Quantum-Centric Supercomputing with Sample-Based Quantum Diagonalization and Qiskit Addons

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IBM Quantum

Tutorial Agenda

Quantum-Centric Supercomputing with Sample-Based Quantum Diagonalization (SQD) and Qiskit Addons

Session 1
10:00-11:30 am MDT

1. **Intro to SQD**
2. **Tour of the software and Qiskit addons**: `qiskit-addon-sqd`
3. **Code demonstration** for a chemistry application: Nitrogen molecule

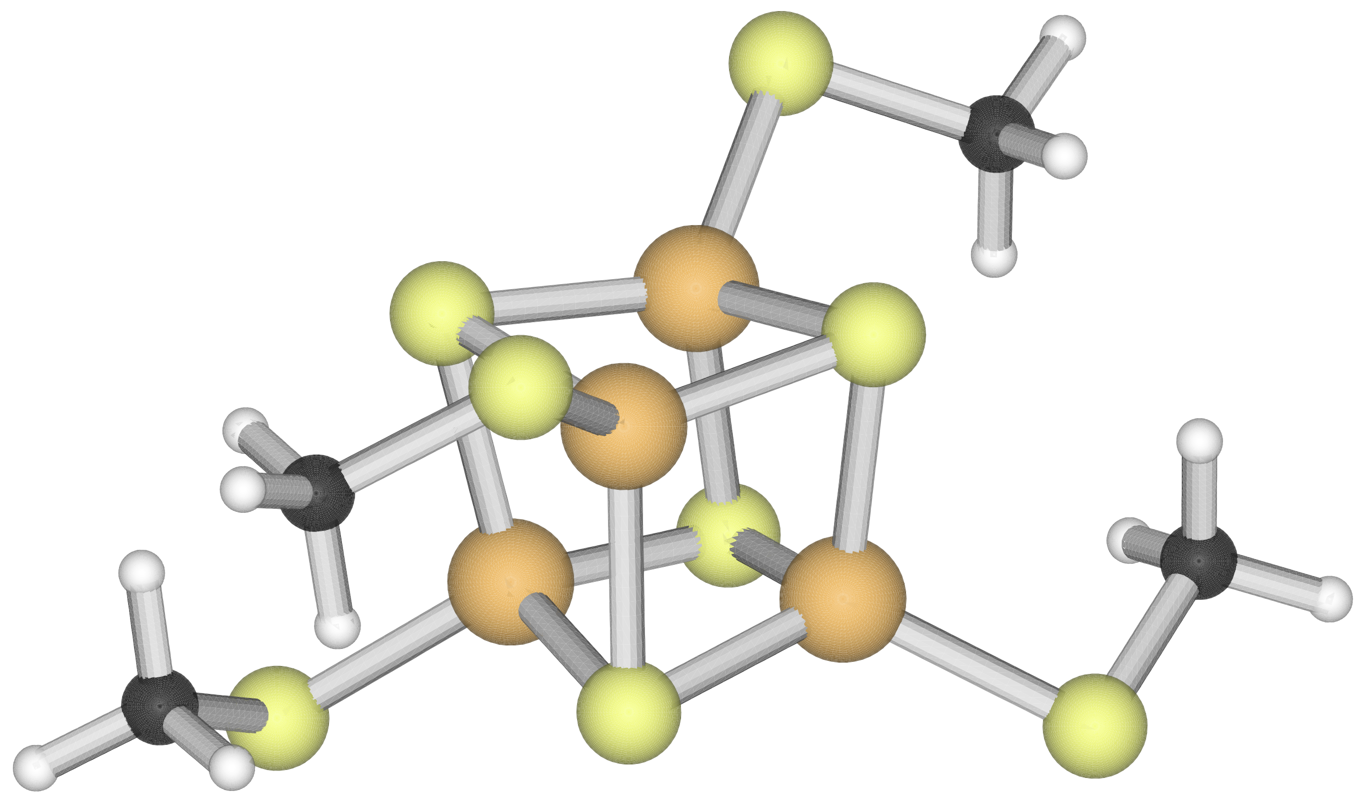
Session 2
1:00-2:30 pm MDT

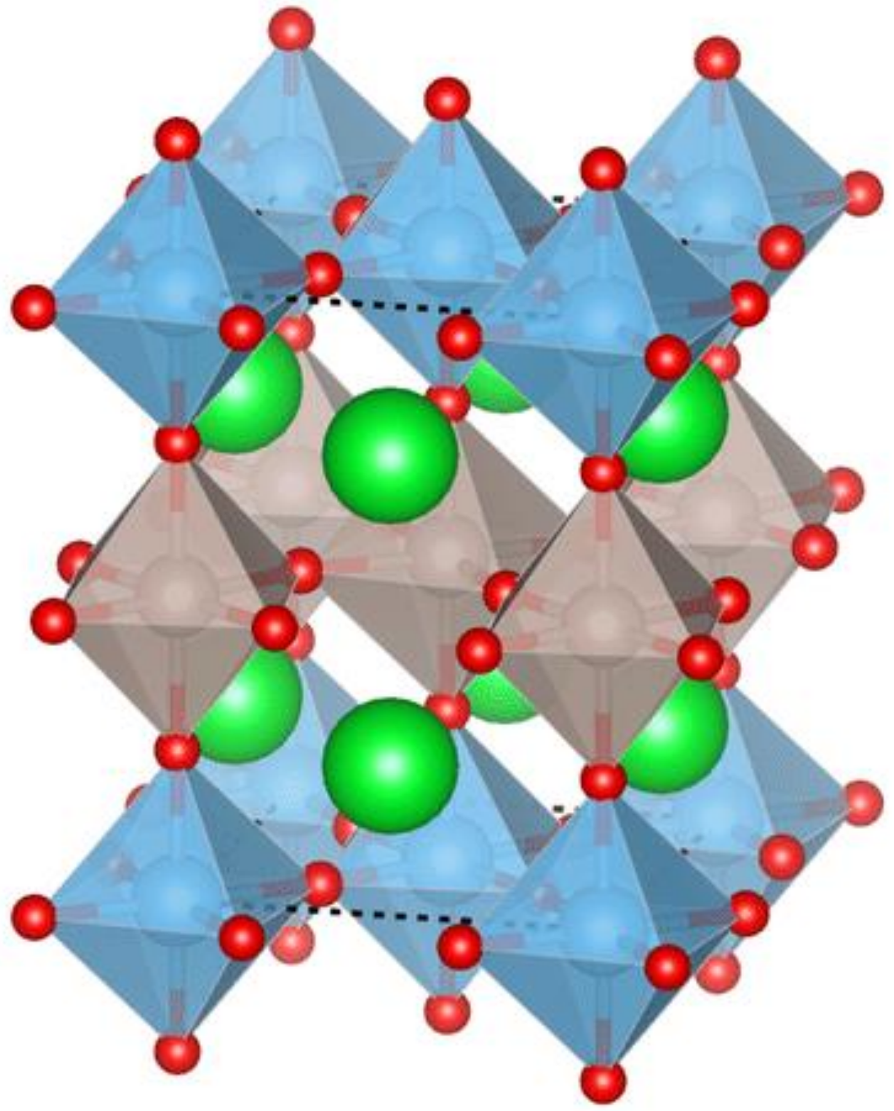
1. Intro to SQD with **quantum Krylov states**
2. **Code demonstration** for a physics application: Anderson impurity model

Quantum Algorithms for ground states

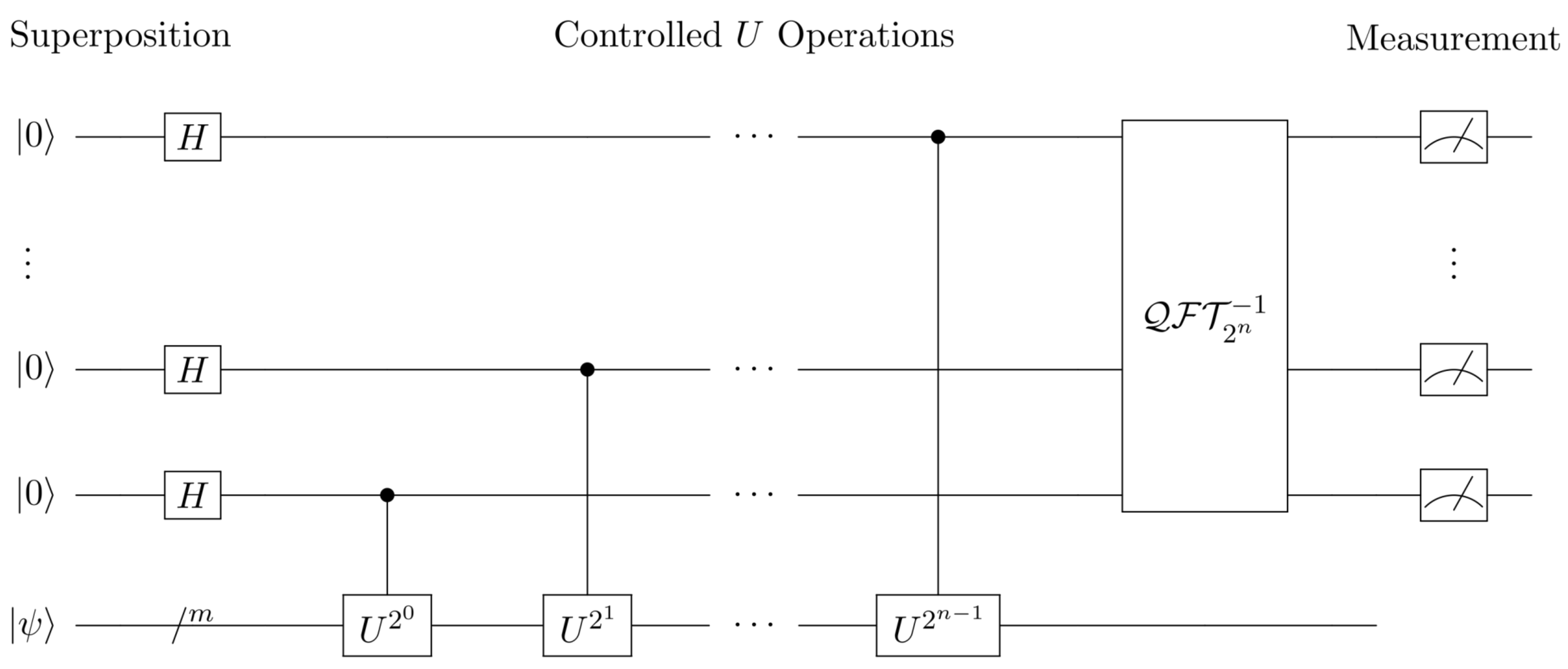
- Goal: solving computationally challenging energy-estimation problems in quantum chemistry and materials

