

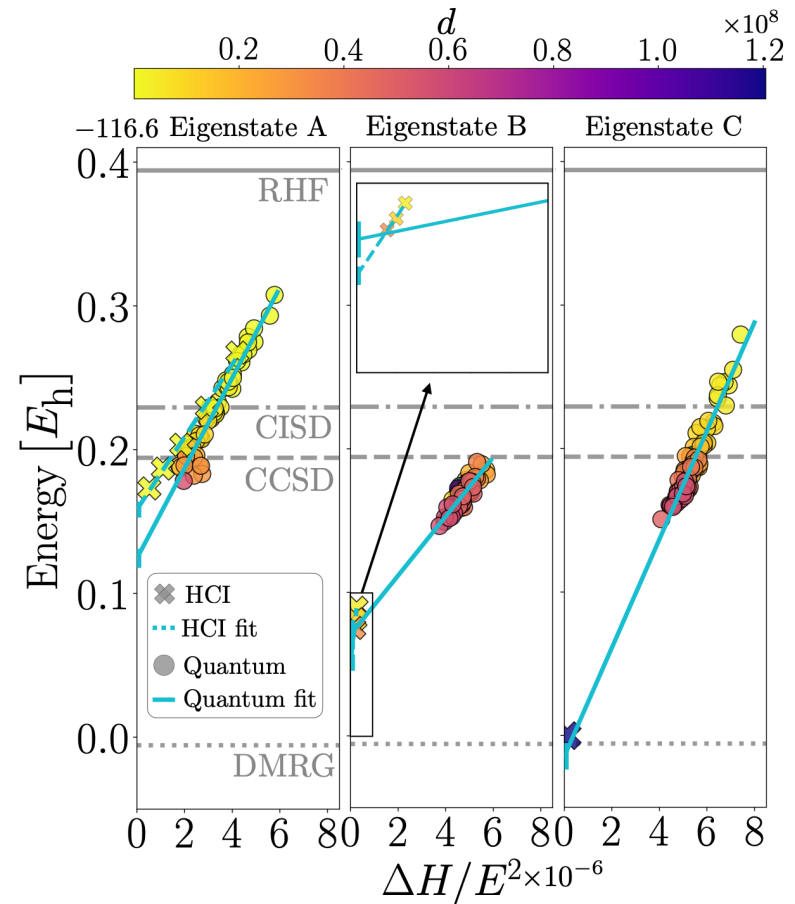
Sample-based quantum algorithms in theory and practice

Will Kirby

IBM Quantum

william.kirby@ibm.com

OSU 10/28/25



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william.kirby@ibm.com

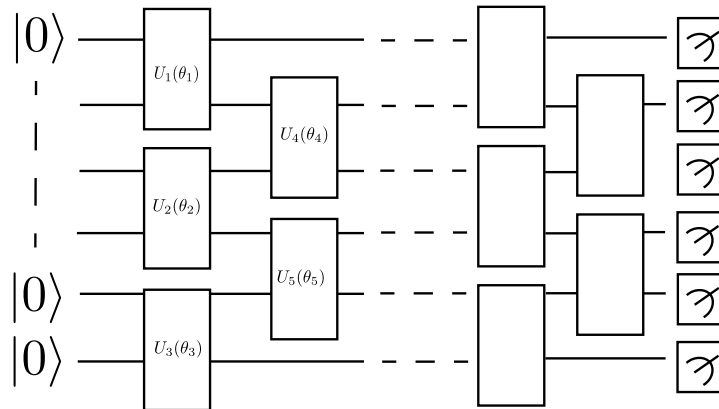
Topics

1. Quantum circuits and sampling
2. Estimating ground state energies
3. Aside: on quantum advantage
4. Two algorithms

Quantum circuits and sampling

Foundational process in every quantum algorithm:

1. Prepare initial state e.g. $|000\dots 0\rangle$
2. Transform state under some unitary operation $\rightarrow U|000\dots 0\rangle$
3. Measure all qubits: Born rule $\text{prob}(| \underbrace{b}_{\in \{0,1\}^n} \rangle) = |\langle b|U|000\dots 0\rangle|^2$



Two sides of coin:

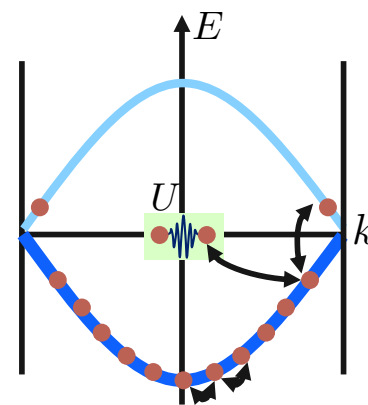
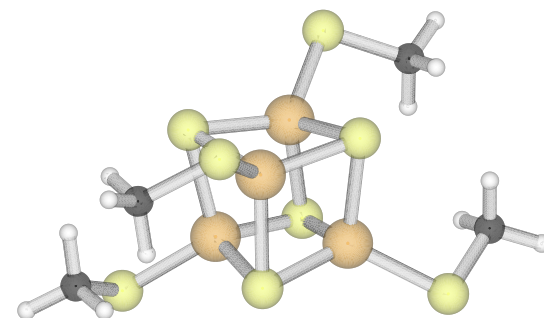
1. Identify hard problems and try to solve with quantum
2. Identify what quantum does well and try to fit hard problems into that

Quantum Algorithms for ground states

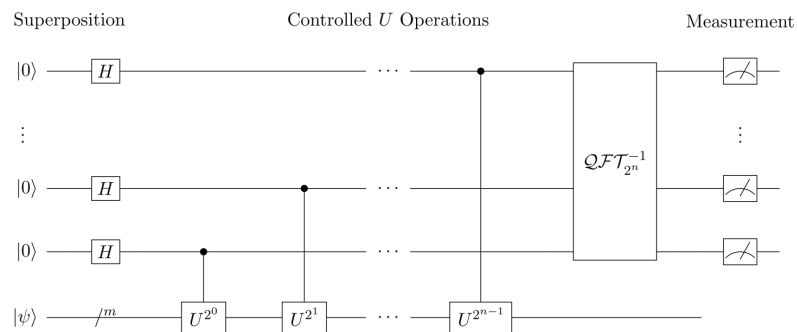
Goal: solving computationally challenging energy-estimation problems in quantum chemistry and materials

This is a *first step* towards...

Applications: development of new materials, drug discovery, battery design, etc.



