Adaptive quantum simulation algorithms

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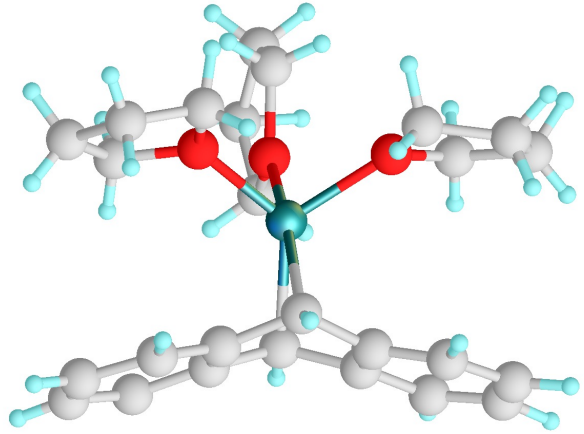
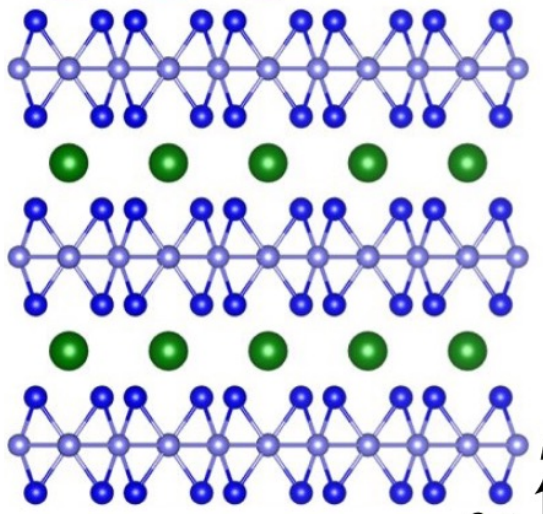
CQCWS3, IPAM, Nov. 6, 2023

Quantum simulation

- Predicting and designing properties of chemicals important for industry, medicine, agriculture, …
- Understanding/designing physical systems with interesting properties: superconductivity, …





The electrons in molecules and crystals behave quantum mechanically

→ The size of the space scales exponentially with the number of electrons

Quantum simulation

In general, representing n interacting two-level systems involves storing $2 * 2^n$ real numbers. Scaling is exponential.

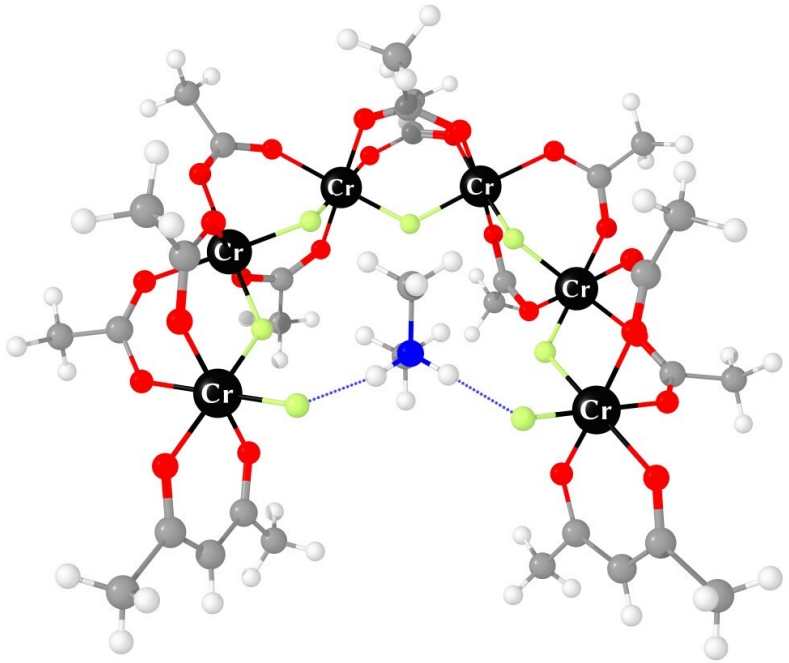
Even storing moderately-sized quantum states is infeasible with classical hardware

# of qubits	RAM required to store state
1	32 B
10	16 kiB
20	16 MiB
30	16 GiB
40	16 TiB
46	1 PiB

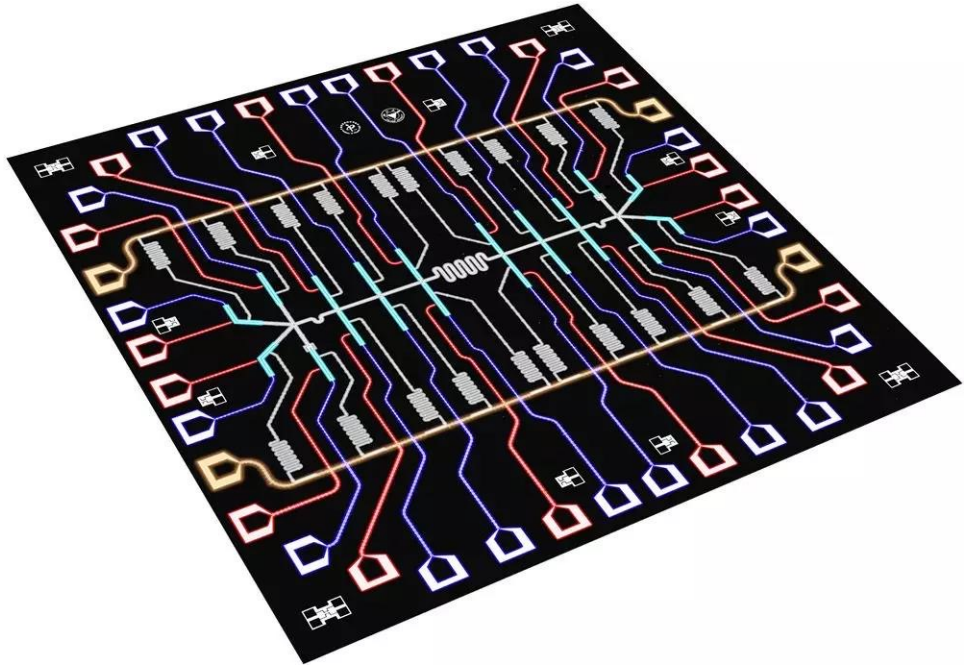
Use quantum systems that can be controlled to simulate other quantum systems

Digital simulation

System to be simulated



Quantum computer



Observable (Hamiltonian) in second quantized form

- Fermionic Hamiltonian $$H = -\sum_i \frac{\nabla_{r_i}^2}{2} - \sum_{i,j} \frac{Z_i}{|R_i - r_j|} + \sum_{i,j>i} \frac{Z_i Z_j}{|R_i - R_j|} + \sum_{i,j>i} \frac{1}{|r_i - r_j|}$$

- Second quantization (basis chosen, Coulomb integrals computed—*classical preprocessing step*)

$$\hat{H} = \sum_{i,j} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

- Wavefunction antisymmetric under exchange of two particles → fermionic operators satisfy anticommutation relations

$$\left\{\hat{a}_\alpha, \hat{a}_\beta\right\} = 0, \quad \left\{\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger\right\} = 0, \quad \left\{\hat{a}_\alpha, \hat{a}_\beta^\dagger\right\} = \delta_{\alpha,\beta}$$

In second quantization, the states correspond to occupation numbers of the spin-orbitals in the basis:

E.g. 1 electron in state $\phi_2(\vec{x})$, 1 electron in state $\phi_4(\vec{x})$

$$\frac{1}{\sqrt{2}}\left(\phi_2(\vec{x}_1)\phi_4(\vec{x}_2) - \phi_4(\vec{x}_1)\phi_2(\vec{x}_2)\right) \rightarrow |0,1,0,1,0,0,\ldots\rangle$$

A natural mapping to qubits: Jordan-Wigner

- We associate one qubit with each of our single-particle states

  Unoccupied $\rightarrow |0\rangle$, occupied $\rightarrow |1\rangle$

- Map creation/annihilation operators onto qubit raising/lowering operators, being careful to preserve anticommutation relations

$$a_i \rightarrow \prod_{j<i} Z_j \frac{1}{2}(X_i - i\,Y_i) \qquad a_i^\dagger \rightarrow \prod_{j<i} Z_j \frac{1}{2}(X_i + i\,Y_i)$$

Now, we can represent molecular electronic states/operators with states/operators on our quantum computer!

Review: Rev. Mod. Phys. **92**, 015003 (2020)

What is the objective of quantum simulation?

- Create the state of interest (often ground or low excited state)
- Measure properties (total energy, correlation functions, response to fields, …)
- Do this accurately and definitely better than classical approaches

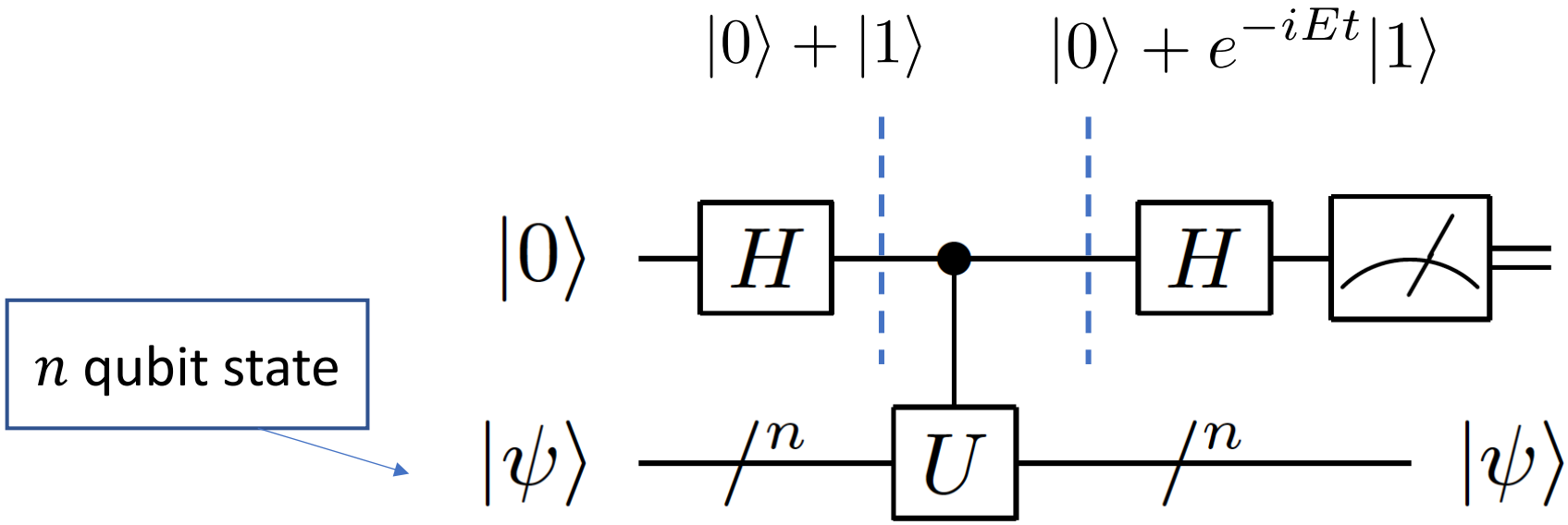
Analog vs digital simulation

- Analog quantum simulation
  - Create Hamiltonian of system on simulator
  - Simulator has tunable parameters, study various regimes
  - Limited by native interactions of simulator

