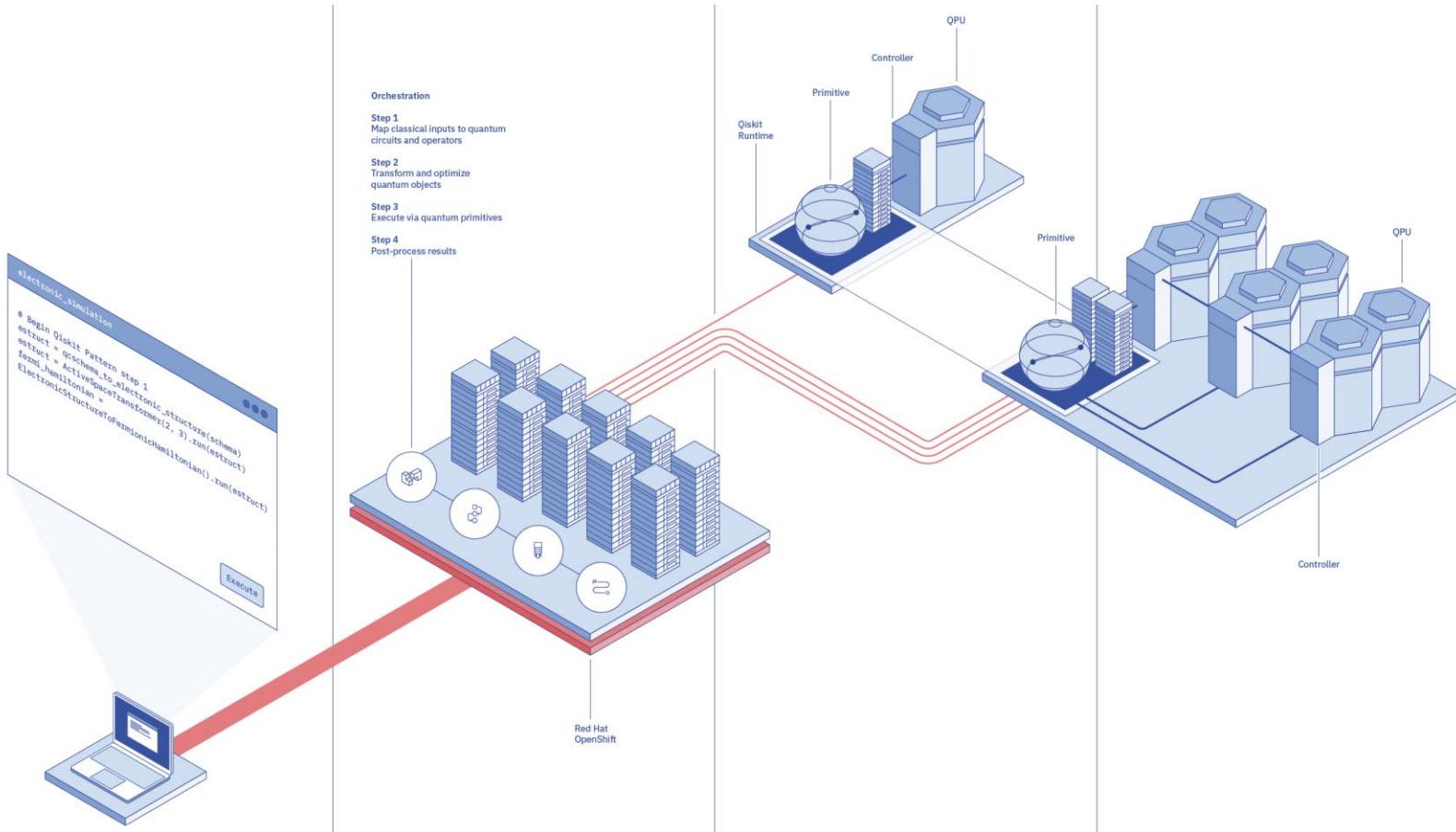


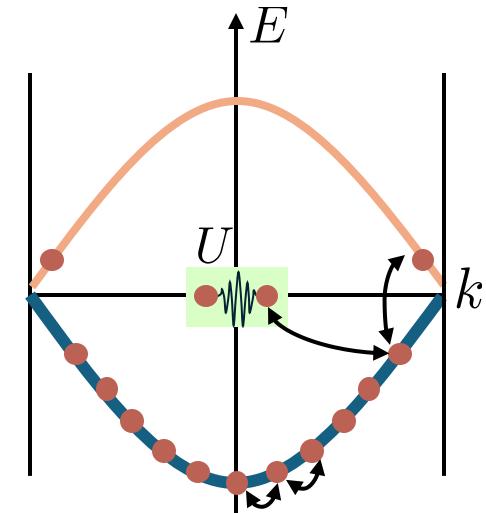
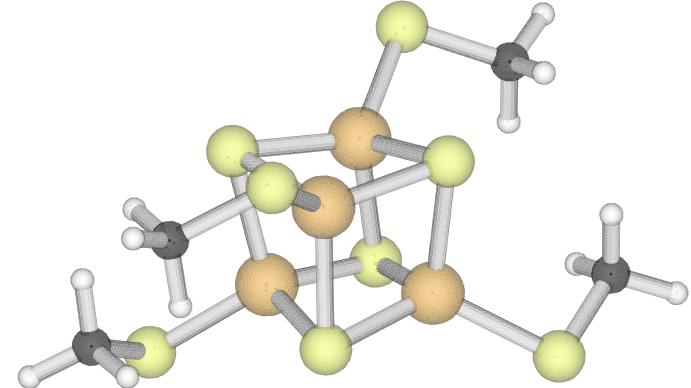
A deep dive into Sample-Based Quantum Diagonalization Methods



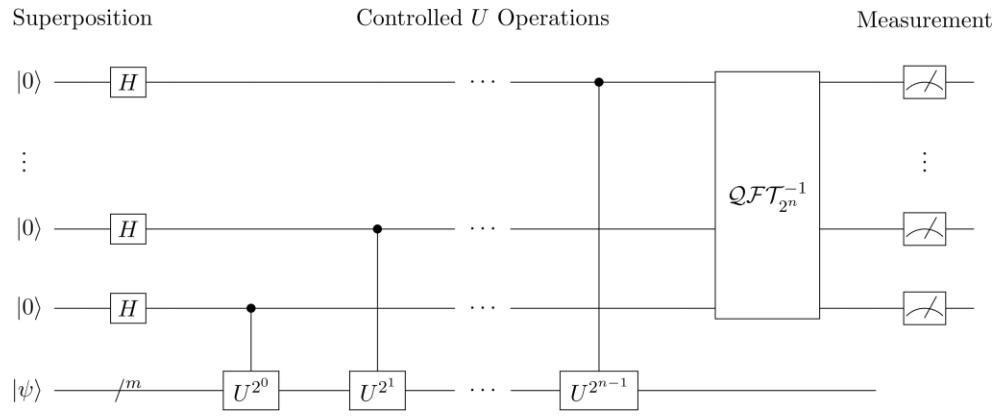
Javier Robledo Moreno
Research Scientist

Quantum Algorithms for ground states

- Goal: solving computationally challenging energy-estimation problems in quantum chemistry and materials
- Applications: development of new materials, drug discovery, battery design



Prior algorithms in fault-tolerant era



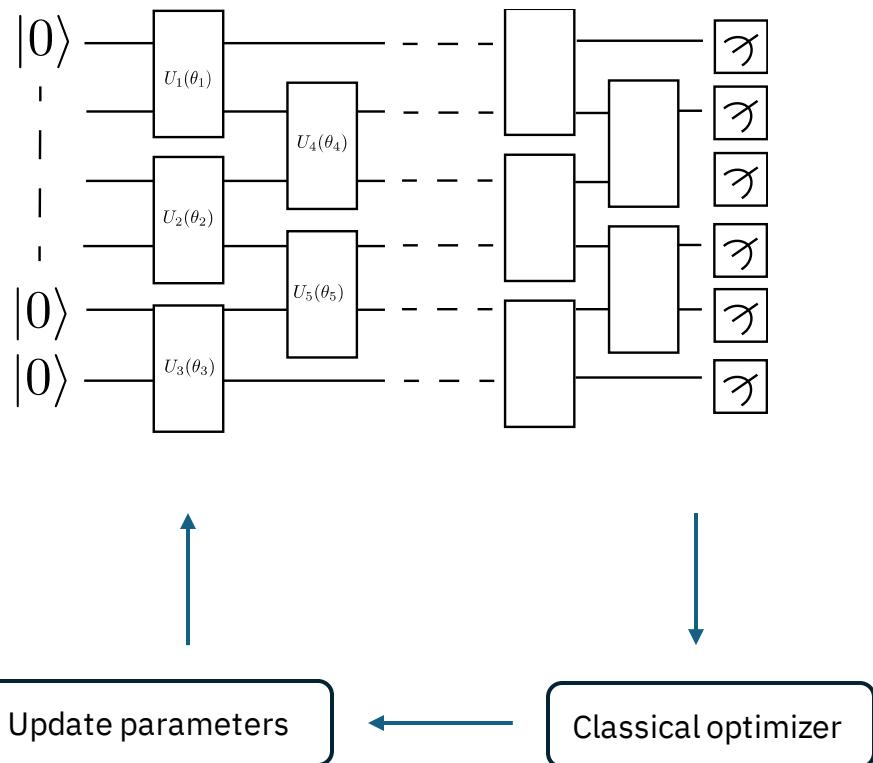
Quantum Phase Estimation (QPE)

- Convergence guarantees when initial state has $1/\text{poly}(n)$ overlap with the true ground state

Key Challenges

- Requires deep quantum circuits and fault-tolerant quantum processors

Prior algorithms in near term



Variational Quantum Algorithms (VQA)