Prior algorithms in fault-tolerant era - example



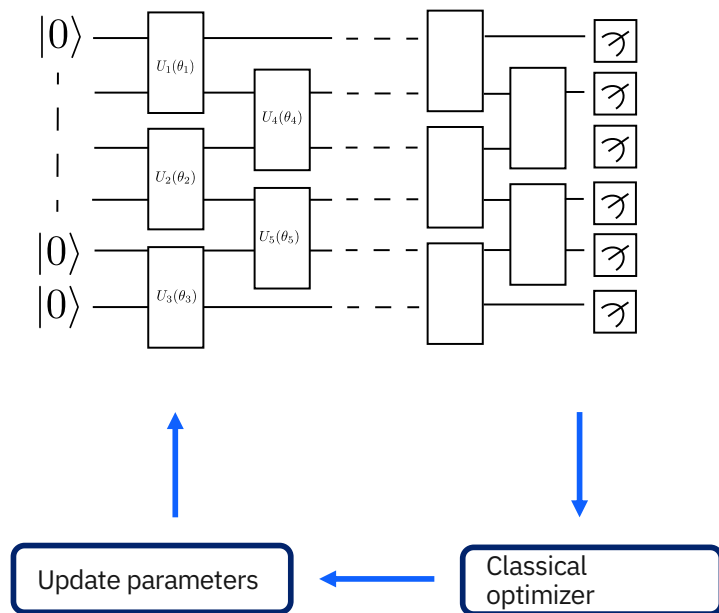
Quantum Phase Estimation (QPE)

- Convergence guaranteed 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 - example



Variational Quantum Algorithms (VQA)

- Shallow-depth circuits

Key challenges

- No convergence guarantee
- Measurement overhead for chemistry problems

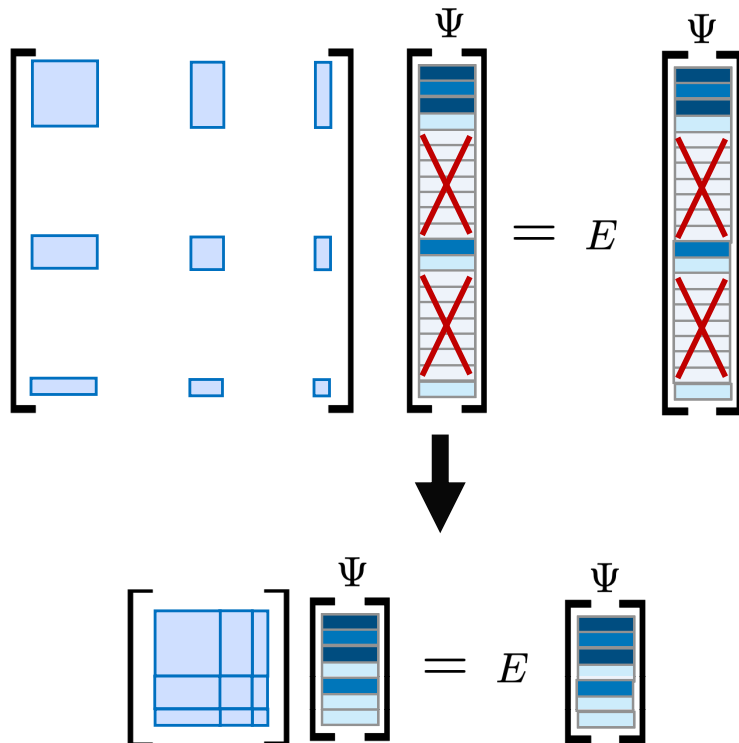
Eigenstate approximation

Sparse eigenvector problem

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

- Vector space dimension is exponential
- Hamiltonian matrix has classical representation
- e.g. Pauli decomposition
- **Assume sparse trial solution:** eigenvectors have polynomial support

Sparse eigenvector problem

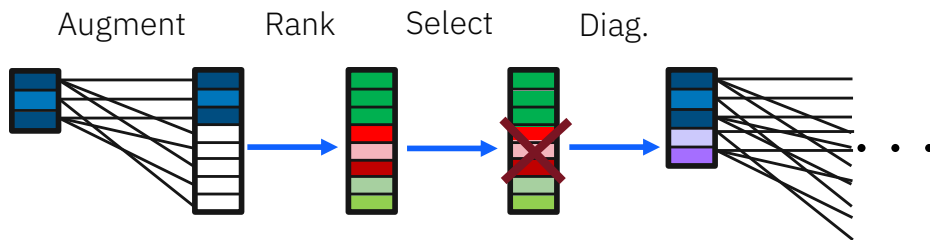


- Suppose we are given the subspace of relevant amplitudes
- We can remove “less relevant” remainder
- Tractable eigenvalue problem

Searching for relevant dimensions

Classical

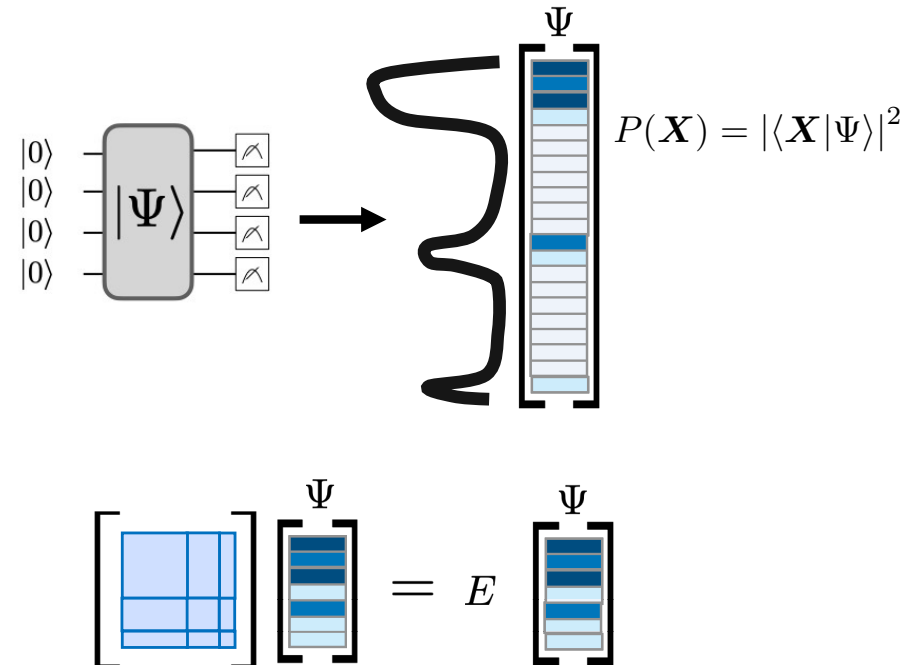
- Tree-like search (Selected Configuration Interaction)
- Heuristic methods that rely on physics intuition and or perturbation theory