- Digital quantum simulation
  - Evolution decomposed in elementary gates
  - Any problem can in principle be solved

Phase estimation algorithm

- Find eigenenergy of many-body state with $H_{tot} = H_a + H_b + \cdots + H_k$
- n qubits to encode eigenstate $|\Psi\rangle$ & ancilla qubits
- Conditionally apply time evolution $U = \ldots e^{-iH_{tot}t}$



- Conditional-U through Trotterization: $U = (e^{-iH_a t/N} e^{-iH_b t/N} \ldots e^{-iH_k t/N})^N$
- Exact for N→ ∞

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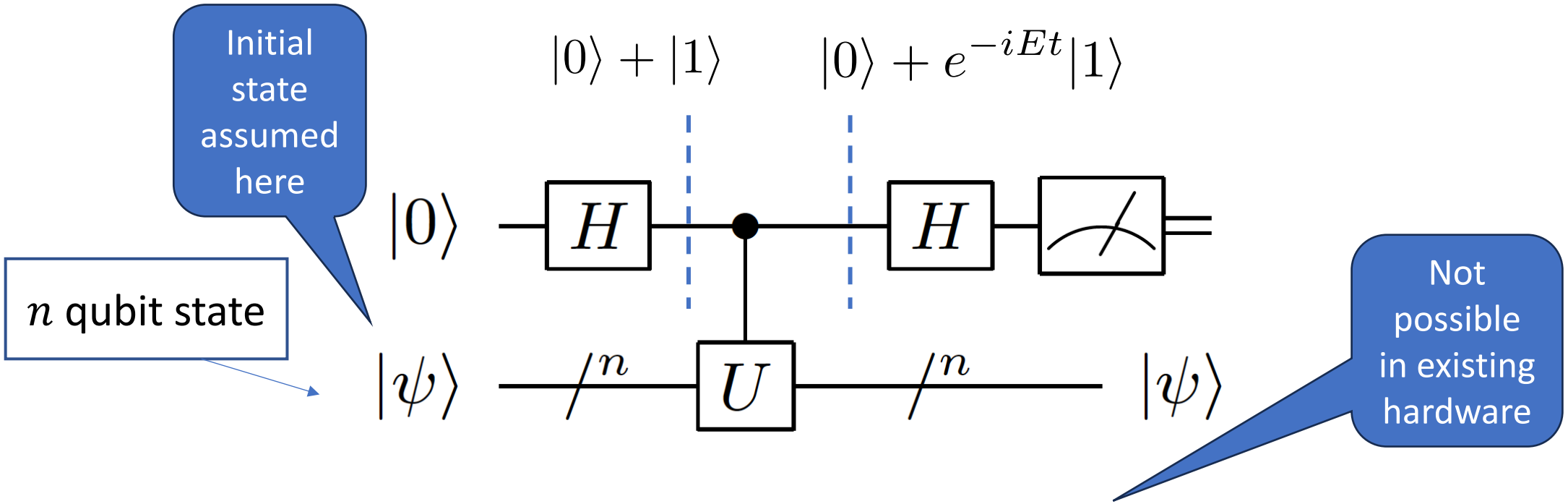

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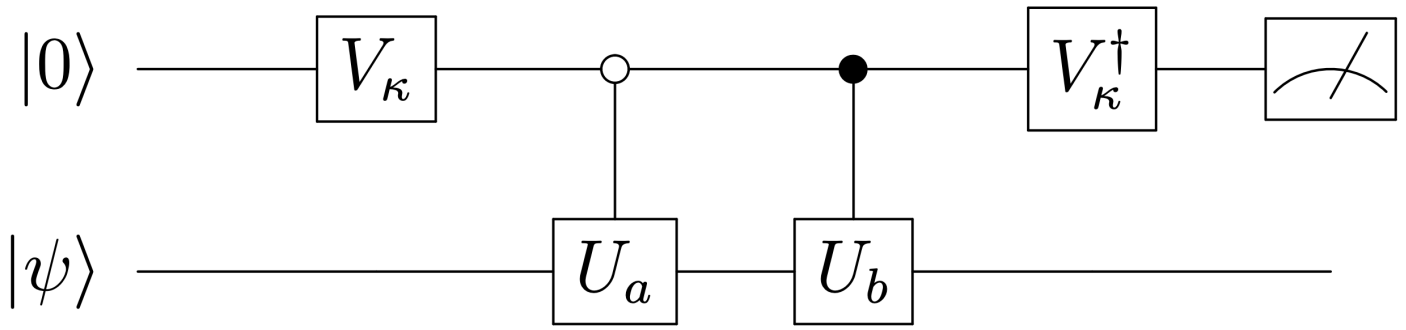
Linear combination of unitaries



Initial state assumed here too

Variational Quantum Eigensolver (VQE)

Variationally change $\vec{\theta}$

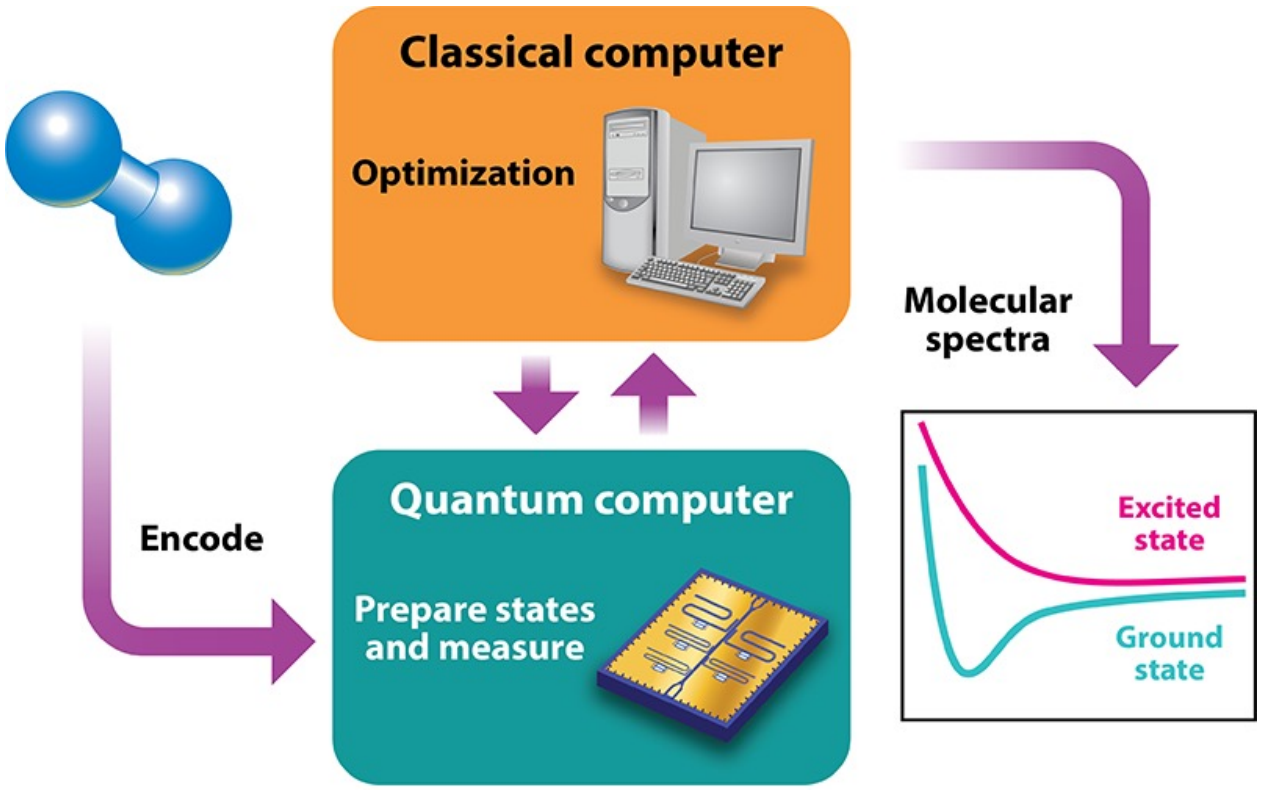
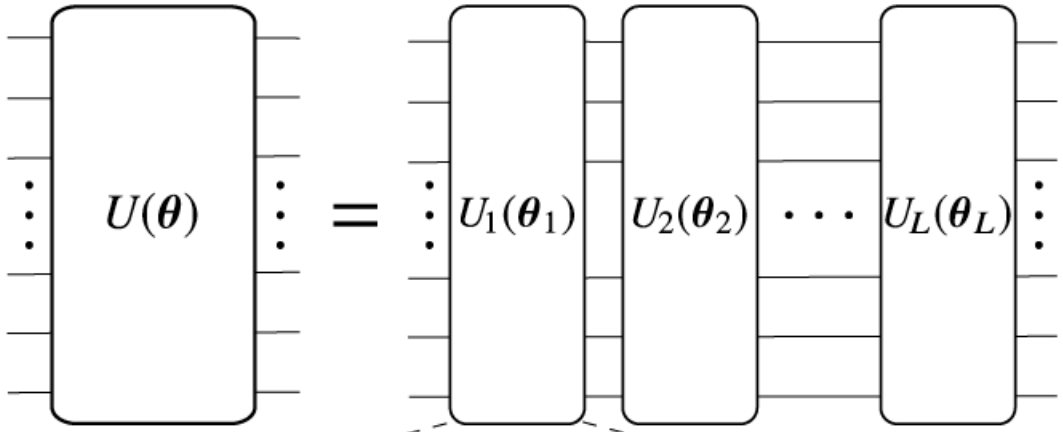


Image from Physics **11**, 14 (2018)

Ansatz $|\Psi(\vec{\theta})\rangle = U(\vec{\theta})|\Psi_{ref}\rangle$

Measured energy $E(\vec{\theta}) = \langle\Psi(\vec{\theta})|H|\Psi(\vec{\theta})\rangle$

