Observation of Improved Accuracy over Sparse Ground State Solvers using a Quantum Computer

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Based on arxiv:2603.03496

Observation of Improved Accuracy over Classical Sparse Ground State Solvers using a Quantum Computer

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Quantum diagonalization algorithms

Many quantum algorithms for approximating ground states (and energies)

Quantum Phase Estimation

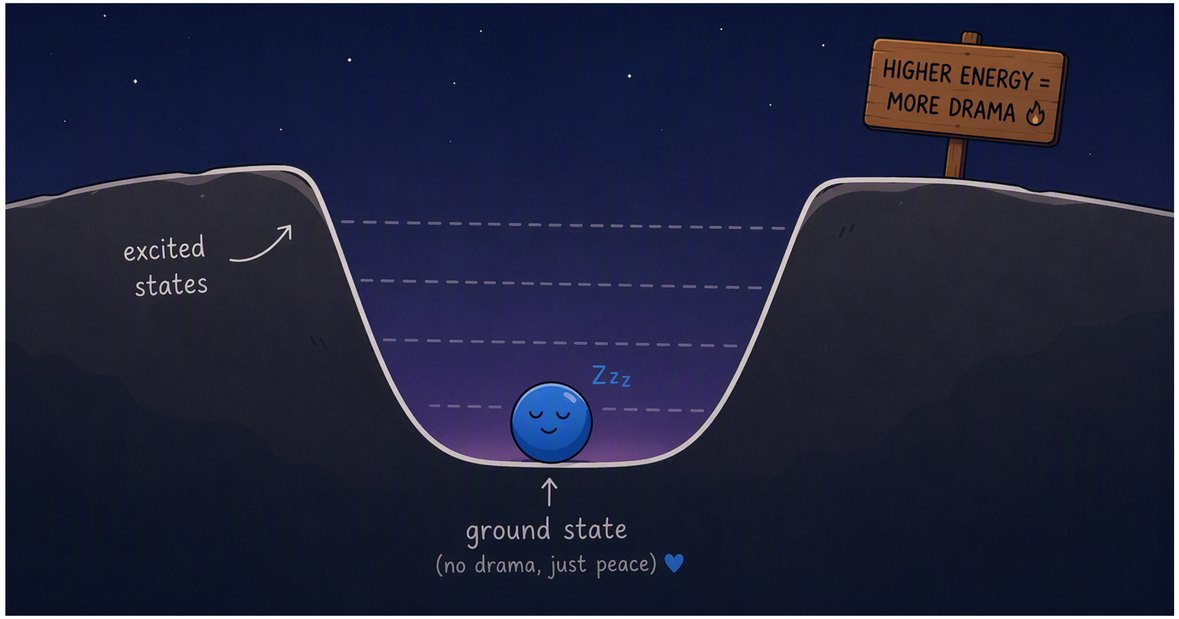
Variational Quantum Eigensolver

Adiabatic State Preparation

…and endless variations, extensions, and other approaches

Commonly touted as the first useful application of quantum computers…

And yet…



Quantum advantage

Quantum algorithm that verifiably outperforms all known classical methods in:

accuracy,

runtime,

or energy usage/cost

- We have seen early examples of plausible quantum advantage for dynamics tasks
- **We have not yet seen it for ground state energies**

Motivating question: what is a constructive path towards quantum advantage for ground state energy?

Quantum advantage

Scaling advantage

Is there evidence for exponential quantum advantage in quantum chemistry?

Seunghoon Lee[1], Joonho Lee[2], Huanchen Zhai[1], Yu Tong[3], Alexander M. Dalzell[4], Ashutosh Kumar[5,9], Phillip Helms[1], Johnnie Gray[1], Zhi-Hao Cui[1], Wen-Yuan Liu[1], Michael Kastoryano[4,6], Ryan Babbush[7], John Preskill[10,4], David R. Reichman[2], Earl T. Campbell[11], Edward F. Valeev[5], Lin Lin[3,8], and Garnet Kin-Lic Chan *[1]

https://arxiv.org/pdf/2208.02199

vs

Advantage in practice

Can we identify a slice of *problem instances* where quantum algorithms outperform classical **in practice**?

Sample-based quantum diagonalization algorithms

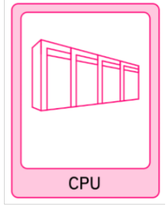
1. Given $2^n \times 2^n$ Hamiltonian ground state problem…

2. Sample configs from quantum circuit(s)

↓

3. Project Hamiltonian onto config basis

4. Diagonalize projected Hamiltonian



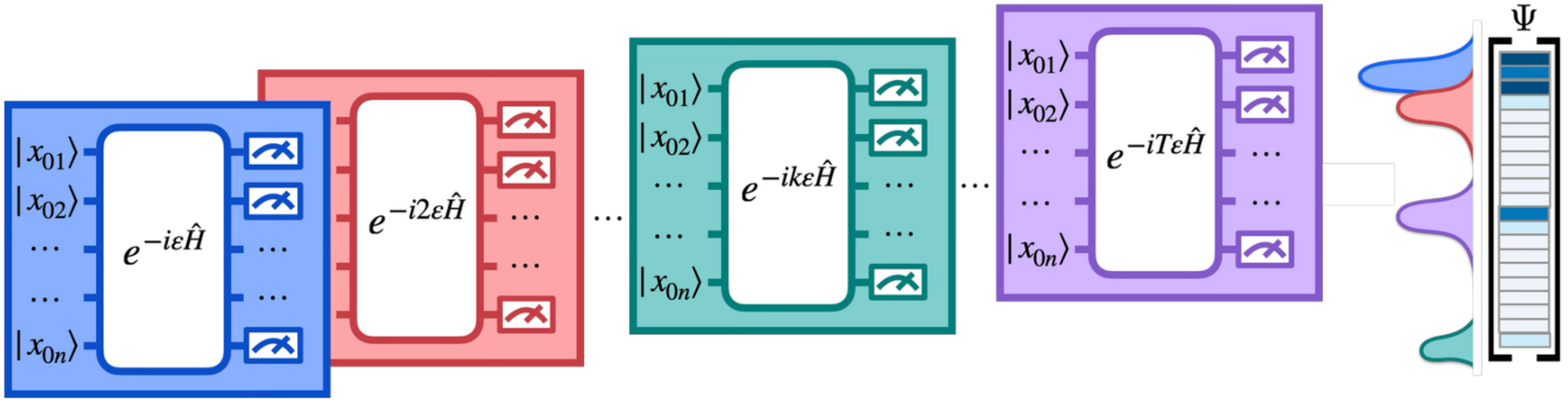
- Require approximately sparse ground state
- Offer variational, classically-verifiable energies

⇓

Potential for verifiable quantum advantage

First proposed in QSCI: https://arxiv.org/abs/2302.11320

Sample-based Krylov Quantum Diagonalization (SKQD)



Overlap of reference state with ground state: $1/\text{poly}(n)$

Spectral gap: $1/\text{poly}(n)$

Ground state approximately sparse

Guided sparse ground state problem

Ground state converges efficiently with # circuits and shots

arxiv:2501.09702

Approximate sparsity

Approximate sparsity required for SKQD to converge: for $|\psi_{\text{g.s.}}\rangle = \sum_i c_i |x_i\rangle$ with comp. basis $|x_i\rangle$ and

$$|c_0| \geq |c_1| \geq |c_2| \geq \cdots,$$

we require there to exist L, α, β such that

$$\sum_{i=0}^{L-1} |c_i|^2 \geq \alpha \text{ and } |c_i|^2 \geq \beta \quad \forall i < L$$

- L should be poly(n)
- $1 - \alpha \ll 1$ controls the energy error
- $\beta \geq 1/\text{poly}(n)$ controls the success probability (to find all L "good configurations")