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SQD

- Quantum circuit produces samples



Aside: on quantum advantage

Quantum advantage

Quantum computer does task we care about verifiably “better” than classical algorithms

Nuances

1. What classical algorithms? *Ideally, any possible; minimum, best we know of now*
2. “Better”? *In appropriate metric(s) for task: accuracy, runtime, energy usage, \$\$\$, ...*
3. “Verifiably”? *The hard one*

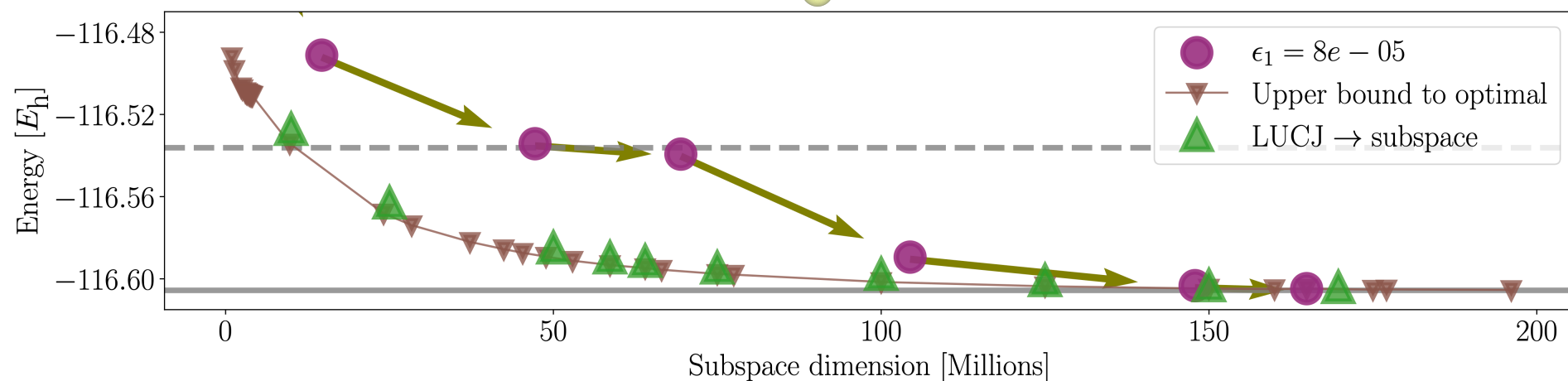
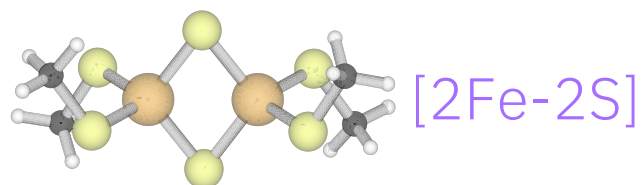
Most use-cases will require some trust (from benchmarking and tractable verification)

Advantage for sample-based diagonalization

“Verifiably” gets much easier

- Output of quantum algorithm: set of bitstrings to project and diagonalize on
- Estimate is lower bounded by true value (“variational” up to *classical* machine precision)
- Many classical algorithms have same guarantee (SCI, CISD, DMRG, ...)
- ⇒ Lower energy estimate wins!
- Set of bitstrings is a *classical witness* of the output energy

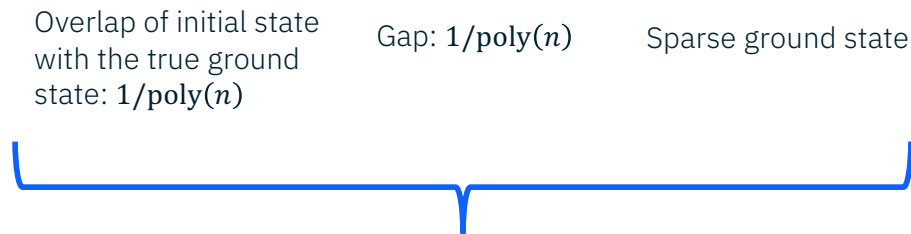
Why quantum? (heuristic version)



Numerics on 40 qubits | Quantum circuits can produce subspaces of better quality than classical heuristics (HCI)

Why quantum? (provable version)

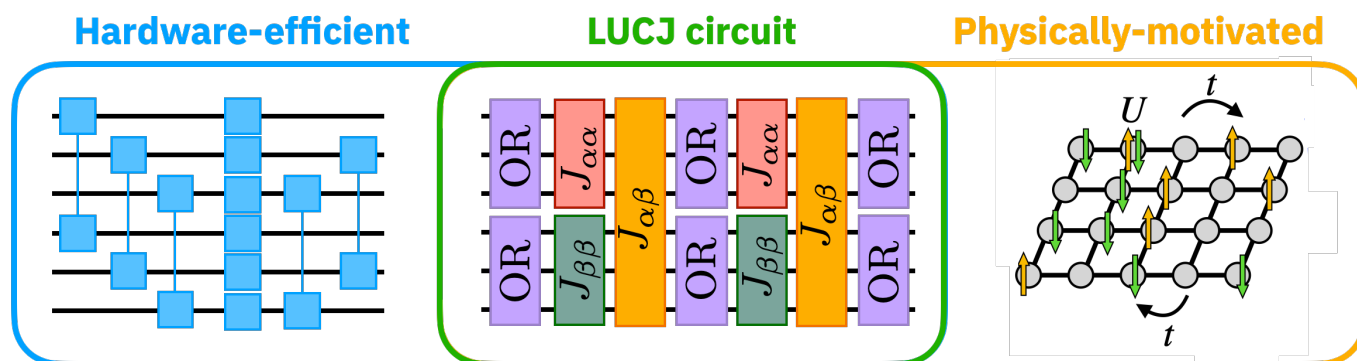
- Sample from time-evolved states
- Time-evolution circuits are (relatively) easy to execute
- Three conditions required for probably efficient convergence:



Ground state error converges efficiently with
increasing # circuits and shots

Heuristic circuits

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

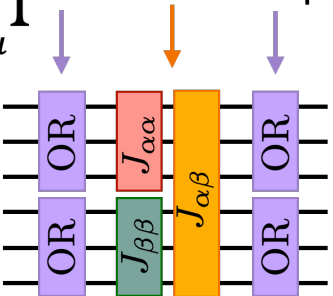
- Unitary coupled-cluster singles and doubles (UCCSD)

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

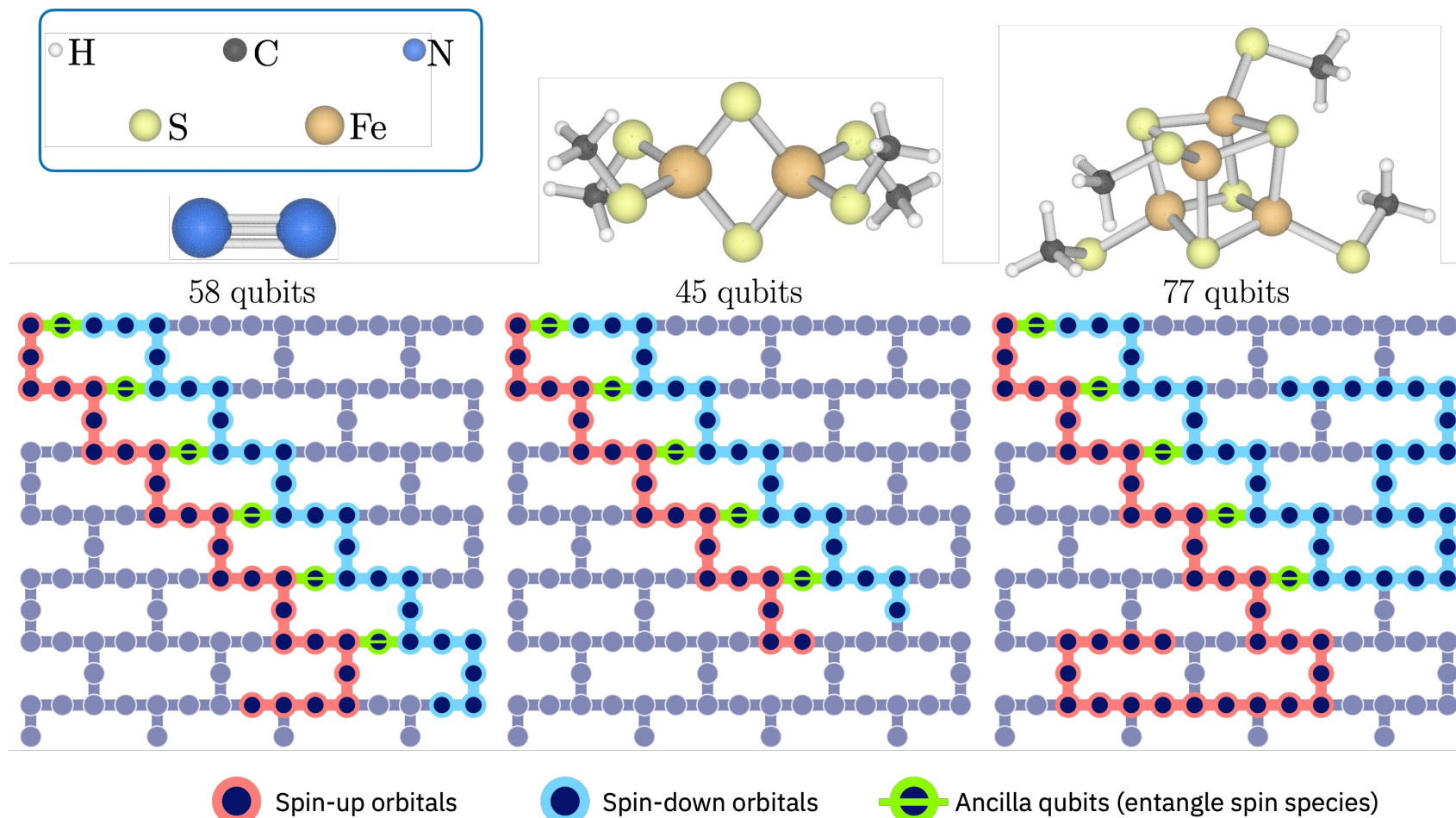
- Jastrow form of the UCCSD:

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

- Local Unitary Cluster Jastrow ansatz*

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


Circuits for chemistry: Local Unitary Cluster Jastrow

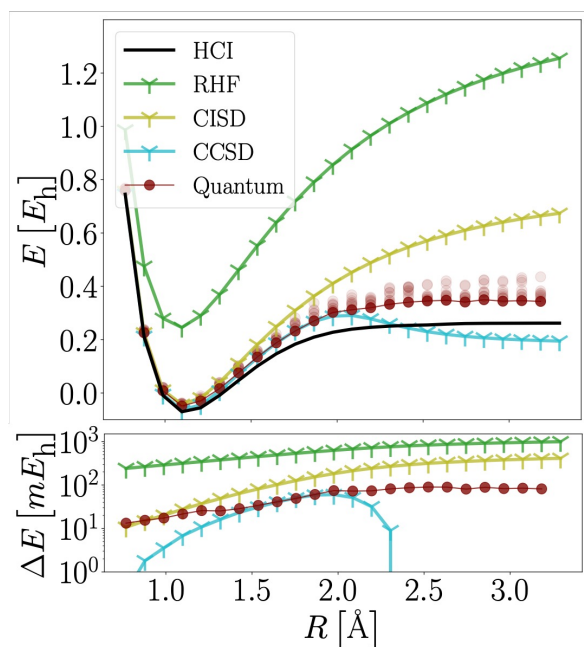


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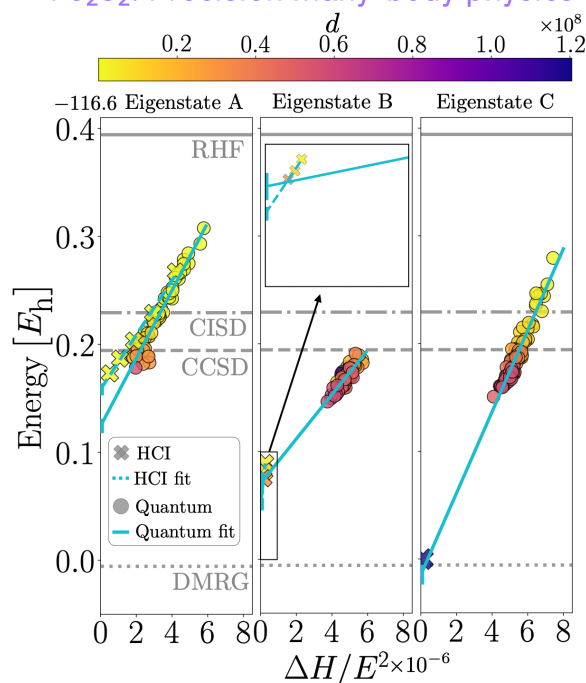
Science Advances 11 (25), eadu9991 (2025)