- Applications: development of new materials, drug discovery, battery design





Prior algorithms in **fault-tolerant** era



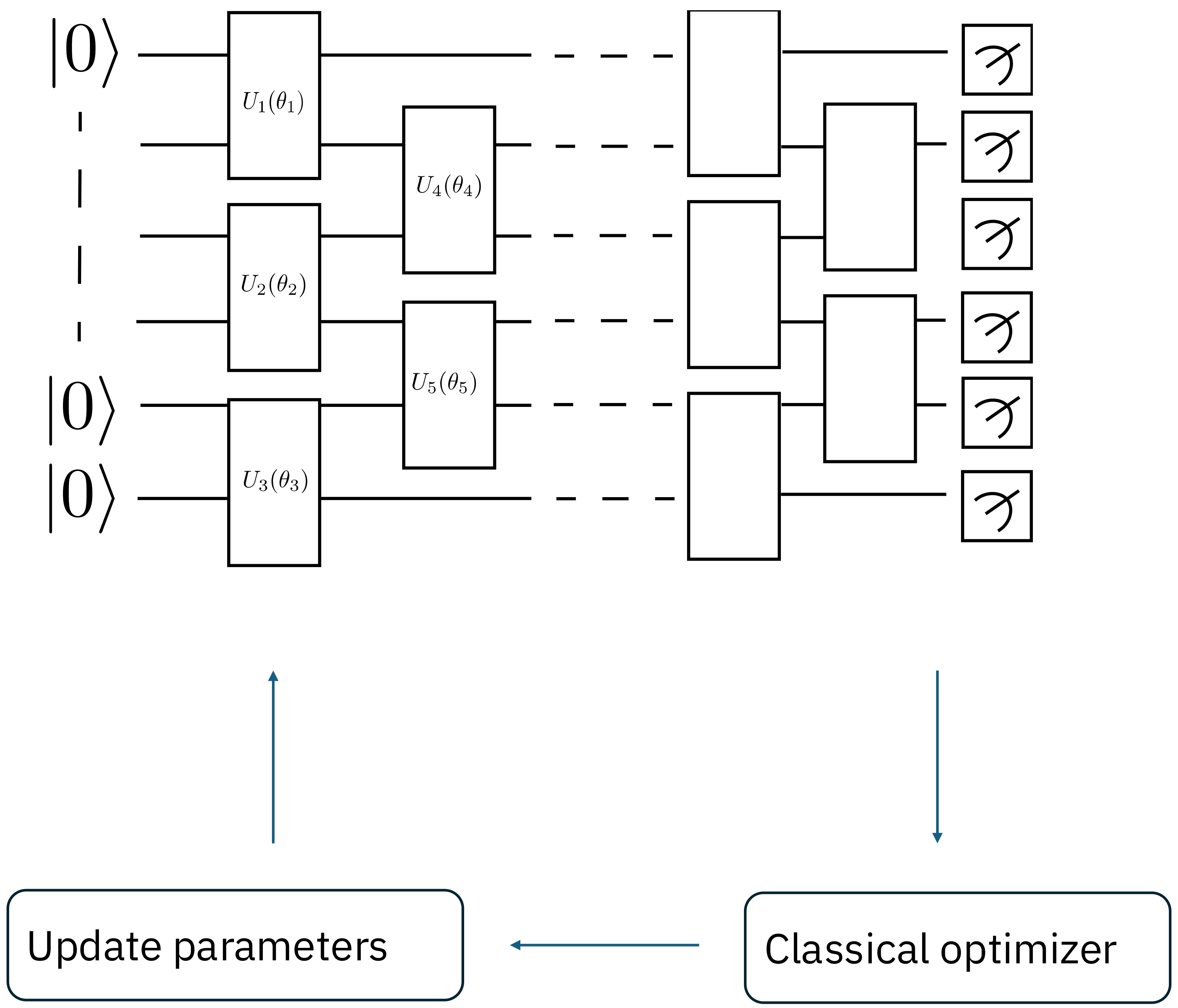
Quantum Phase Estimation (QPE)

- Convergence guarantees when initial state has $1/\mathrm{poly}(n)$ 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

Quantum-centric supercomputing

Can we perform reliable simulation of nature with *provable convergence* before fault-tolerant quantum computers?

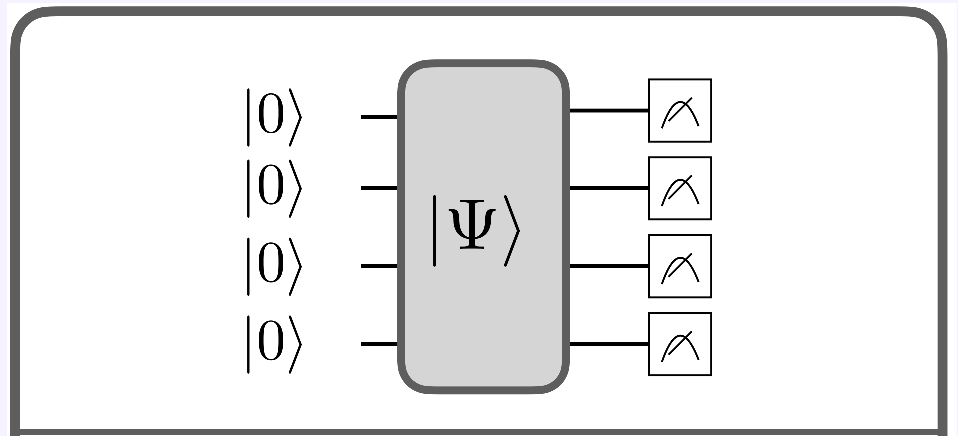
Sample-based Quantum Diagonalization (SQD)

Sample-based Quantum Diagonalization (SQD)

Science Advances 11 (25), eadu9991 (2025)

Quantum compute generates samples from an exponentially large space

Sampler()