From here on, we focus on exact sparsity: $|c_i| = 0 \quad \forall i \geq L$

Sparsity and classical simulability

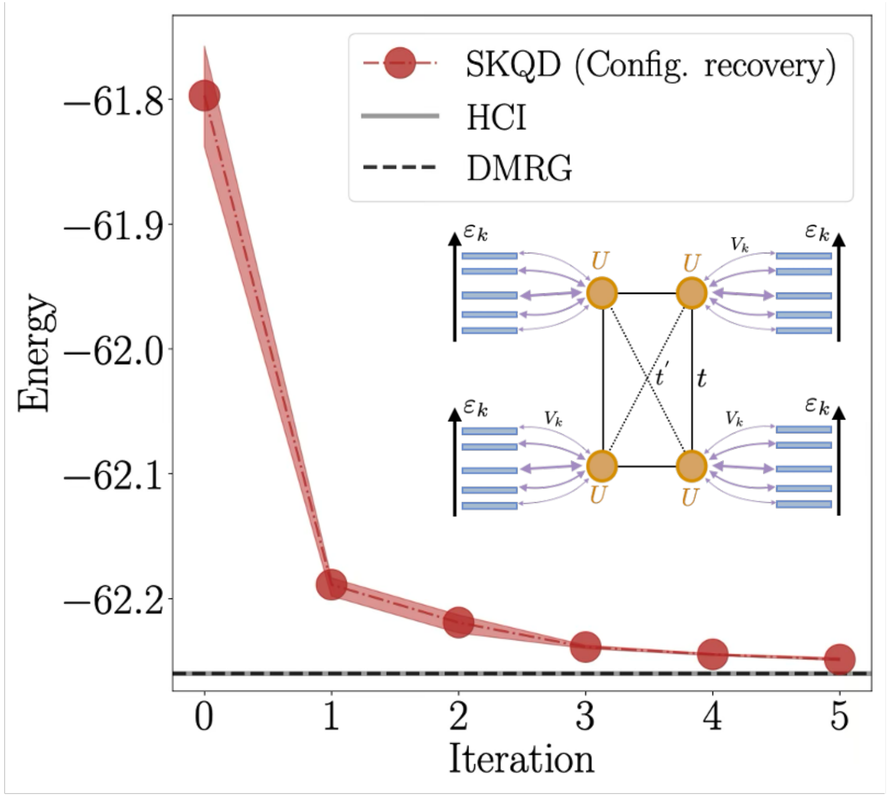
Two primary worries about sparse ground states:

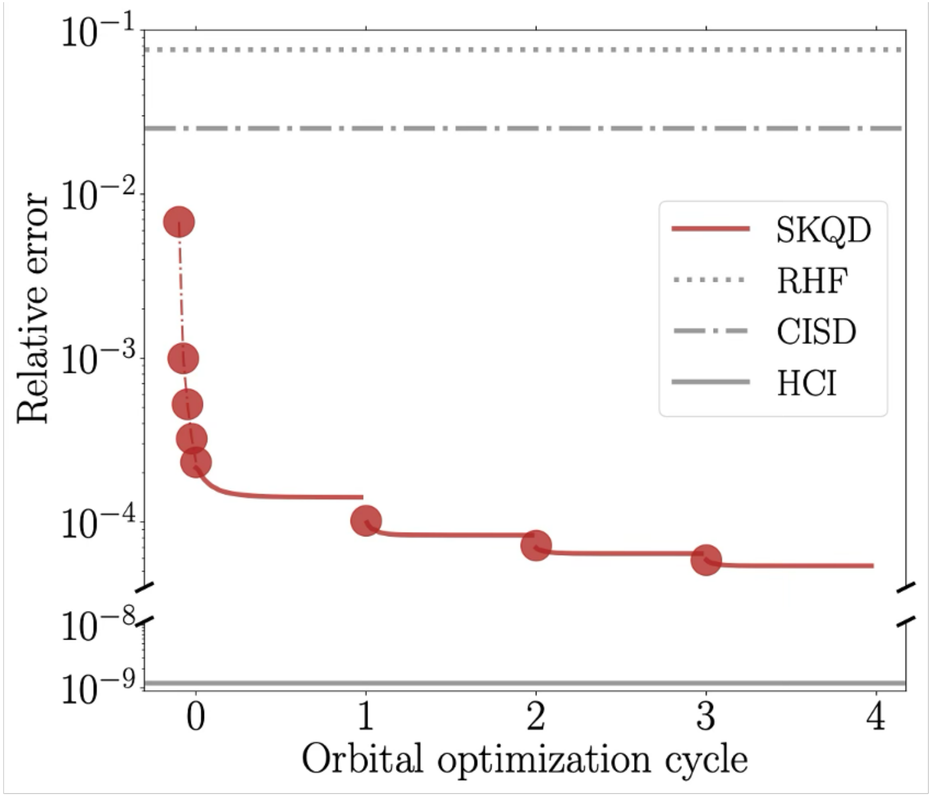
1. Guided sparse ground state problem (*with sparse initial state) is classically efficiently simulable
   - Algorithm is a truncated variant of power method [1]
   - Asymptotic total runtime scaling is identical to SKQD up to polylog factors
   - $\Rightarrow$ best we can hope for with SKQD* is speedup *in practice*

2. Many classical heuristics exist to produce sparse ground state approximations efficiently in practice
   - Selected configuration interaction heuristics
   - Truncated variant of Arnoldi's method
   - DMRG (MPS can represent sparse vector with bond dim'n = sparsity)

[1] arxiv:1112.2679

First experiments: impurity models





$\varepsilon \sim \text{Uniform}(-2,2)$
$t = -1$
$t' = -0.5$
$U = 10$
$V = 0.16$

Fact that SCI (HCI) converges indicates sparsity is perturbative

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

arxiv:2501.09702

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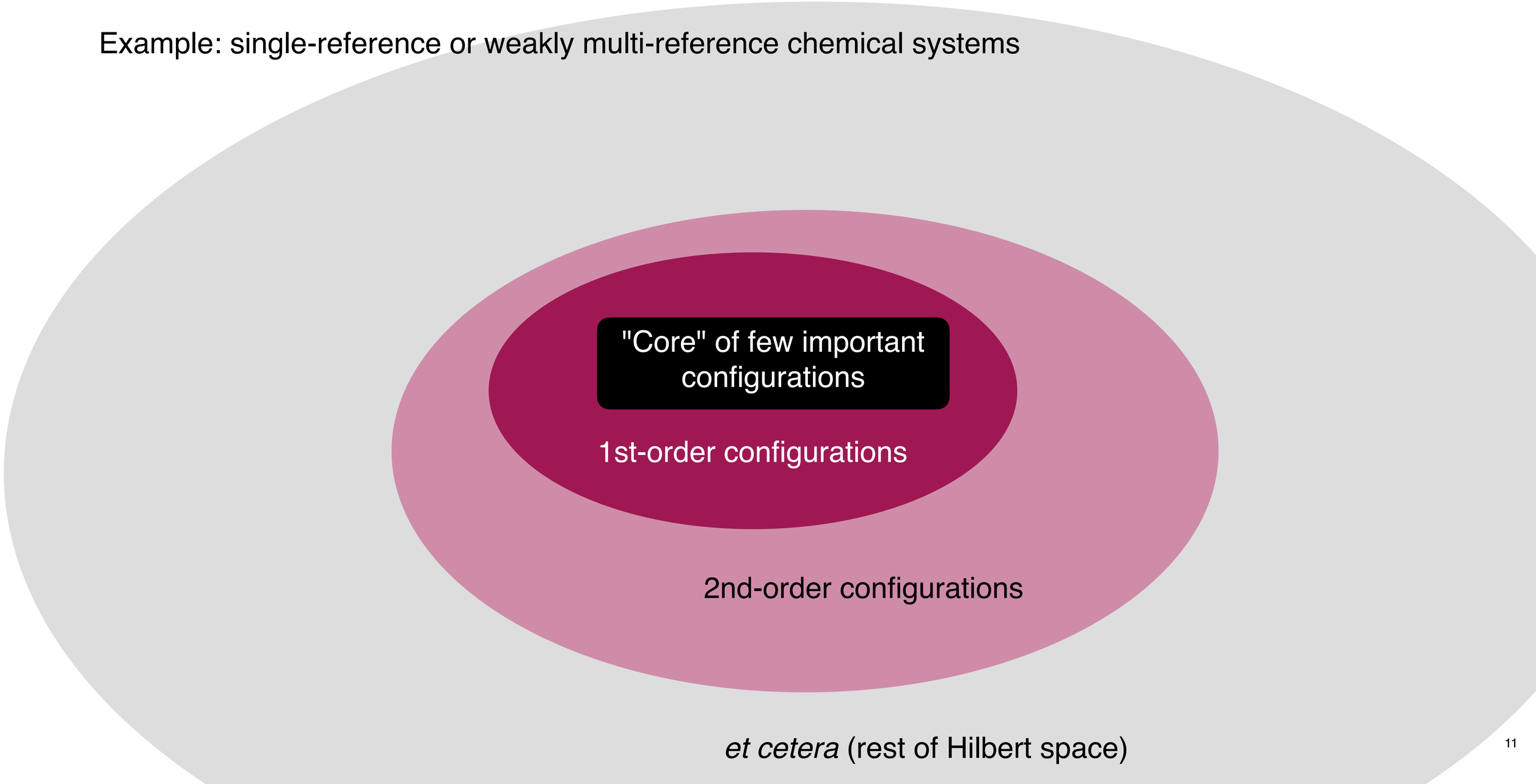
Cartoon: perturbative sparsity