Results Highlights

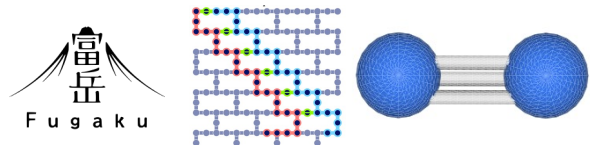
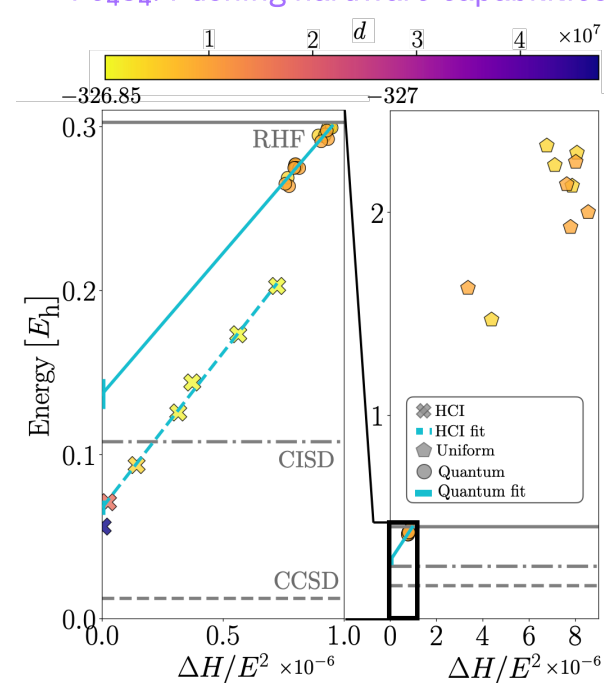
N_2 : Bond breaking on large basis set



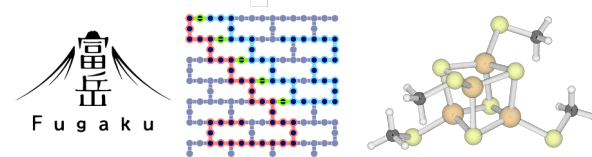
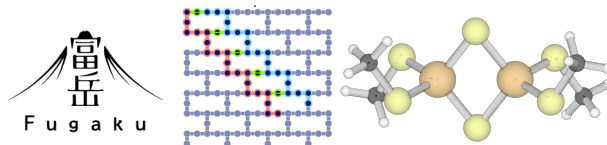
Fe_2S_2 : Precision many-body physics



Fe_4S_4 : Pushing hardware capabilities



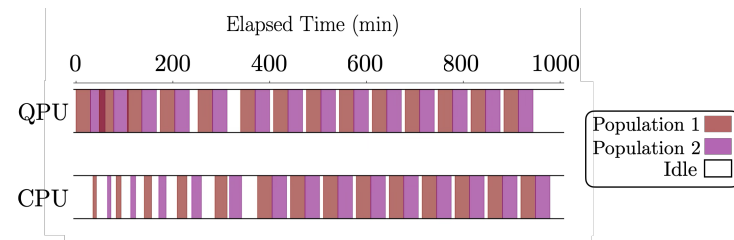
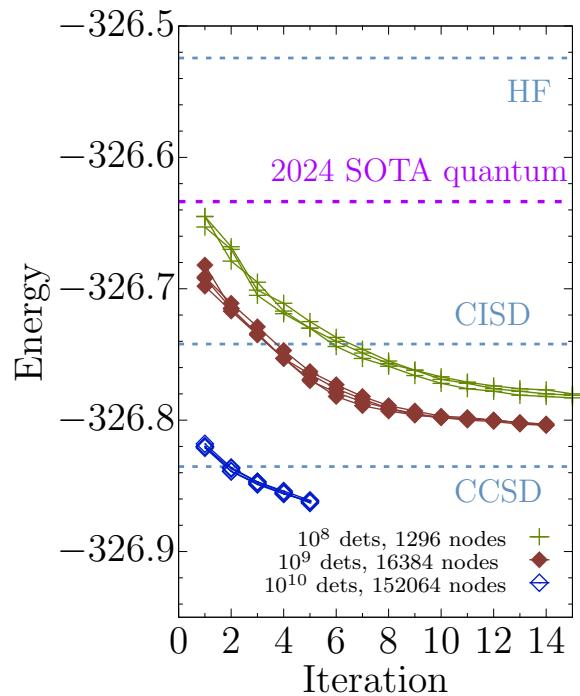
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Large-scale SQD circuit optimization

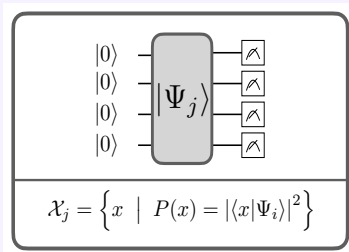
Differential-evolution optimization with two populations:
no idle time



Algorithm(s) with provable convergence

SKQD

Sampler()



Simple states to prepare that have good overlap with ground states

$$|\Psi_j\rangle = |\phi_{\text{ref}}\rangle \exp(-ij\Delta t H)$$

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

Aside: Krylov quantum diagonalization

High-level idea:

1. H = Hamiltonian, $U = e^{-iH\Delta t}$ = time evolution
2. Initial guess $|\psi_0\rangle$
3. $(\mathbf{H}, \mathbf{S})$ = project H onto $\text{span}[|\psi_0\rangle, U|\psi_0\rangle, U^2|\psi_0\rangle, \dots, U^{D-1}|\psi_0\rangle]$

Krylov space

$$\begin{matrix} \boxed{V^\dagger} & \boxed{H} & \boxed{V} & = & \boxed{\mathbf{H}} & , & \boxed{V^\dagger} & \boxed{V} & = & \boxed{\mathbf{S}} \end{matrix}$$