$$\mathcal{X} = \{x | P(x) = |\langle x|\Psi\rangle|^2\}$$

Classical component:
Approximation of the ground state energy of H

Configuration recovery

↓

Projection and subspace diagonalization

↓

Ground state properties

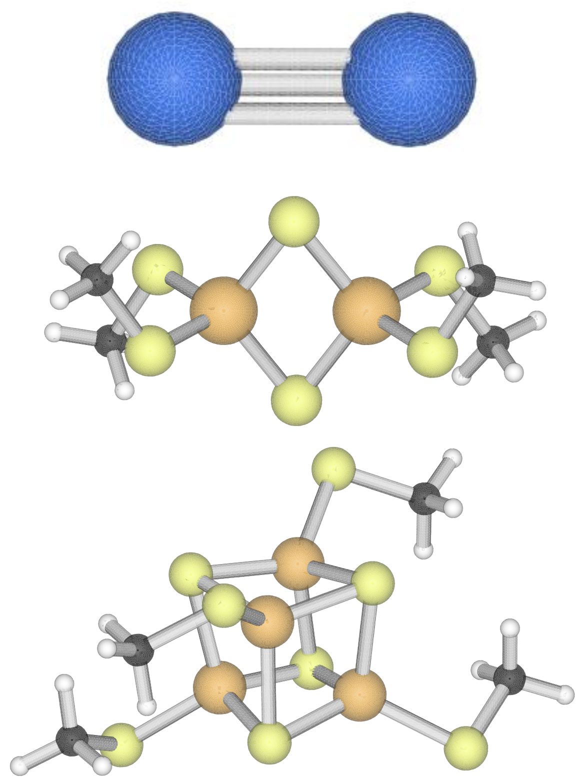
Fugaku

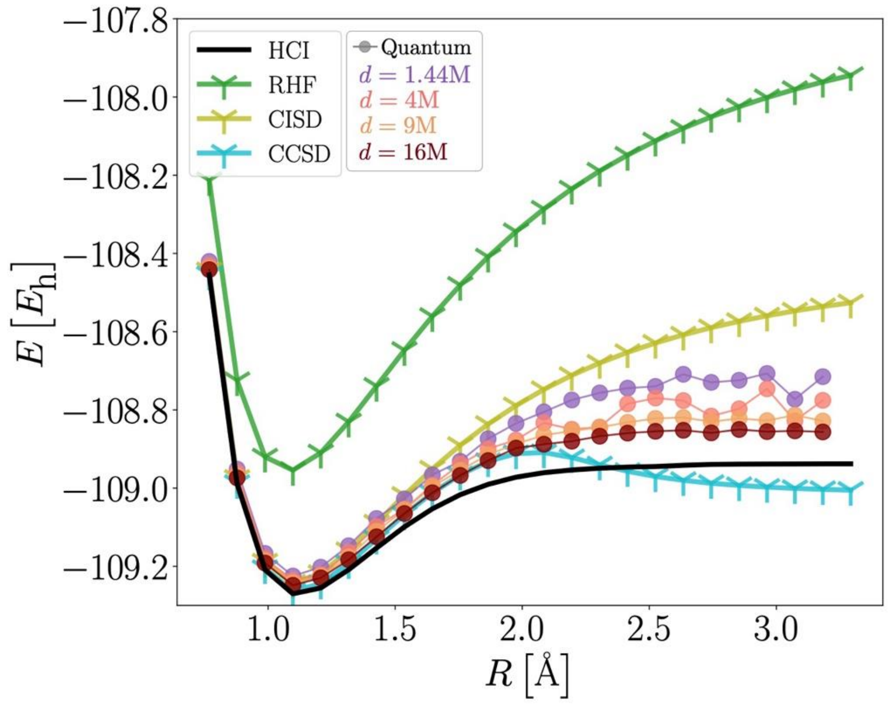
SQD for chemistry

check that all these examples are public

Remove 5k challenge box at bottom?

Chemistry beyond exact solutions...





77 qubits
3500 2-qubit gates

RIKEN

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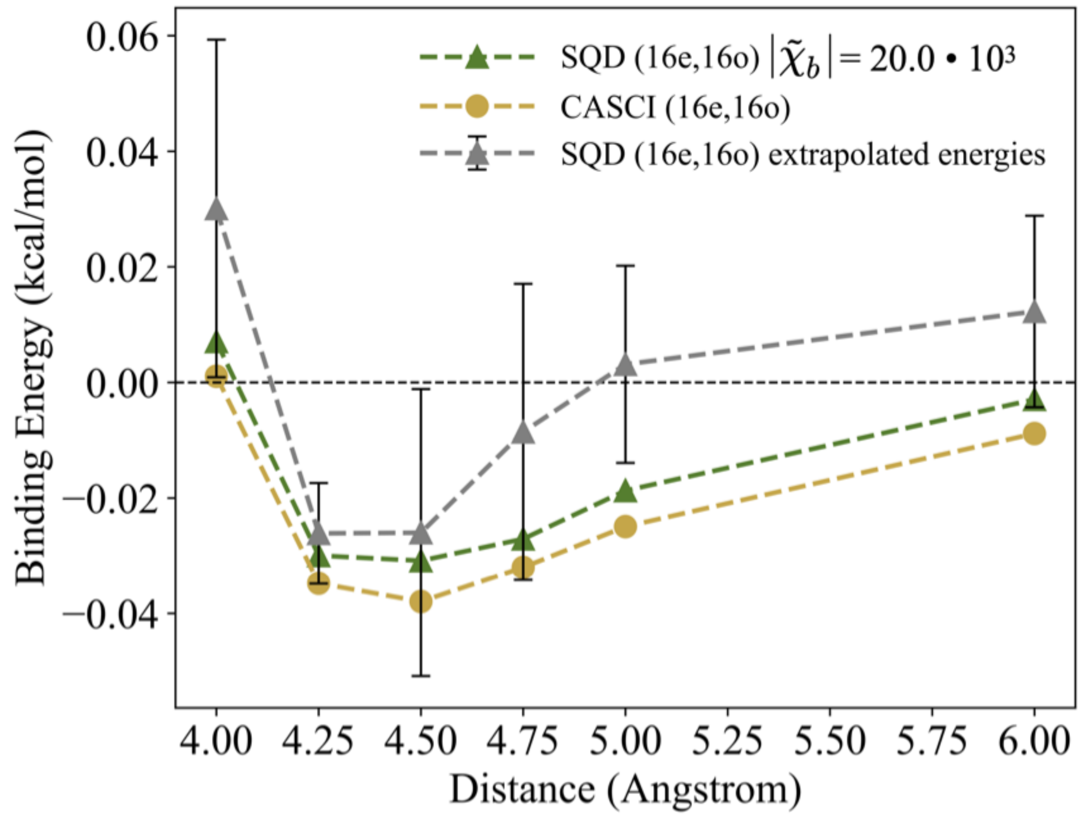
High-precision SQD applied to supramolecular interactions

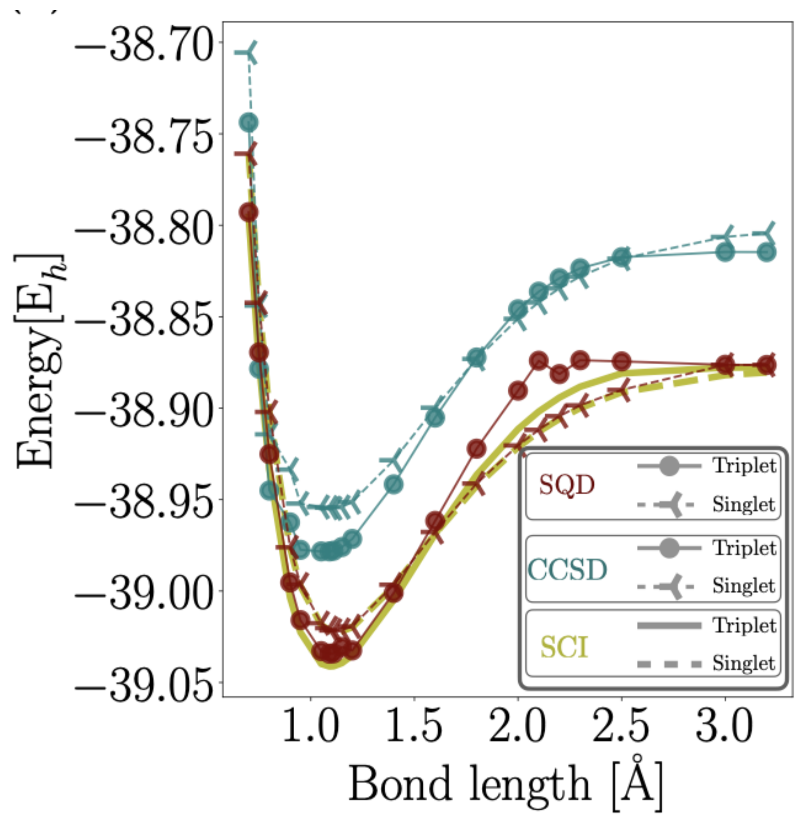


52 qubits
1600 2-qubit gates

Cleveland Clinic

IBM **Quantum**

SQD … te



52 qubits
3500 2-qubit gates

LOCKHEED MARTIN

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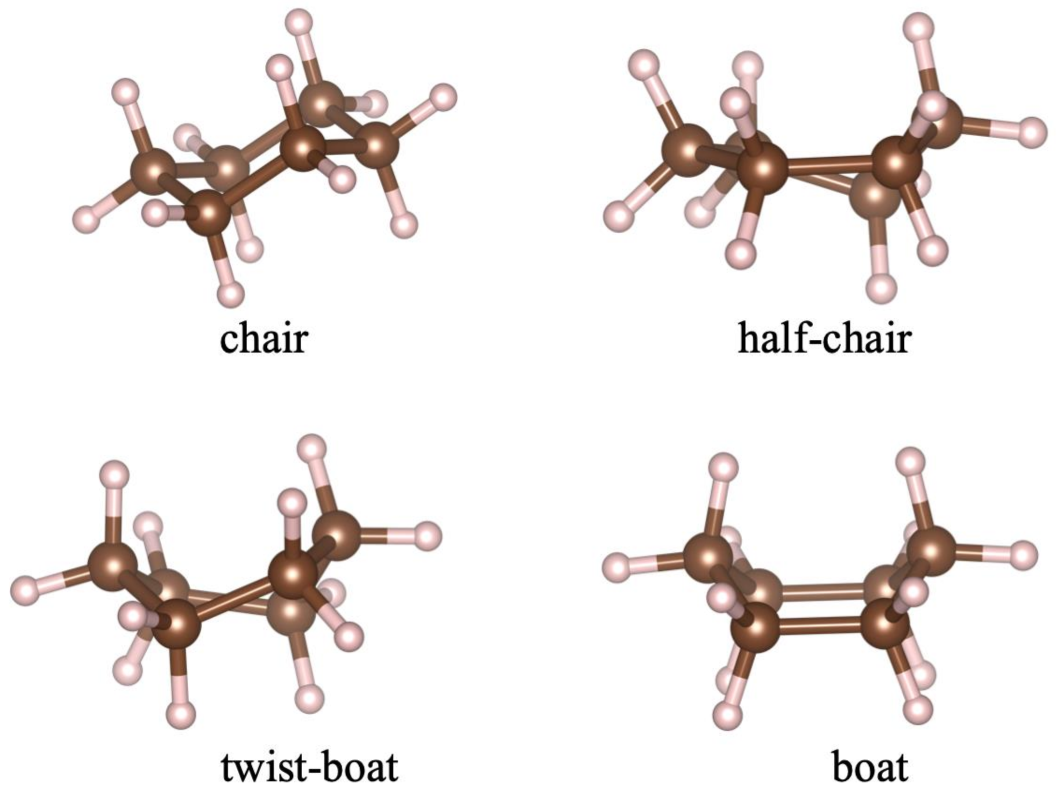
DMET + SQD for organic chemistry