Example: single-reference or weakly multi-reference chemical systems



Strategy

Design ground state problems to be “easy” for SKQD

and “hard” for classical methods

“Standard” approach

Choose challenging, interesting physics → Try to get quantum advantage

This project

Design ideal physics for quantum advantage → Work backward towards physical interest

Strategy

Design ground state problems to be “easy” for SKQD

and “hard” for classical methods

Build a family of Hamiltonians such that…

1. Conditions for guided sparse ground state problem hold:
   - sparse ground state
   - good initial state overlap (guiding state)
   - nonzero spectral gap (for finite sized instances)
2. Support of ground state is challenging to find by perturbation theory

Classical target for this phase

Selected configuration interaction (SCI)

1. **Input:** Hamiltonian H, initial configuration $|x_0\rangle$
2. $S \leftarrow \{|x_0\rangle\}$
3. $\Pi_S :=$ projector onto S
4. **For** $i = 1,2,...:$
5. Expand S to configurations connected by H
6. Truncate S according to cost function f_i
7. **Return** lowest eigenvalue of $\Pi_S H \Pi_S$

Example cost function (CIPSI/ASCI):

$$f_i(x) = \frac{\langle x|H|\psi_{\text{g.s.}}^{(i-1)}\rangle}{|\langle x|H|x\rangle - E_{\text{g.s.}}^{(i-1)}|}$$

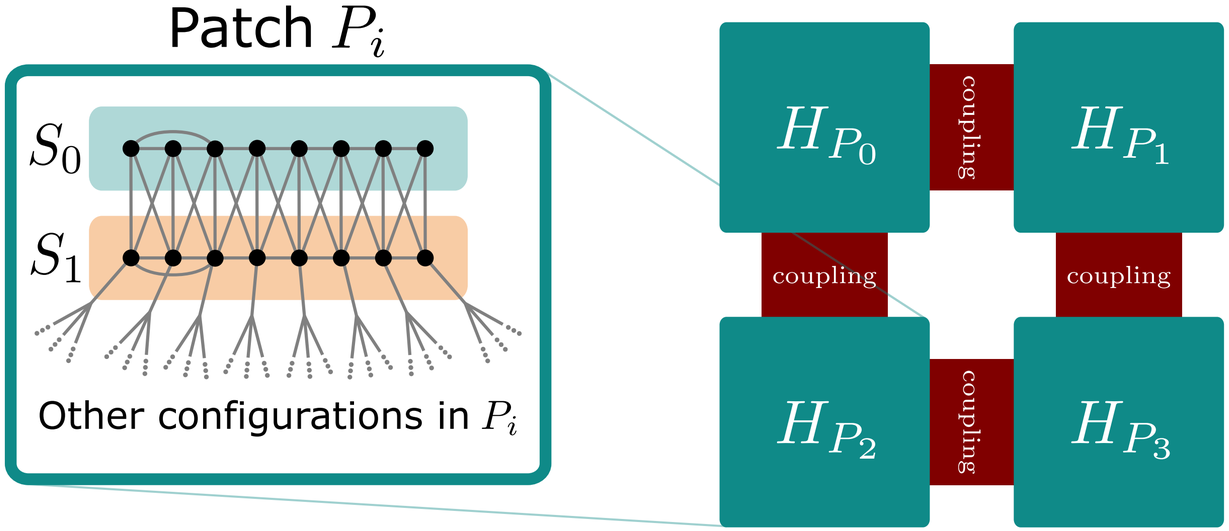
Truncation to k highest ranked or all above $\epsilon > 0$

Construction sketch

1. Partition qubits into equal-sized “patches”
2. Within patch, choose “path” S_0 of configurations
   - E.g. 10000000, 01000000, …, 00000001
3. Engineer interactions within S_0 such that

   SCI struggles to traverse path
4. Engineer outgoing interactions from S_0 such that

   lowest energy state of patch = lowest on S_0



Result:

(1) global ground state is product of patch ground states, each supported on S_0

(2) other eigenstates are entangled across patches

Construction: key component #1

$$H_{S_0} = \begin{pmatrix} a+\frac{1}{2} & 1 & b & 0 & 0 & 0 & 0 & 0 \\ 1 & a & c & 0 & 0 & 0 & 0 & 0 \\ b & c & a+2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & a+2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & a+1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & a+1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & a+1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & a \end{pmatrix},$$

$$a \approx 0.907,\ b \approx -0.788,\ c \approx -0.615$$

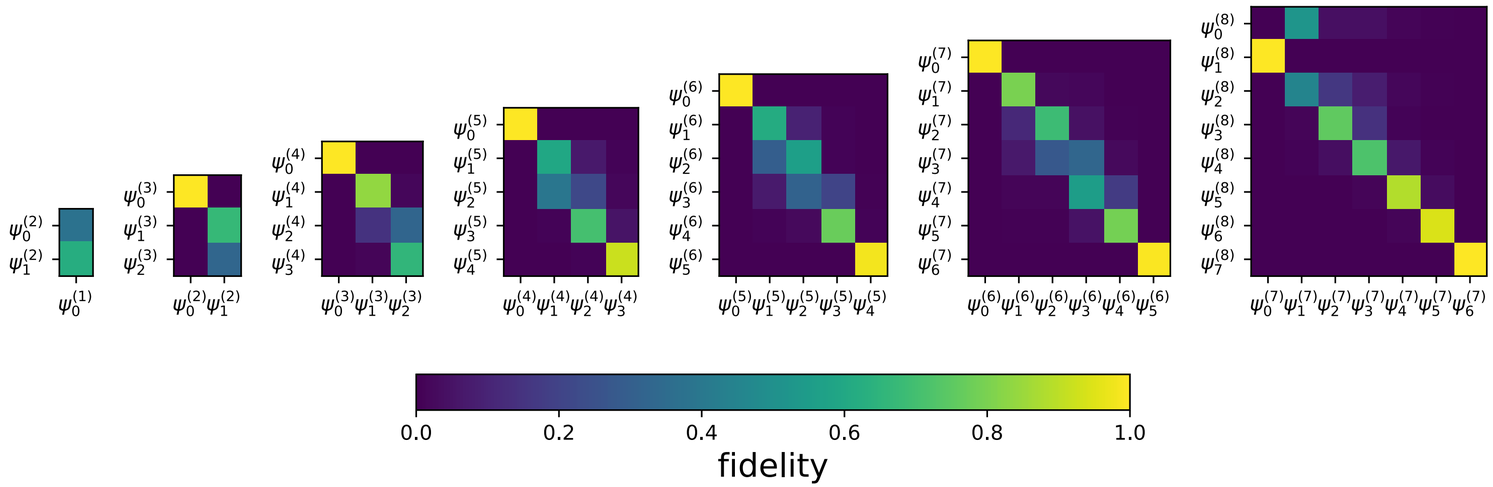
Let $\psi_i^{(j)}$ denote ith lowest eigenvector of $j \times j$ principal submatrix.