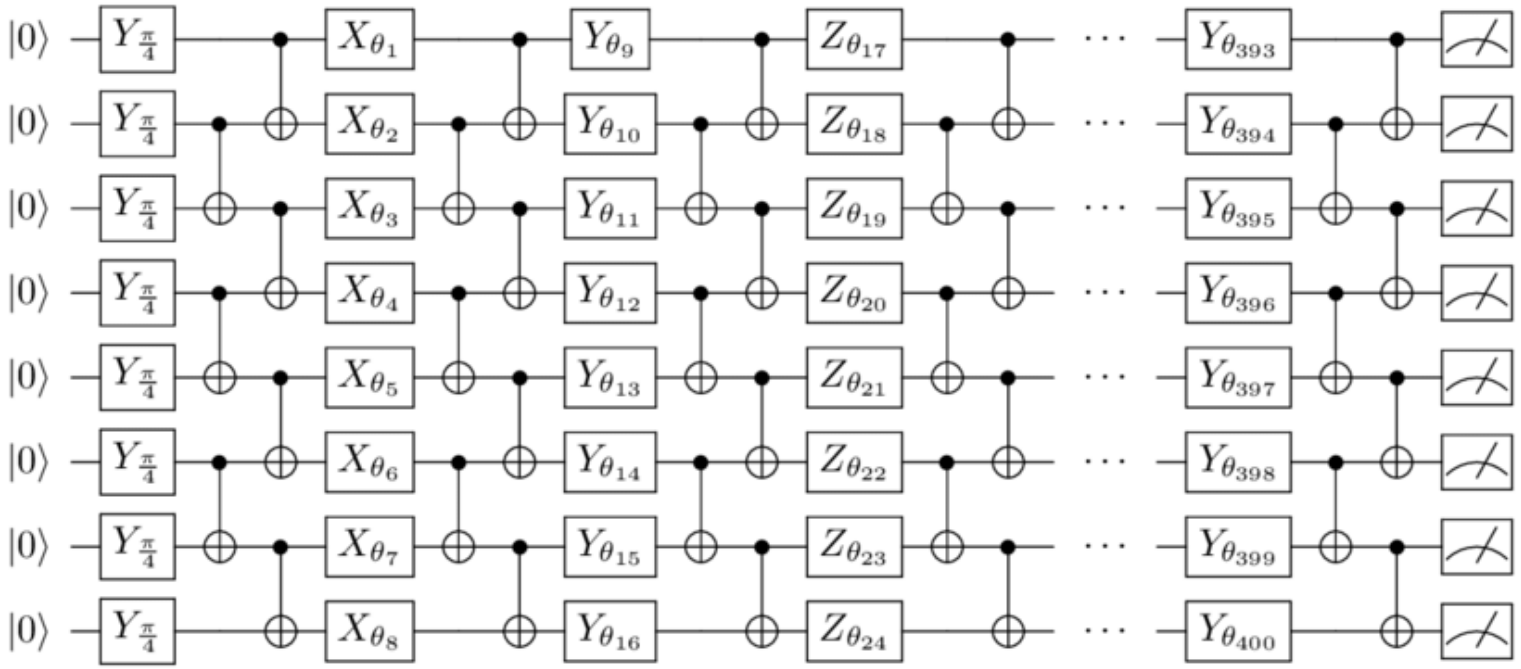
Parametrized circuit



Recent reviews:
Cerezo et al, Nat. Rev. Phys. 3, 625 (2021)
Bharti et al, RMP 94, 015004 (2022)
Tilly et al, arXiv:2111.05176

How do the parameterized circuits look?

- Generally, there is a lot of freedom in selecting the gates (unitary operators) that enter the circuit
- Example:



Outline

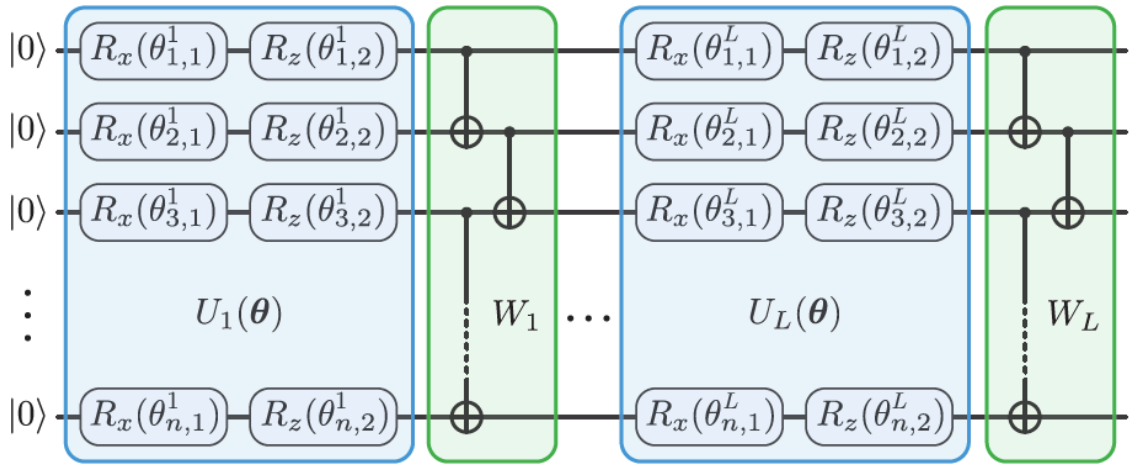
- Typical ansatze & issues
- Our approach: Adaptive quantum simulation
- Control-VQE: optimizing at the pulse level

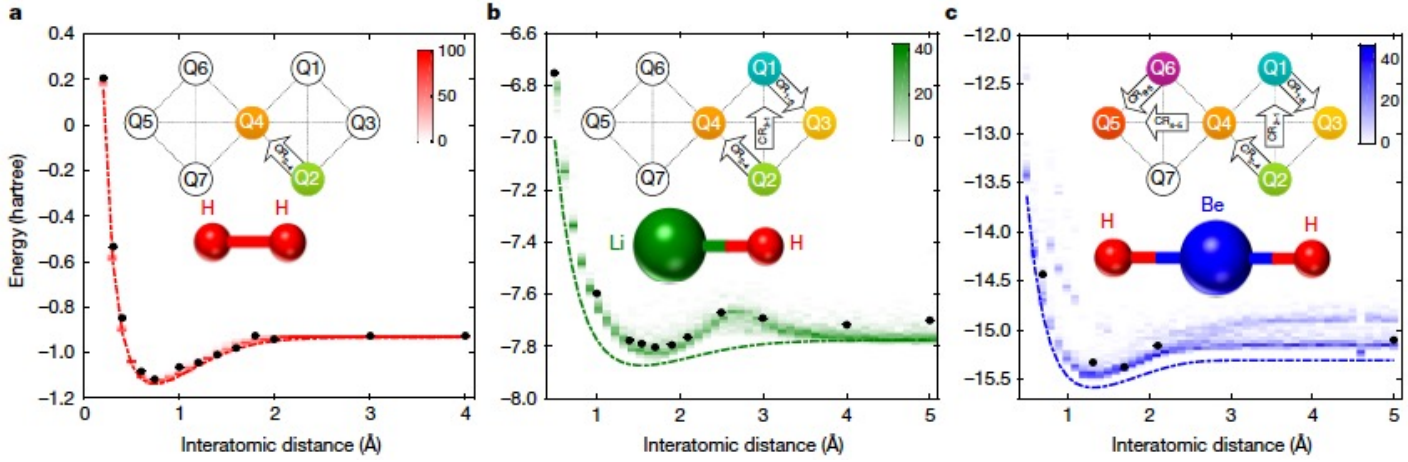
Most widely considered ansatze

I. Hardware-efficient ansatz

- Tailored to chosen platform
- Inefficient—too much of the Hilbert space sampled
- Difficult to optimize (barren plateaus)

McClean et al., Nat. Commun. 9, 4812 (2018)





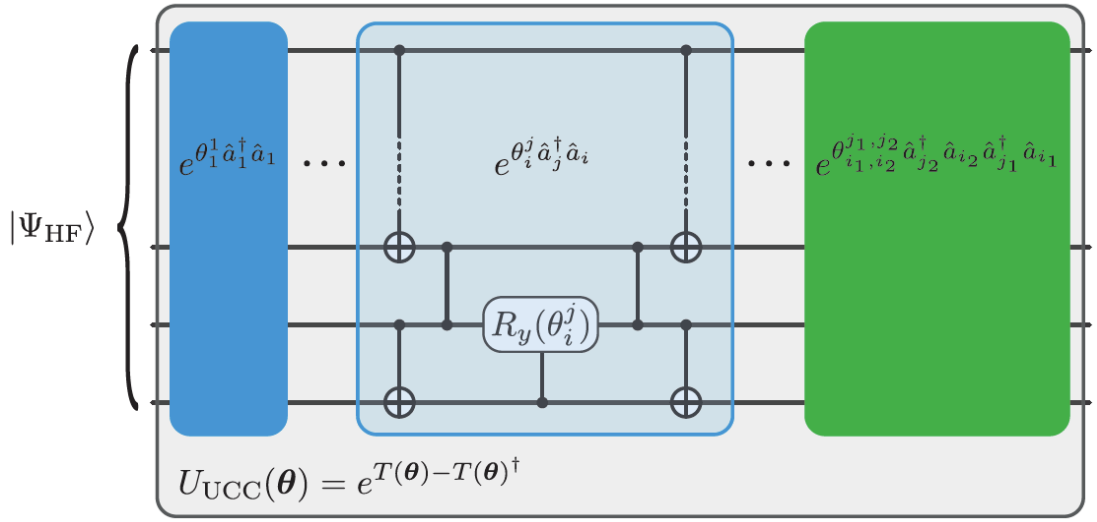
Kandala et al, Nature **549**, 242 (2017)

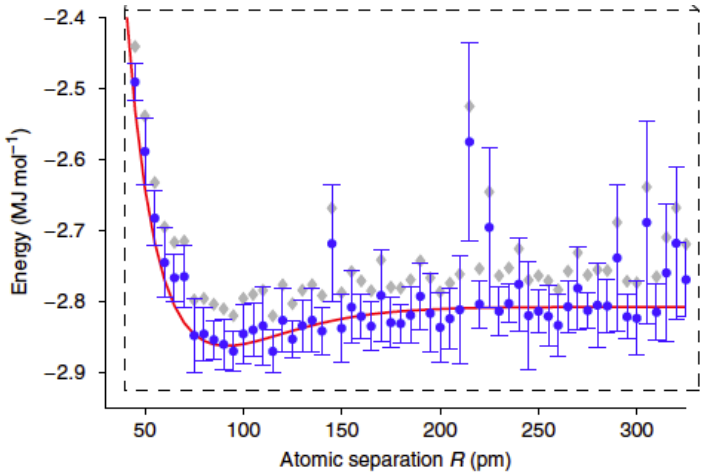
Most widely considered ansatze

II. Chemistry-inspired ansatz (UCC)

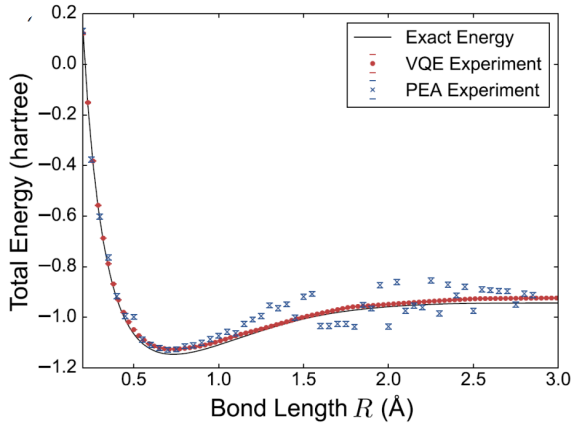
- Generalizes classical simulations
- Impractically long circuits
- Inconsistent under low-order Trotterization