- May require shallow-depth circuits

Key challenges

- No convergence guarantees
- Measurement overhead for chemistry problems

Problem statement: eigenstate approximation

Problem statement

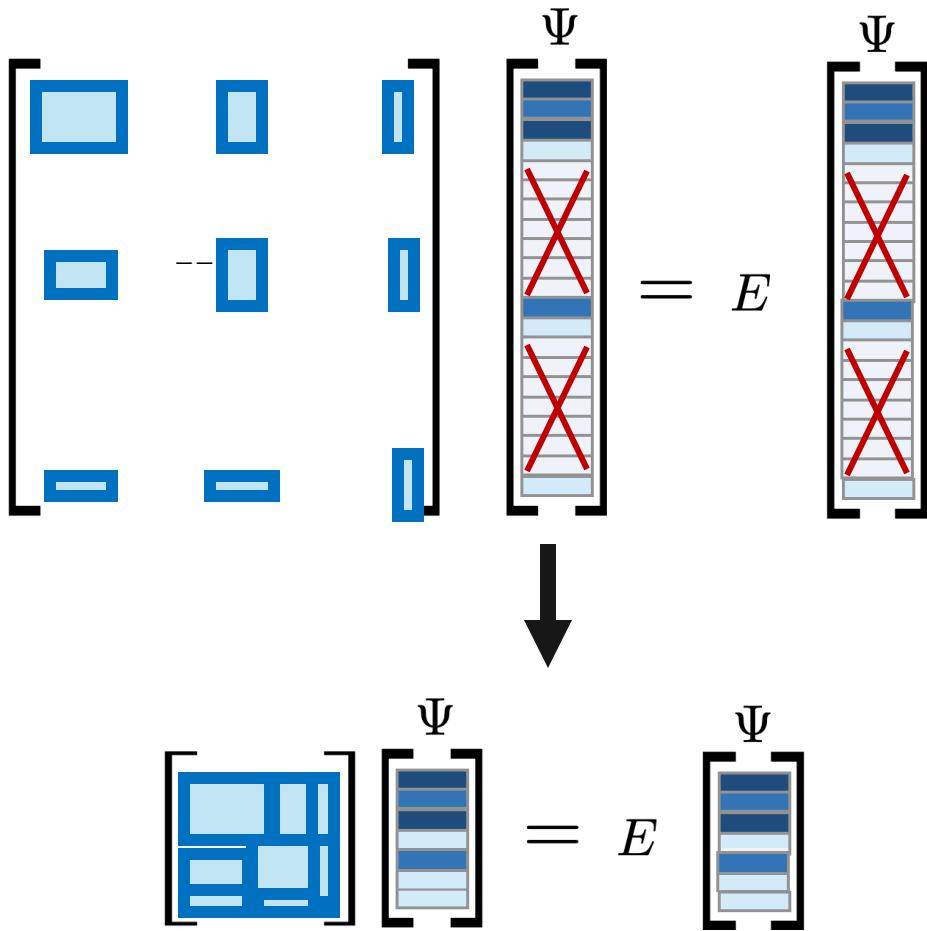
$$H_{x,x'} \begin{bmatrix} \Psi \end{bmatrix} = E \begin{bmatrix} \Psi \end{bmatrix}$$

$$I = \sum_{\mathbf{X}} |\mathbf{X}\rangle\langle\mathbf{X}|$$
$$\mathbf{X} \in \{0, 1\}^N$$

- Extremal eigenvalue problem
- Vector space dimension is exponential
- “Hamiltonian” matrix is exponentially sparse
- The eigenvectors have poly. support (physical intuition)

Diagram showing that high-energy configurations may contribute little to the GS.

Problem statement



- Thought experiment: we are given the subspace of relevant amplitudes
- We can remove “useless dimensions”
- Tractable eigenvalue problem

Searching for relevant dimensions

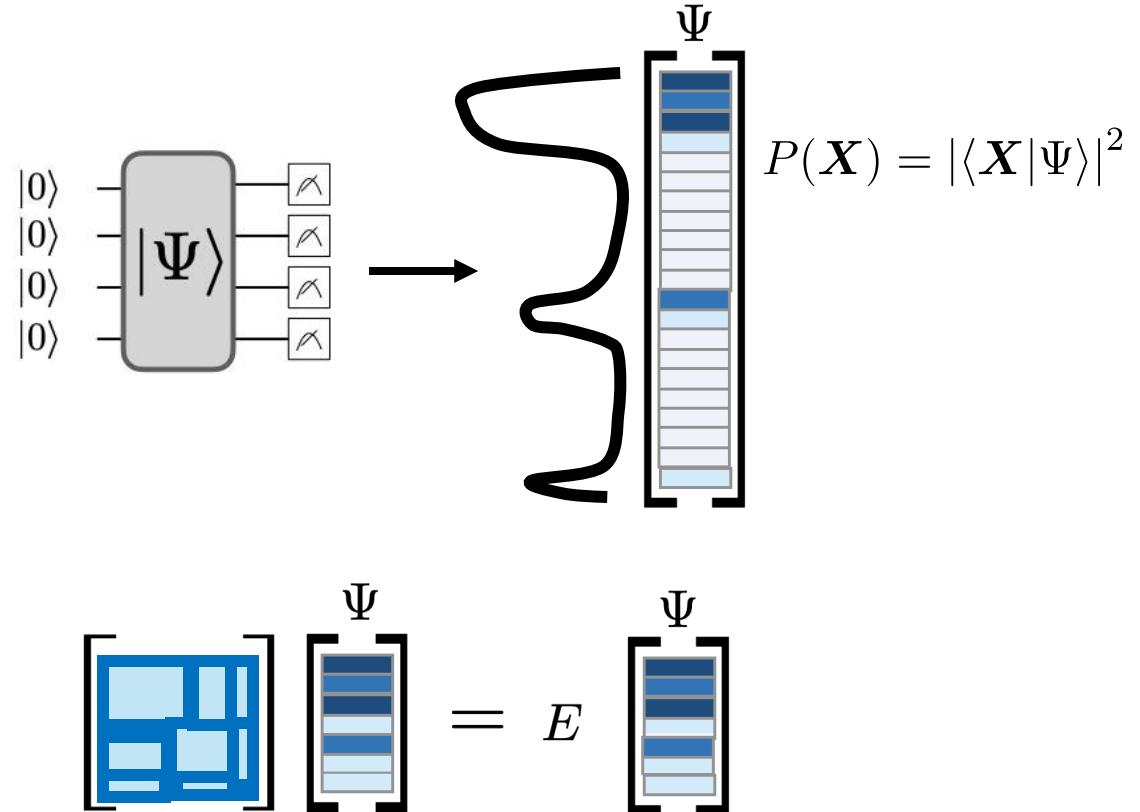
Classical

- Tree-like search (Selected Configuration Interaction)
- Heuristic methods that rely on physics knowledge and or perturbation theory

Diagram showing a high-level schematic of SCI

SQD

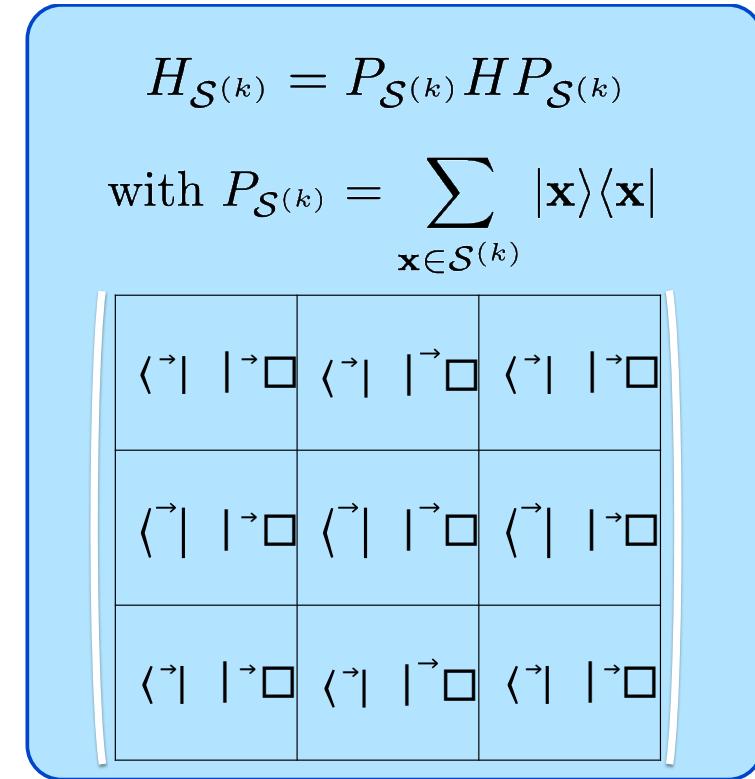
- Quantum circuit produces samples



Effect of noise and config. recovery

Subspace diagonalization and noise tolerance

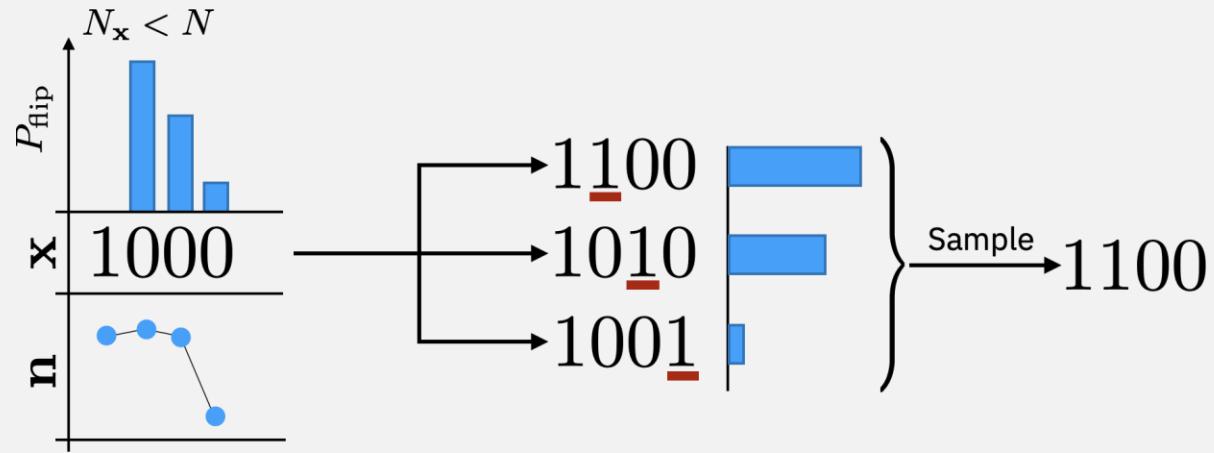
$\vec{a} = 0011$
 $\vec{b} = 1010 \longrightarrow$
 $\vec{\epsilon} = 1100$



$$H_{\mathcal{S}^{(k)}} \mid \psi^{(k)} \rangle = E^{(k)} \mid \psi^{(k)} \rangle$$
$$\mid \psi^{(k)} \rangle = p \frac{1}{2} \vec{a} + 0 \cdot \vec{b} + p \frac{1}{2} \vec{\epsilon}$$

$$|\text{GroundTruth}\rangle = \frac{|\psi^{(k)}\rangle + |\psi^{(k)}\rangle}{\sqrt{2}}$$

