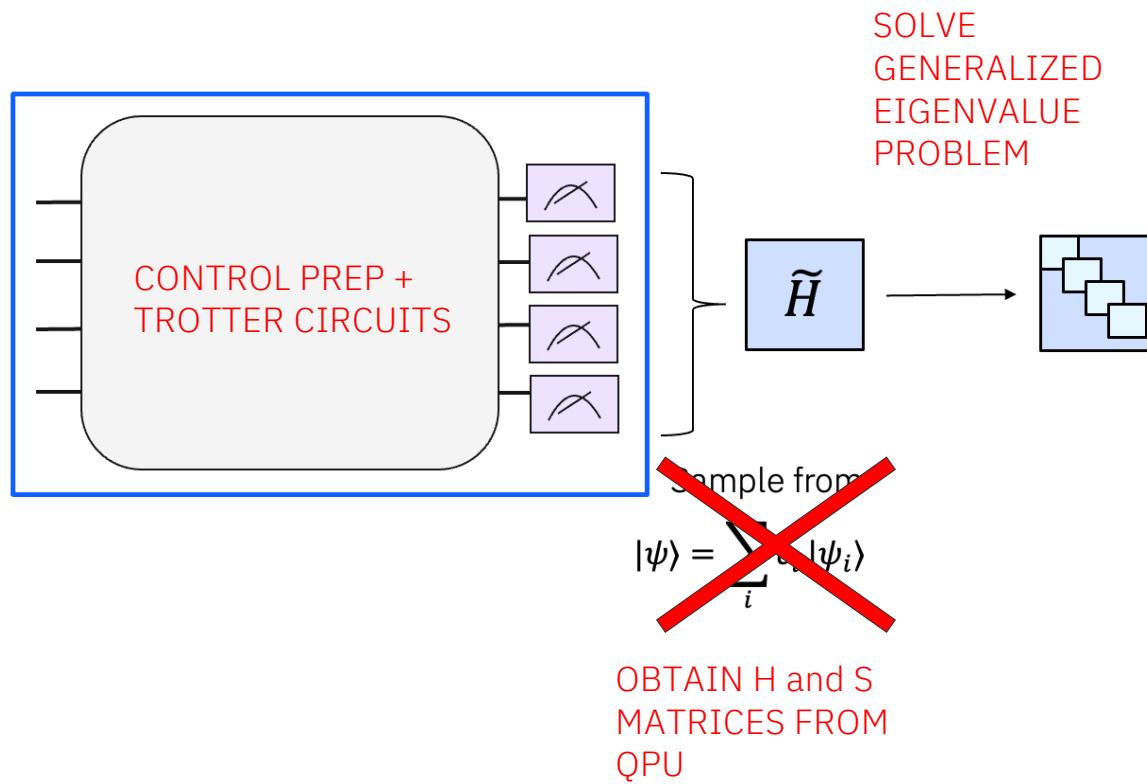
Krylov Quantum Diagonalization (KQD)

One can make circuits shorter by absorbing the reference state un-preparation in the measurement:



$$\tilde{P} = (C - \text{Prep } \psi_0)X/Y \otimes P(C - \text{Prep } \psi_0)^\top$$

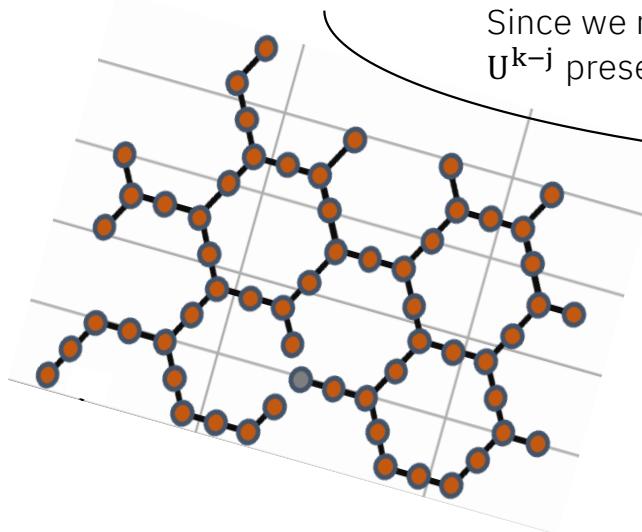
Krylov Quantum Diagonalization (KQD)



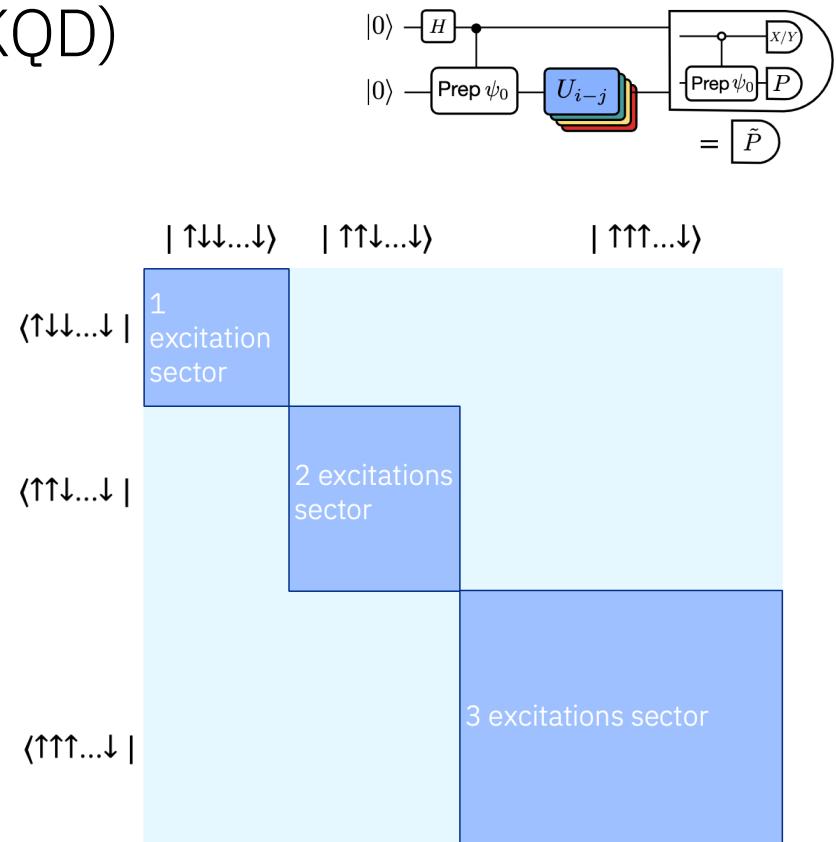
Krylov Quantum Diagonalization (KQD)