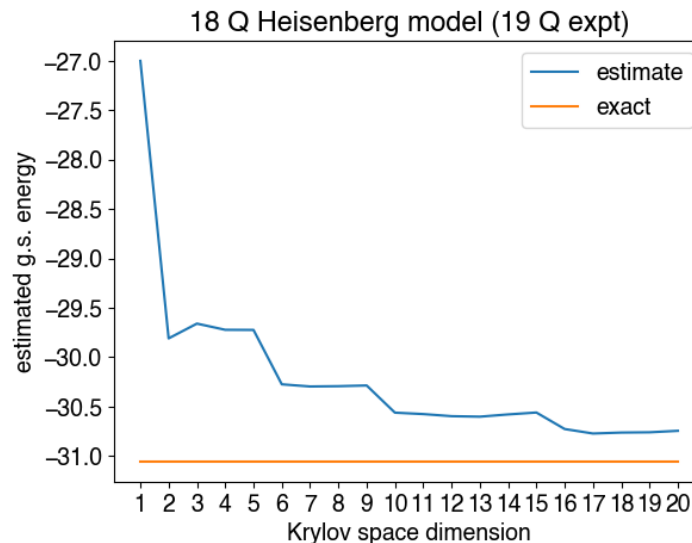
3. Lowest eigenvalue of $(\mathbf{H}, \mathbf{S})$ i.e., of $\mathbf{H}\mathbf{v} = \lambda\mathbf{S}\mathbf{v}$, approximates lowest eigenvalue of H

Aside: Krylov quantum diagonalization

Can show¹ that energy error from a noisy quantum Krylov experiment is bounded as

$$\text{energy error} \leq O \left(\underbrace{\delta' \mathbf{1}(\delta' > \Delta)}_{\text{from free parameter}} + \frac{\|H\|}{|\gamma_0|^2} \left[\underbrace{\left(\frac{1}{\delta' - \delta} + D \right) \eta}_{\text{from noise}} + \underbrace{\left(1 + \frac{\pi \delta}{2 \|H\|} \right)^{-D}}_{\text{from Krylov projection}} \right] \right)$$

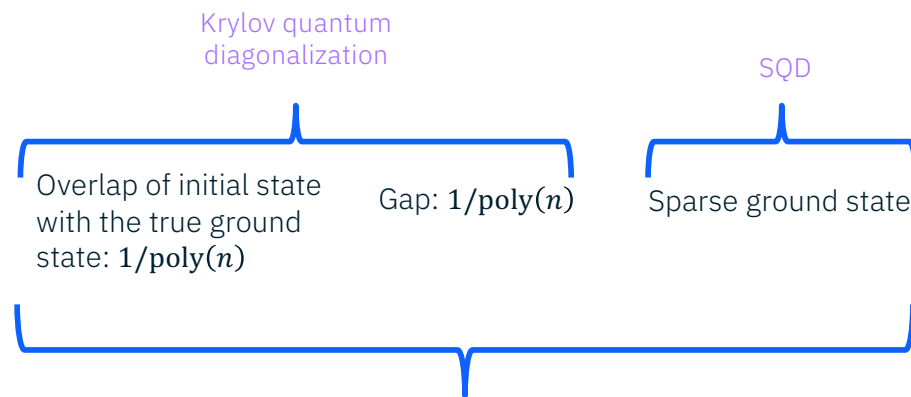
So one expects a result with this overall shape:



- η = noise rate
- γ_0 = initial state overlap
- Δ = spectral gap
- D = Krylov dimension
- δ, δ' = positive free parameters

¹Epperly *et al.*, <https://arxiv.org/abs/2110.07492>,
Kirby, <https://arxiv.org/abs/2401.01246>

SKQD convergence guarantees



Ground state error converges efficiently with increasing # circuits and shots

First SKQD experiments: impurity models

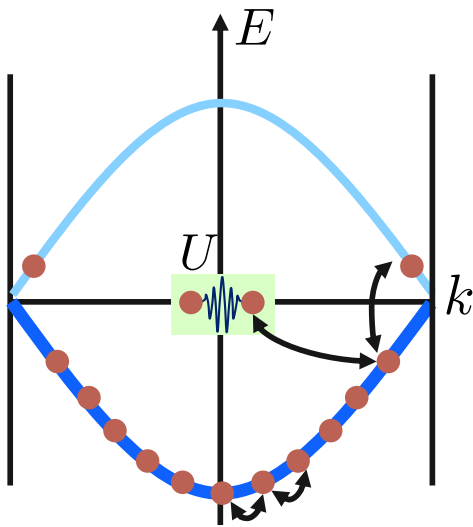
Free electrons coupled to interacting impurities