Grimsley et al., JCTC 2020, 16, 1, 1-6

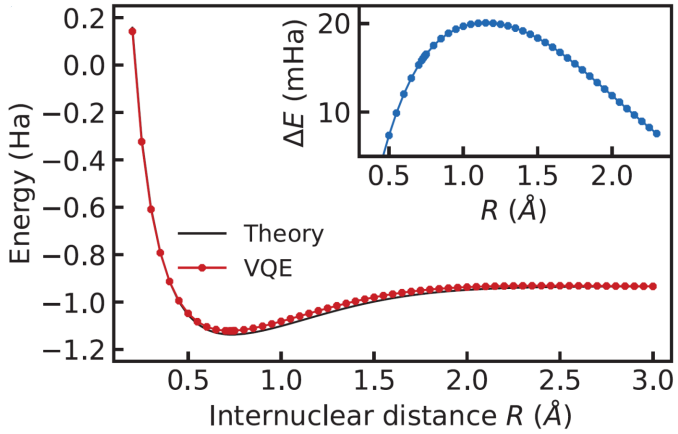




*Peruzzo et al, Nature Comm. **5**, 1 (2014)*



*O'Malley et al, PRX **6**, 031007 (2016)*



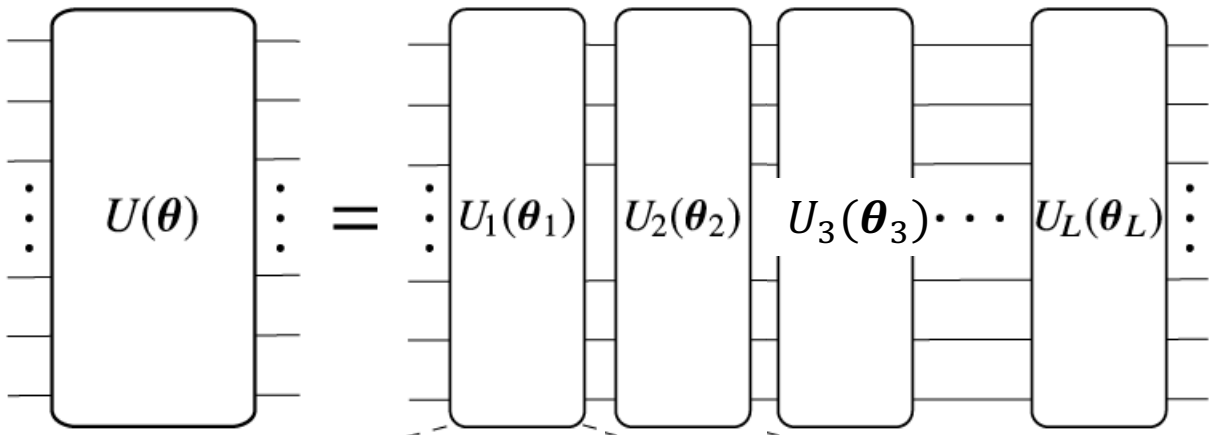
Xue et al, Nature 601, 343 (2022)

Most widely considered ansatze

- *Quantum-resource inefficient: long circuits*
- *Not problem-tailored*
- *Possible trainability issues*

Adaptive, problem-tailored VQE (ADAPT-VQE)

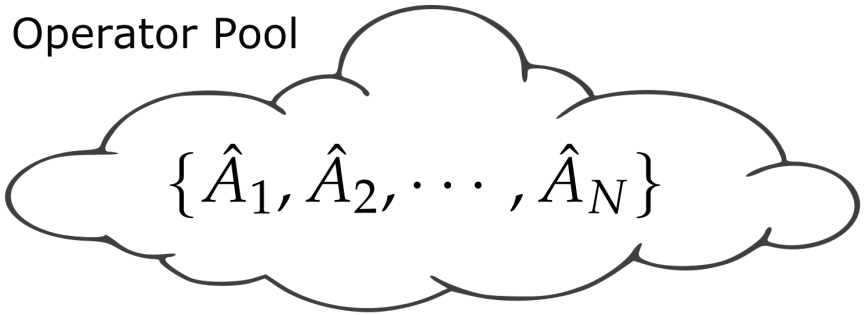
- Start from a simple reference state
- Quantum resources are precious: Only add as many operators as needed
- Problem-tailor the ansatz: Use the QC to determine how to grow the ansatz further



Grimsley, Economou, Barnes, Mayhall, Nature Communications **10**, 3007 (2019)

ADAPT-VQE ingredients: (i) operator pool

- ADAPT-VQE uses a pool of operators, A_m
- Applies unitaries one by one : $U_m = \exp(\theta_m A_m)$ to a reference state



ADAPT-VQE ingredients: (ii) update criterion

- Identify which $e^{\theta_j A_j}$ to apply to reference state $|\Psi_0\rangle$
- Take gradient of mean energy wrt θ_j

$$\frac{\partial}{\partial \theta_j} \langle \Psi_0 | e^{-\theta_j A_j} H e^{\theta_j A_j} | \Psi_0 \rangle |_{\theta_j = 0}$$

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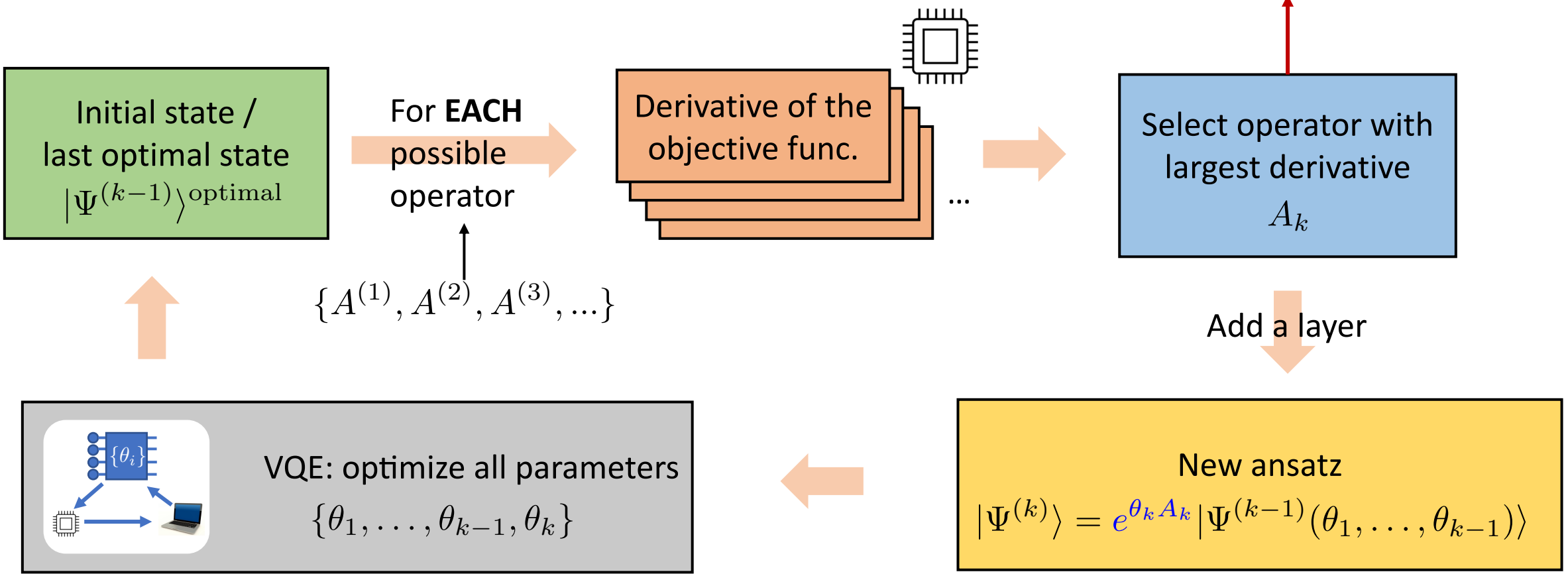
New operator → measure on hardware

ADAPT-VQE overview

Inputs:

- Hamiltonian
- Initial state
- Operator pool



Grimsley, Economou, Barnes, Mayhall, Nature Communications **10**, 3007 (2019)

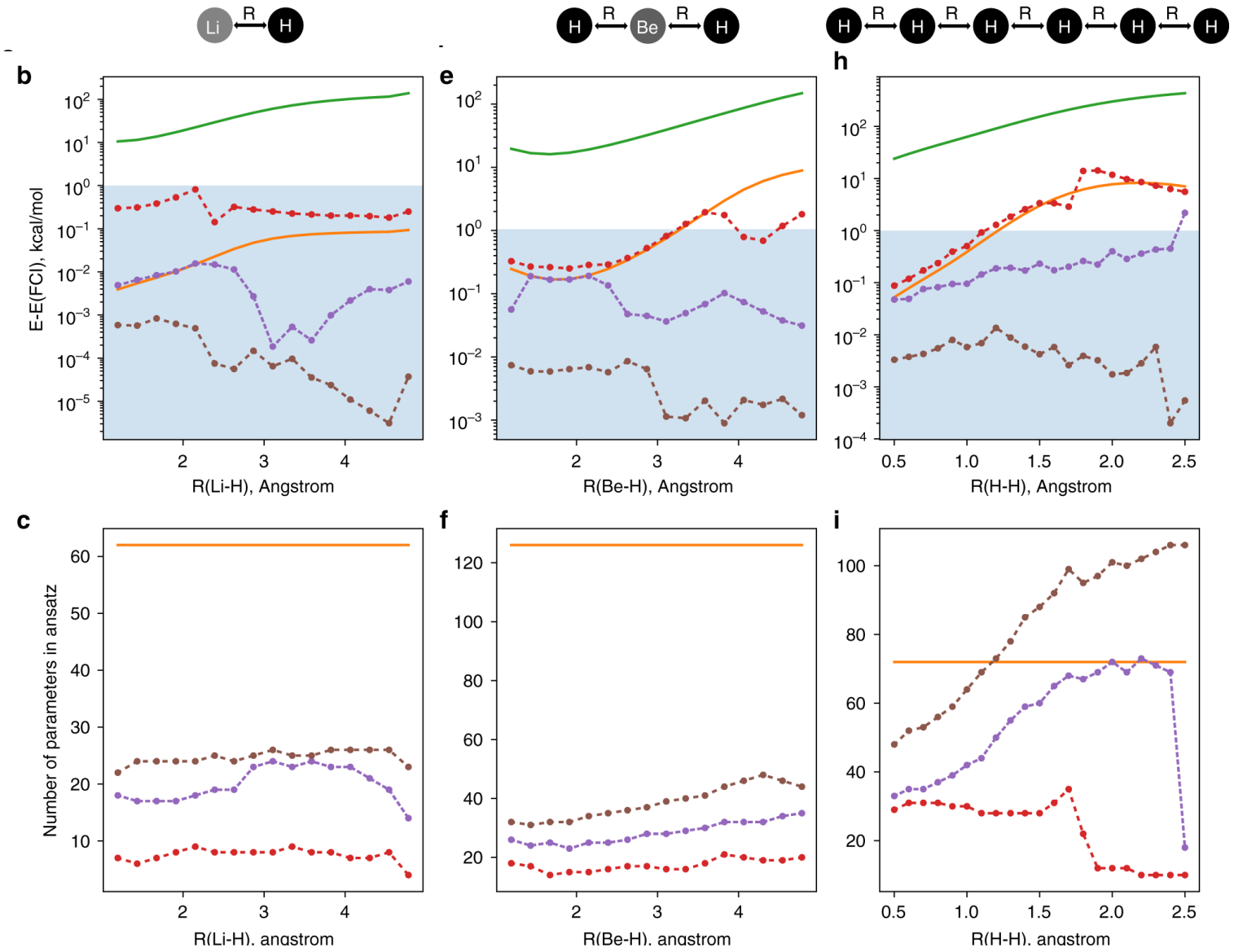
Convergence in ADAPT-VQE

$$\frac{\partial}{\partial \theta_j} \langle \Psi_0 | e^{-\theta_j A_j} H e^{\theta_j A_j} | \Psi_0 \rangle |_{\theta_j = 0} = \underbrace{\langle \Psi_0 | [H, A_j] | \Psi_0 \rangle}$$

The algorithm terminates when this is zero (i.e., very small)

- This is satisfied by any energy eigenstate
- Strictly speaking, ADAPT finds energy eigenstates (not necessarily the g.s.)
- In practice, it always finds the g.s. given a proper pool

ADAPT-VQE with fermionic pool (classical simulations)