Let's look at the Heisenberg model on a heavy-hex lattice:

$$H = J \sum_{\langle i,j \rangle} (X_i X_j + Y_i Y_j + Z_i Z_j)$$

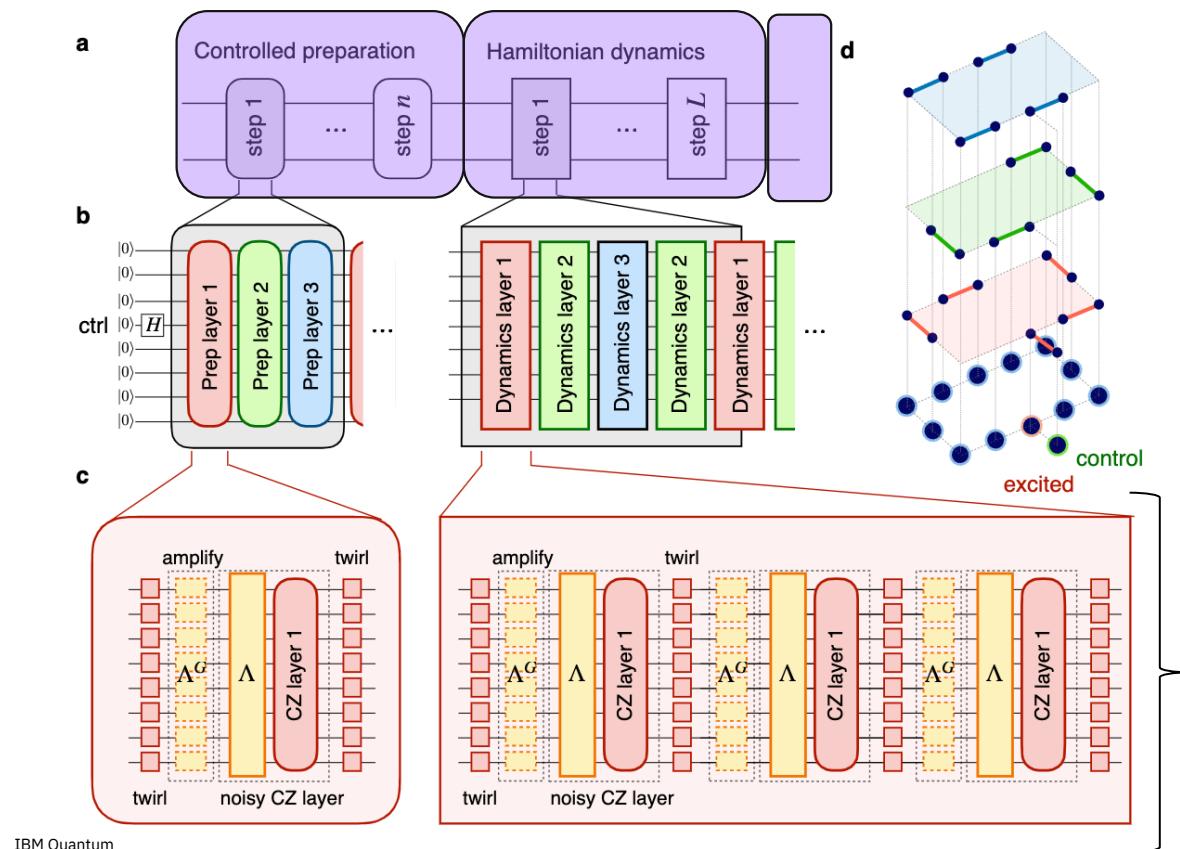


Since we need to assume that U^{k-j} preserves particle number

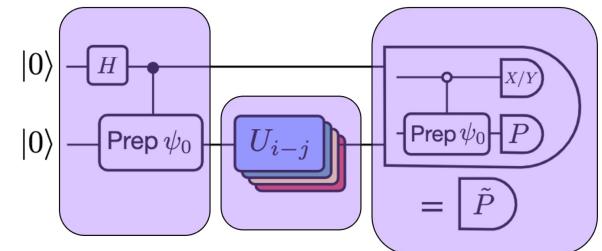


We can be block-diagonalize the Hamiltonian by number of excitations

Krylov Quantum Diagonalization (KQD)



IBM Quantum

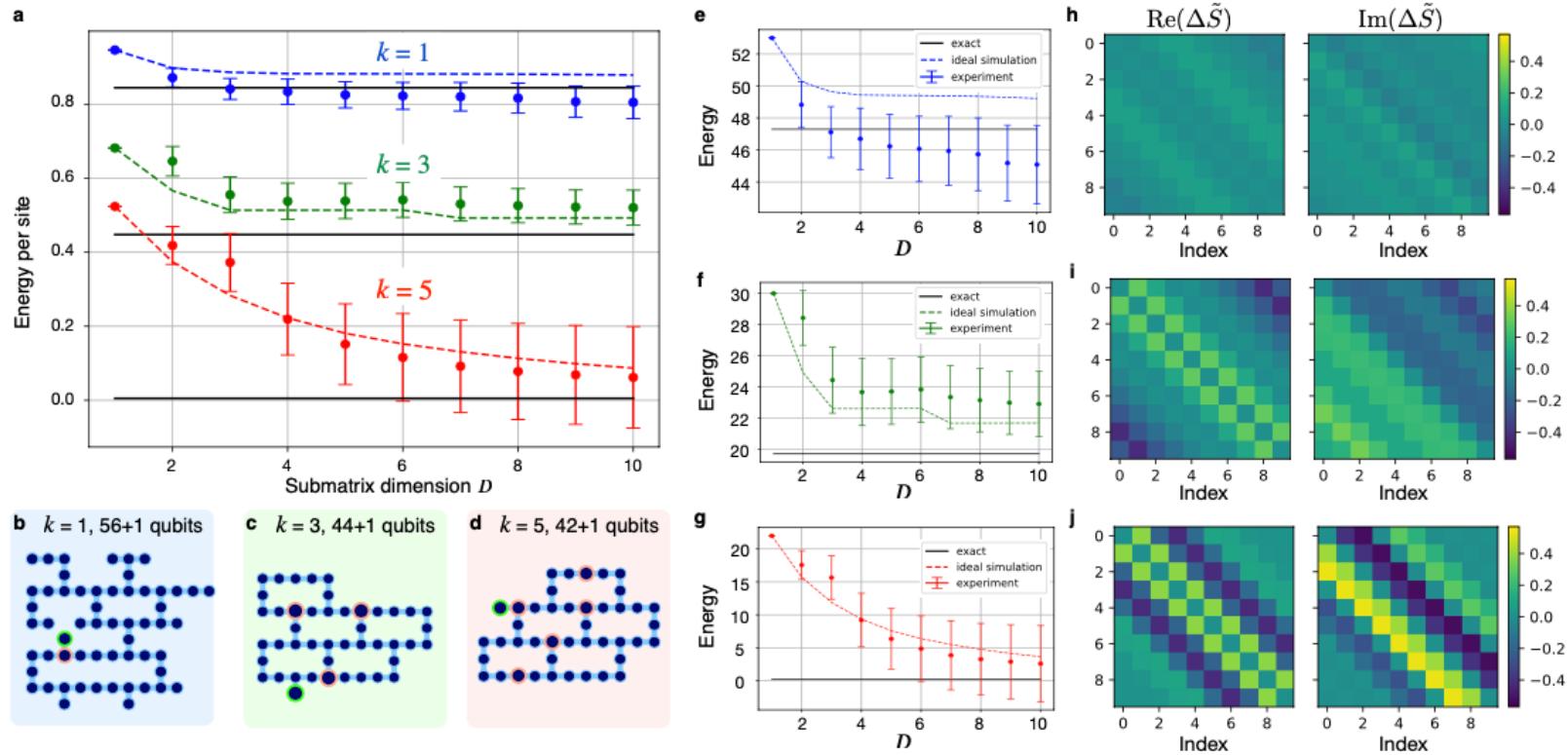


This allows for the implementation of error mitigation techniques:

- Pauli Twirling
- ZNE with PEA

(+ dynamical decoupling, measurement error mitigation)

Krylov Quantum Diagonalization (KQD)



Krylov Quantum Diagonalization (KQD)

Modest resource requirements

Short-depth Trotterized time evolution circuits are enough to get good accuracy

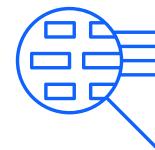
Efficient for large systems

Capable of handling large many-body systems and any interaction types without assumption on the system or sparsity of the ground state

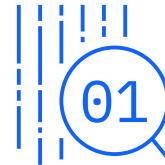
Fast and provable convergence

Quickly converges to the extremal eigenvalues with theoretical guarantees

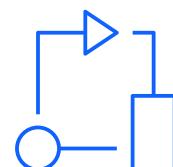
But...



Numerical instabilities



Accuracy affected by
Trotter error and
hardware noise



Hadamard test (&
alternatives) are still
complicated – need to
estimate H and S.

SQD vs KQD → SKQD

SQD

- Well-suited for quantum chemistry ✓
- Only sampling, no expectation values ✓
- Method like configuration recovery can help reduce the effect of noise ✓
- Good accuracy if one can prepare a **good approximation of the ground state support** such that all bitstrings can be sampled with high probability (**sparse but concentrated**) !

KQD

- Needs approximate **time evolution**, well-suited for spin systems instead ✓
- Theoretical guarantee of good accuracy provided the **initial state has a nontrivial overlap with GS** and the **spectrum of H is well-behaved** ✓
- Requires estimating the matrix elements of H and S (expectation values and controlled operations!) !
- Noise has a large effect on the output and noise mitigation can represent a large overhead !

SKQD

Quantum-centric Supercomputing

- Sample-based Quantum Diagonalization (**SQD**) May 2024

Chemistry Beyond Exact Solutions on a Quantum-Centric Supercomputer

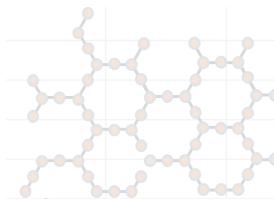
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- Krylov Quantum Diagonalization (**KQD**) October 2024

Diagonalization of large many-body Hamiltonians on a quantum processor

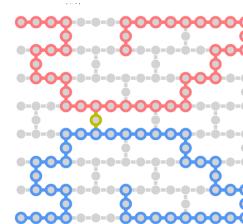
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- Sample-based Krylov Quantum Diagonalization (**SKQD**) January 2025

Sample-based Krylov Quantum Diagonalization

Jeffery Yu,^{1,2,3,*} Javier Robledo Moreno,^{1,†} Joseph Iosue,^{1,2,3} Luke Bertels,⁴ Daniel Claudino,⁴ Bryce Fuller,¹ Peter Groszkowski,⁵ Travis S Humble,⁶ Petar Jurcevic,¹ William Kirby,⁷ Thomas A. Maier,⁸ Mario Motta,¹ Bibek Pokharel,¹ Alireza Seif,¹ Amir Shehata,⁶ Kevin J. Sung,¹ Minh C. Tran,¹ Vinay Tripathi,¹ Antonio Mezzacapo,^{1,‡} and Kunal Sharma^{1,§}



Sample-based Krylov Quantum Diagonalization (KQD)

Recall KQD:

$$H \rightarrow U = e^{-iHt}$$

$$K_r^U = \{|\psi_0\rangle, U|\psi_0\rangle, U^2|\psi_0\rangle, U^3|\psi_0\rangle, \dots, U^{r-1}|\psi_0\rangle\}$$

$$\tilde{H}_{jl} = \langle \psi_j | H | \psi_l \rangle = \langle \psi_0 | U^{j\dagger} H U^l | \psi_0 \rangle$$

$$\tilde{S}_{jl} = \langle \psi_j | \psi_l \rangle$$

solve generalized
eigenvalue problem

$$\tilde{H}\vec{c} = E\tilde{S}\vec{c}$$

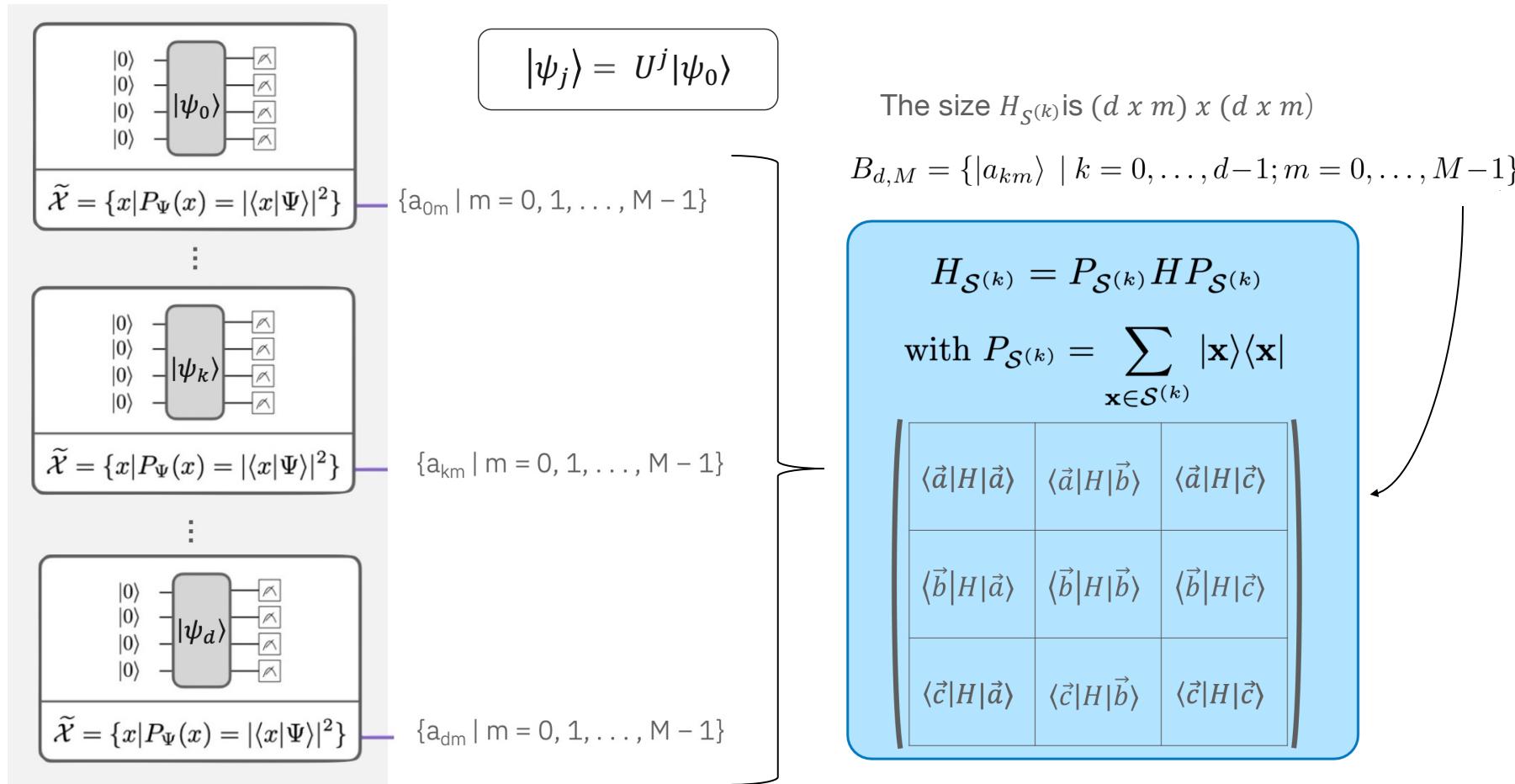
SKIP THIS PART!