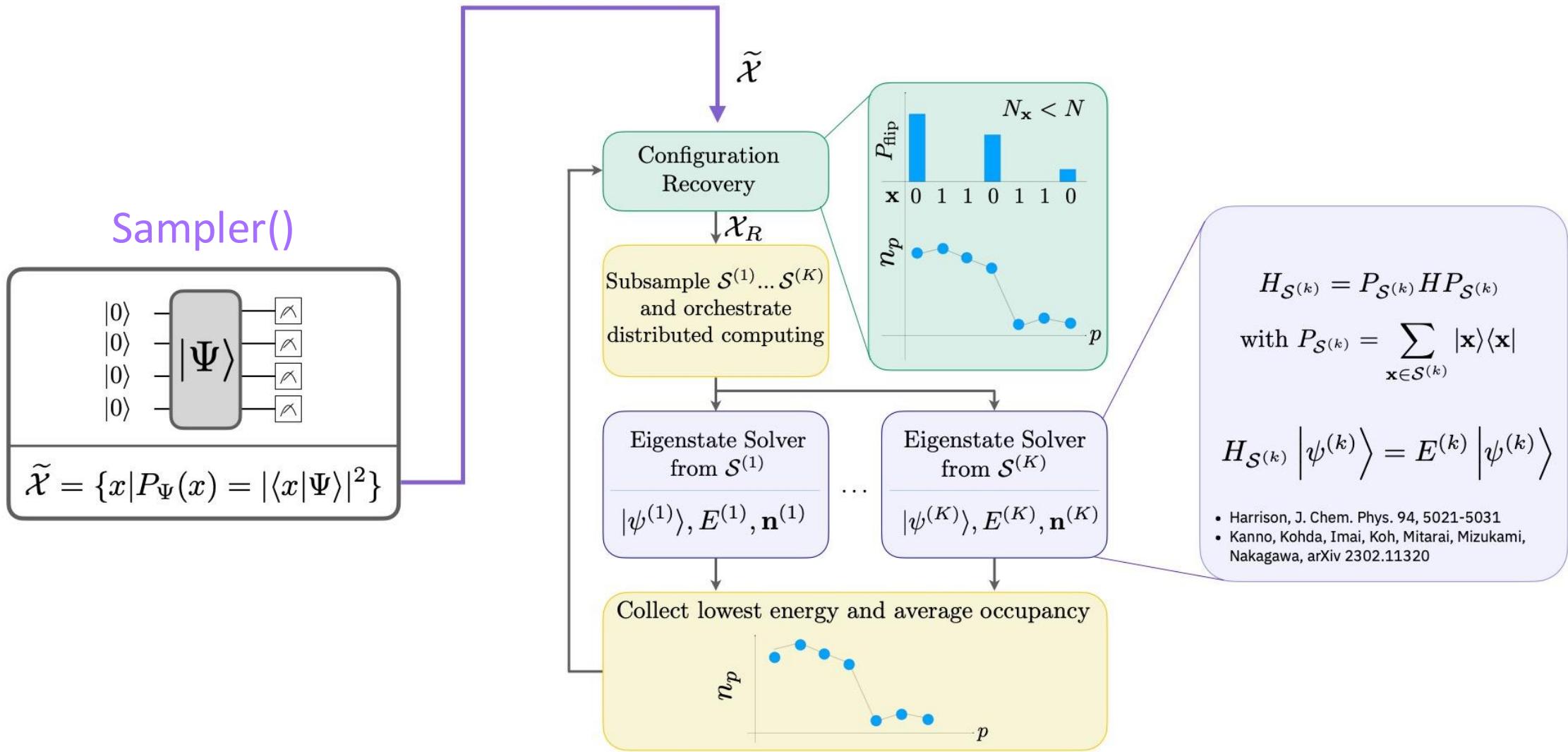
Self-consistent configuration recovery



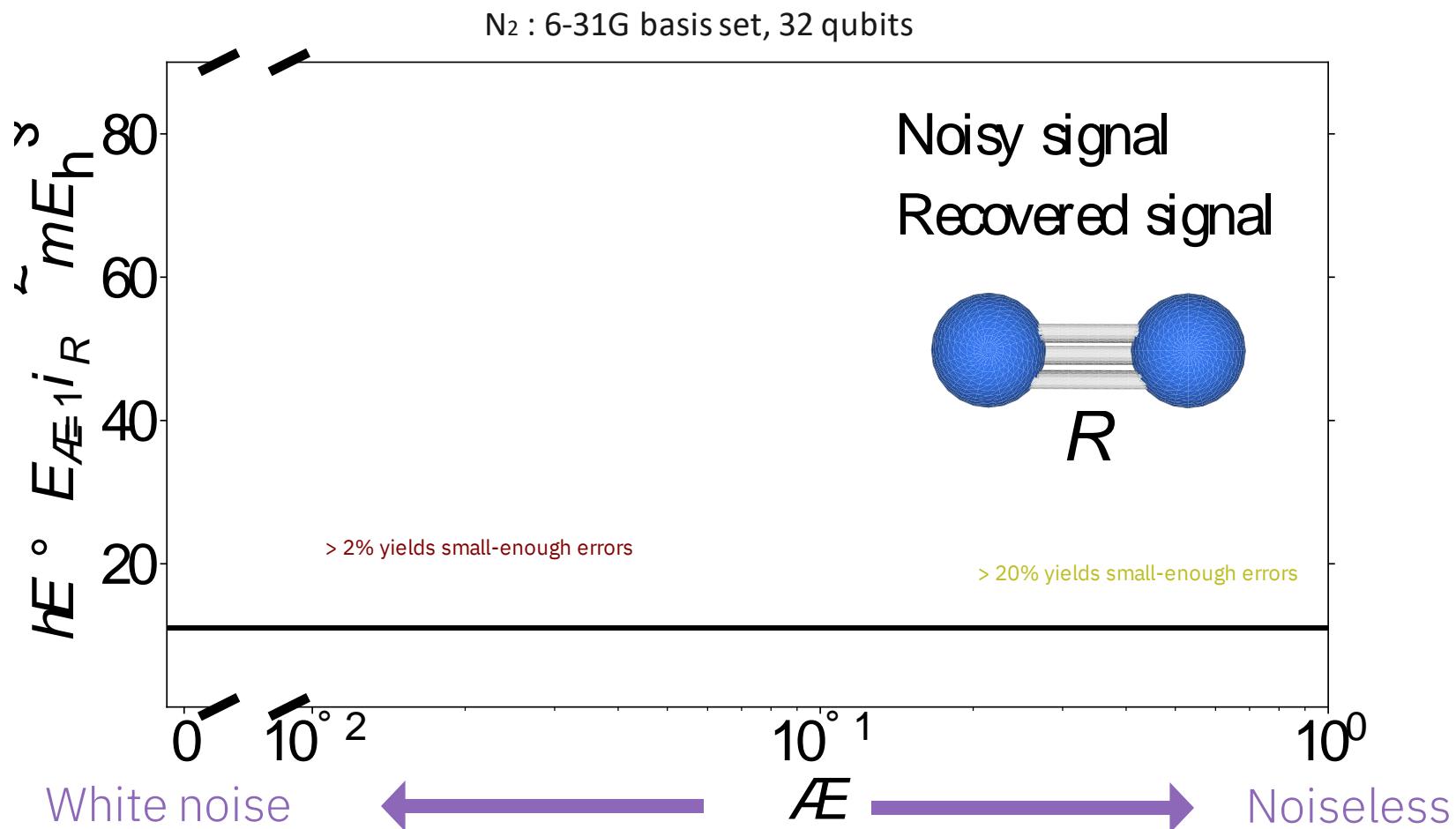
$$n_{p\sigma} = \langle \psi | \hat{n}_{p\sigma} | \psi \rangle = \langle \psi | \hat{c}_{p\sigma}^\dagger \hat{c}_{p\sigma} | \psi \rangle$$

Particle number restored by flipping bits according to a probability informed by the difference between the value of the bit and the average occupancy of the orbital and the filling factor

Complete workflow



Self-consistent configuration recovery in action



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

Quantum circuits

How do we choose the quantum circuits?

Heuristic

- Physically-inspired ansatze (Local Unitary Cluster Jastrow)
- Can either be optimized or initialized from approximate classical electronic structure methods

SQD

arXiv:2405.05068

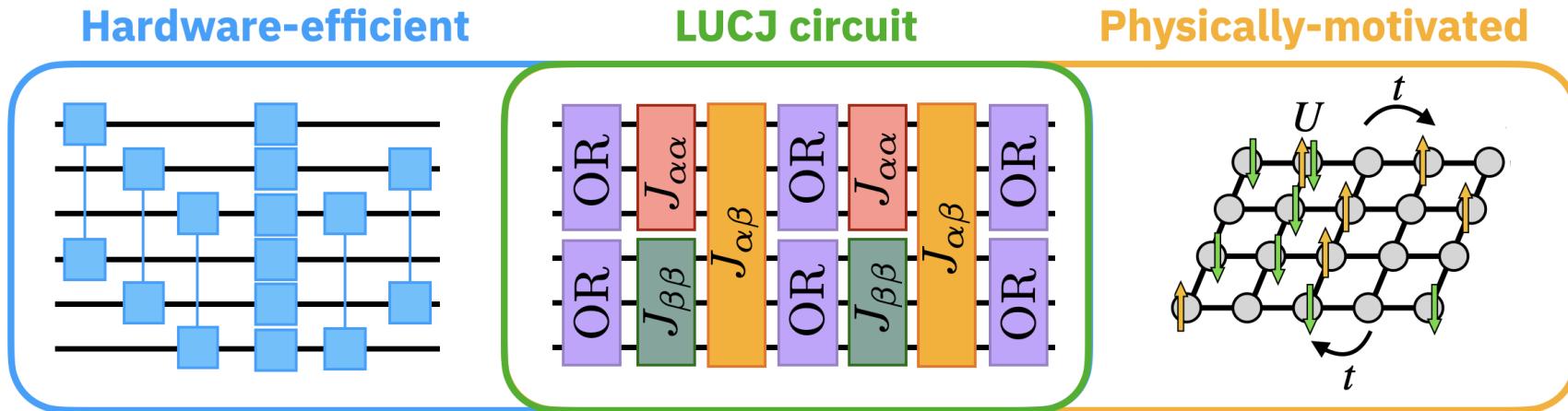
With convergence guarantees

- Sample from the members of a Krylov basis
- Time-evolution circuits may be hardware friendly and are a Krylov basis
- Not suitable for ab-initio

SKQD

arXiv:2501.09702

Circuits for chemistry: Local Unitary Cluster Jastrow



Compatible with hardware
connectivity/gates/depth...
Hard to initialize and optimize

Parameters from classical
calculations, easy to optimize
All-to-all connectivity, high circuit
depth and gate count



Local Unitary Cluster Jastrow

Physical motivation (derived from coupled-cluster)

Hardware friendliness (device-specific connectivity)