UCCSD
HF
ADAPT(ϵ_1)
ADAPT(ϵ_2)
ADAPT(ϵ_3)
Chemical Accuracy

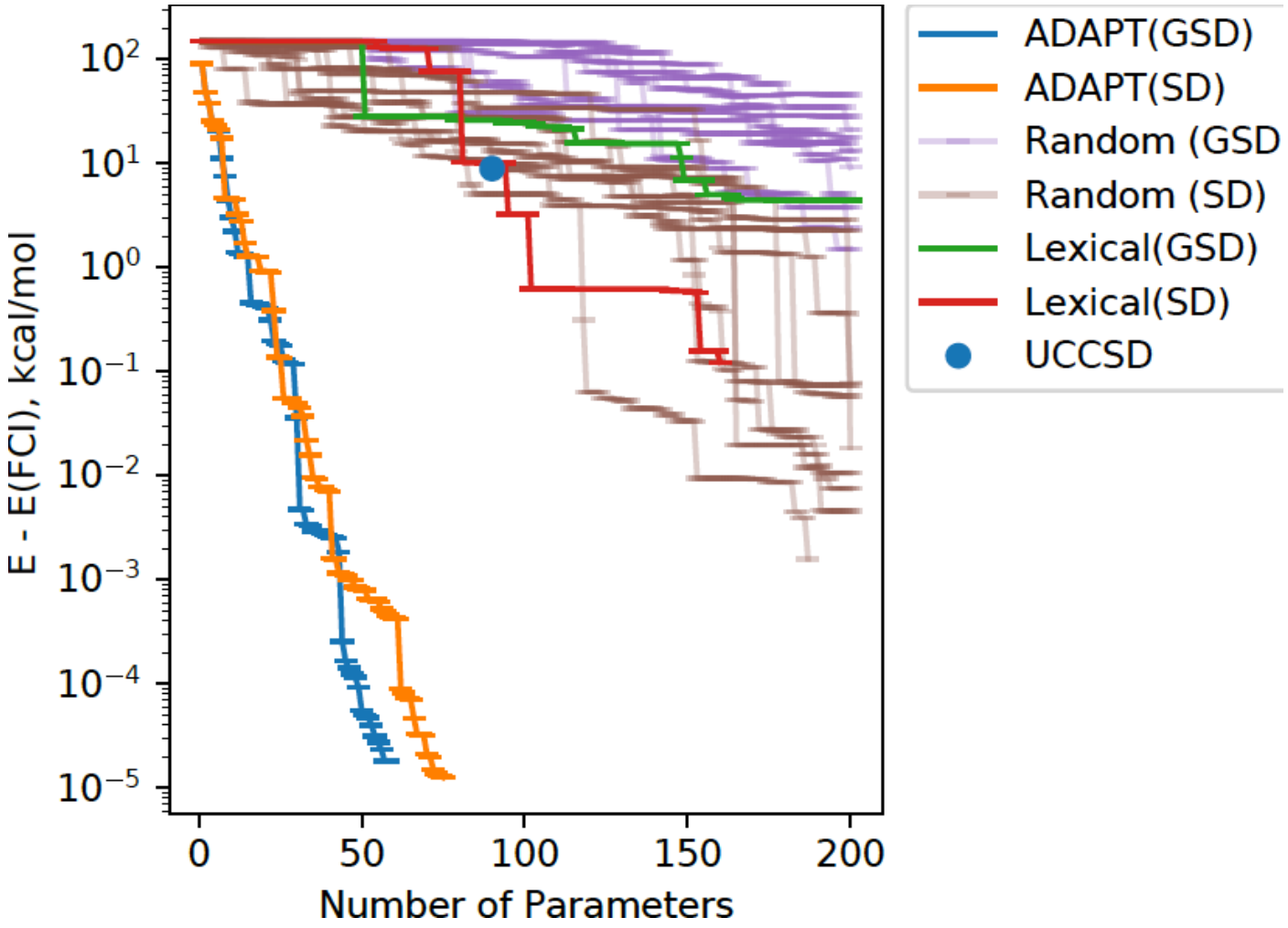
$\epsilon_1 = 0.1$

$\epsilon_2 = 0.01$

$\epsilon_3 = 0.001$

Grimsley, Economou, Barnes, Mayhall, Nature Communications **10**, 3007 (2019)

Comparing ADAPT to other orderings

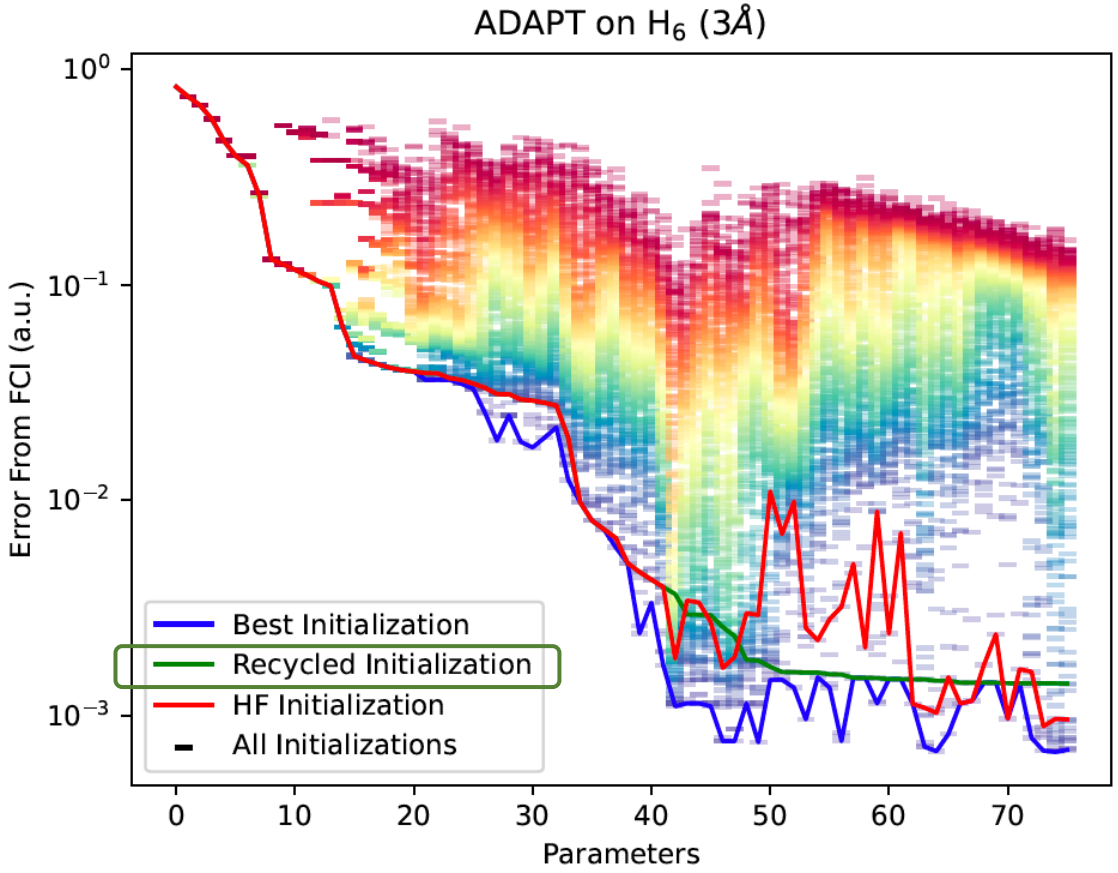


BeH_2
bond distance 2.39 Å

Grimsley, Economou, Barnes, Mayhall, Nature Commun. **10**, 3007 (2019)

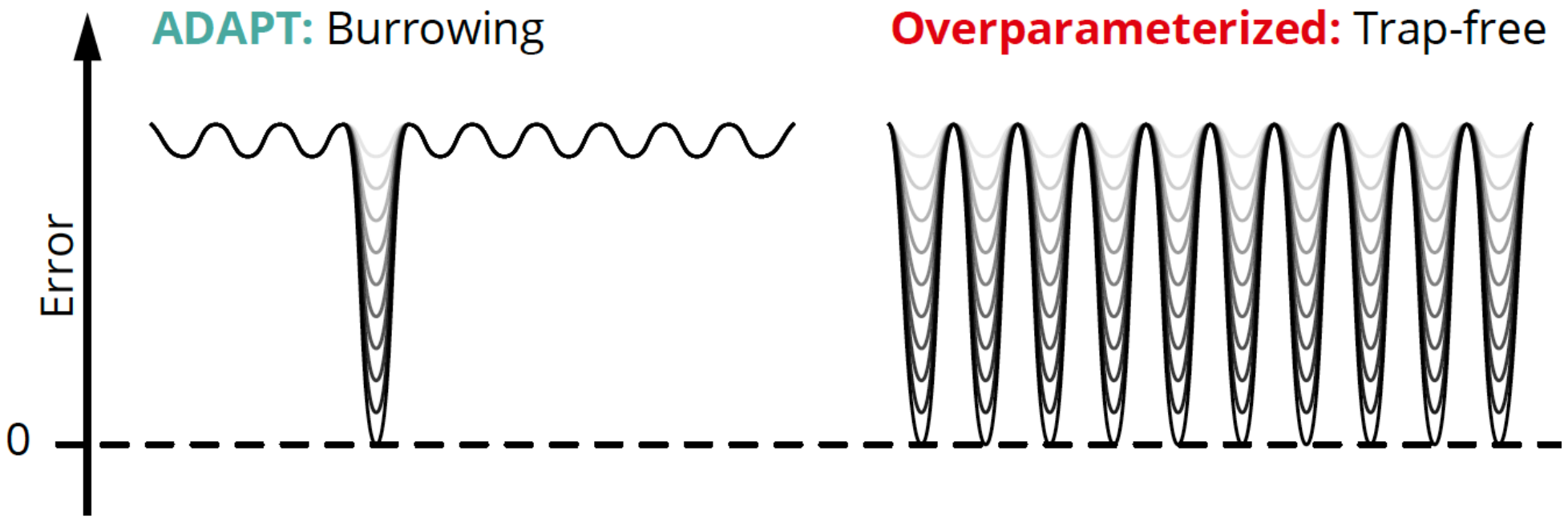
Trainability of ADAPT-VQE

- ADAPT produces compact, problem tailored ansatze
- Shallow circuit → the landscape is generally too rugged
- ADAPT avoids the issues associated with trainability
- By construction resistant to barren plateaus



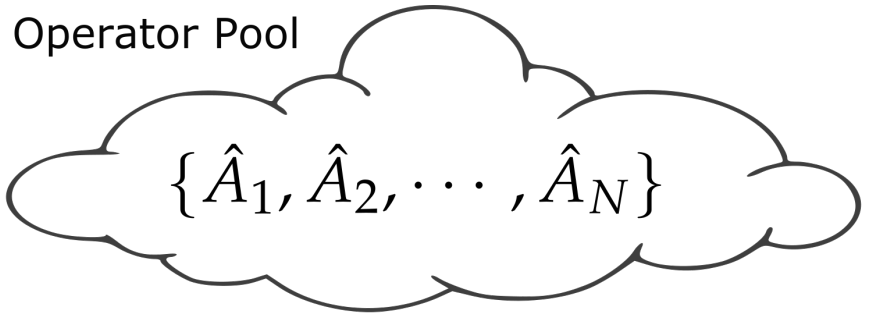
Grimsley et al, npj Quantum Information **9**, 19 (2023)

Intuitive picture



Grimsley et al, npj Quantum Information **9**, 19 (2023)

How should the operator pool be chosen?