Use sample-
based routine
instead!

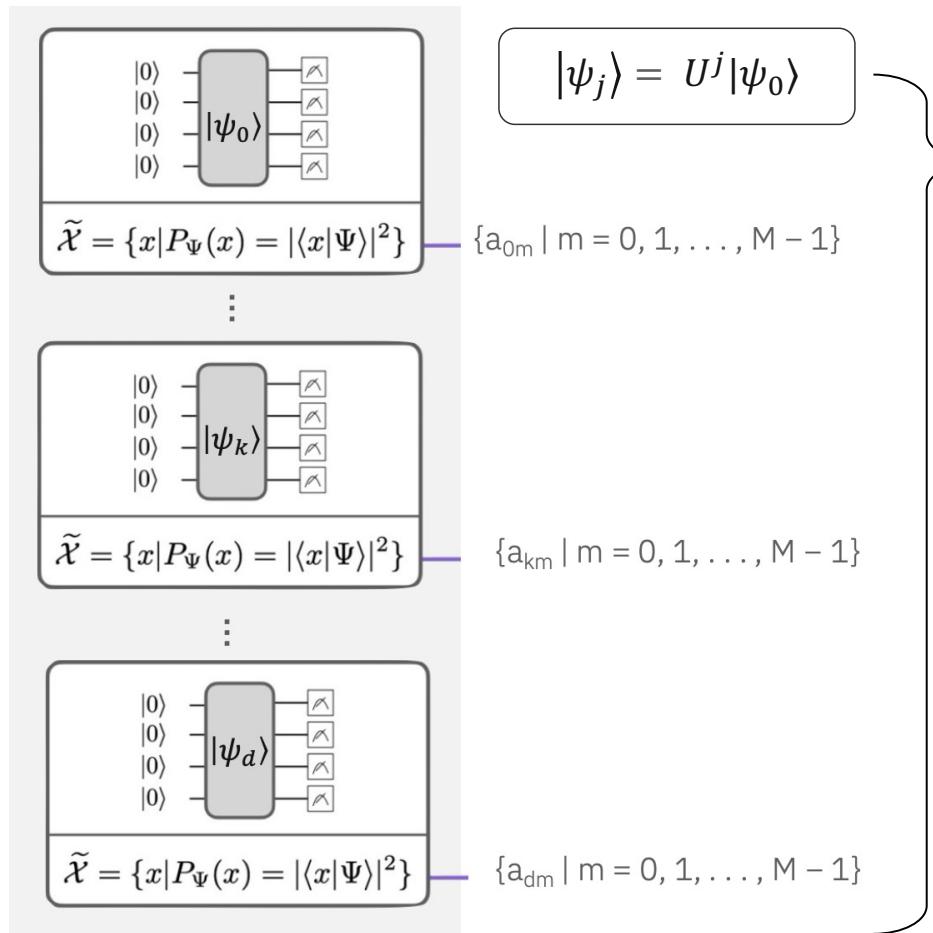
Let's assume that the GS can be expressed as:

$$|\psi\rangle = \sum_{j=1}^N g_j |b_j\rangle \quad \left. \begin{aligned} \sum_{j=1}^L |g_j|^2 &\geq \alpha_L \\ |g_1|^2, \dots, |g_L|^2 &\geq \beta_L \end{aligned} \right\} (\alpha_L, \beta_L)\text{-sparsity}$$

Krylov Quantum Diagonalization (KQD)



Krylov Quantum Diagonalization (KQD)