41 qubits
1500 2-qubit gates

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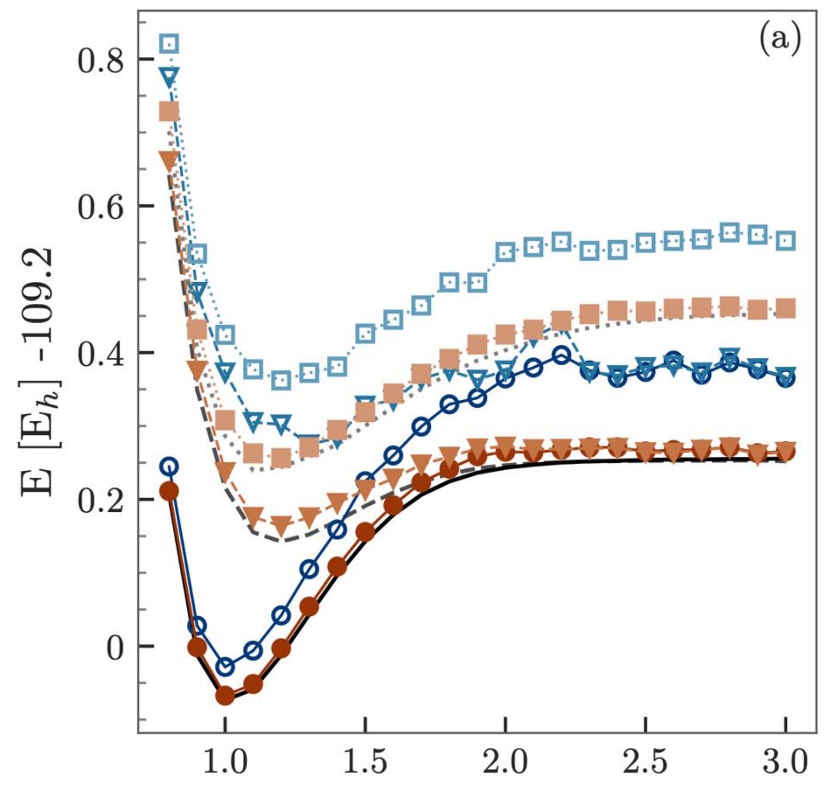
Ext-SQD: excited states



58 qubits
1792 2-qubit gates

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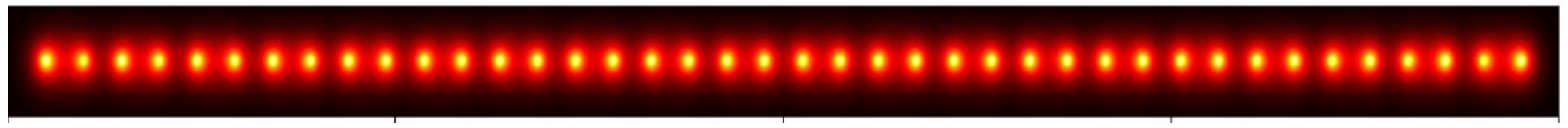
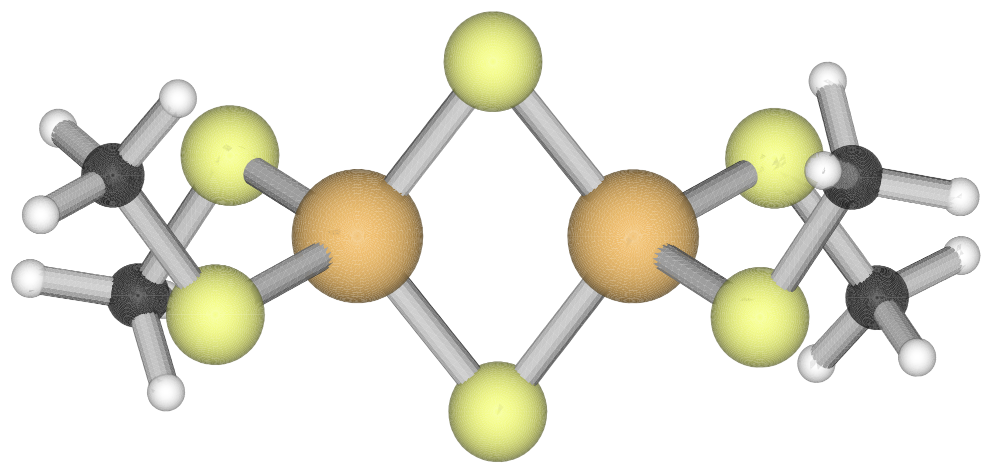
5k challenge on hydrogen chains

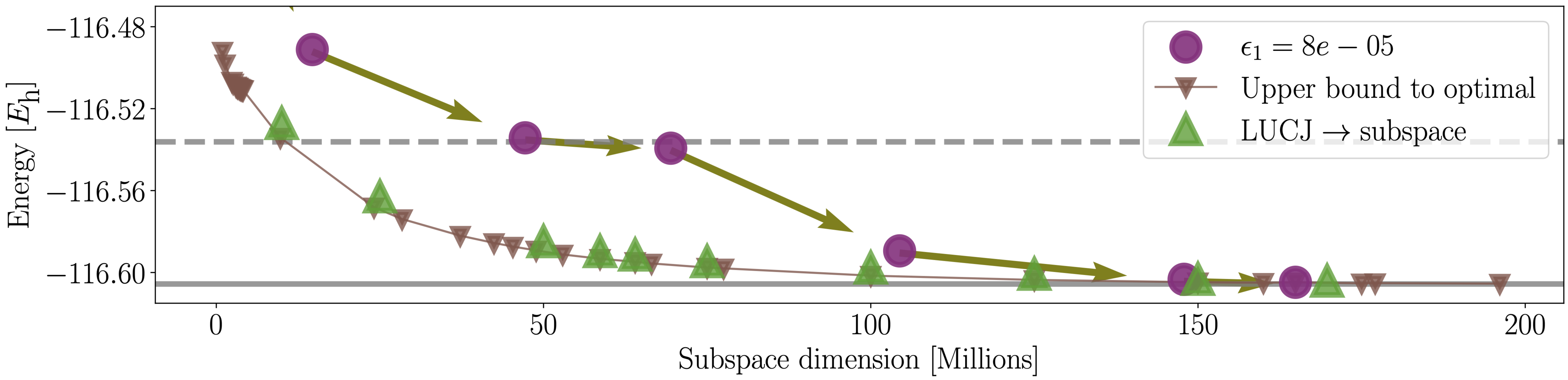


84 qubits
5000 2-qubit gates

Looking forward | quality of the subspaces

No false positives





Numerics | Quantum circuits can produce subspaces of better quality than classical heuristics

Quantum algorithms for spectrum estimation

	SQD	?
Circuits	Depends on the ansatz state $\|\psi\rangle$	Session 2
Recovery from noisy bitstrings	Configuration recovery	
Current experiments	Chemistry	
Convergence proof	NO	
Good use cases	Chemistry	

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

Science Advances 11 (25), eadu9991 (2025)

SQD

With convergence guarantees

- ?

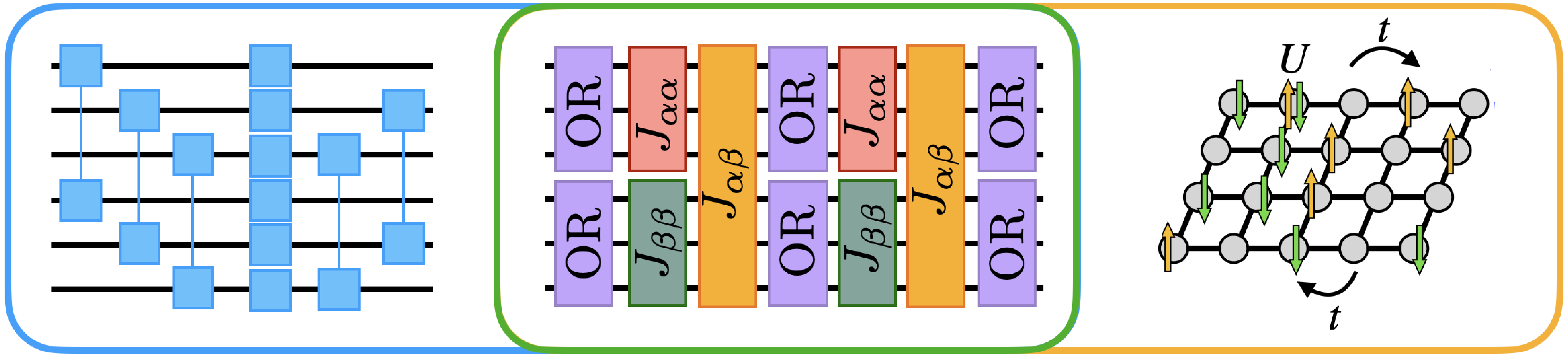
Session 2

?