- We can choose it according to hardware constraints

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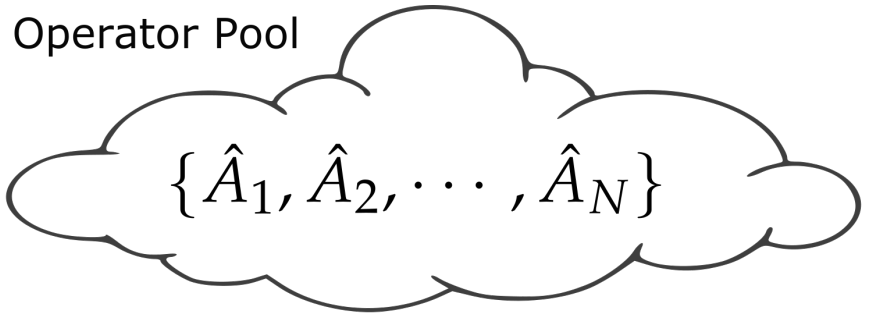
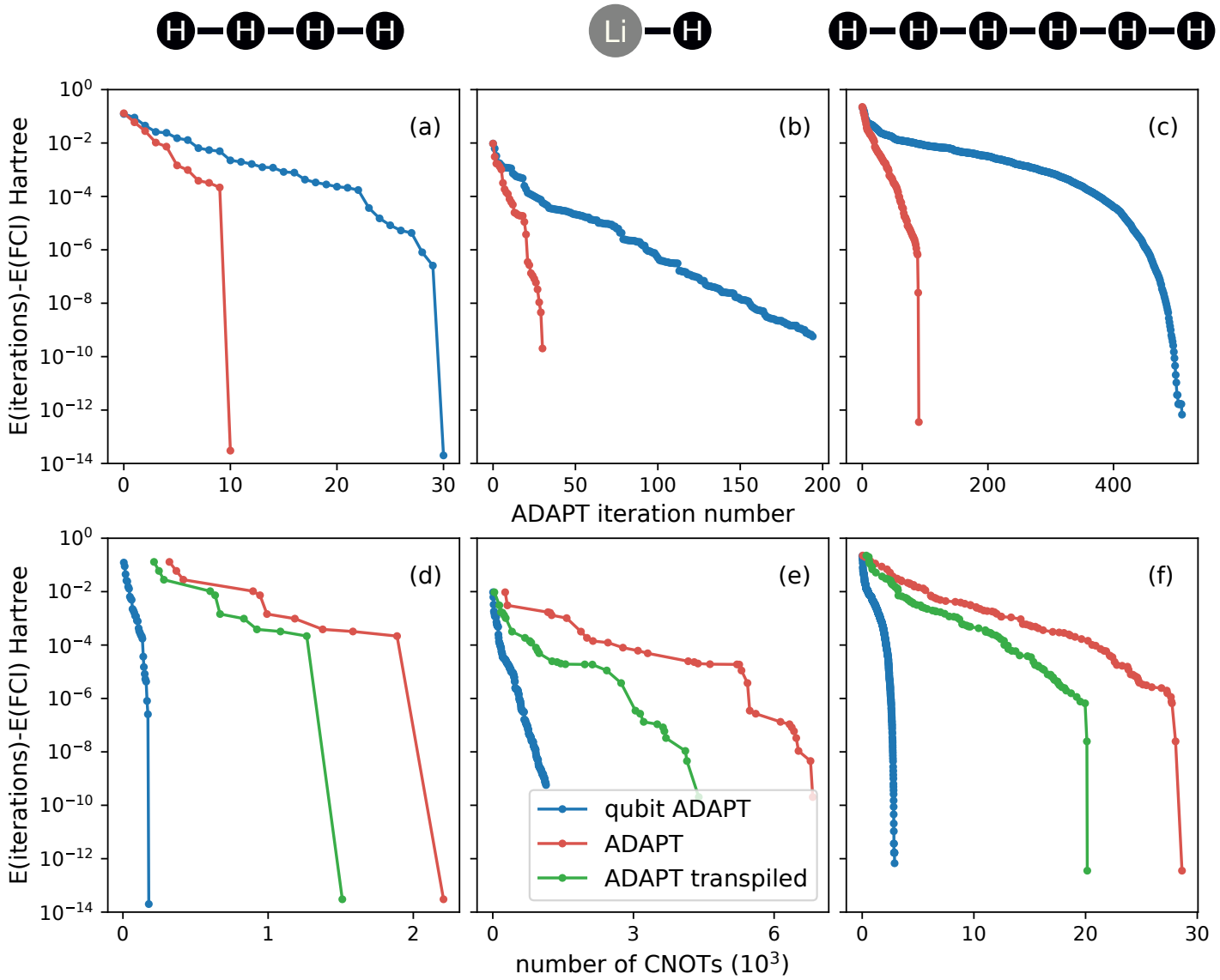


- We can choose it according to hardware constraints
  - Hardware-efficient pool $\{e^{i\theta_j P_j}\}$, where P_j is a Pauli string with up to 4 Paulis
  - For simplicity, take doubles and drop Z's: $XYYY, XXXY$ ("qubit-ADAPT-VQE")

Qubit ADAPT-VQE—results

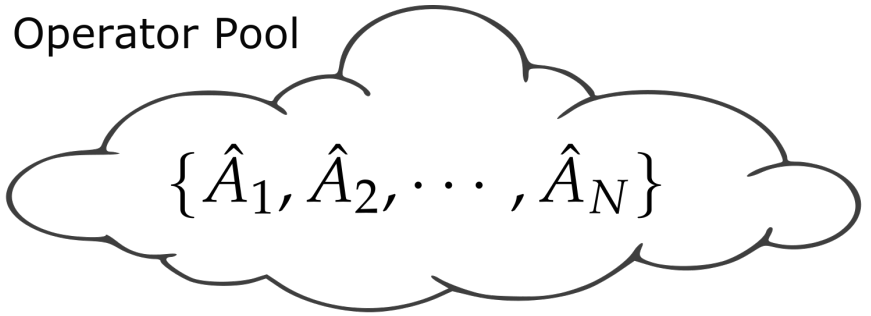


See also follow-up work by Cambridge group Arvidsson-Shukur et al *Communications Physics 4 (1), 228 (2021)*

- 8, 12, 12 qubits respectively
- bond distances 1.5, 2, 1.5 Å

Tang, Shkolnikov, Barron, Grimsley, Mayhall, Barnes, Economou, PRX Quantum 2, 020310 (2021)

How should the operator pool be chosen?



- We can choose it according to hardware constraints

- Ideally, the pool size should be as small as possible, to reduce quantum resources
- How can we guarantee that it contains enough and the right type of operators?

Complete pools

$$|\psi^{ADAPT}(\vec{\theta})\rangle = e^{\theta_n A_n} ... e^{\theta_2 A_2} e^{\theta_1 A_1} |\psi^{ref}\rangle = e^{\sum_i \phi_i B_i} |\psi^{ref}\rangle$$

where $\{B_i\} = \{A_1, A_2, ..., [A_1, A_2], ..., [A_1, [A_2, A_3]], ...\}$

We have a complete pool when states $B_i|\psi\rangle$ form a complete basis (where $|\psi\rangle$ is an arbitrary state)

Minimal complete pools (MCPs)

Minimal complete pool: smallest sized complete Pauli pool

The minimal size of complete pools is linear in the nr of qubits: *2n-2*

Example of min complete pool

$$\begin{aligned} &G_1 = ZYII\ldots I, \quad G_2 = IZYII\ldots I, \\ &\quad G_3 = IIZYII\ldots I, \quad \ldots, \quad G_{n-2} = II\ldots IZYI, \quad G_{n-1} = II\ldots IZY, \\ &G_n = YII\ldots I, \quad G_{n+1} = IYII\ldots I, \\ &\quad G_{n+2} = IIYII\ldots I, \quad \ldots, \quad G_{2n-3} = II\ldots IYII, \quad G_{2n-2} = II\ldots IYI \end{aligned}$$

We also have a simple criterion to determine whether a minimal pool is complete that scales polynomially with system size

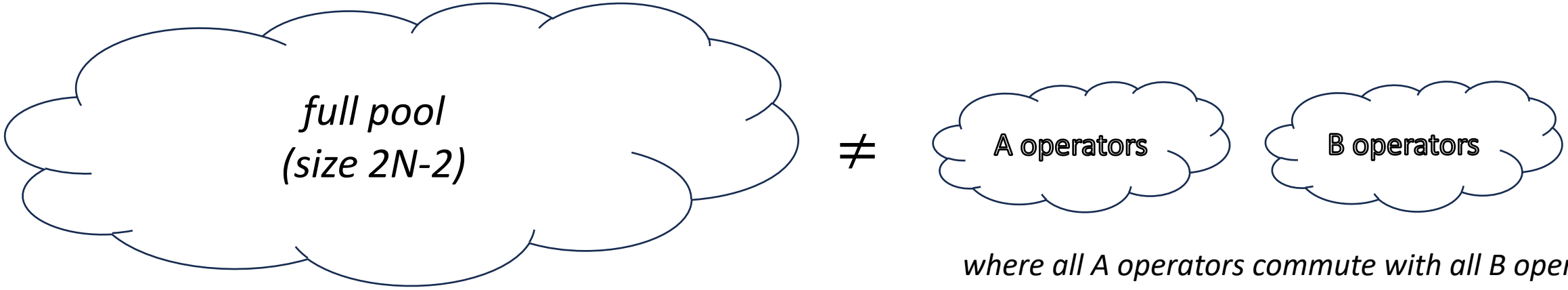
Shkolnikov, Mayhall, Economou, Barnes, Quantum **7**, 1040 (2023)

Minimal complete pools—cont.

Given a pool of size *2n-2,* how do we know it's complete?

- Taking all the commutators to check the full algebra scales exponentially with system size
- We have a simple, polynomially scaling criterion to determine whether a minimal Pauli pool is complete:

If the pool operators cannot be split into two fully mutually commuting sets, then the MCP is complete



where all A operators commute with all B operators

Shkolnikov, Mayhall, Economou, Barnes, Quantum **7**, 1040 (2023)

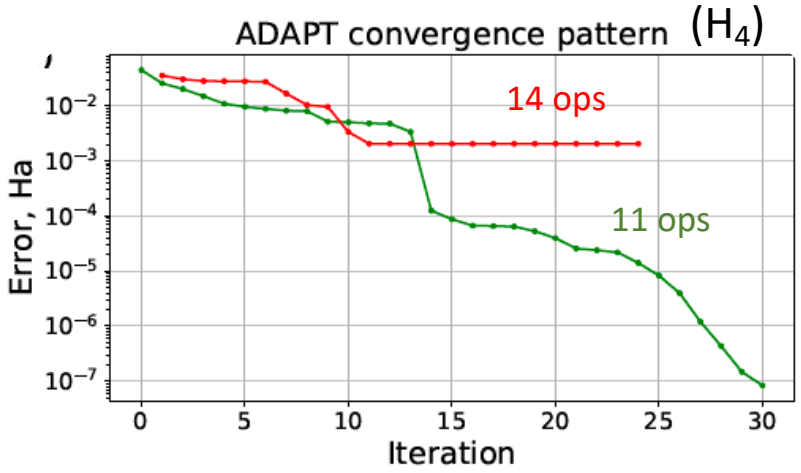
Incorporating symmetries

- Using random MCPs not aware of symmetries can cause convergence issues

- This can be addressed using symmetry-preserving MCPs

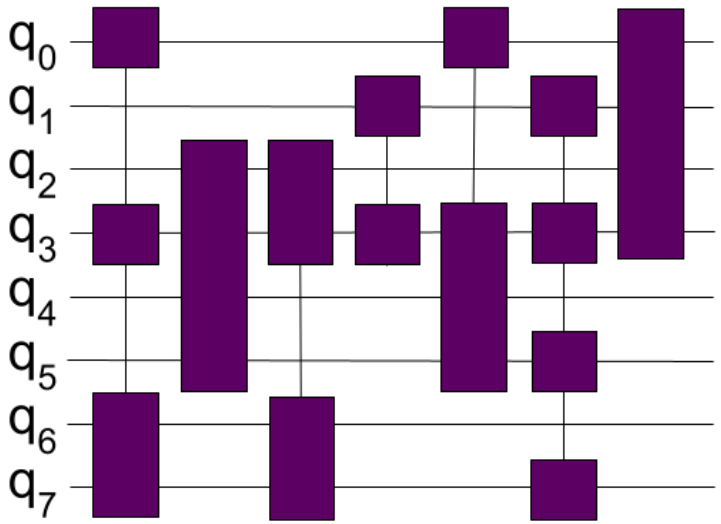
- For starting the algorithm, include “starters”, operators that preserve symmetries
- These need to involve two-particle excitations (four nontrivial Paulis), since HF is the lowest-energy product state

- Symmetry-preserving MCPs have fewer than $2n - 2$ operators
- This is because we do not need to span the full Hilbert space



Shkolnikov, Mayhall, Economou, Barnes, Quantum **7**, 1040 (2023)

Is ADAPT-VQE the most efficient way to construct circuits?