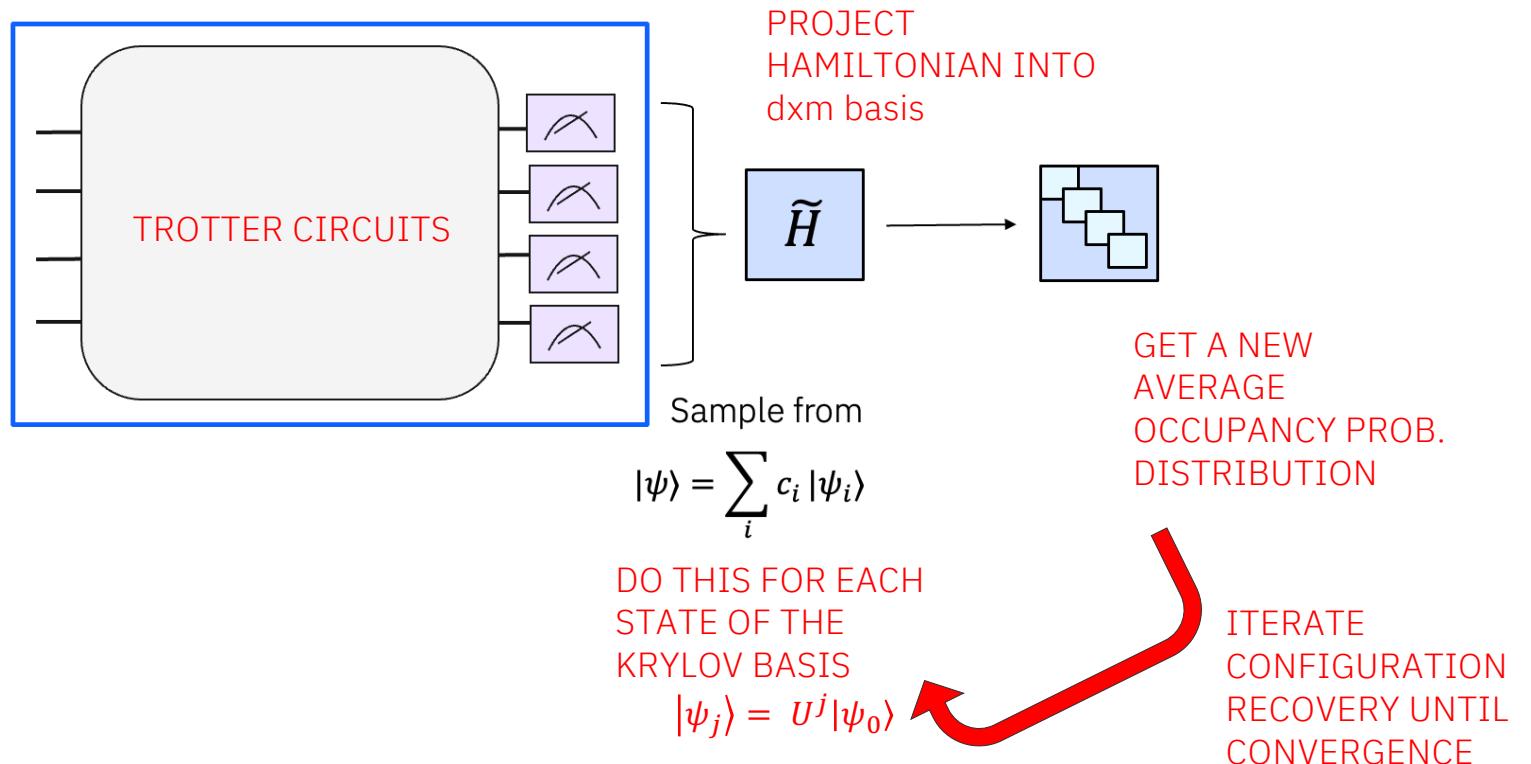


Theoretical guarantees:

- The initial state $|\psi_0\rangle$ has a nontrivial ground-state overlap ($1/\text{poly}(n)$)
- H has a well-behaved spectrum (i.e., ΔE_{N-1} not growing too quickly and ΔE_1 not too small)
- The groundstate is (α_L, β_L) -sparse with $L = \mathcal{O}(\text{poly}(n))$.

A constant error ε in approximating the ground-state energy can be achieved by setting $d = \mathcal{O}(\log(1/\varepsilon))$ and $M = \mathcal{O}(\text{poly}(n))$

Sample-based Krylov Quantum Diagonalization (SKQD)



Sample-based Krylov Quantum Diagonalization (SKQD)

SKQD implementation for the:

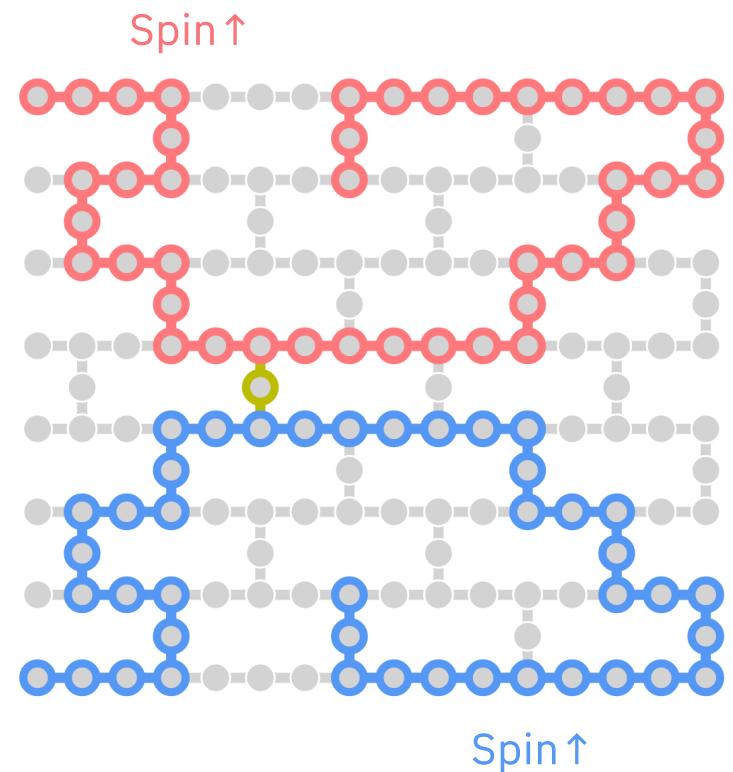
one-dimensional single-impurity Anderson (SIAM) model

$$H = H_{\text{imp}} + H_{\text{bath}} + H_{\text{hyb}}$$

$$H_{\text{imp}} = \varepsilon (\hat{n}_{d\uparrow} + \hat{n}_{d\downarrow}) + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$$

$$H_{\text{bath}} = -t \sum_{\mathbf{j}=0}^{L-1} \sum_{\sigma \in \{\uparrow, \downarrow\}} \left(\hat{c}_{\mathbf{j},\sigma}^\dagger \hat{c}_{\mathbf{j}+1,\sigma} + \hat{c}_{\mathbf{j}+1,\sigma}^\dagger \hat{c}_{\mathbf{j},\sigma} \right)$$

$$H_{\text{hyb}} = V \sum_{\sigma \in \{\uparrow, \downarrow\}} \left(\hat{d}_\sigma^\dagger \hat{c}_{0,\sigma} + \hat{c}_{0,\sigma}^\dagger \hat{d}_\sigma \right)$$



Sample-based Krylov Quantum Diagonalization (SKQD)

SKQD implementation for the SIAM model:

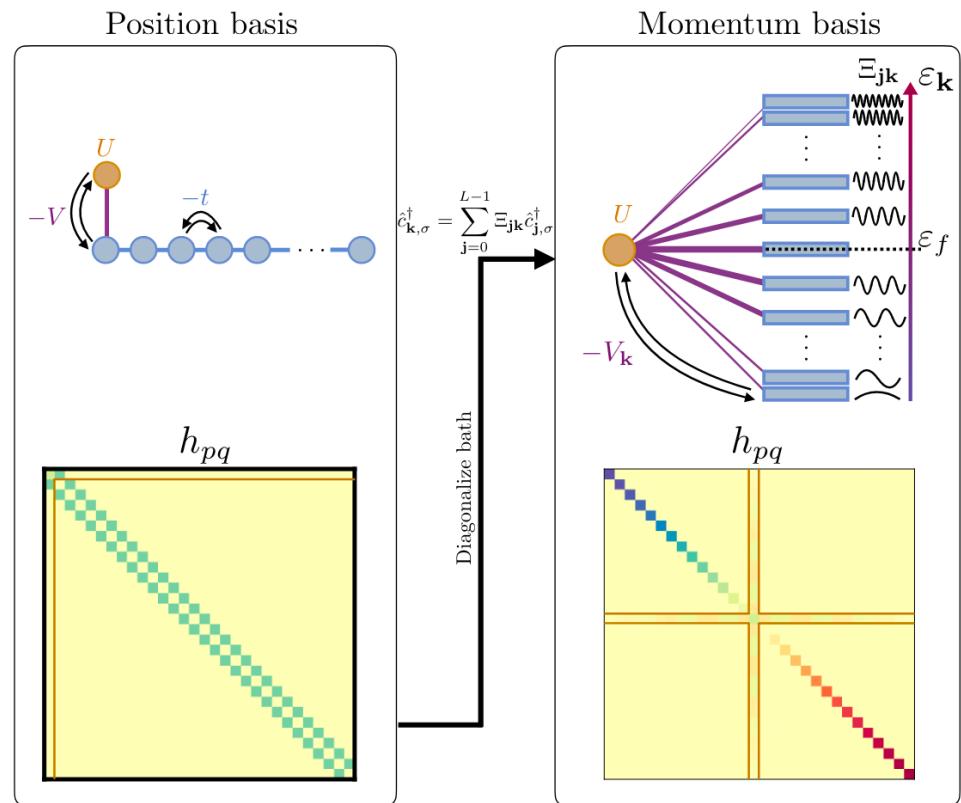
$$H = H_{\text{imp}} + H_{\text{bath}} + H_{\text{hyb}}$$