Key facts:

1. $\psi_0^{(j)}$ is supported on first two entries for $j = 2,...,7$
2. $\Rightarrow \langle j | H_{S_0} | \psi_0^{(j)} \rangle = 0$ for $j = 2,...,7$
3. $\psi_0^{(8)}$ (g.s. of H_{S_0}) is supported everywhere

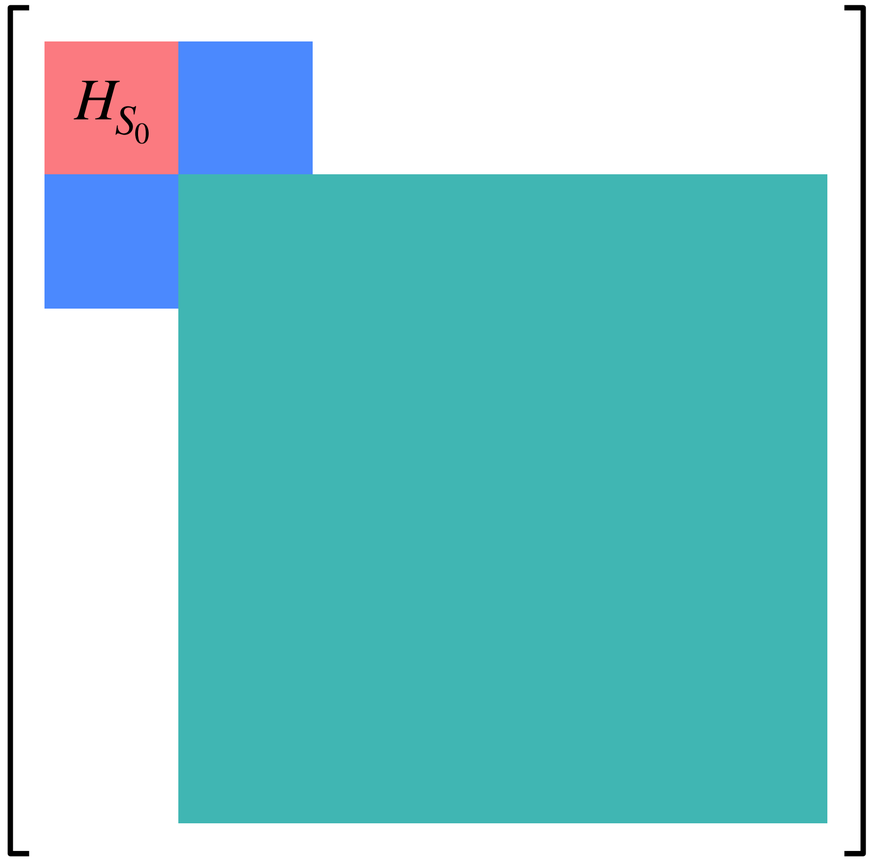
Recall: CIPSI cost function

$$f_i(x) = \frac{\langle x | H | \psi_{\text{g.s.}}^{(i-1)} \rangle}{|\langle x | H | x \rangle - E_{\text{g.s.}}^{(i-1)}|}$$



Construction: key component #2

$H_{\text{patch}} =$



Choose interactions such that

$\cdot\, |\psi_0^{(8)}\rangle = 0$

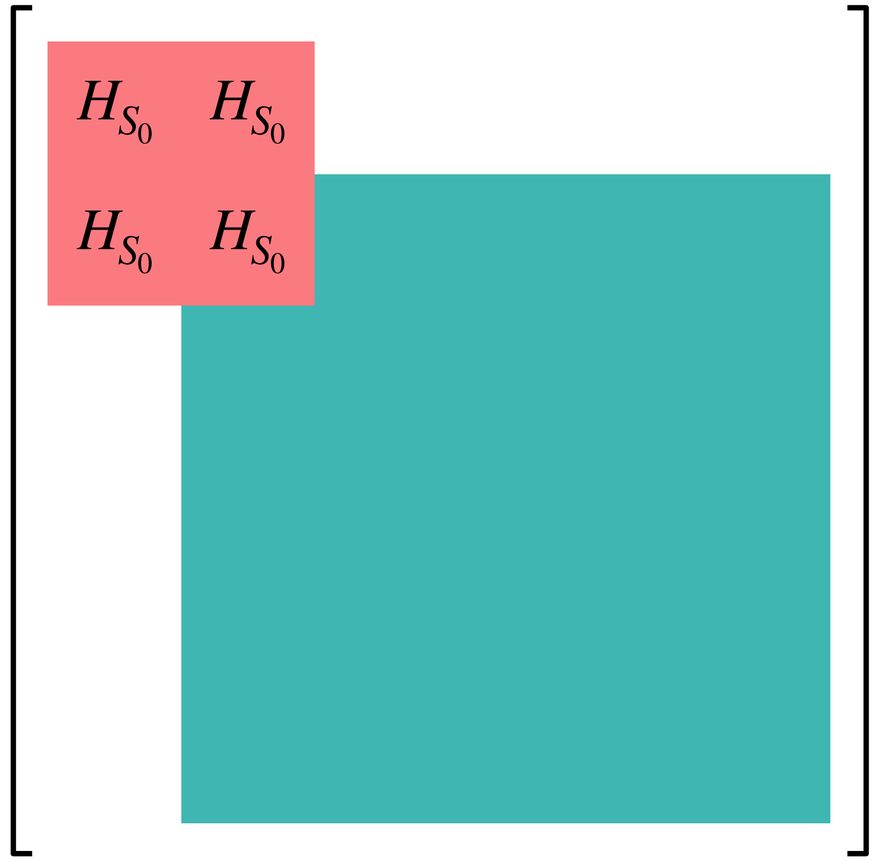
lowest eigenstate of H_{S_0}

$\Rightarrow |\psi_0^{(8)}\rangle$ padded with zeros is eigenstate of H

Choose remaining interactions (defining ) such that $|\psi_0^{(8)}\rangle$ has lowest energy

Construction: key component #2

$H_{\text{patch}} =$



Conveniently,

$$H_{S_0} \cdot |\psi_0^{(8)}\rangle = 0$$

lowest eigenstate of H_{S_0}

$\Rightarrow |\psi_0^{(8)}\rangle$ padded with zeros is eigenstate of H

Choose remaining interactions (defining ■) such that $|\psi_0^{(8)}\rangle$ has lowest energy

Construction: specifics

- "Support configurations" S_0 of patch ground state:

$$\underbrace{|1000000000000000\rangle}_{16 \text{ qubit path}}, |0010000000000000\rangle, \ldots, |0000000000000010\rangle$$

- Configurations S_1 coupled at first-order:

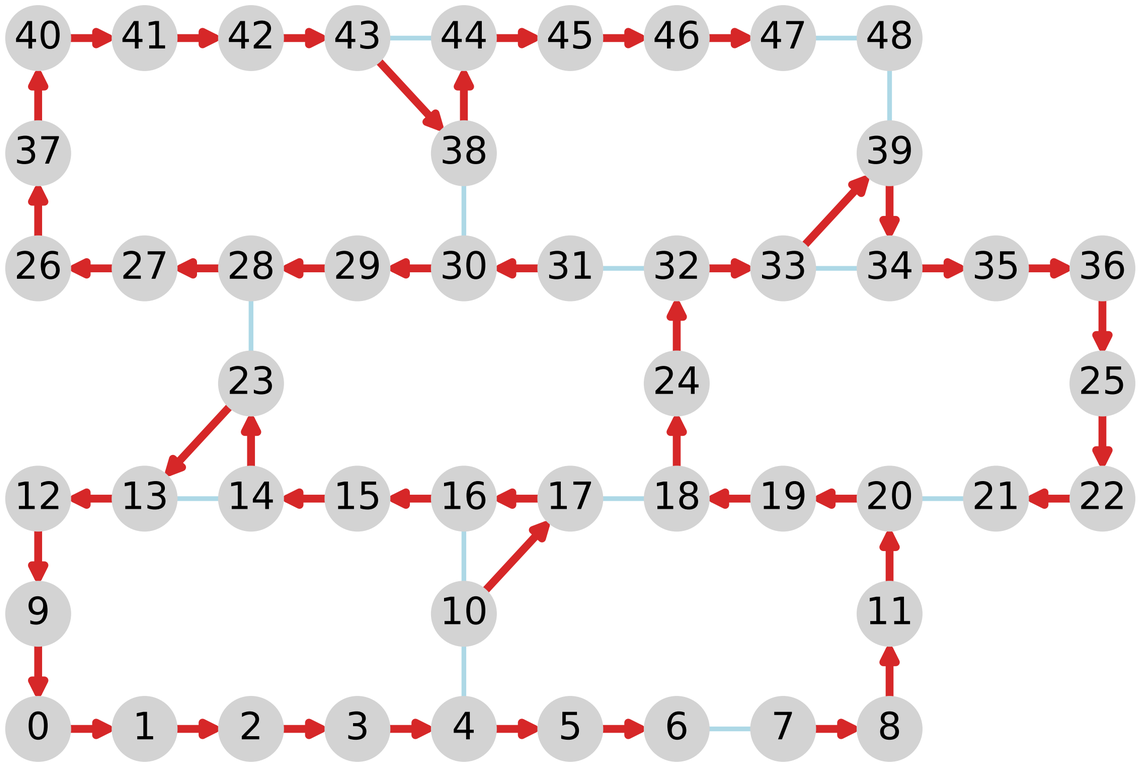
$$|0100000000000000\rangle, |0001000000000000\rangle, \ldots, |0000000000000001\rangle$$

$\Rightarrow$ $\begin{pmatrix} H_{S_0} & H_{S_0} \\ H_{S_0} & H_{S_0} \end{pmatrix}$ acting on $S_0 \cup S_1$ becomes local-ish along path (since H_{S_0} is nearly tridiagonal)

"controlled" on $|1\rangle$ in S_1

- Other configurations couple to S_1 via transitions like $|10\rangle \leftrightarrow |11\rangle$

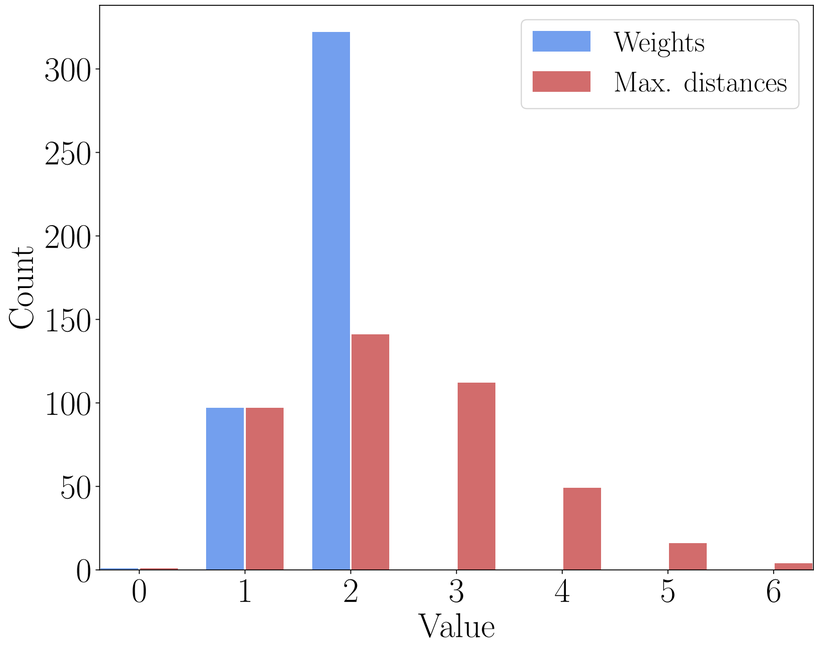
49Q experimental instance



3 patches ⇒ ground state sparsity $8^3 = 512$

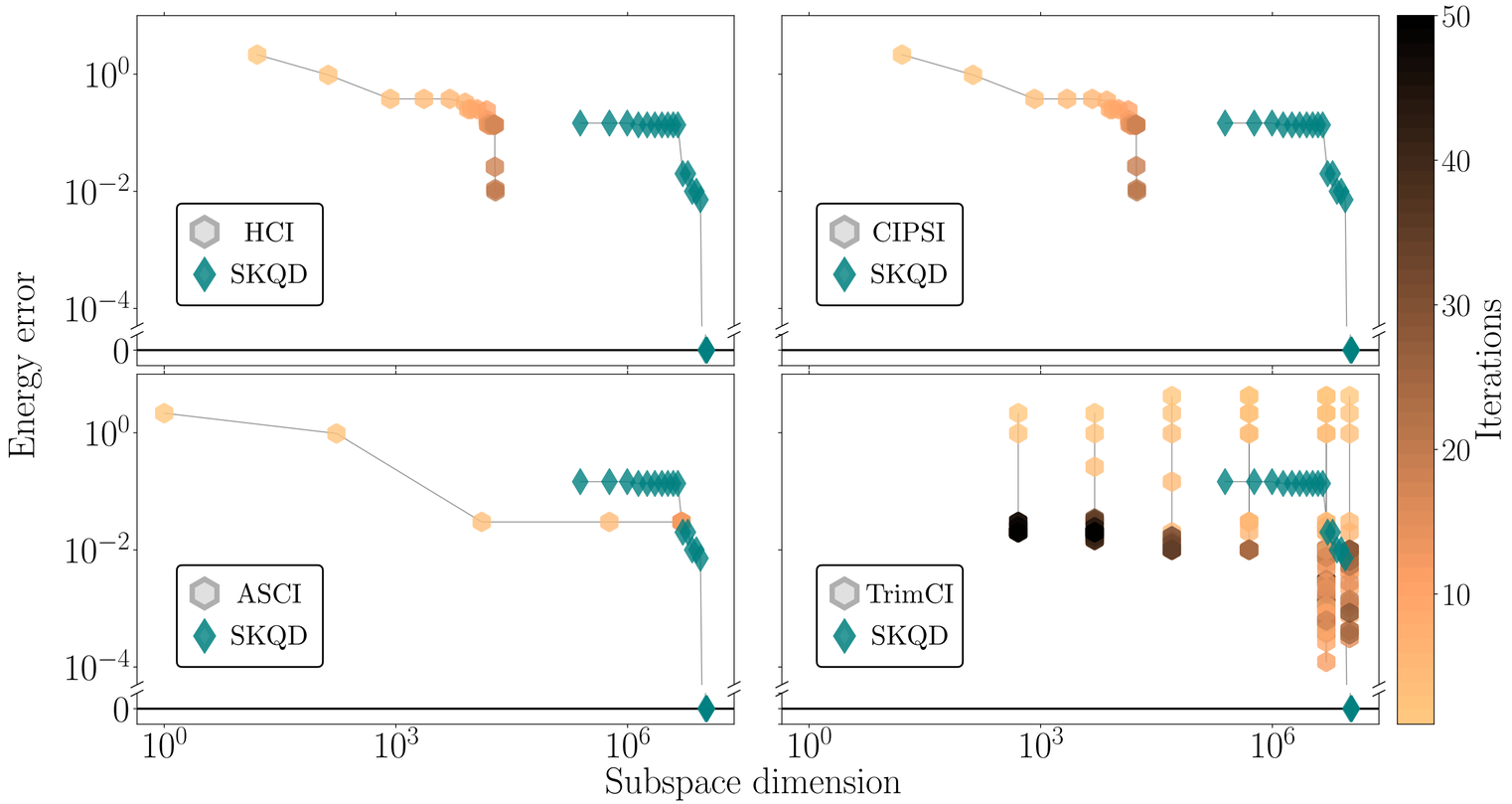
S_0 and configs coupled to S_0 at 1st-order are Hamming-wt-1, alternating along paths