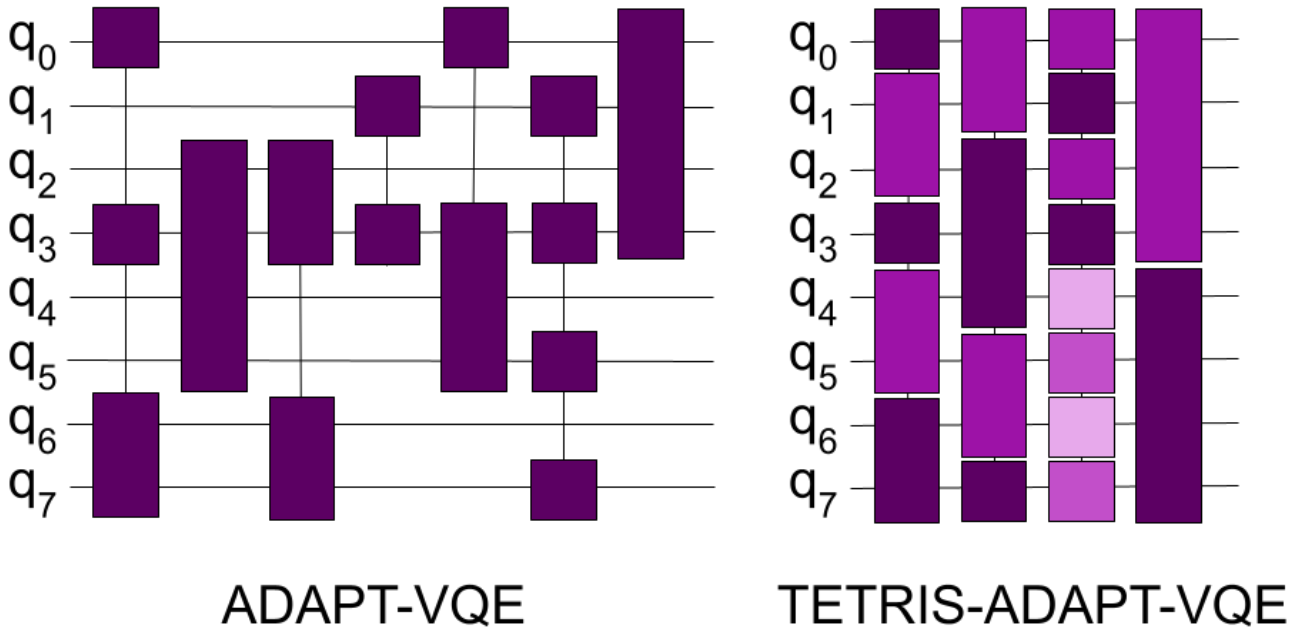


ADAPT-VQE

TETRIS-ADAPT-VQE: concept

Tiling Efficient Trial circuits with Rotations Implemented Simultaneously

Instead of one-at-a-time, add multiple operators at each step



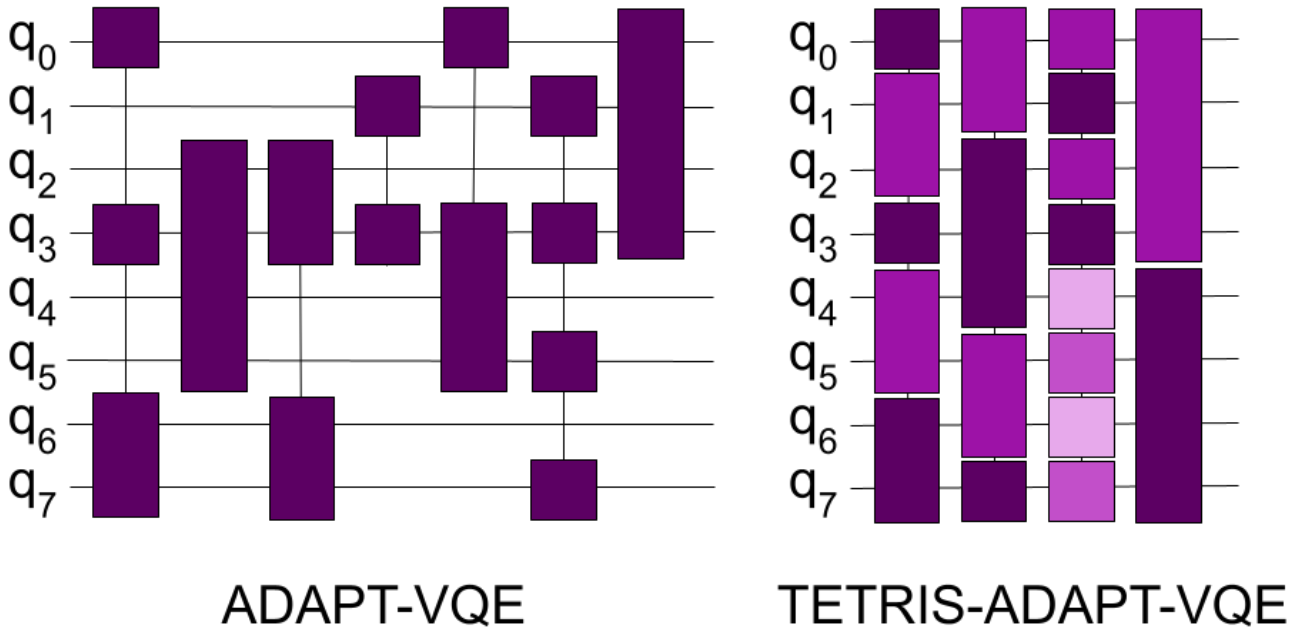
Anastasiou, Chen, et al, arXiv:2209.10562

TETRIS-ADAPT-VQE: concept

Tiling Efficient Trial circuits with Rotations Implemented Simultaneously

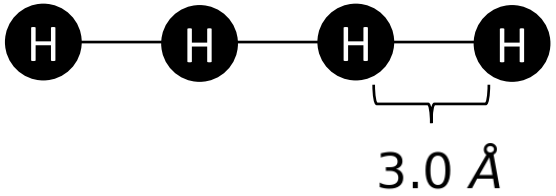
Instead of one-at-a-time, add multiple operators at each step according to:

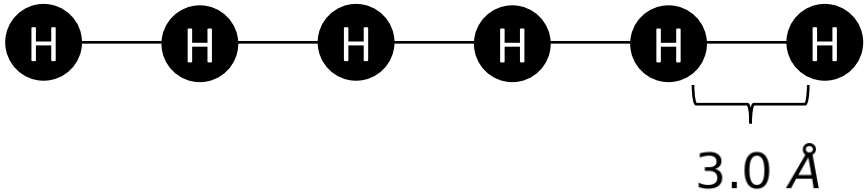
- Gradient magnitude
- $\mathcal{N}$th operator acting on different set of qubits from $(\mathcal{N}-j)$th

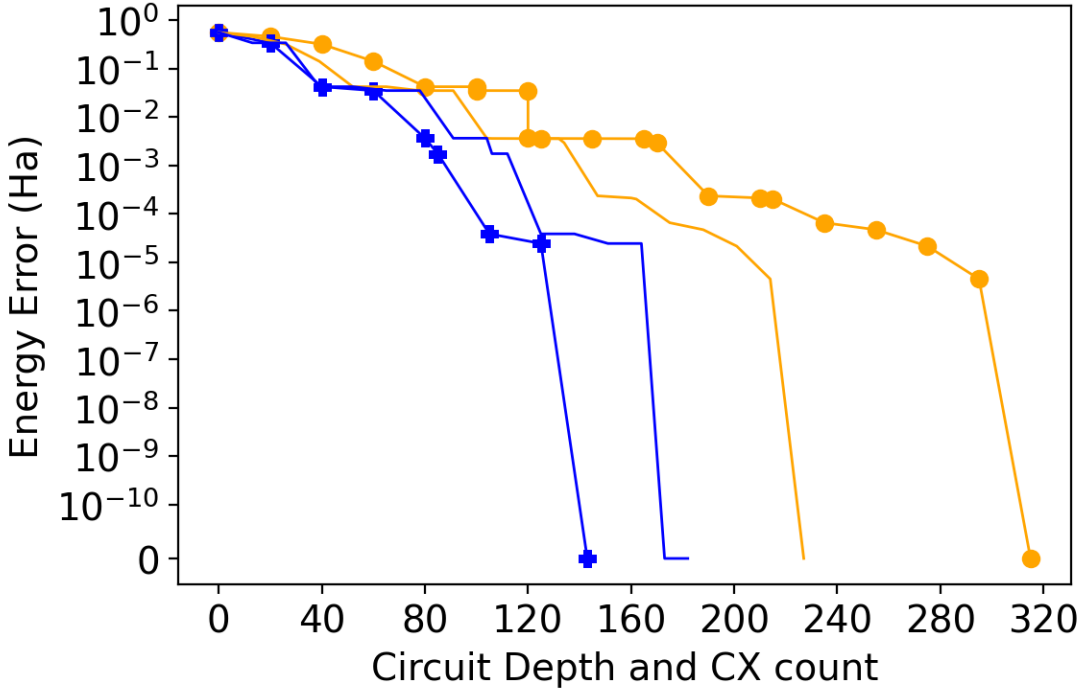


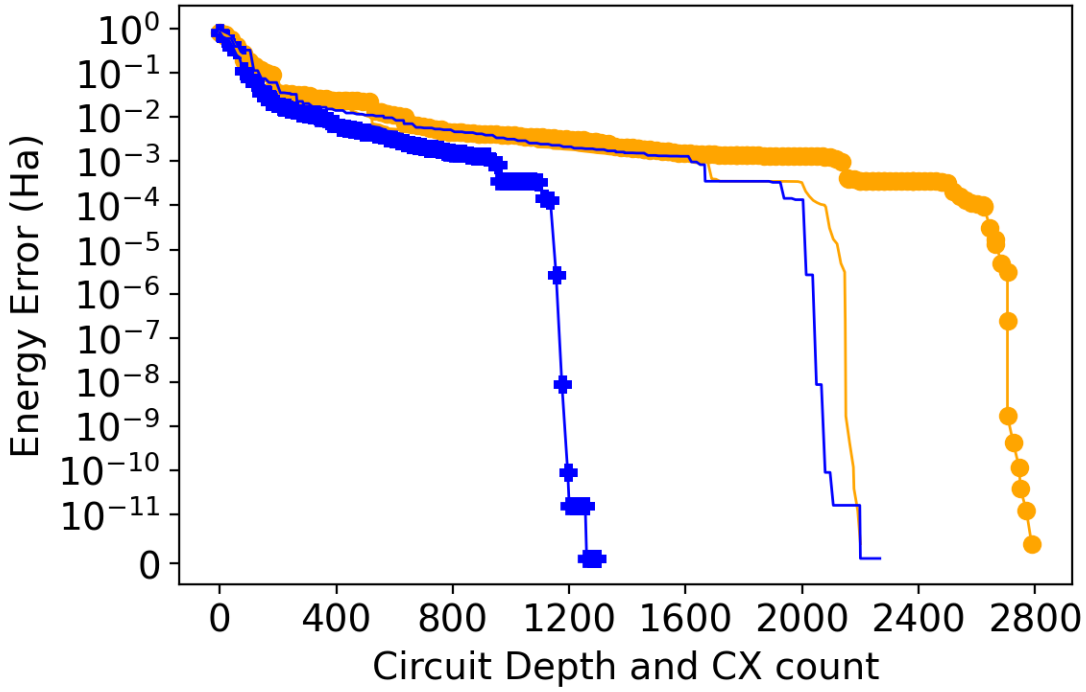
Anastasiou, Chen, et al, arXiv:2209.10562