Circuits for chemistry: Local Unitary Cluster Jastrow

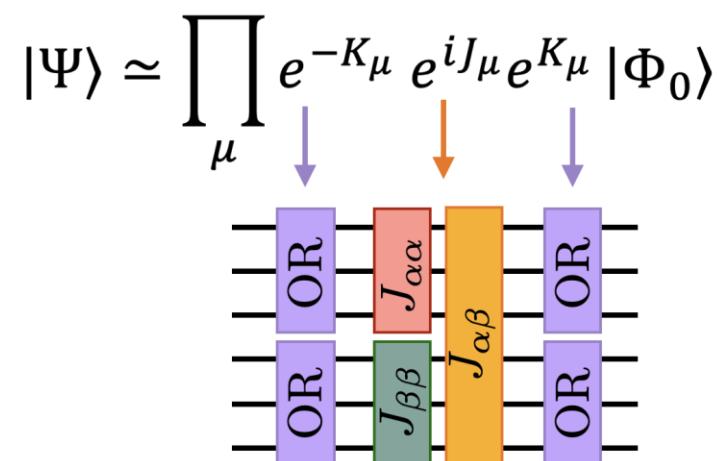
- Unitary coupled-cluster singles and doubles (UCCSD)

$$|\Psi\rangle = e^{T-T^+} |\Phi_0\rangle \quad T = \sum_{ai} t_i^a \hat{c}_a^\dagger \hat{c}_i + \sum_{abij} t_{ij}^{ab} \hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_j \hat{c}_i$$

- Jastrow form of the UCCSD:

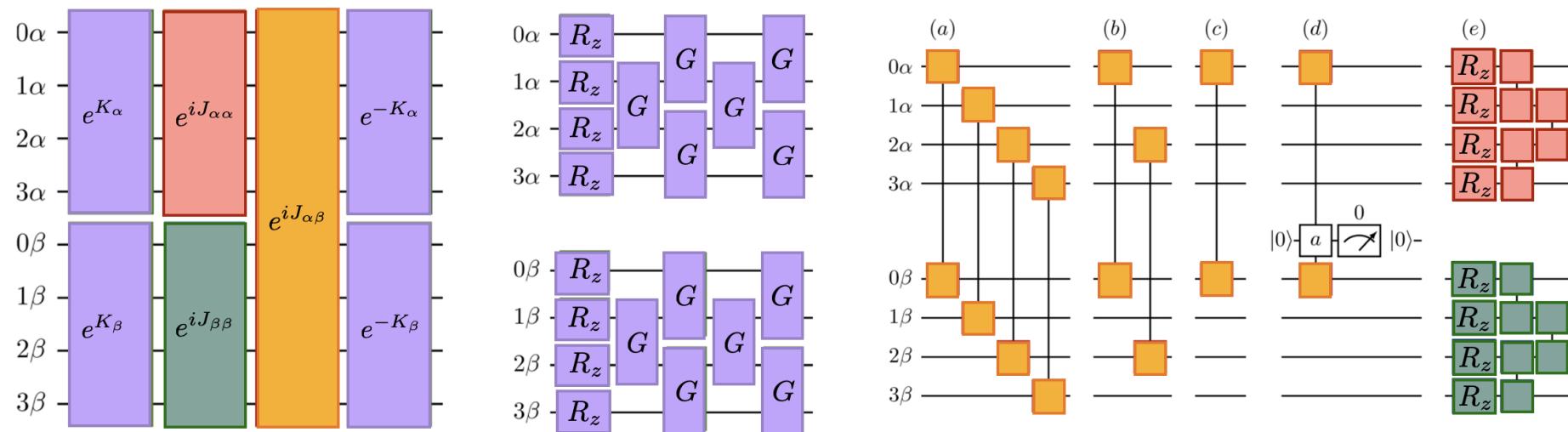
$$T - T^+ \simeq \sum_{\mu} e^{-K_{\mu}} iJ_{\mu} e^{K_{\mu}}, \quad K_{\mu} = \sum_{pr,\sigma} K_{pr}^{\mu} \hat{c}_{p\sigma}^\dagger \hat{c}_{r\sigma}, \quad J_{\mu} = \sum_{pr,\sigma\tau} J_{pr}^{\sigma\tau} \hat{n}_{p\sigma} \hat{n}_{r\tau}$$

- Local Unitary Cluster Jastrow ansatz*

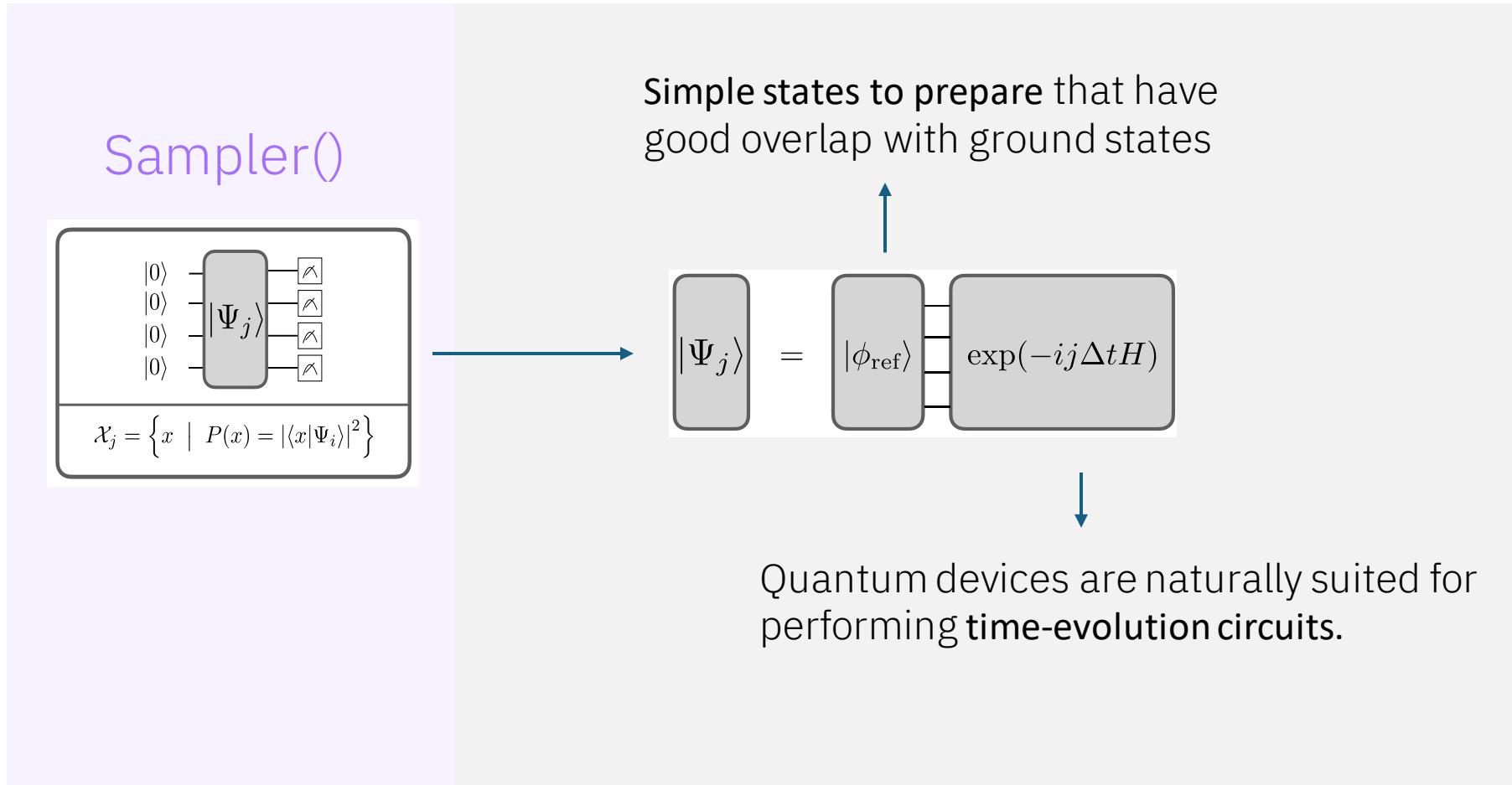


Circuits for chemistry: Local Unitary Cluster Jastrow

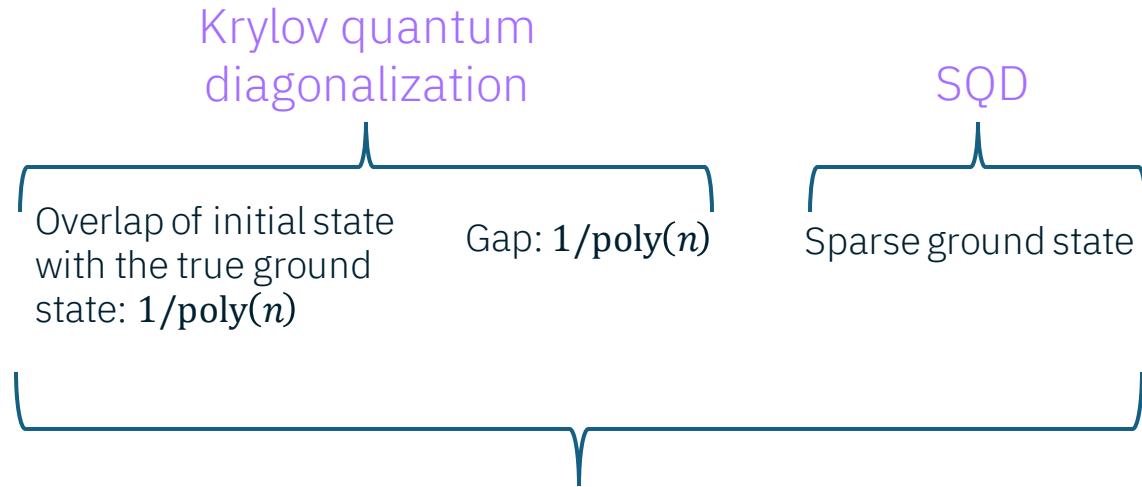
- These circuits can take as input parameters from classical solutions
- There is evidence that they can perform better than their classical counterpart*
- The circuits are hard to simulate classically
- Compatible with quantum hardware