Heuristic circuits

Circuits for chemistry: Local Unitary Cluster Jastrow

Hardware-efficient | **LUCJ circuit** | **Physically-motivated**



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

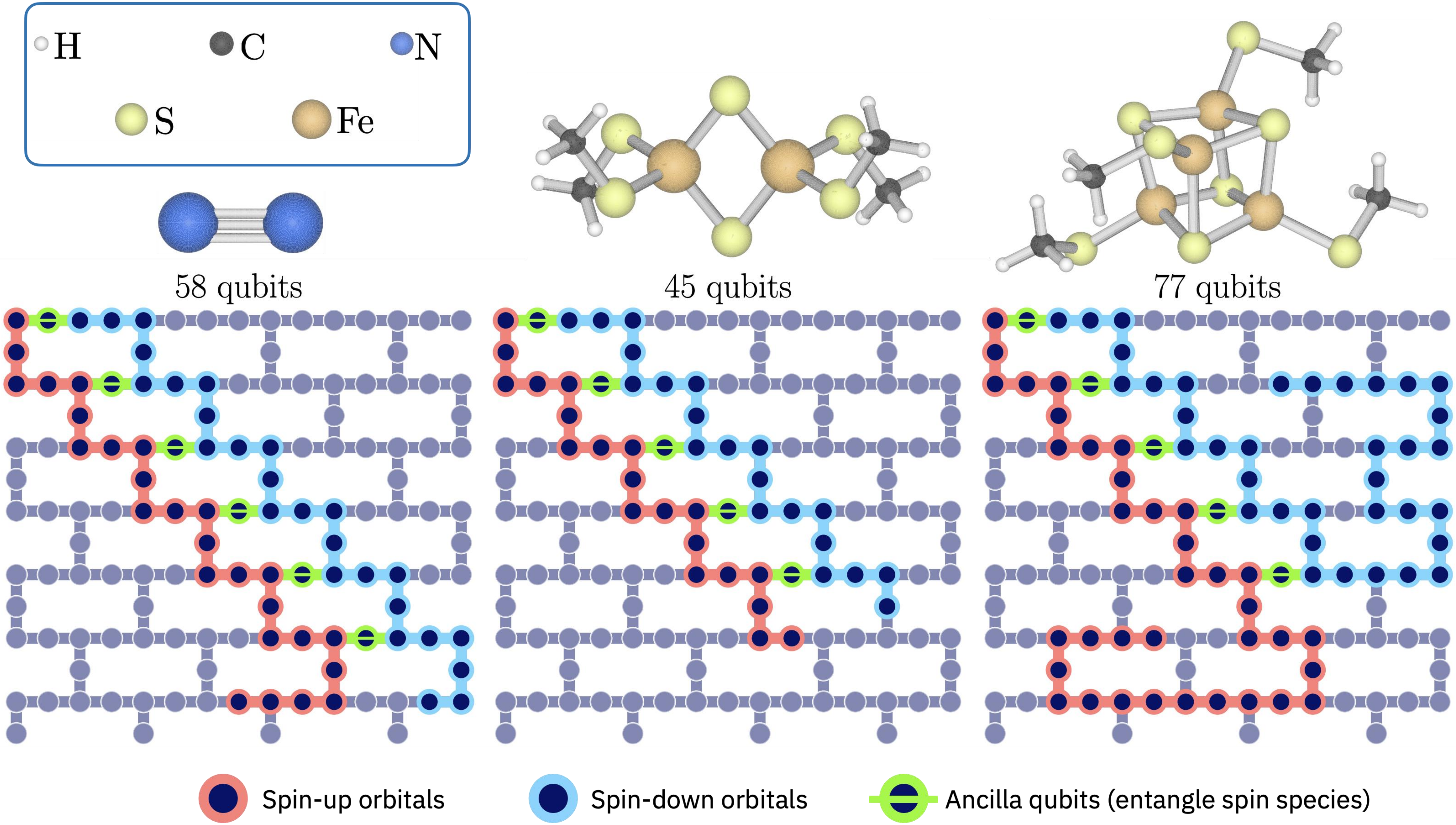
Local Unitary Cluster Jastrow

Physical motivation (derived from coupled-cluster)

Hardware friendliness (device-specific connectivity)

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

Circuits for chemistry: Local Unitary Cluster Jastrow



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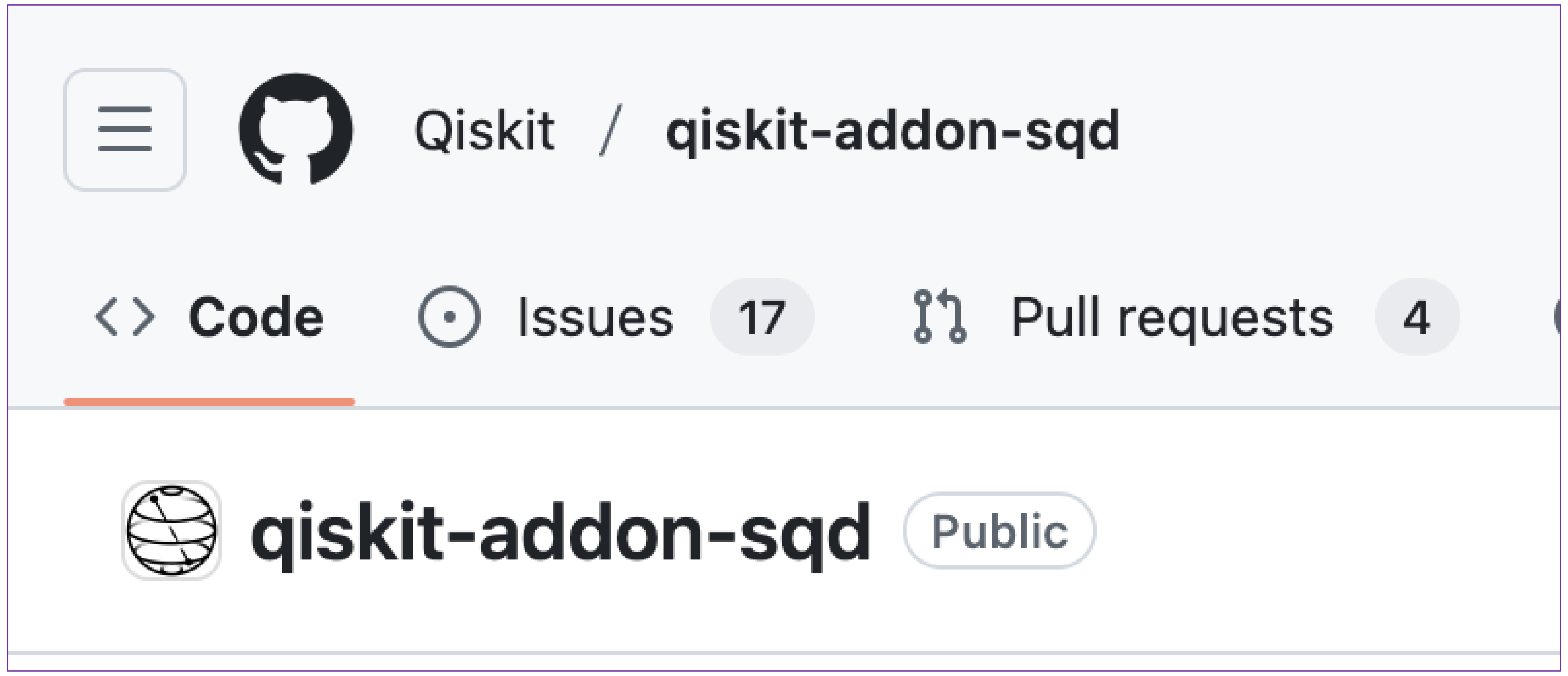
Science Advances 11 (25), eadu9991 (2025)

Brute-force requirements for chemistry and materials

Systems	Basis	Qubits	Memory vector storage	Reference
BeH	STO-3G	6	1KiB	*Nature 549, 242 (2017)*
Fe_2S_2	Cc-pvtz (DKH)	40	2 GiB	SQD paper
N_2	Cc-pvdz	52	33 GiB	SQD paper
C_3H_8	STO-3G	Classical	7TiB	*J. Chem. Theory Comput. 20, 1185 (2024)*
Fugaku Storage	-	-	4.85PiB	-
Front. Storage	-	-	700 PiB	-
Fe_4S_4	Cc-pvtz (DKH)	72	63 PiB	SQD paper

Classical SOTA

SQD as an open-source Qiskit addon



ibm.biz/addon-sqd

Qiskit addons build on the Qiskit SDK

A collection of research capabilities developed as modular tools that can plug into a workflow to design new algorithms at the utility scale

Map	Optimize	Execute	Post-Process
AQC-Tensor	OBP		SQD
MPF	Circuit cutting		M3
Qiskit Circuit Library	Transpiler	Primitives	Quantum Info
Input: Domain inputs	Input: Circuits, observable	Input: ISA circuit, observable	Input: Expectation value/samples
Output: Circuits, observable	Output: ISA circuit, observable	Output: Expectation value/samples	Output: Data objects/visualizations

Overview of the SQD Qiskit addon

finish me!