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

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

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

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

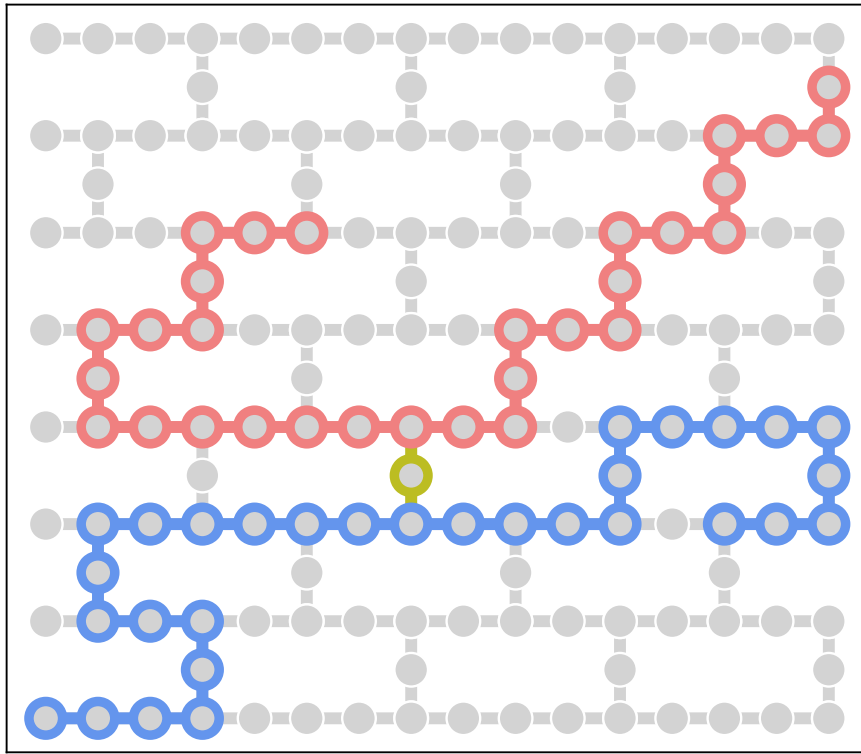


Relevant to **simplify real materials calculations** on DMFT workflows

Extensively used to **benchmark numerical techniques**

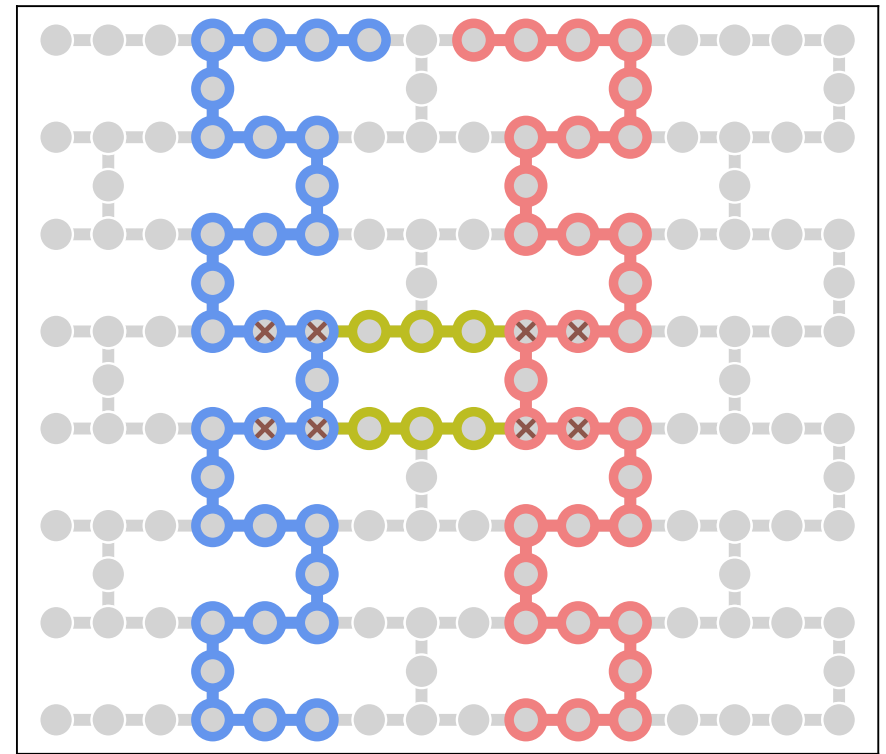
First SKQD experiments: impurity models

1 Imp. 41 Bath modes $\rightarrow$ 84+1 qubits



[arXiv:2501.09702](https://arxiv.org/abs/2501.09702)

4 Imp. 28 Bath modes $\rightarrow$ 64+6 qubits



unpublished

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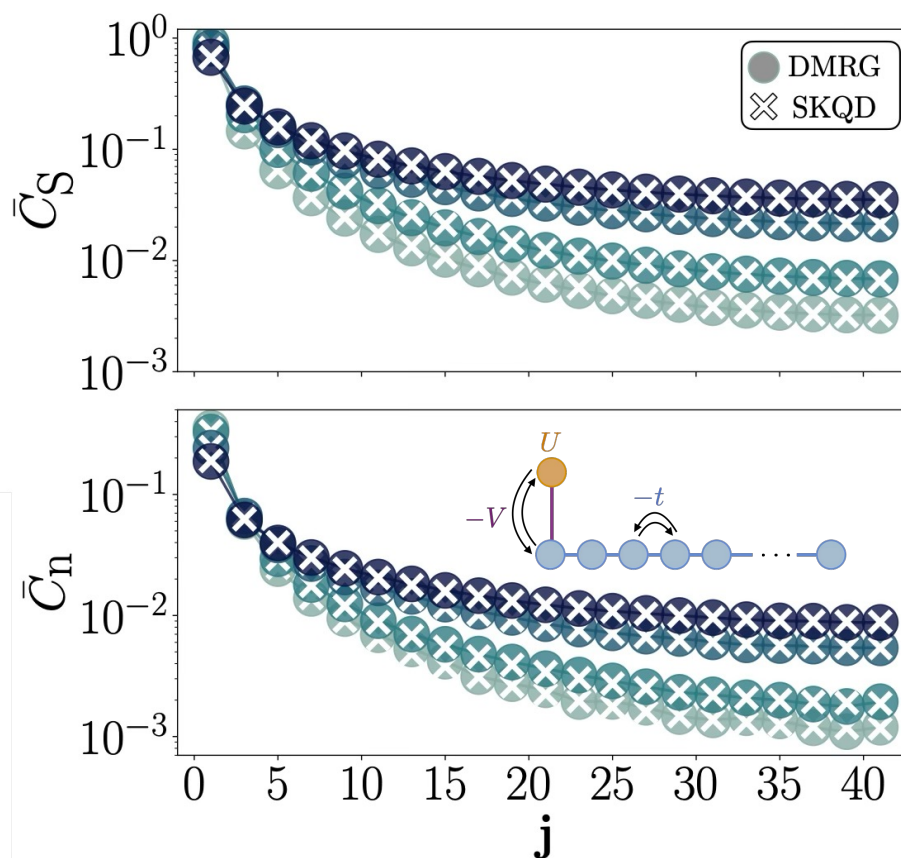
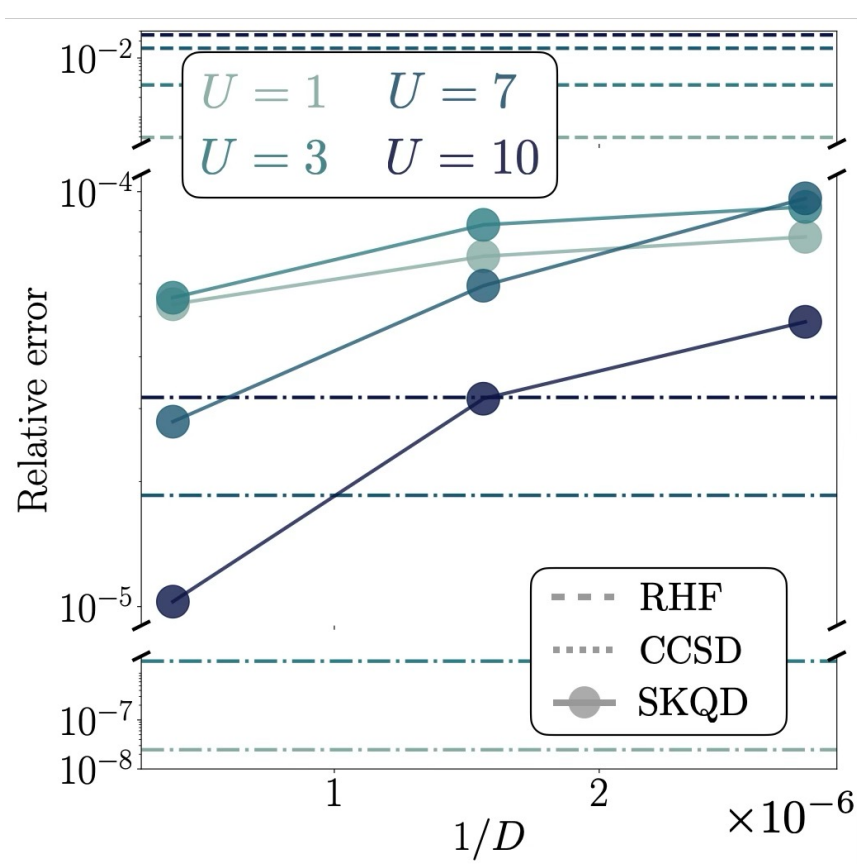
Spin-up orbitals