Sample-based Krylov quantum diagonalization

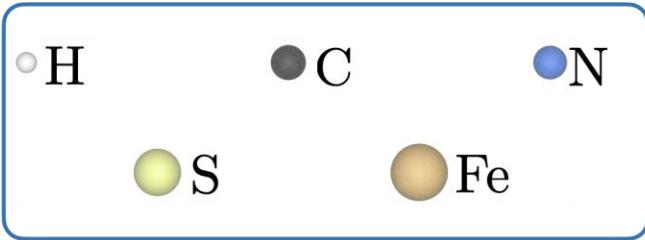


Convergence guarantees

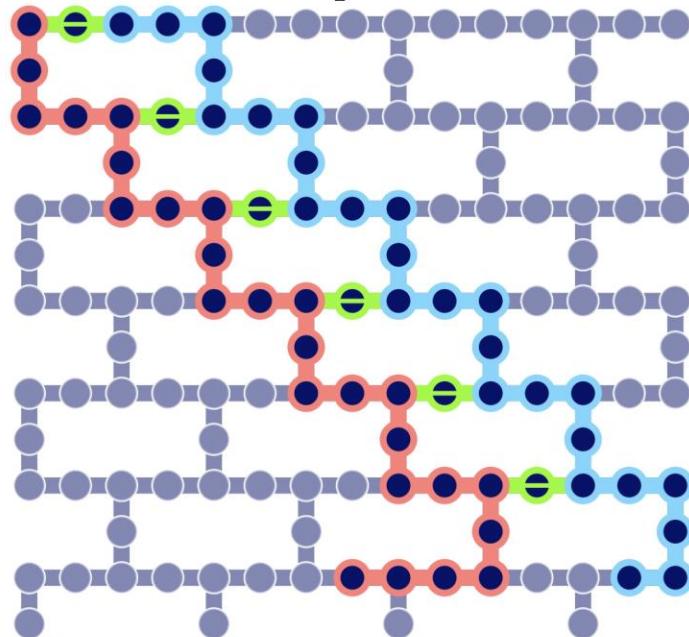


Applications

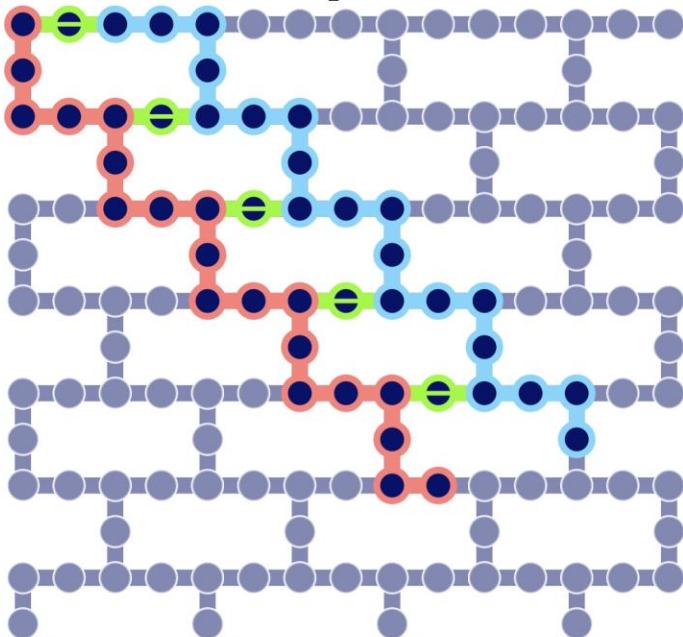
Chemistry



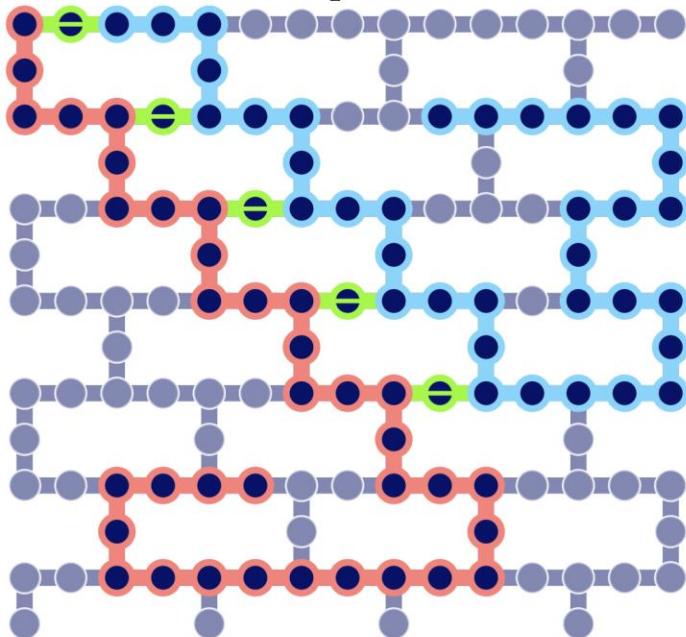
58 qubits



45 qubits



77 qubits



Spin-up orbitals



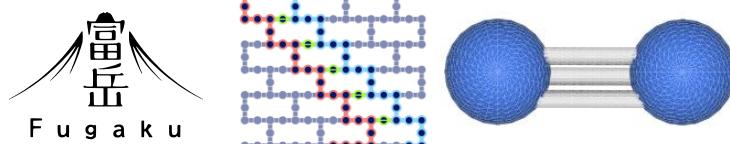
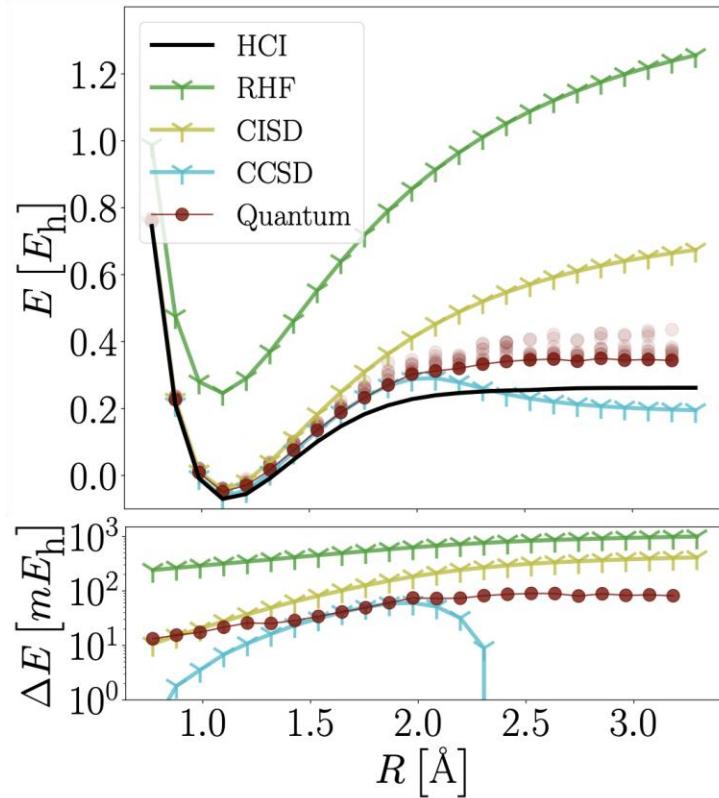
Spin-down orbitals



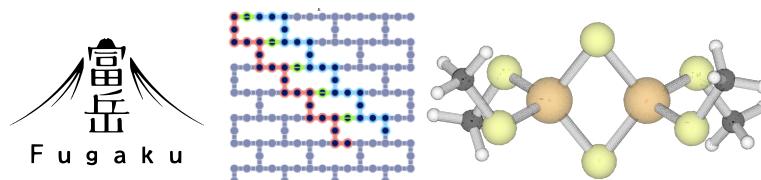
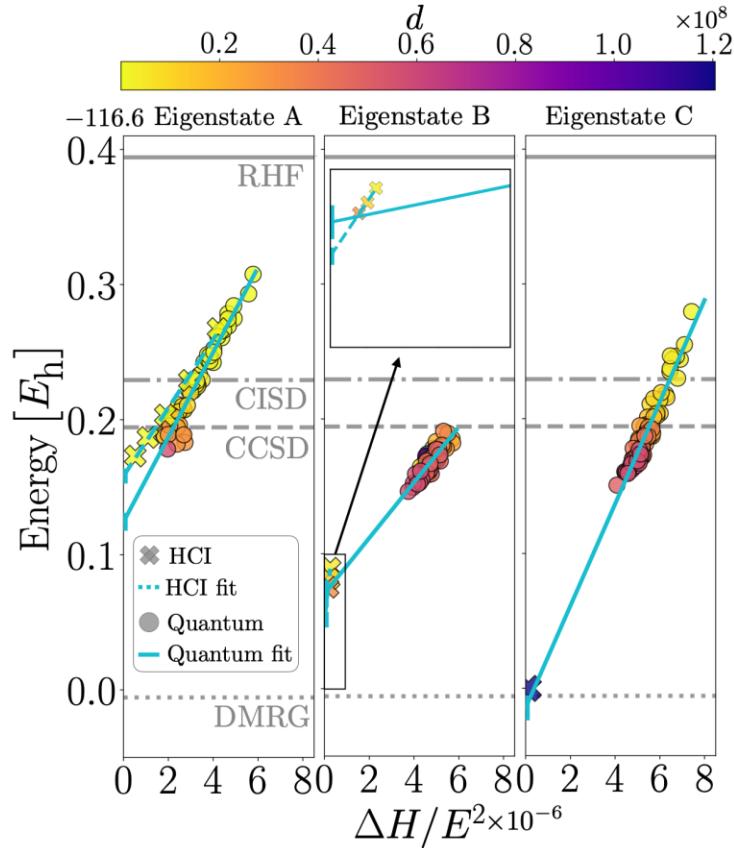
Ancilla qubits (entangle spin species)

Chemistry Results: Highlights

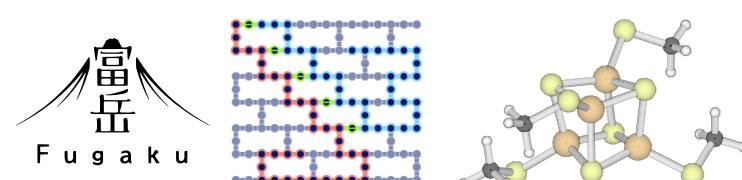
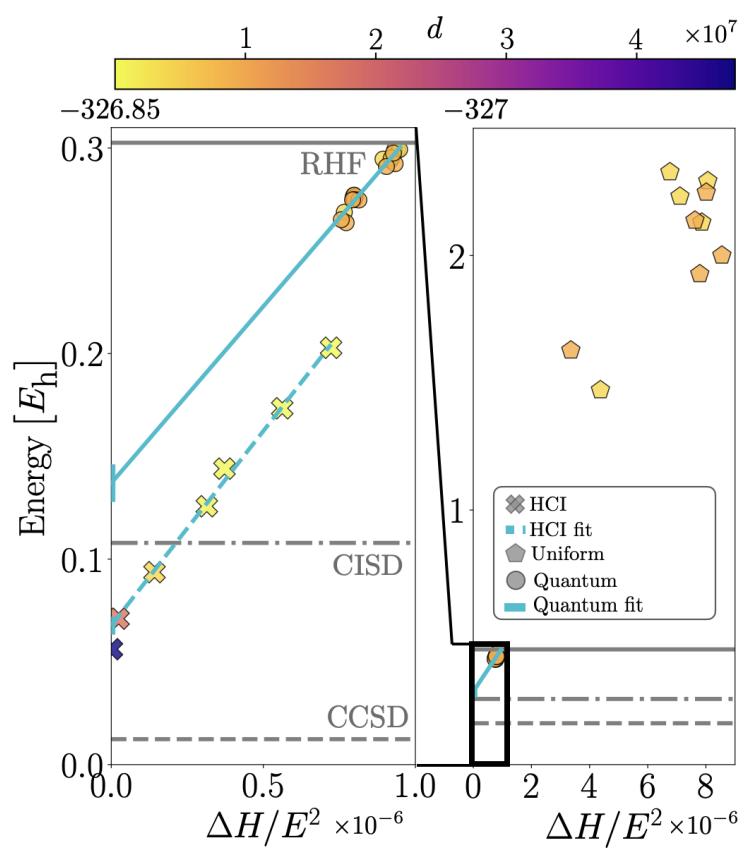
N_2 : Bond breaking on large basis set