<summary of main features>

Code demonstration for a chemistry application: Ground state of the nitrogen molecule

ibm.biz/sqd-tutorial-chemistry

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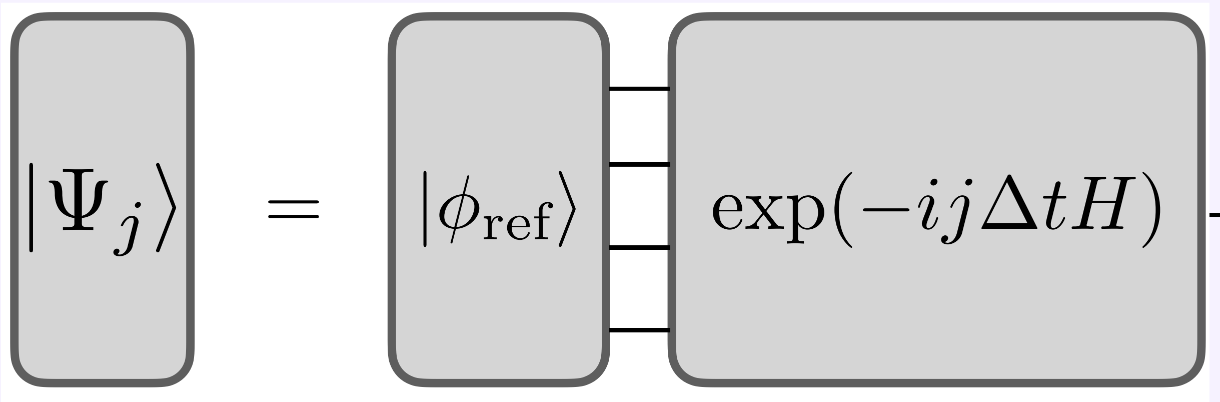
Sample-based Krylov Quantum Diagonalization (SKQD)

Preliminaries: Krylov quantum diagonalization

Quantum component

Krylov quantum states



for $j = 1$ to d

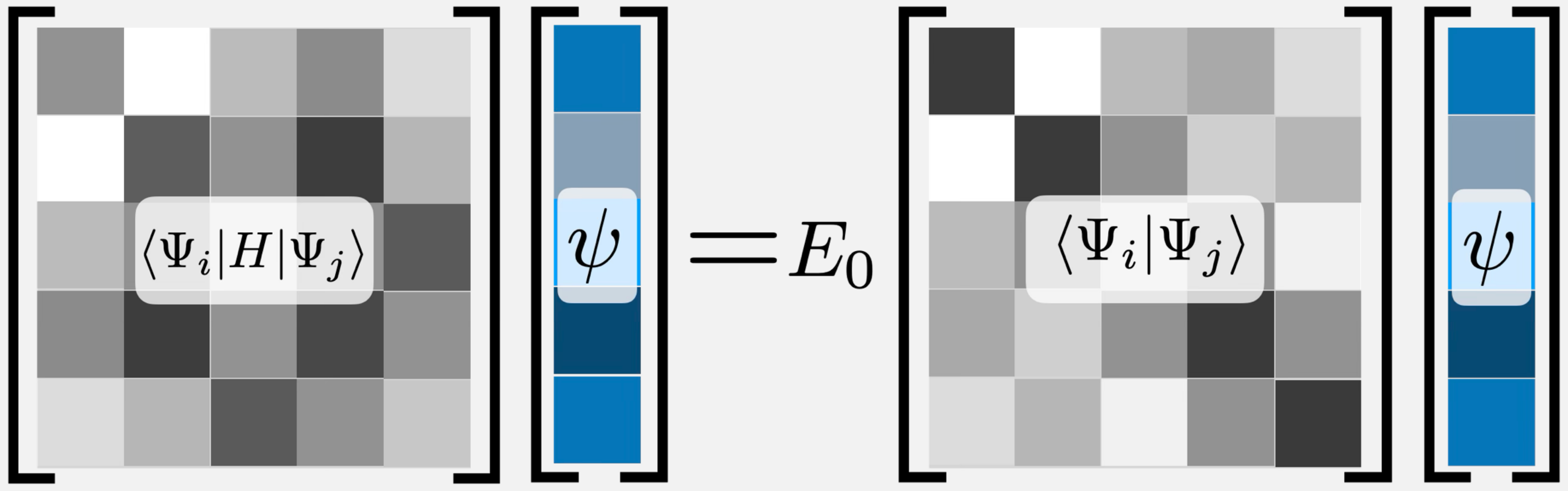
Reference state

Projection in the Krylov subspace

Classical component: Approximation of the ground state energy of H

subspace diagonalization in the Krylov subspace

Ground state properties



Preliminaries: Krylov quantum diagonalization

$$\underbrace{\text{Overlap of initial state with the true ground state: } 1/\mathrm{poly}(n) \qquad \text{Gap: } 1/\mathrm{poly}(n)}$$

Ground state error converges efficiently with increasing # circuits and shots

Experimental result (arxiv:2407.14431): computed eigenenergies of quantum many-body systems on two-dimensional lattices of up to 56 sites

Motivating questions

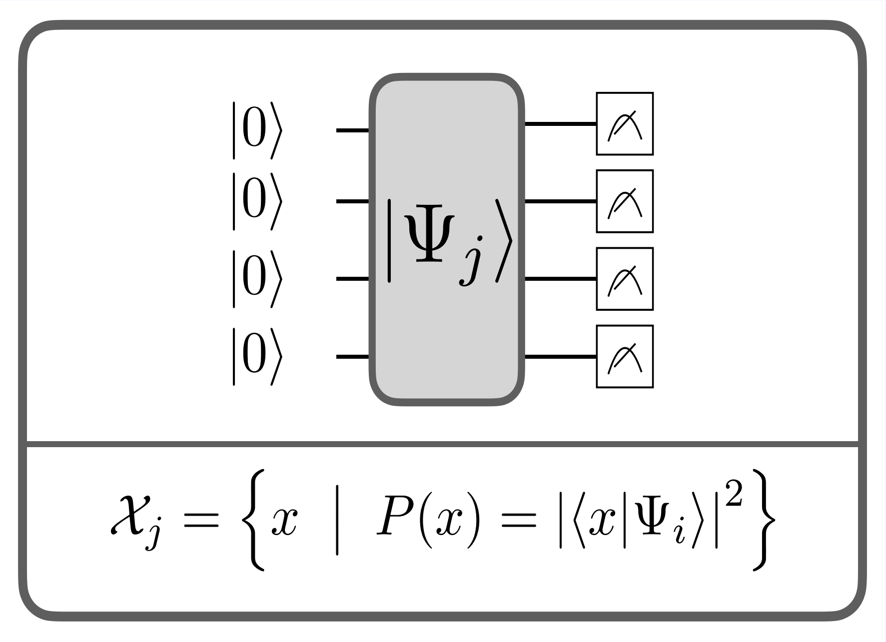
Can we leverage the strengths of SQD and Krylov to approximate the ground state energies of interesting Hamiltonians?

↓

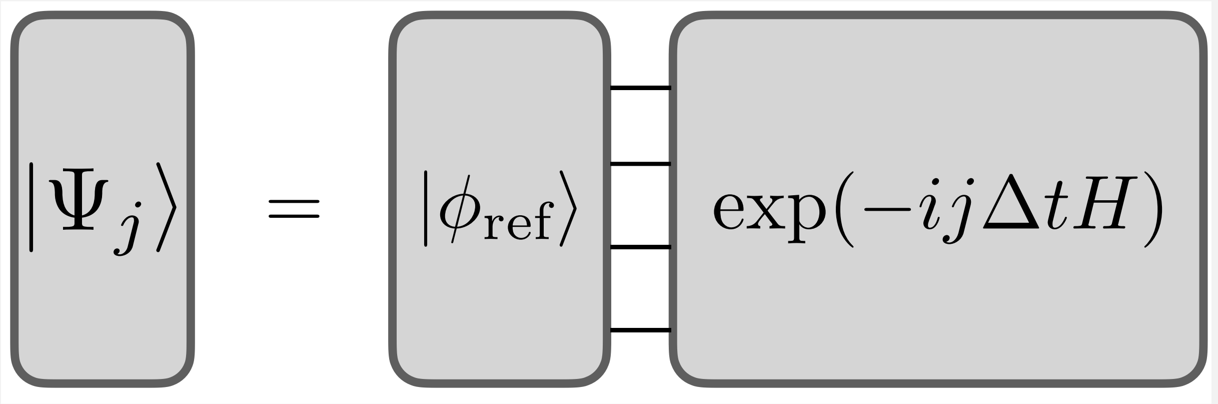
Can we perform reliable and verifiable simulation of nature with provable convergence on pre-fault-tolerant quantum computers?

Sample-based Krylov Quantum Diagonalization (SKQD)

Sampler()



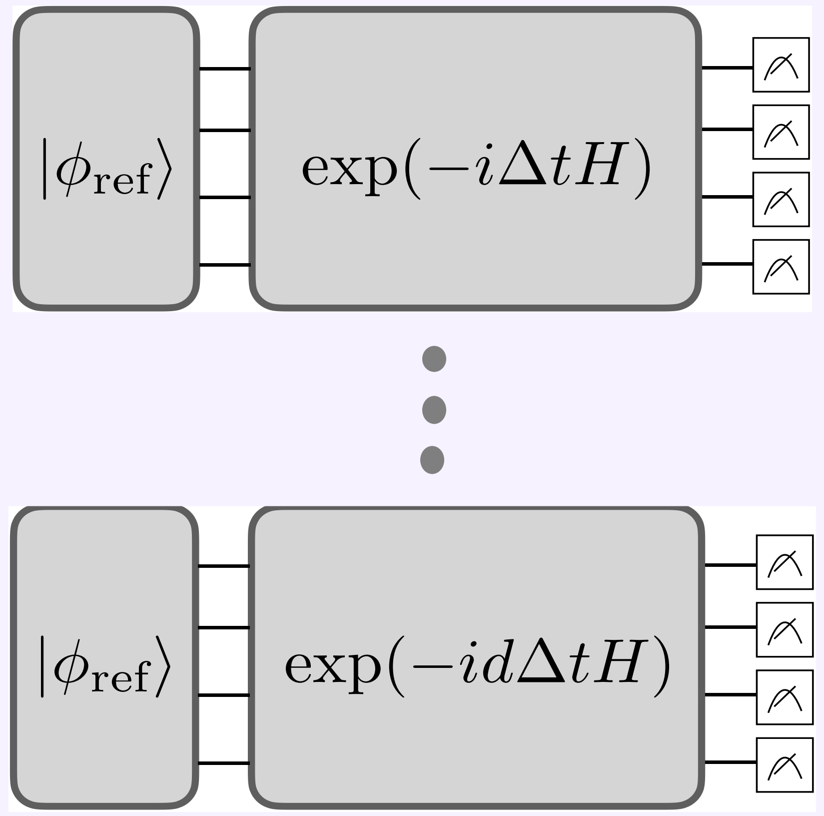
Simple states to prepare that have good overlap with ground states