Resulting 419 Pauli terms have weight ≤ 2 and distance ≤ 6

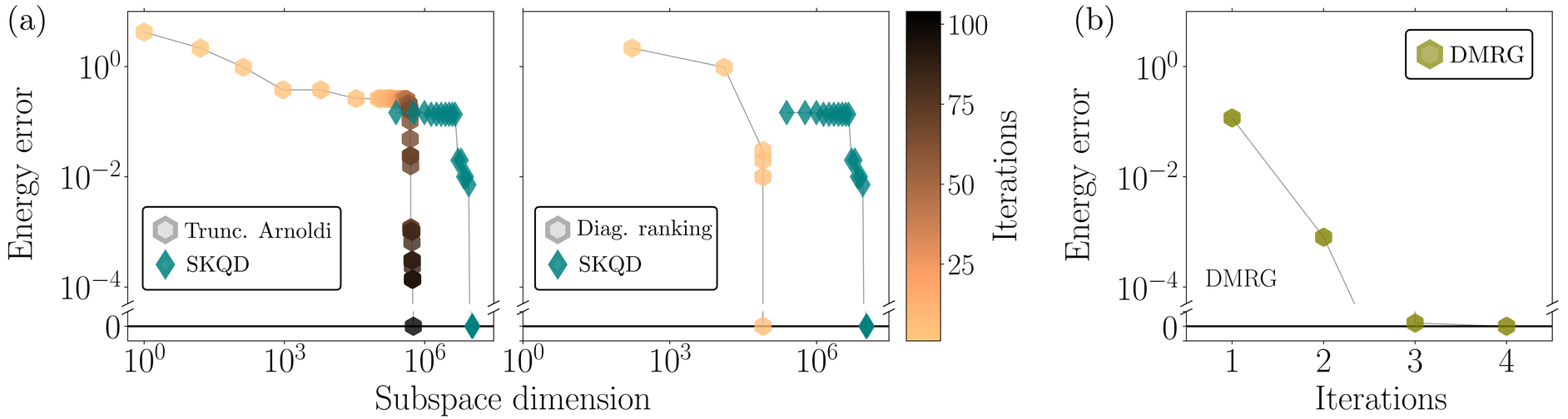


Experimental results: 49 qubit test

Quantum vs SCI methods:



vs other classical:



Experimental results: 49 qubit test

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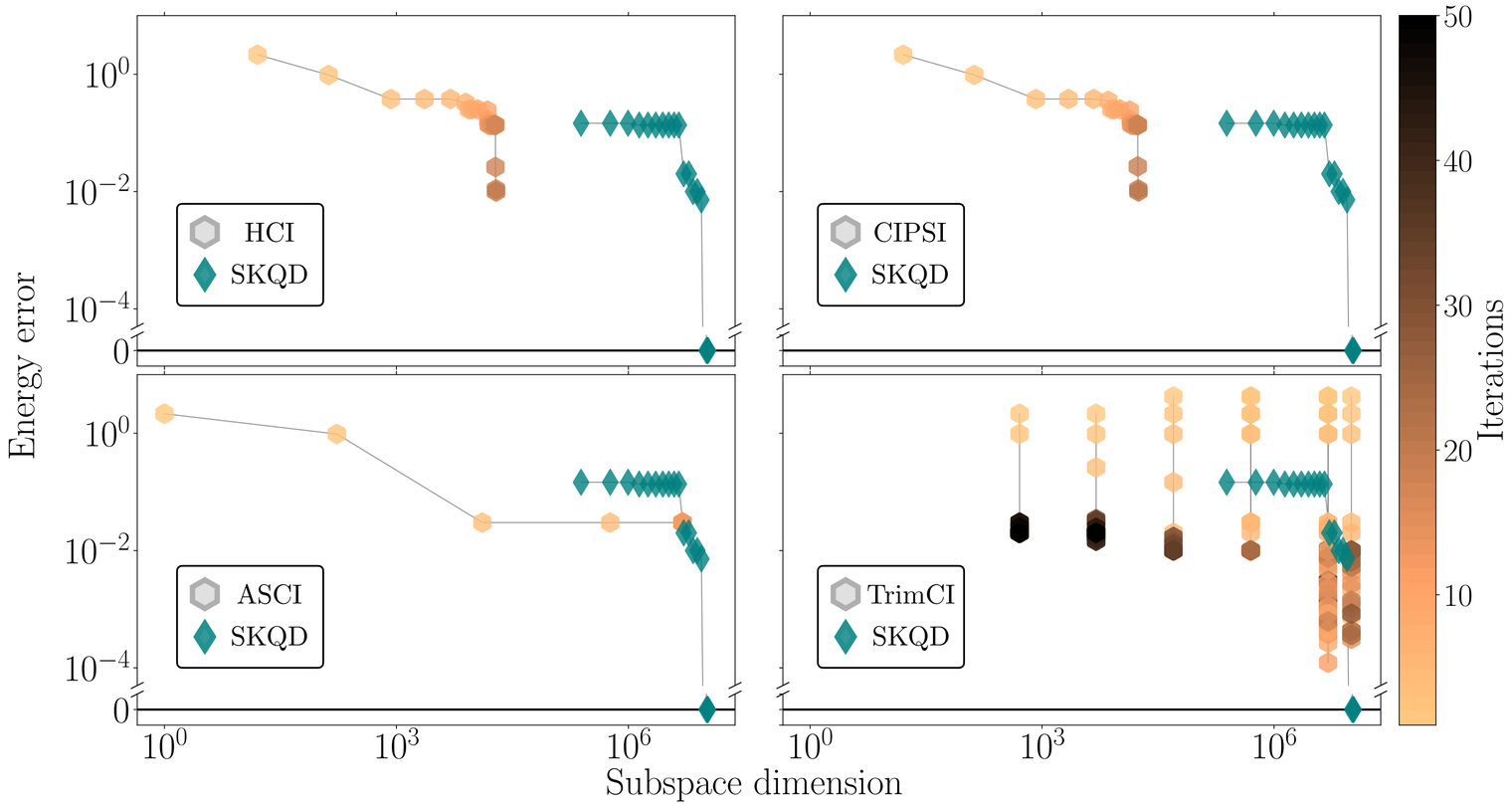
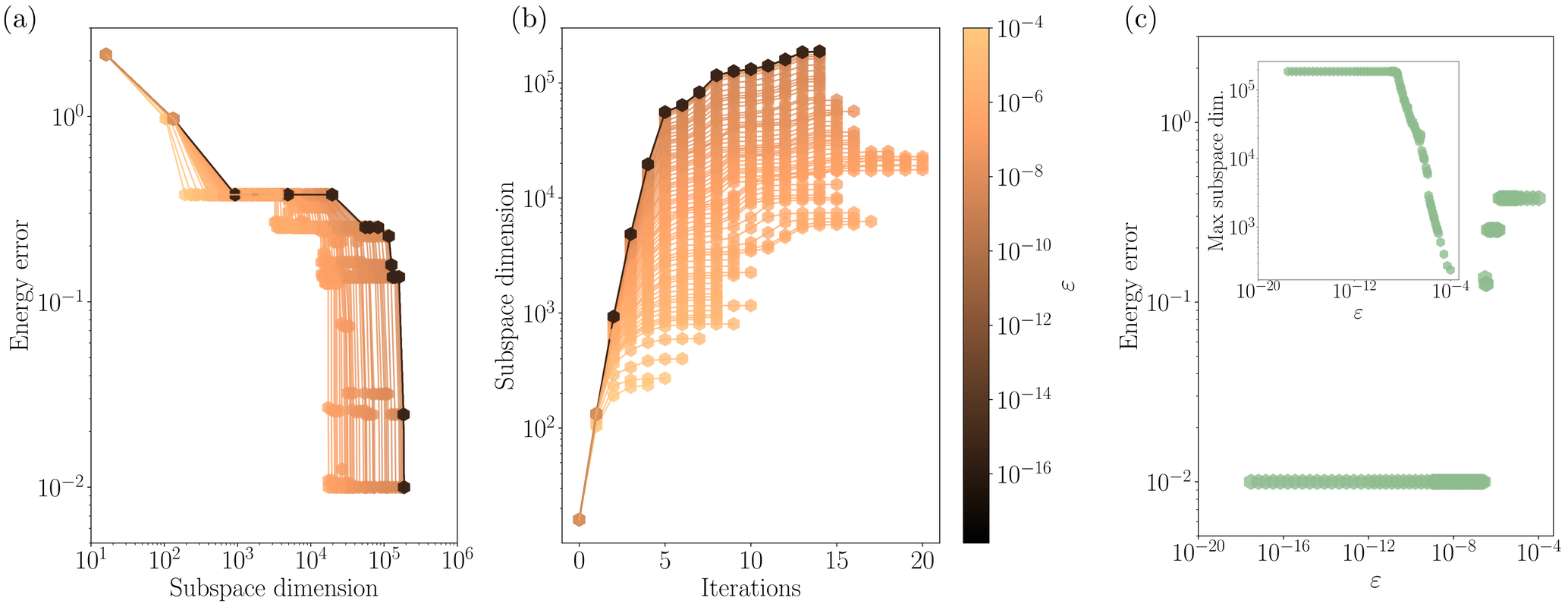