Fe_2S_2 : Precision many-body physics



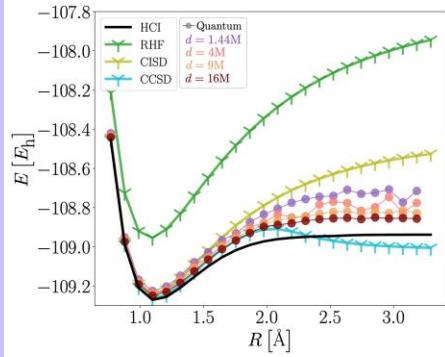
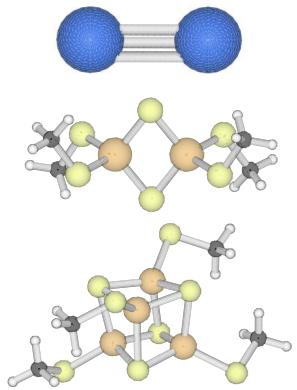
Fe_4S_4 : Pushing hardware capabilities



arXiv:2405.05068

Chemistry Results: Highlights

Chemistry beyond exact solutions...

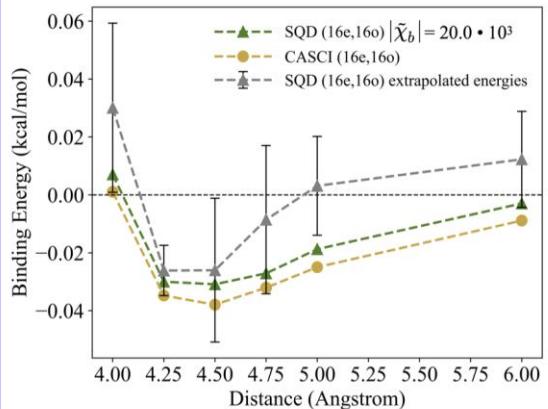


77 qubits
3500 2-qubit gates



IBM Quantum

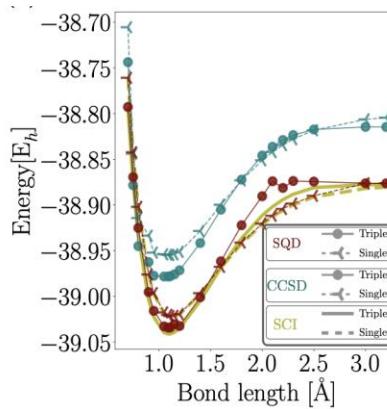
High-precision SQD applied to supramolecular interactions



52 qubits
1600 2-qubit gates

Cleveland Clinic
IBM Quantum

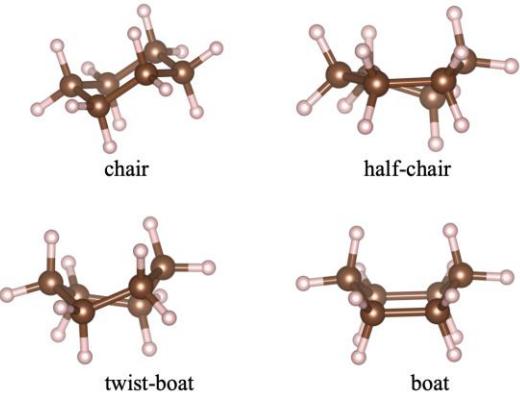
SQD applied to open-shell systems



52 qubits
3500 2-qubit gates

LOCKHEED MARTIN
IBM Quantum

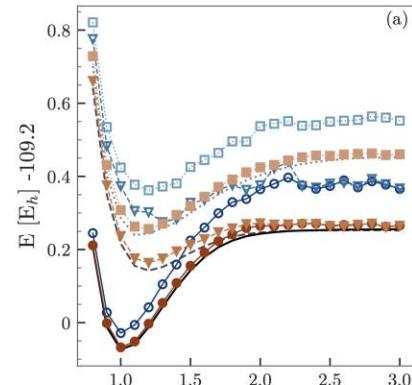
DMET + SQD for organic chemistry



41 qubits
1500 2-qubit gates

Cleveland Clinic
IBM Quantum

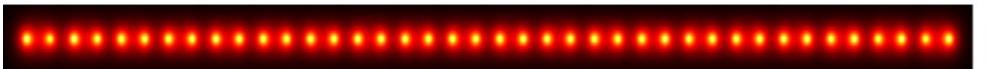
Ext-SQD: excited states



58 qubits
1792 2-qubit gates

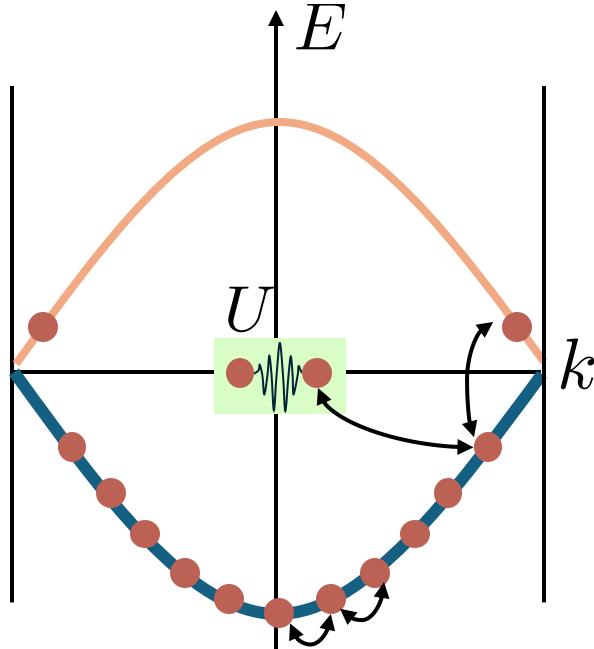
IBM Quantum

5k challenge on hydrogen chains



84 qubits
5000 2-qubit gates

Lattice models: SKQD



Free electrons coupled to interacting impurities

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

$$H_{\text{bath}} = \sum_{k\sigma} \varepsilon_k \hat{c}_{k\sigma}^\dagger \hat{c}_{k\sigma}$$

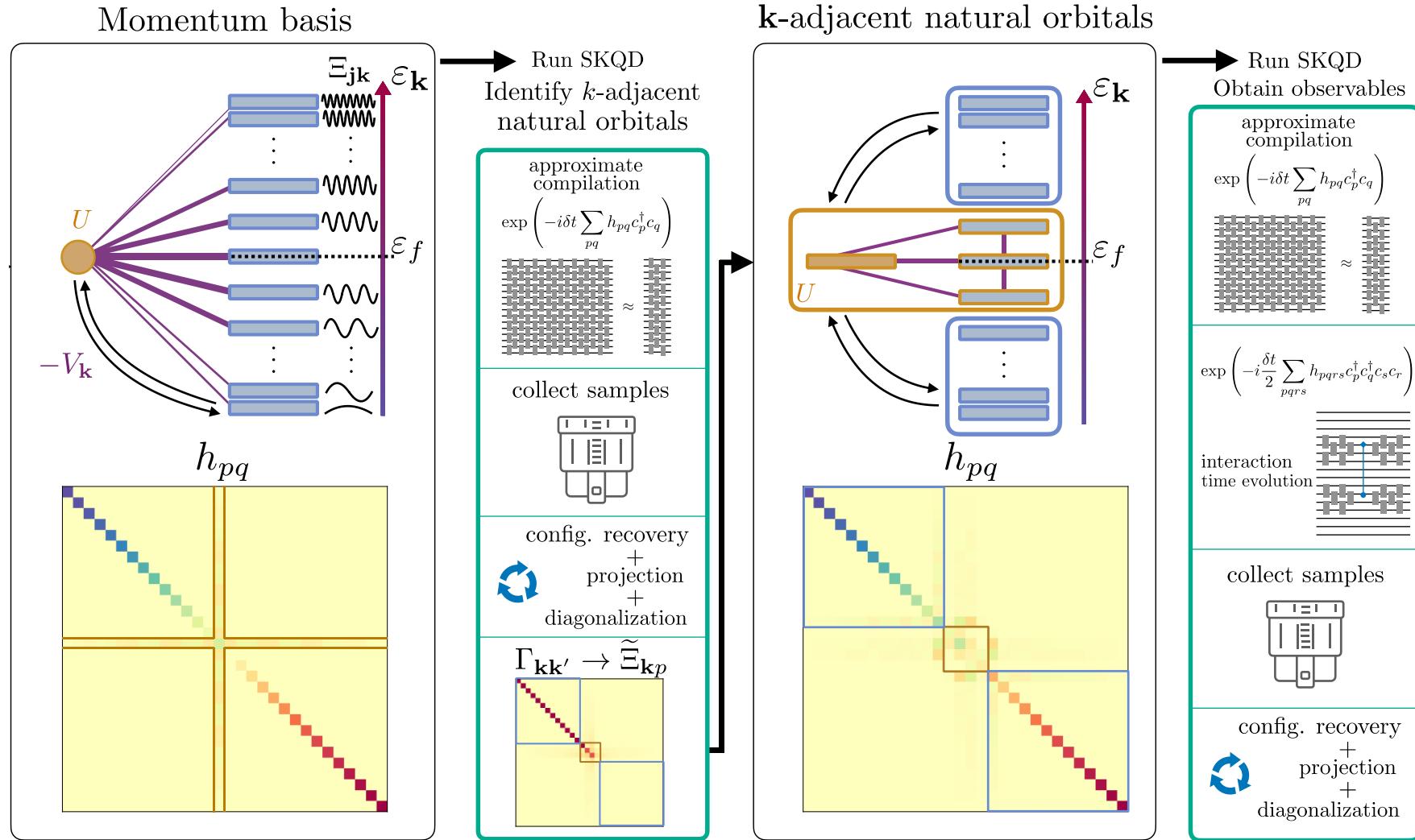
$$H_{\text{hyb.}} = \sum_{k\sigma} V_k \left(\hat{c}_{k\sigma}^\dagger \hat{d}_\sigma + \hat{d}_\sigma^\dagger \hat{c}_{k\sigma} \right)$$

$$H_{\text{imp.}} = U \hat{d}_\uparrow^\dagger \hat{d}_\uparrow \hat{d}_\downarrow^\dagger \hat{d}_\downarrow$$