Quantum devices are naturally suited for performing **time-evolution circuits.**

SKQD: algorithm

Sampler()



$\{|b_j^k\}_{j=1}^{M}$

For $k = 1$ to d

Krylov time-evolved states

Approximation of the ground state energy of H

Configuration recovery

Projection and subspace diagonalization

Ground state properties

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OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

arXiv:2501.09702

SKQD: convergence guarantees

Krylov quantum diagonalization

SQD

Overlap of initial state with the true ground state: $1/\mathrm{poly}(n)$

Gap: $1/\mathrm{poly}(n)$

Sparse ground state

Ground state error converges efficiently with increasing # circuits and shots

arXiv:2501.09702

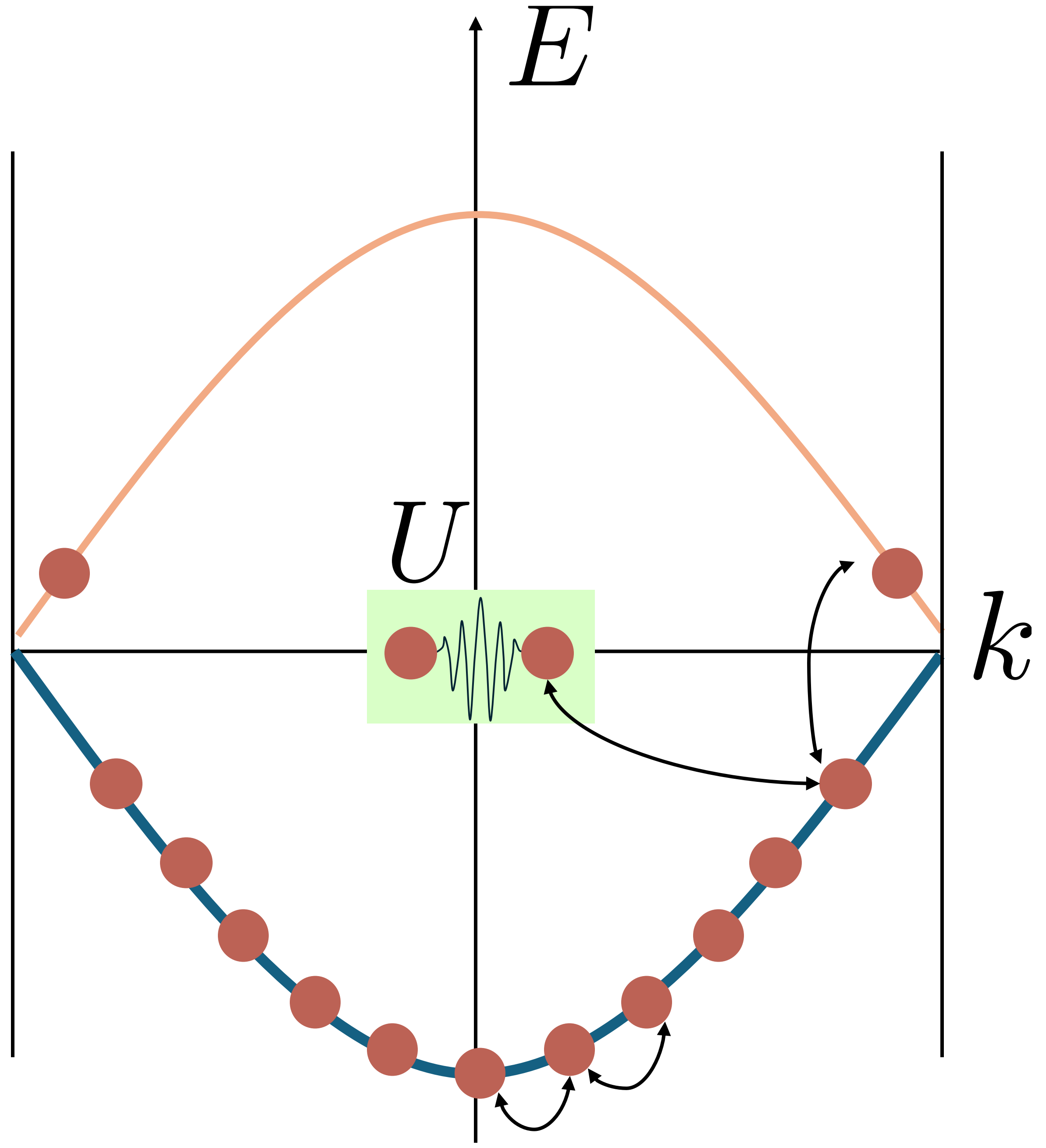
SKQD: key takeaways

- No false positives for ground states: estimations are always upper bounds on the true ground-state energy
- Its performance has a provable convergence for sparse ground states given good initial reference state
- No ansatz required: wavefunction ansatz is replaced with a reference state, followed by time evolution circuits

SKQD: first experiments

arXiv:2501.09702

Single-impurity Anderson model



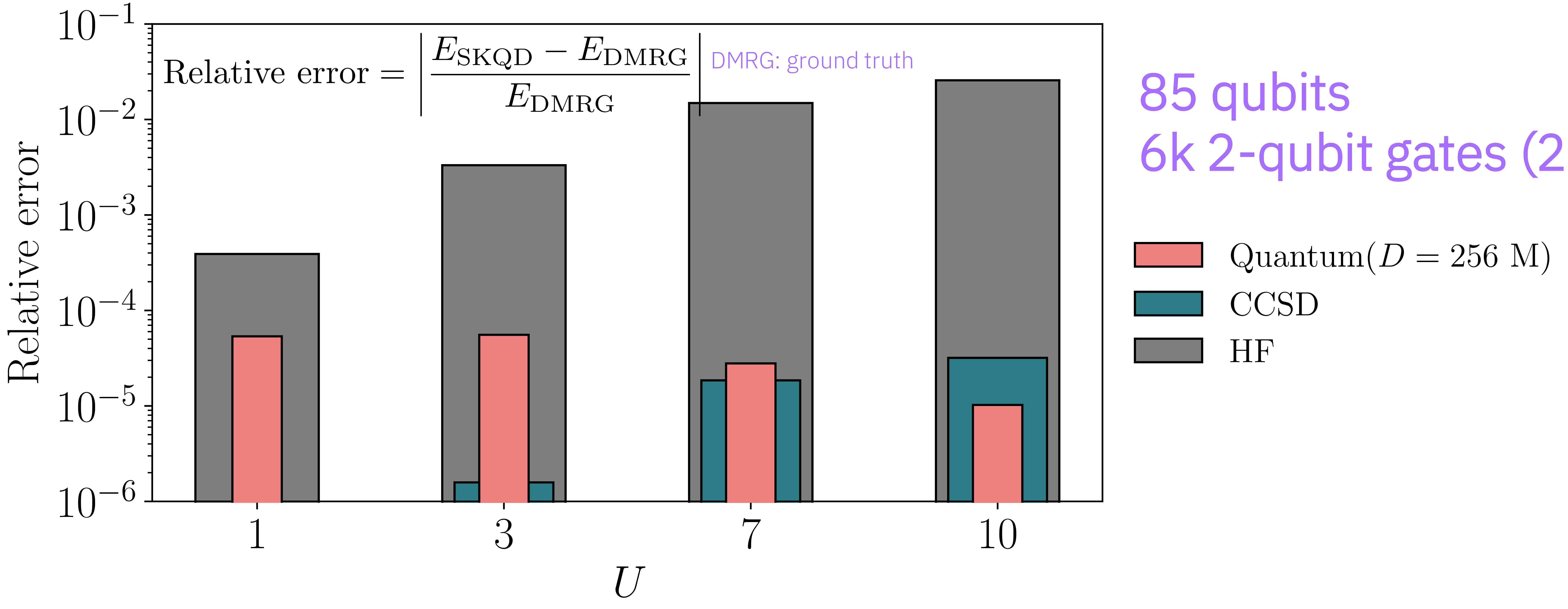
Free electrons coupled to interacting impurities

Relevant to simplify real materials calculations on DMFT workflows

Extensively used to benchmark numerical techniques

SKQD: first experiments

arXiv:2501.09702



85 qubits
6k 2-qubit gates (25 Trotter)