SKQD finds exact ground state, while SCI does not
⇒ advantage over SCI in accuracy

Example hyperparameter sweep - CIPSI, threshold ε

Observation: CIPSI and HCI can't reach as high *total dimension* as SKQD

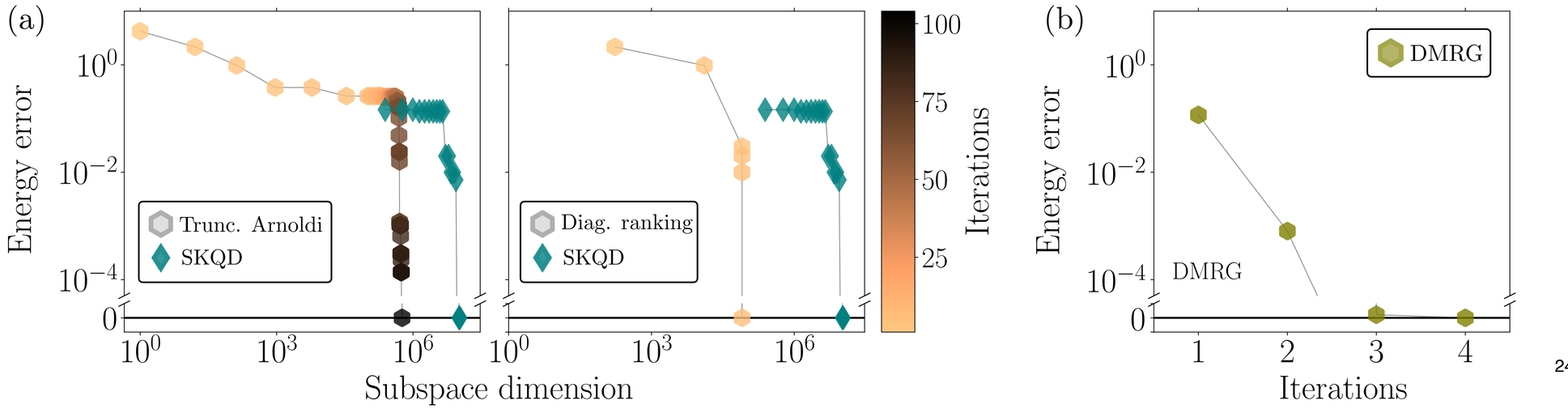


Recall: truncation condition is $f_i(x) = \dfrac{\langle x \,|\, H \,|\, \psi_{\text{g.s.}}^{(i-1)} \rangle}{|\, \langle x \,|\, H \,|\, x \rangle - E_{\text{g.s.}}^{(i-1)} \,|} \leq \varepsilon$

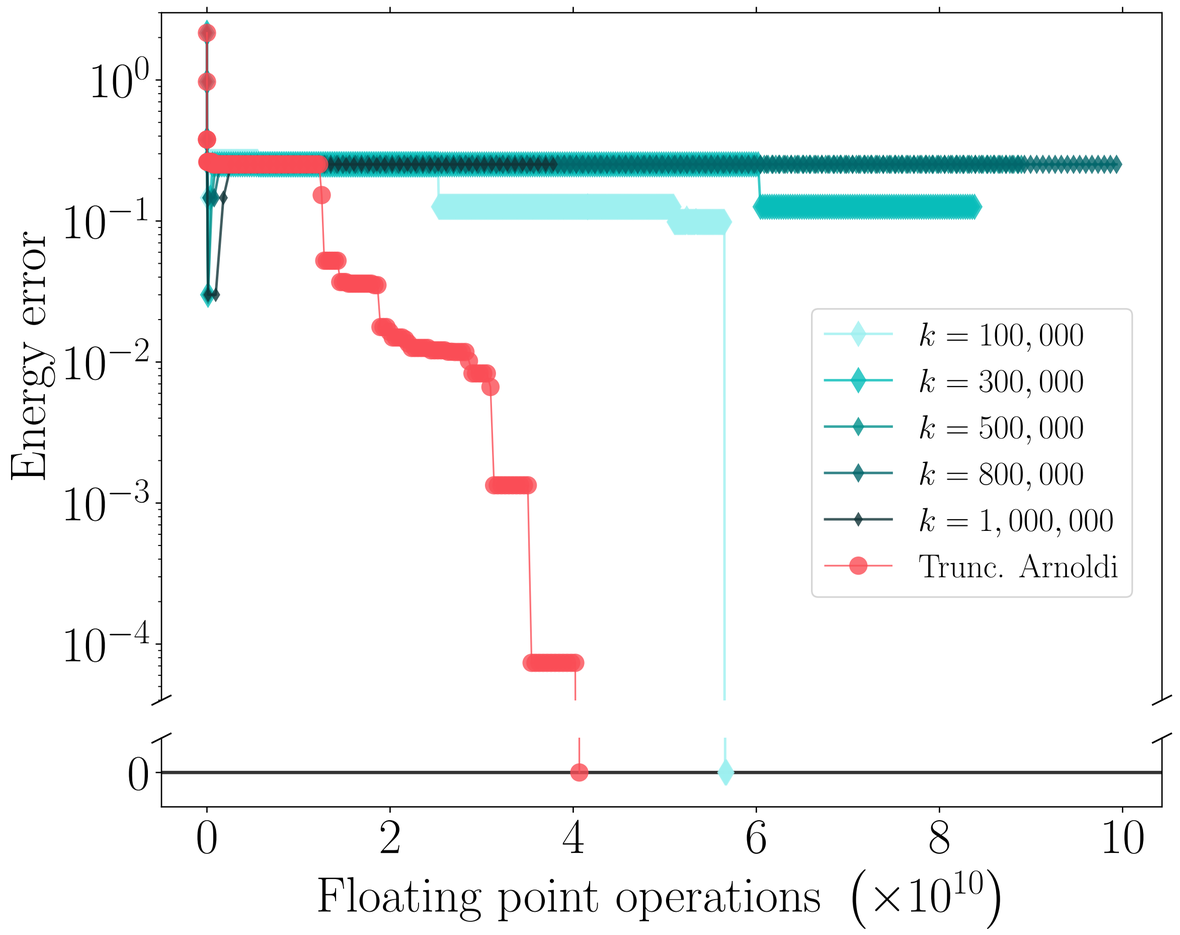
Experimental results:
49 qubit test

Not yet quantum advantage:
our “bespoke” iterative solvers + DMRG still win

vs other classical:



Recall: classical method with provable convergence



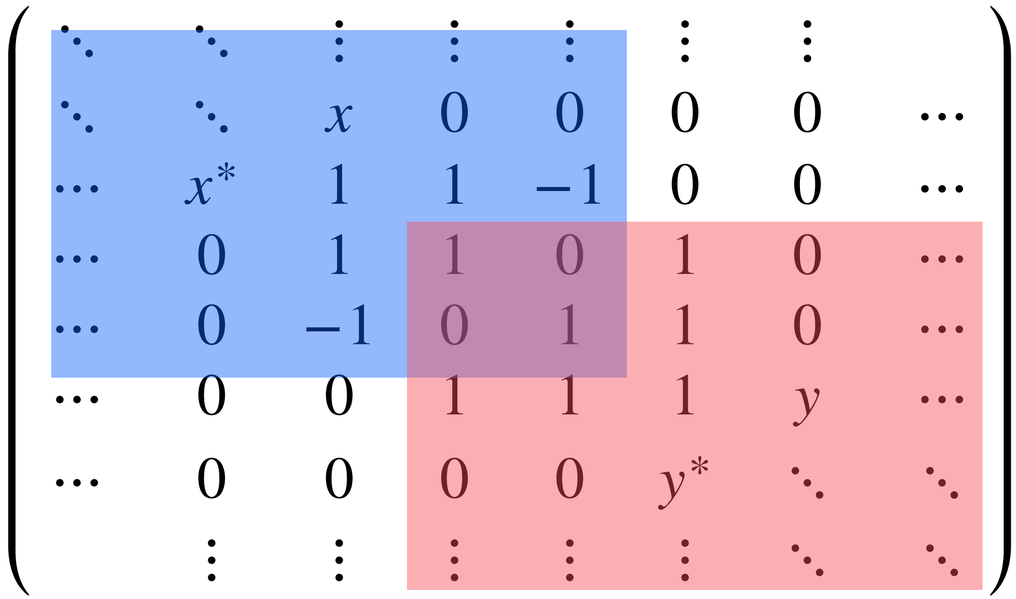
Truncated power method converges

- Polynomial dep. on all parameters
- Requires sufficiently large truncation cutoff k
- For our instance, this $k^* \sim 10^{23}$
- Not feasible, so we try smaller k as heuristic
- Not as performant as truncated Arnoldi's method

What have we learned, physically?

Key property to look for SCI hardness:

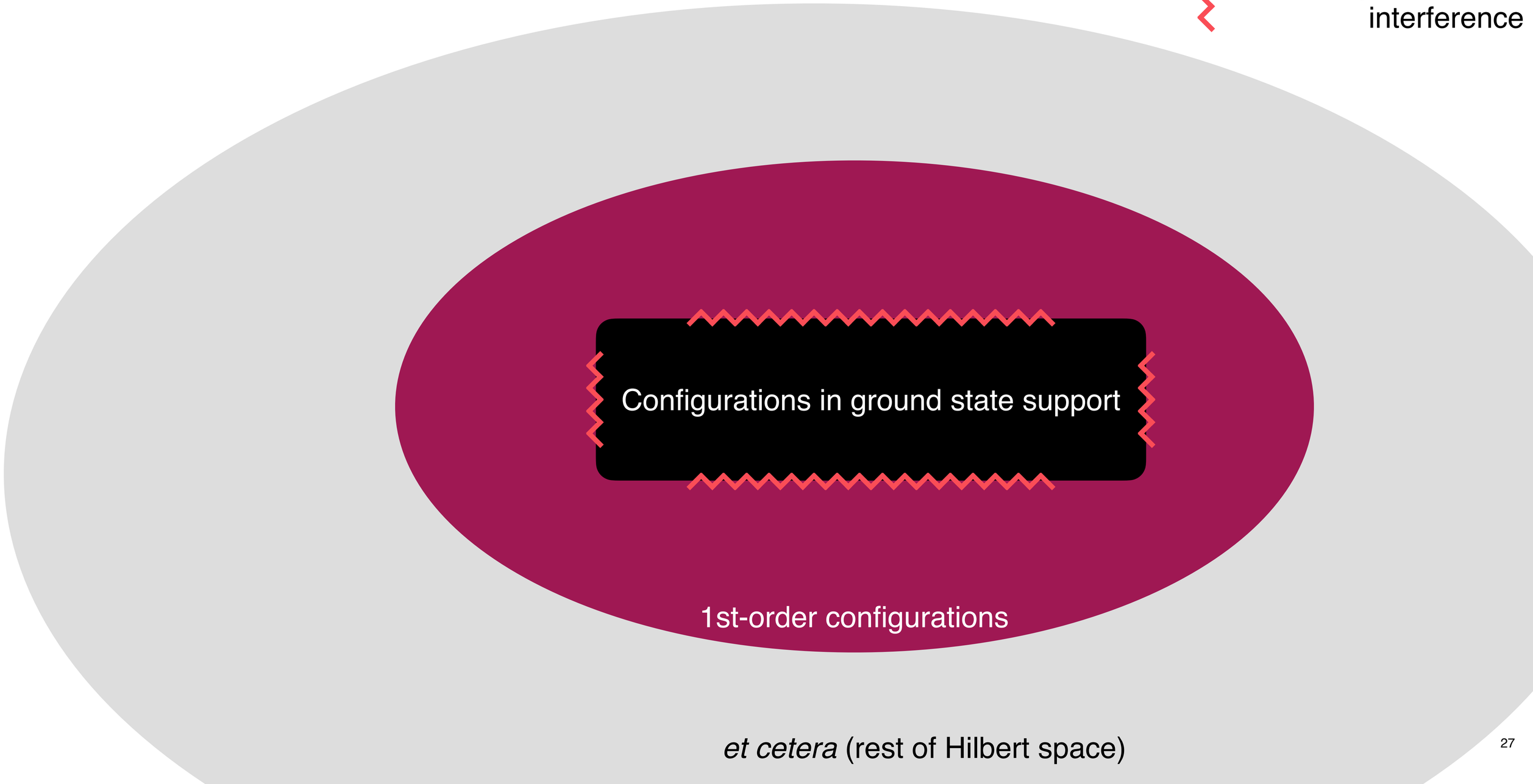
- Need support of ground state to be strongly sensitive to which subset of configurations we project on
- Concrete example:



- ∃ eigenvectors with support: everywhere, only in red, and only in blue
  - *Compact localized states with boundary destructive interference*
- Order of eigenvalues determined by exactly which rows and cols are included

Cartoon: non-perturbative sparsity

= boundary destructive interference



Conclusion

- Aim for practical speedups on finite-sized sparse ground state problems
- SCI solvers have previously matched or outperformed SKQD
- We construct problem instances where SKQD achieves higher accuracy
- Quantum advantage over other classical methods (esp. DMRG) remains the target

You can find the Hamiltonian and take a stab at it here!

https://quantum-advantage-tracker.github.io/trackers/variational-problems