Relevant to **simplify** real materials calculations
on DMFT workflows

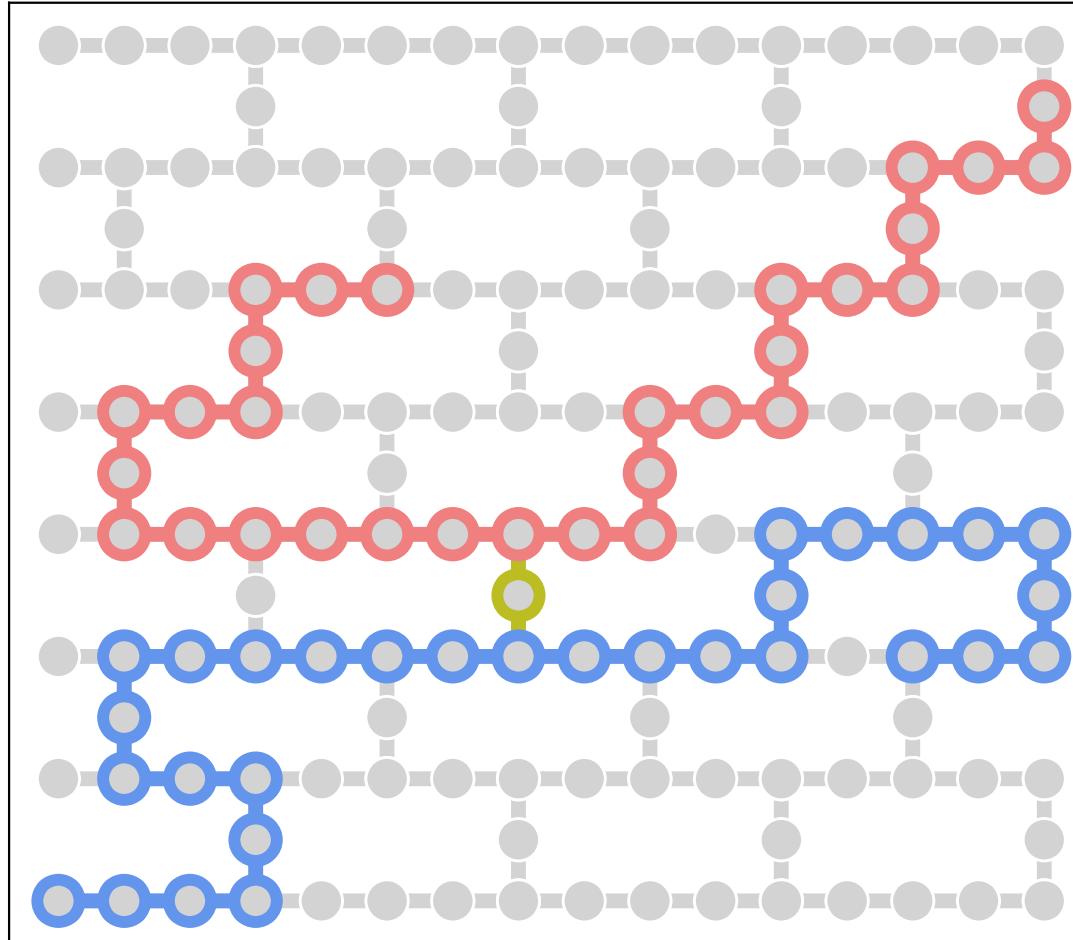
Extensively used to **benchmark** numerical techniques

Time evolution circuits



Circuit layouts

41 Bath modes -> 84 + 1 qubits



Spin-up orbitals



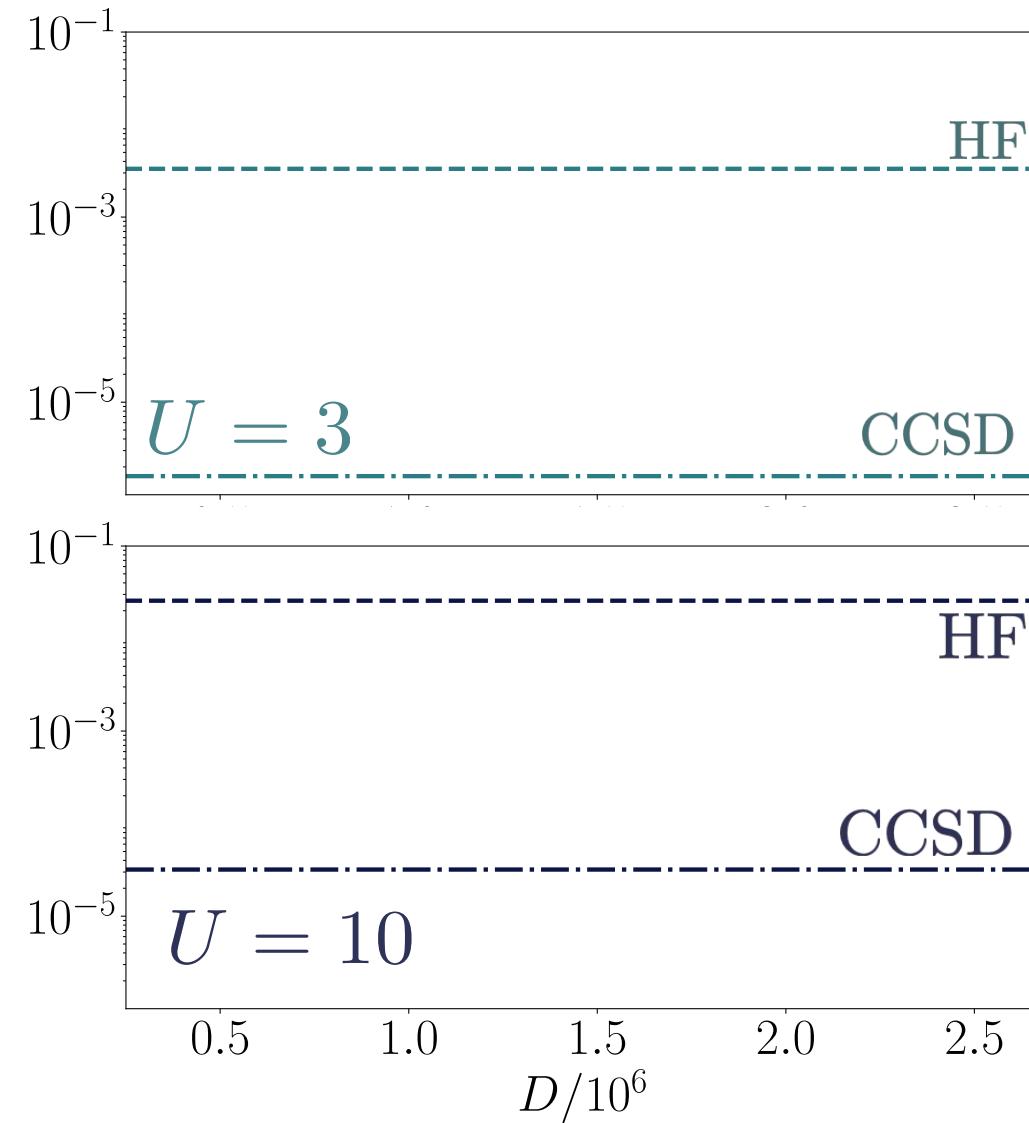
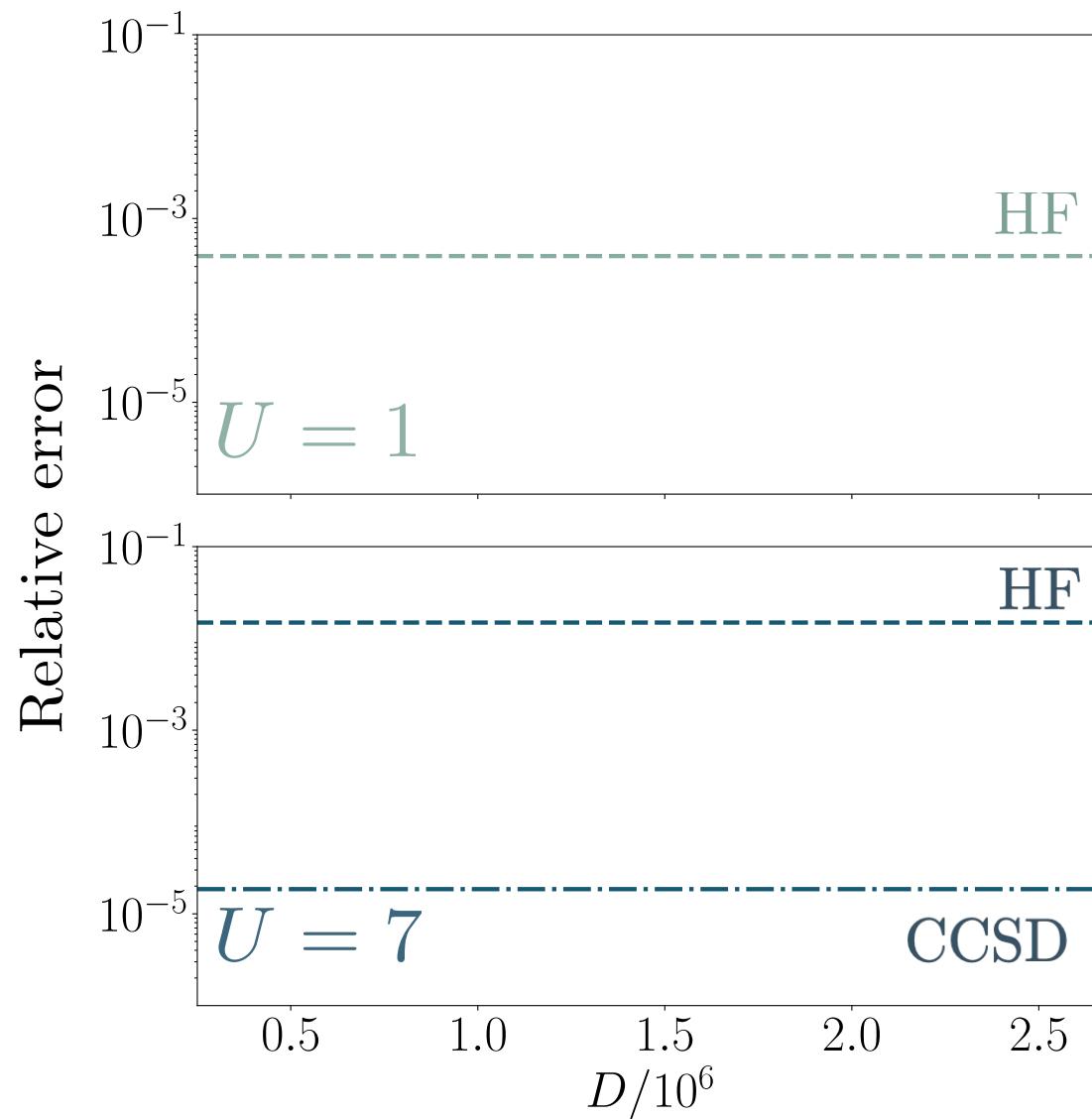
Spin-down orbitals