Spin-down orbitals

Ancilla qubits

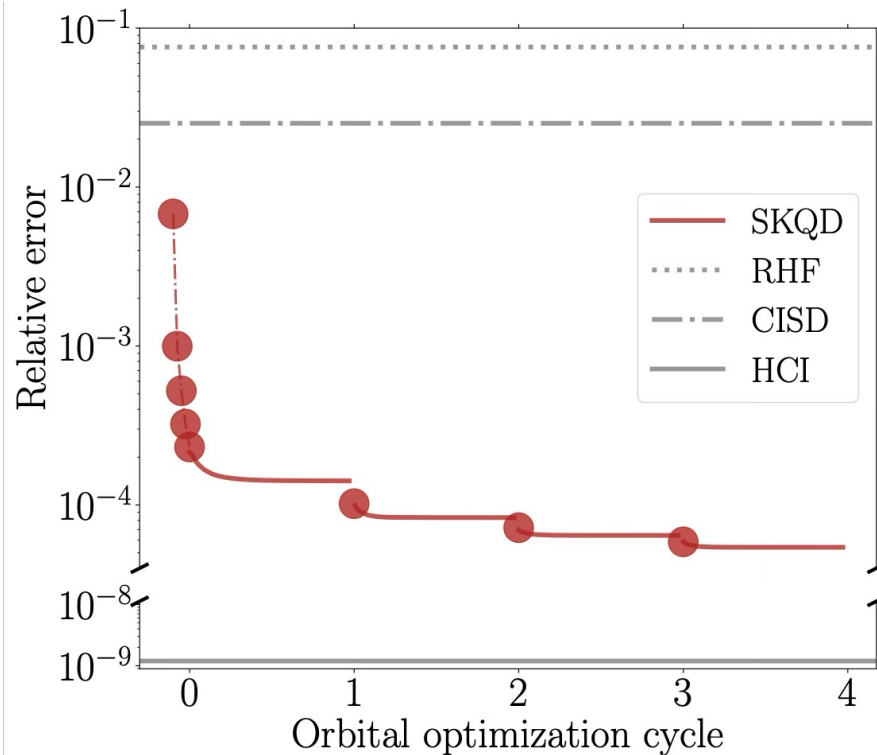
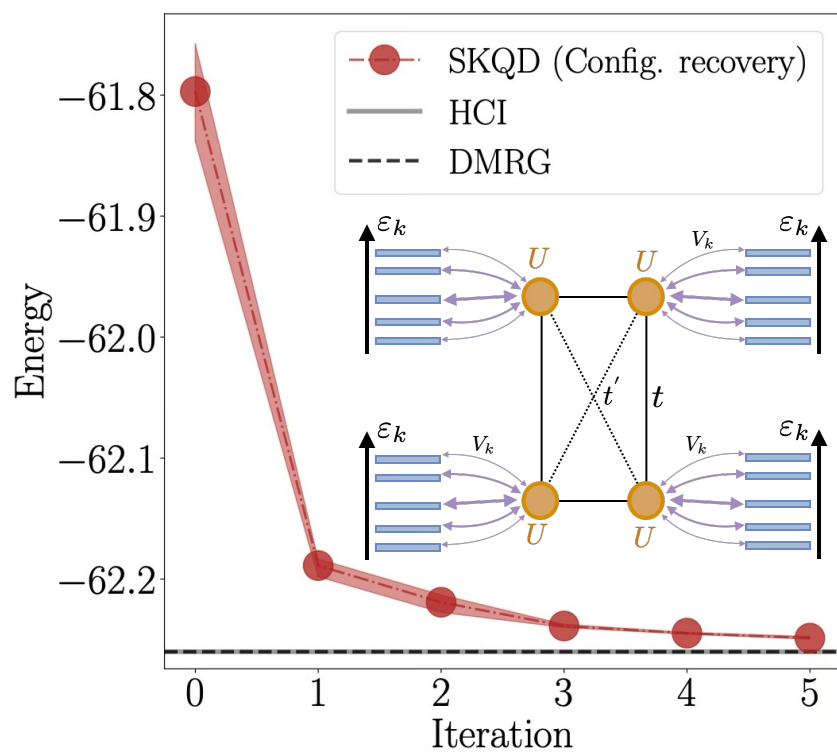
SKQD experiments: 1 impurity

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



SKQD experiments: 4 impurities

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



Main Takeaways

(1) Use quantum for what it's best at – sampling. (2) Large (but not exponential) diagonalizations on high-performance classical. (3) Accurate results even with noisy quantum hardware!

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Framework yields variational energies (no false positive solutions) and any future quantum advantage will be classically verifiable

We have both variational heuristic and provable Krylov-based versions of the algorithm (another talk: new hybrid of the two for chemistry)

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

[arXiv:2405.05068](https://arxiv.org/abs/2405.05068)

[arXiv:2501.09702](https://arxiv.org/abs/2501.09702)

[arXiv:2508.02578](https://arxiv.org/abs/2508.02578)

Thank you!