Excellent agreement in the ground-state energy estimation

Accuracy increases as interactions increase | higher sparsity

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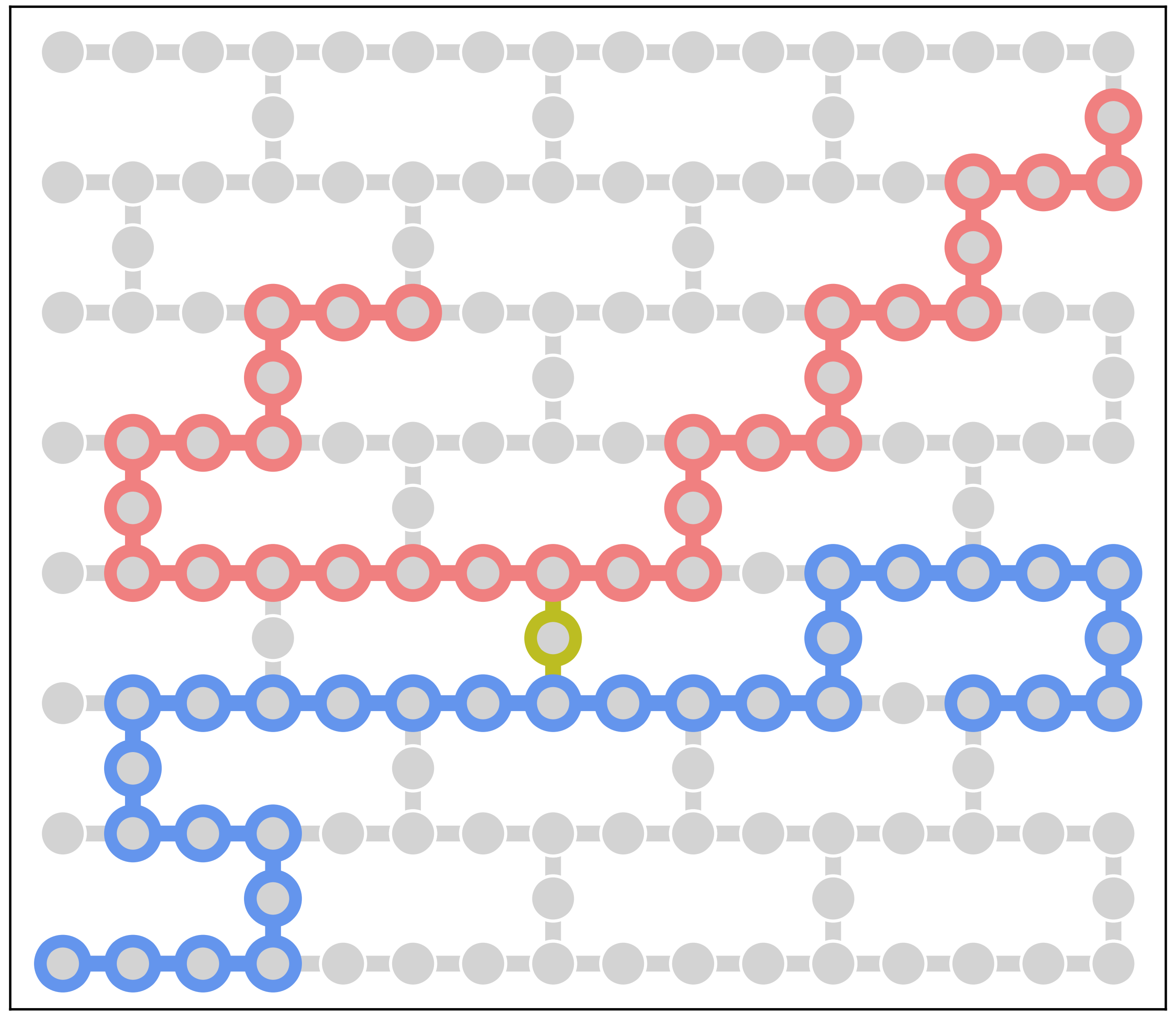
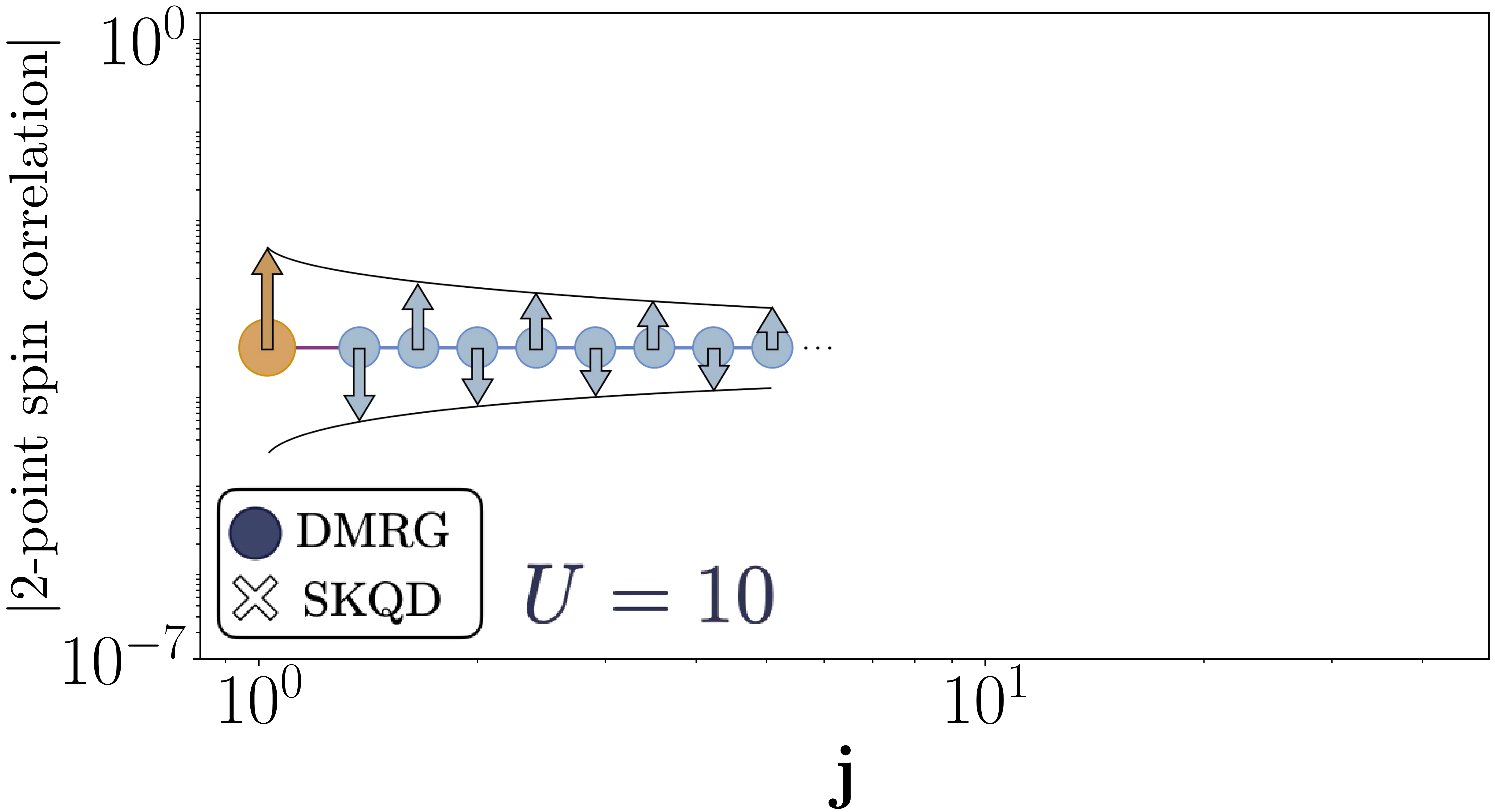
SKQD: first experiments

arXiv:2501.09702





Excellent agreement in other physical properties

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Oak Ridge National Laboratory | Leadership Computing Facility

Brute-force requirements for chemistry and materials

Systems	Basis	Qubits	Memory vector storage	Reference
BeH	STO-3G	6	1KiB	*Nature 549, 242 (2017)*
Fe_2S_2	Cc-pvtz (DKH)	40	2 GiB	SQD paper
N_2	Cc-pvdz	52	33 GiB	SQD paper
C_3H_8	STO-3G	Classical	7TiB	*J. Chem. Theory Comput. 20, 1185 (2024)*
Fugaku Storage	-	-	4.85PiB	-
Front. Storage	-	-	700 PiB	-
Fe_4S_4	Cc-pvtz (DKH)	72	63 PiB	SQD paper
SIAM (41 bath)	Lattice model	84	$2.06 * 10^9$ PiB	SKQD paper

Classical SOTA

Quantum algorithms for spectrum estimation

	SQD	SKQD
Circuits	Depends on the ansatz state $\|\psi\rangle$	Reference state and time evolution circuits
Recovery from noisy bitstrings	Configuration recovery	Configuration recovery
Current experiments	Chemistry	Single-impurity Anderson model
Convergence proof	NO	YES, with the sparsity assumption
Good use cases	Chemistry	Lattice models

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

Science Advances 11 (25), eadu9991 (2025)

SQD

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

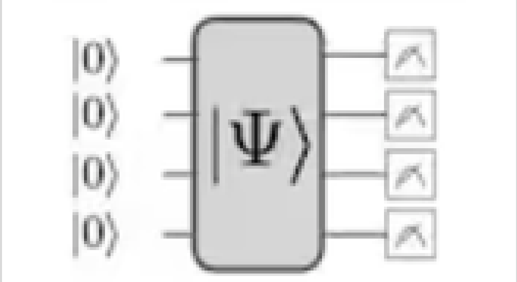
arXiv:2501.09702

SKQD

Code demonstration for a physics application: Anderson impurity model

ibm.biz/sqd-tutorial-physics

SQD workflow



```
0011...0011
0110...0100
1101...0110

...

1011...1110
```

Process samples with SQD

Eigenvectors
Eigenvalues

SQD workflow