$$H_{\text{bath}} = -t \sum_{j=0}^{L-1} \sum_{\sigma \in \{\uparrow, \downarrow\}} \left(\hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma} + \hat{c}_{j+1,\sigma}^\dagger \hat{c}_{j,\sigma} \right)$$

non-interacting

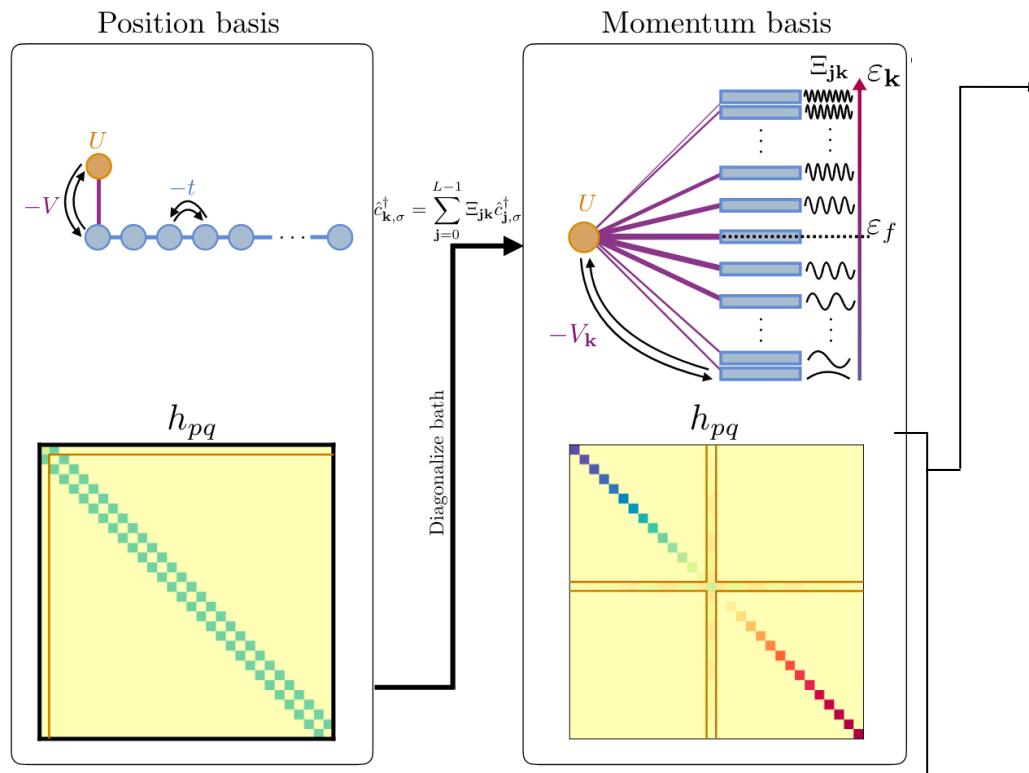
The bath can be diagonalized in momentum space

Note: now the bath modes become approximately plane-wave states, but the impurity is connected to all of them (very non-local!)



Sample-based Krylov Quantum Diagonalization (SKQD)

SKQD implementation for the SIAM model:



This hamiltonian can be expressed in the form

$$H = \sum_{p,q} h_{pq} \hat{a}_{p\sigma}^\dagger \hat{a}_{q\sigma} + \sum_{p,q,r,s} \frac{h_{pqrs}}{2} \hat{a}_{p\sigma}^\dagger \hat{a}_{q\tau}^\dagger \hat{a}_{s\tau} \hat{a}_{r\sigma},$$

But this is highly non-local!

One needs to identify the **basis of natural orbitals**.

Sample-based Krylov Quantum Diagonalization (SKQD)

SKQD implementation for the SIAM model:

This hamiltonian can be expressed in the form

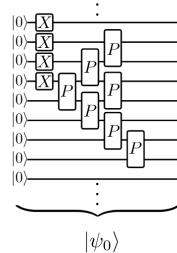
$$H = \sum_{\substack{p,q \\ \sigma}} h_{pq} \hat{a}_{p\sigma}^\dagger \hat{a}_{q\sigma} + \sum_{\substack{p,q,r,s \\ \sigma\tau}} \frac{h_{pqrs}}{2} \hat{a}_{p\sigma}^\dagger \hat{a}_{q\tau}^\dagger \hat{a}_{s\tau} \hat{a}_{r\sigma},$$

But one needs to identify the **basis of natural orbitals**.

Diagonalize it using SKQD.

The idea is to obtain a basis of k -adjacent orbitals so that the impurity only interacts with those.

Initial state:

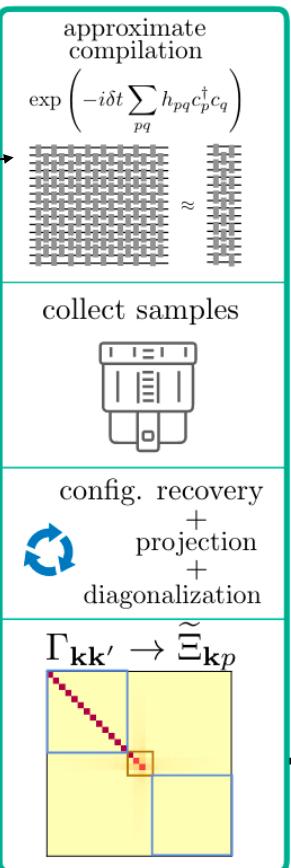


$$P = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Trotter circuits: compile free-fermion time evolution into a shallow circuit of Givens rotations.