Ancilla qubits

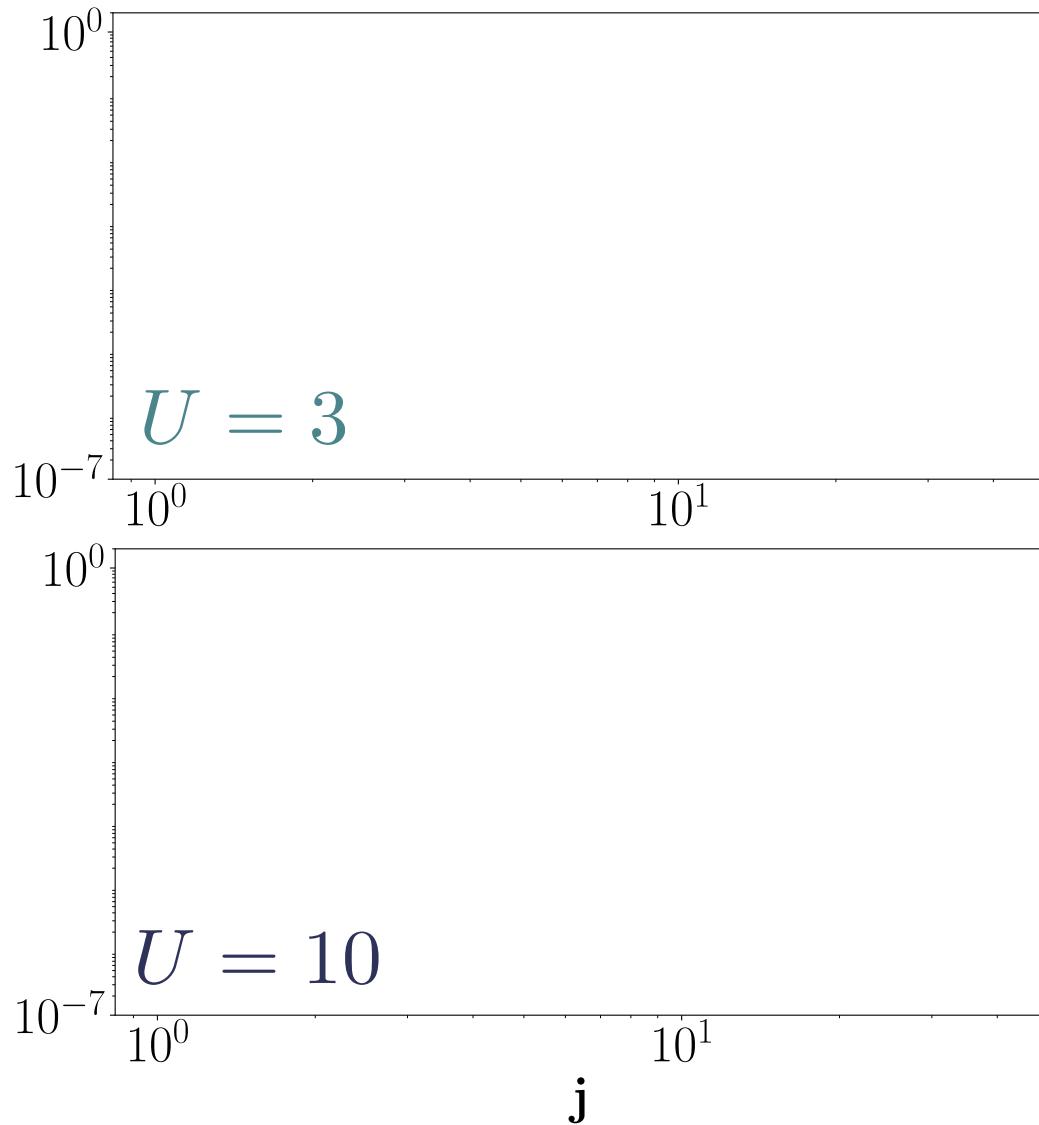
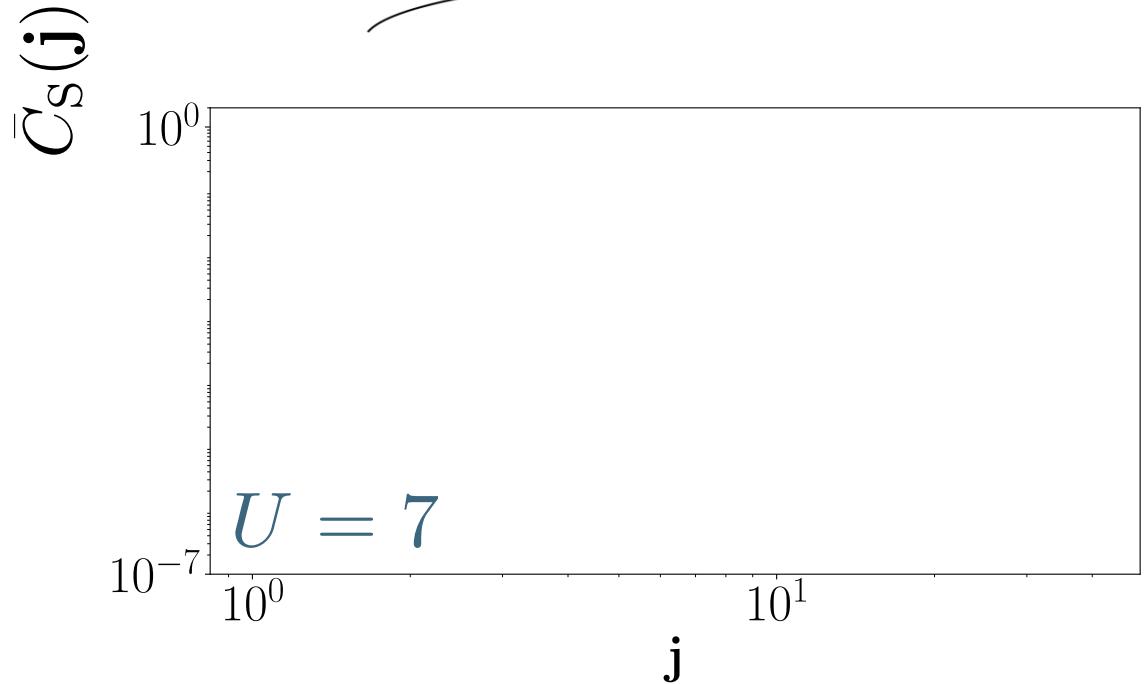
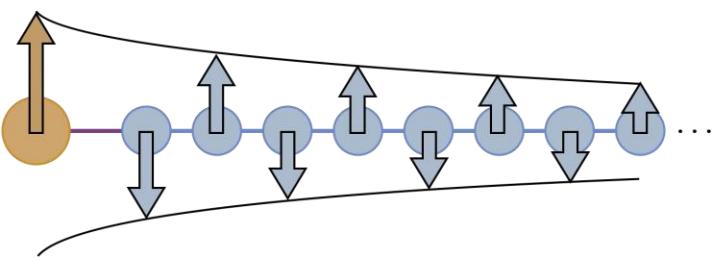
First SKQD experiments: results

$$\text{Relative error} = \left| \frac{E_{\text{SKQD}} - E_{\text{DMRG}}}{E_{\text{DMRG}}} \right|$$



First SKQD experiments: results

$$\bar{C}_S(\mathbf{j}) = \langle \mathbf{S}_d \cdot \mathbf{S}_j \rangle - \langle \mathbf{S}_d \rangle \cdot \langle \mathbf{S}_j \rangle$$



Code and Tools



Qiskit addon: sample-based quantum diagonalization (SQD)
0.10.0

Q Search



Qiskit addon: sample-based quantum diagonalization (SQD)

[Qiskit addons](#) are a collection of modular tools for building utility-scale workloads powered by Qiskit.

This package contains the Qiskit addon for sample-based quantum diagonalization (SQD) – a technique for finding eigenvalues and eigenvectors of quantum operators, such as a quantum system Hamiltonian, using quantum and distributed classical computing together [1-5]. This technique can be run on current quantum computers and has been shown to scale to problem sizes beyond what was possible with variational methods and even beyond the reach of exact classical diagonalization methods [1,2].

Tutorials



Qiskit addon: sample-based quantum diagonalization (SQD)
0.10.0

Q Search



Improving energy estimation of a chemistry Hamiltonian with SQD

In this tutorial we implement a [Qiskit pattern](#) showing how to post-process noisy quantum samples to find an approximation to the ground state of a chemistry Hamiltonian: the N_2 molecule at equilibrium in the 6-31G basis set. We will follow a [sample-based quantum diagonalization approach](#) to process samples taken from a 36-qubit quantum circuit ansatz (in this case, an LUCJ circuit). In order to account for the effect of quantum noise, the configuration recovery technique is used.

The pattern can be described in four steps:



Qiskit addon: sample-based quantum diagonalization (SQD)
0.10.0

Q Search



Improving energy estimation of a Fermionic lattice model with SQD

In this tutorial we implement a [Qiskit pattern](#) showing how to post-process noisy quantum samples to find an approximation to the ground state of a Fermionic lattice Hamiltonian known as the single-impurity Anderson model. We will follow a sample-based quantum diagonalization approach to process samples taken from a set of 16-qubit Krylov basis states over increasing time intervals. These states are realized on the quantum device using Trotterization of the time evolution. In order to account for the effect of quantum noise, the configuration recovery technique is used. Assuming a good initial state and sparsity of the ground state, [this approach](#) is proven to converge efficiently.

Summary



Qiskit addon: sample-based quantum diagonalization (SQD)
0.10.0

Search

Quantum-centric supercomputing enables realistic applications to chemistry and materials: classical distributed computing processes big classical data, while quantum executes a few large quantum circuits

Quantum simulation of molecules (77 qubits, 3.5K two-qubit gates) and materials (85 qubits, 6K two-qubit gates) beyond the reach of brute-force classical solutions

Provable convergence for SKQD when a wavefunction with a polynomial support gives a good approximation to the ground state energy

Beyond the polynomial support assumption, SQD/SKQD can serve as a heuristic to compare with classical methods

Processing of quantum data at the sample level: no false positive solutions and certifiable advantage

Well-defined conditions under which SKQD is guaranteed to work, making it a strong candidate for quantum a