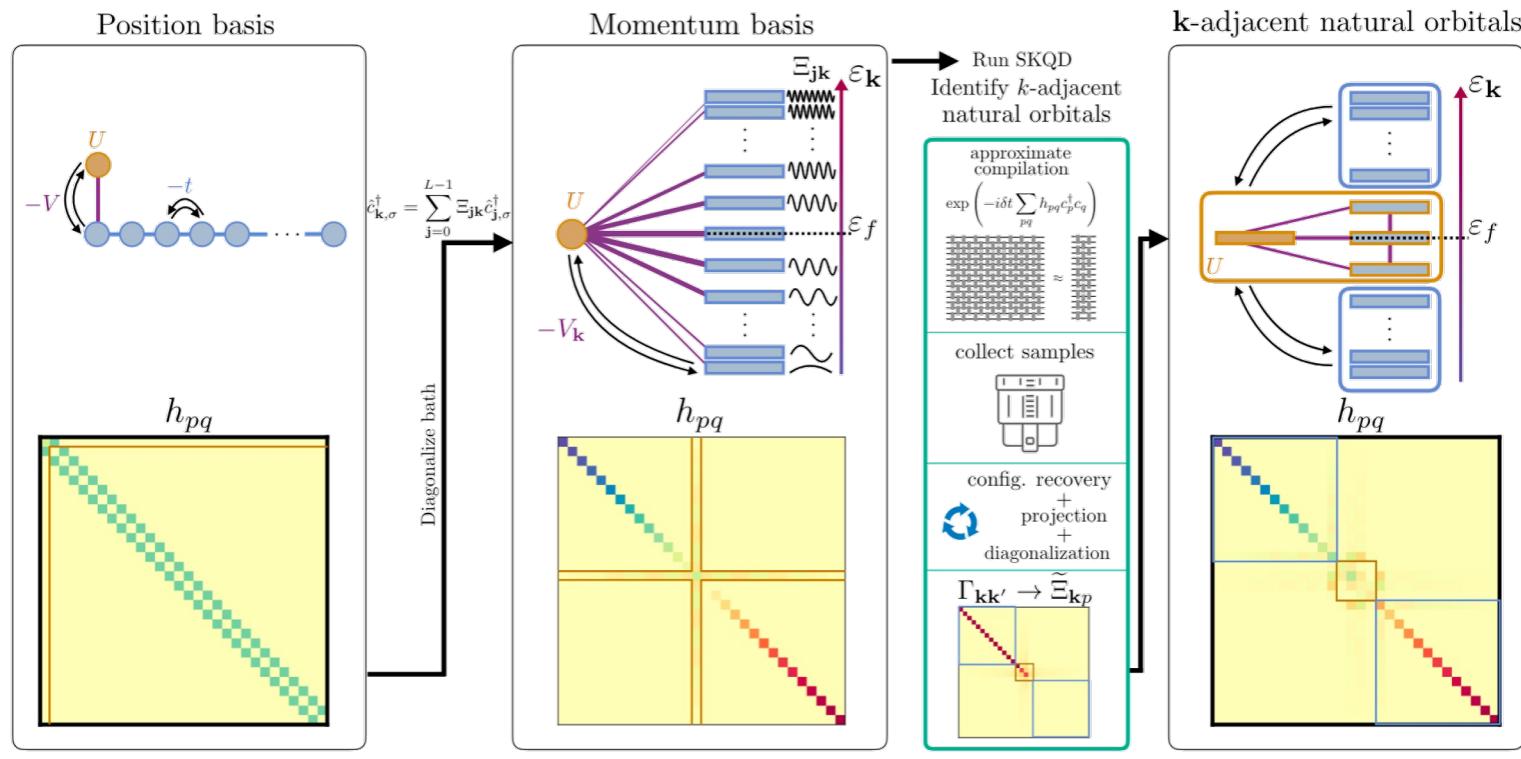
Collect samples and implement **configuration recovery** as in SQD.

One-body reduced density matrix is used to identify k -adjacent natural orbitals.



Sample-based Krylov Quantum Diagonalization (SKQD)

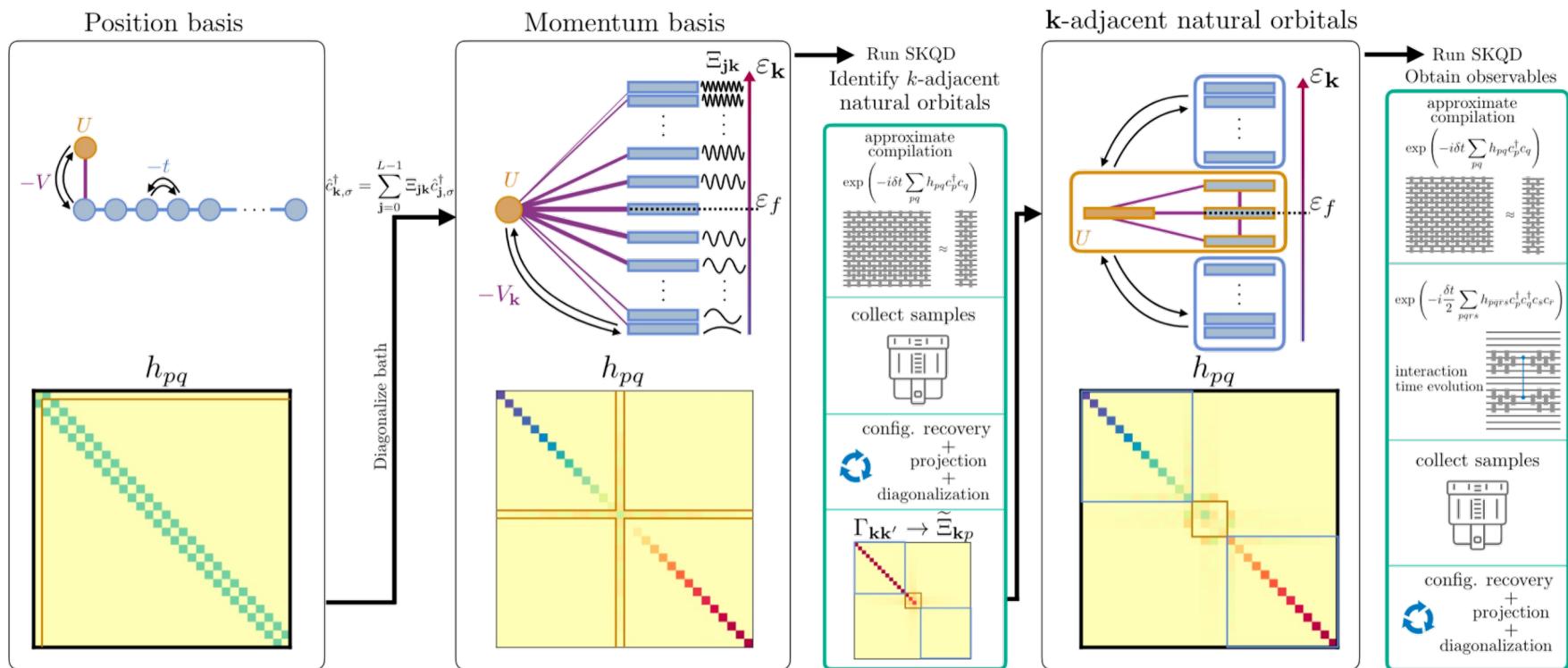
SKQD implementation for the SIAM model:



With this new Hamiltonian we are ready to implement SQKD to estimate the GS

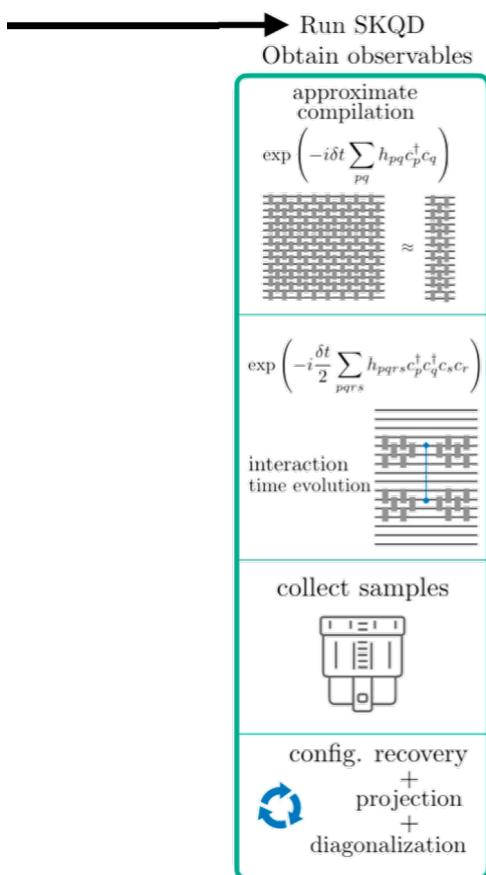
Sample-based Krylov Quantum Diagonalization (SKQD)

SKQD implementation for the SIAM model:



Sample-based Krylov Quantum Diagonalization (SKQD)

SKQD implementation for the SIAM model:



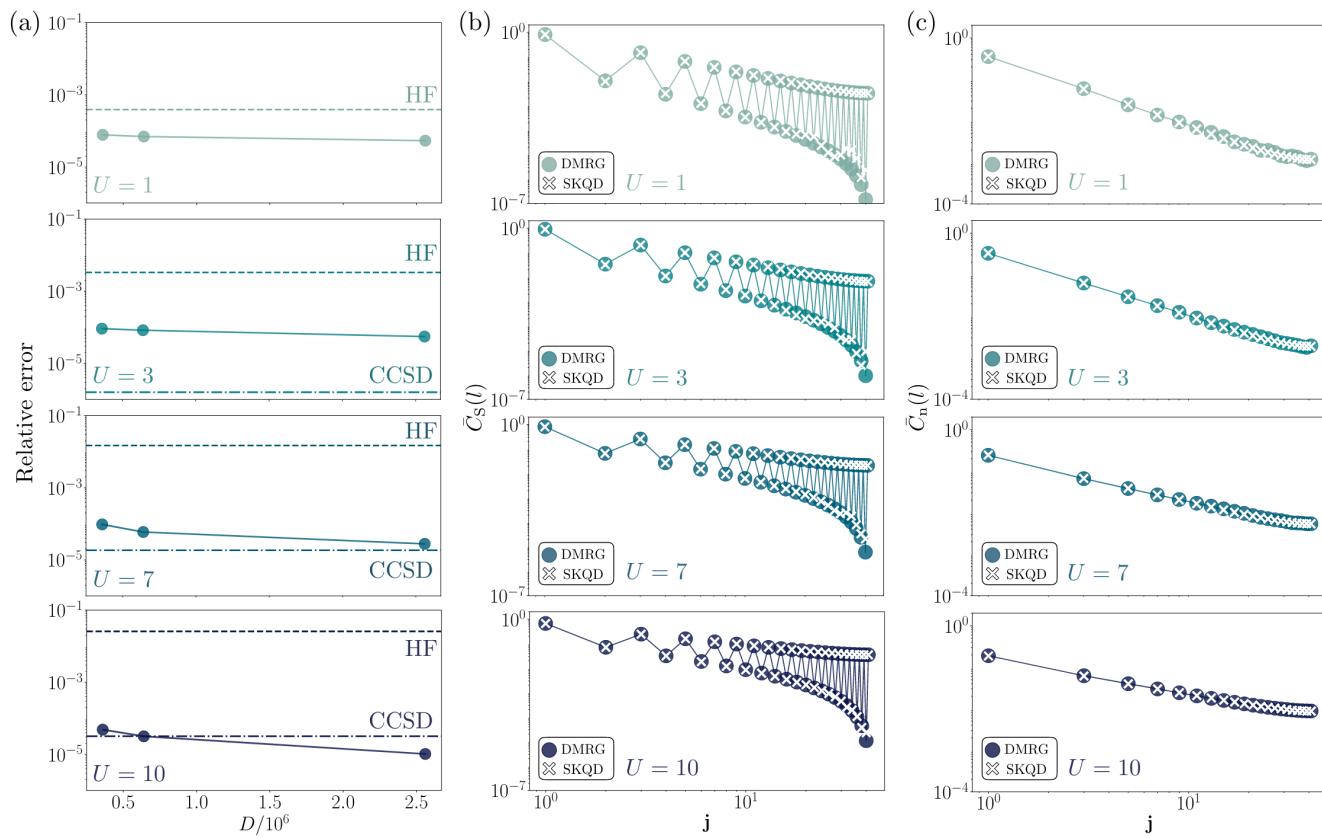
For the experiments, they use $L = 29$ and $L = 41$ bath sites and consider values of the onsite repulsion: $U = 1, 3, 7, 10$.

- $L = 29$ requires 60 qubits under the Jordan-Wigner representation, 30 for each spin species
- $L = 41$ requires 84 qubits, 42 for each spin species.

In all cases they consider $d = 25$ Trotter steps with $\Delta t = 0.1$.

Sample-based Krylov Quantum Diagonalization (SKQD)

SKQD implementation for the SIAM model:



SQD vS KQD → SKQD

SQD

- Well-suited for quantum chemistry ✓
- Only sampling, no expectation values ✓
- Method like configuration recovery can help reduce the effect of noise ✓
- Good accuracy if one can prepare a **good approximation of the ground state support** such that all bitstrings can be sampled with high probability (**sparse but concentrated**) !

KQD

- Needs approximate **time evolution**, well-suited for spin systems instead ✓
- Theoretical guarantee of good accuracy provided the **initial state has a nontrivial overlap with GS** and the **spectrum of H is well-behaved** ✓
- Requires estimating the matrix elements of H and S (expectation values and controlled operations!) !
- Noise has a large effect on the output and noise mitigation can represent a large overhead !

SKQD

- For a **sparse and concentrated** ground state and given an **initial state with polynomial overlap**, one can **approximate the ground state energy in polynomial time** [theoretical guarantees] !
- The only resources needed are: **approximate time evolutions** and **sampling in the computational basis** ✓
- SKQD can outperform KQD in the presence of shot noise+techniques like configuration recovery can help ✓