TETRIS-ADAPT-VQE: results







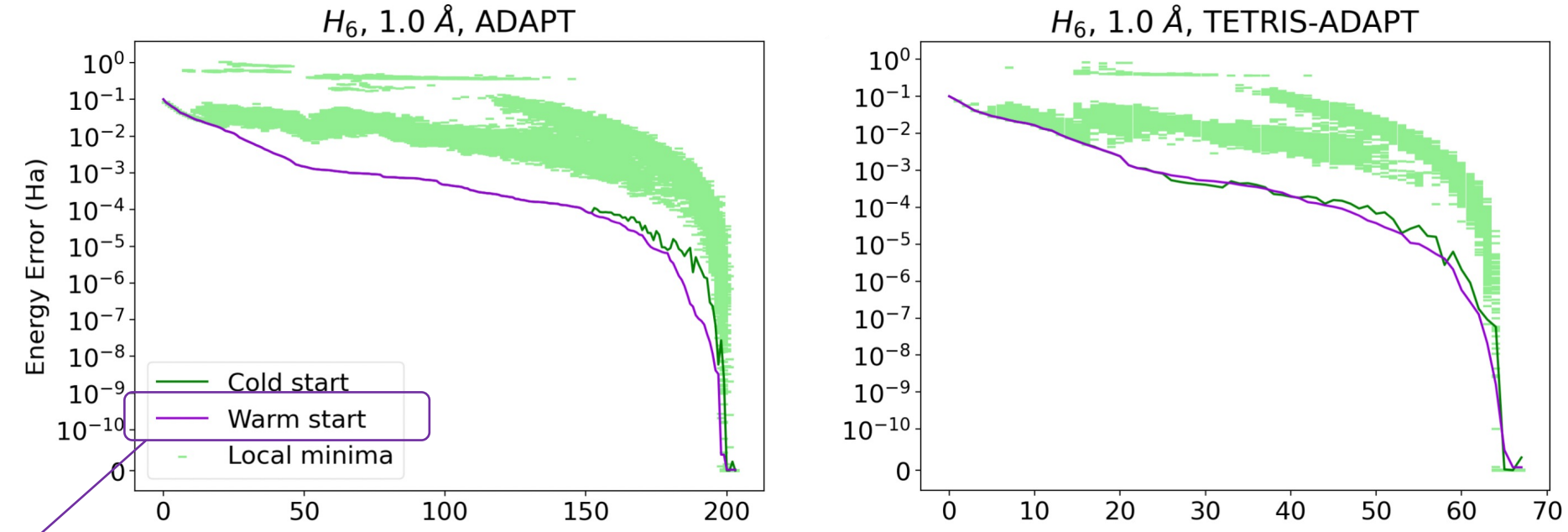


Blue: TETRIS-ADAPT

Orange: standard ADAPT

Anastasiou, Chen, et al, arXiv:2209.10562

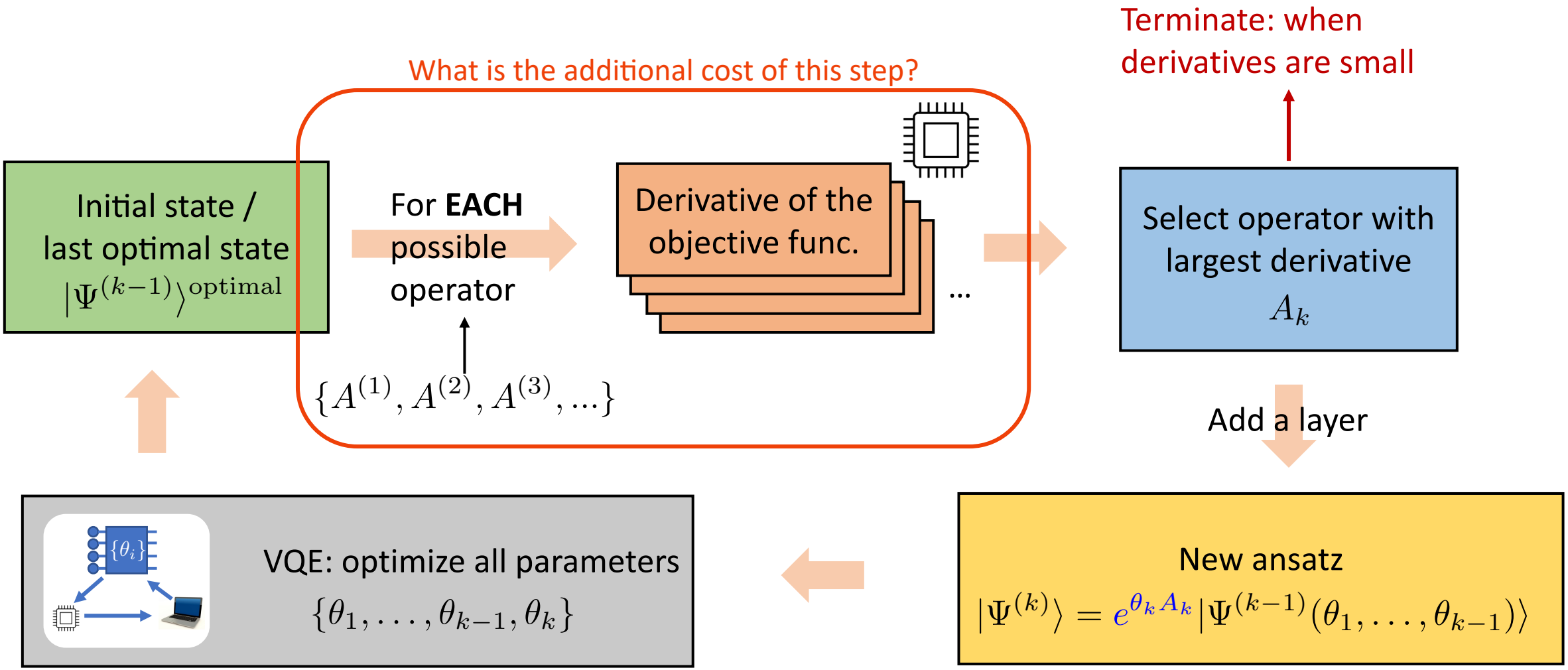
Trainability of TETRIS-ADAPT-VQE



ADAPT strategy

Anastasiou, Chen, et al, arXiv:2209.10562

ADAPT-VQE overview



Measuring gradients in ADAPT

$$\left.\frac{\partial E}{\partial \theta_i}\right|_{\theta_i=0} = \left[\frac{\partial}{\partial \theta_i}\left\langle \Psi^{(k)}\right| e^{-\theta_i P_i} H e^{\theta_i P_i} \left|\Psi^{(k)}\right\rangle\right]\Bigg|_{\theta_i=0} = \left\langle \Psi^{(k)}\right| [H, P_i] \left|\Psi^{(k)}\right\rangle$$

Number of terms goes as $O(N^4)$

Size of Pauli pool also goes as $O(N^4)$

- How can we decrease the number of state preparations?
  Commuting observables can be measured simultaneously

- Which grouping heuristic should we use?
  Not ideal approach, scaling ~$O(N^{16})$

Anastasiou et al, arXiv:2306.03227 (2023)

Measuring gradients in ADAPT—a better approach

For A, B, C Pauli strings:

If $[B, C] = 0$, then $[\,[A, B]\,, [A, C]\,] = 0$

By extension, the commutators of the elements of any mutually commuting set of Pauli strings with any one Pauli string commute!

Anastasiou et al, arXiv:2306.03227 (2023)

Measuring gradients in ADAPT—a better approach

What does this mean for operators of the form $iY_iX_jX_kX_l$?

H term	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
					Y	Z	Y	Y	Z	Y	X	Z	X	X	Z	X
S_1	Y	X	X		X											
S_2	Y	X	X			X										
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
S_3	Y													X	X	X

$O(N^3)$ commutators can be measured simultaneously!

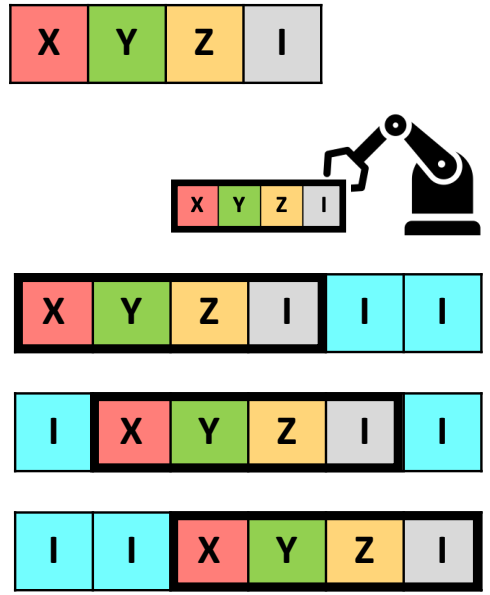
- We can group the commutators of any Hamiltonian term with all qubit operators into $2N$ groups
- Measuring term-by-term of the Hamiltonian means all observables in any given group have the same weight – lower shot-noise
- **Measuring the pool gradient is only $\sim N$ times as expensive as a naïve VQE iteration**

Anastasiou et al, arXiv:2306.03227 (2023)

Beyond molecules: lattice models

Challenge for extended Hamiltonians:

- Full Pauli pool scales as 4^N
- Using ad hoc smaller pool does not respect periodicity



Solution:

- Exploit periodicity (translational symmetry) of lattice

- Algorithm:
  - Run ADAPT with full pool on small tile
  - If there are gradient degeneracies, repeat multiple times
  - Collect operators chosen by ADAPT
  - Tile these operators to larger instances (pad with identities)

- The resulting pool is *linear* in N
- We have identified the conditions for the pool to be *complete*

Van Dyke et al, arXiv:2206.14215
(to be updated soon)

Tiling example: XXZ model

- Use resulting Pauli pool for small instance (1x3 tile for 1D, 2x2 tile for 2D): take chosen operators, tile them to create pool for larger instances
- Run 1000 trials, pick operators randomly in case of degenerate gradients

1D case:

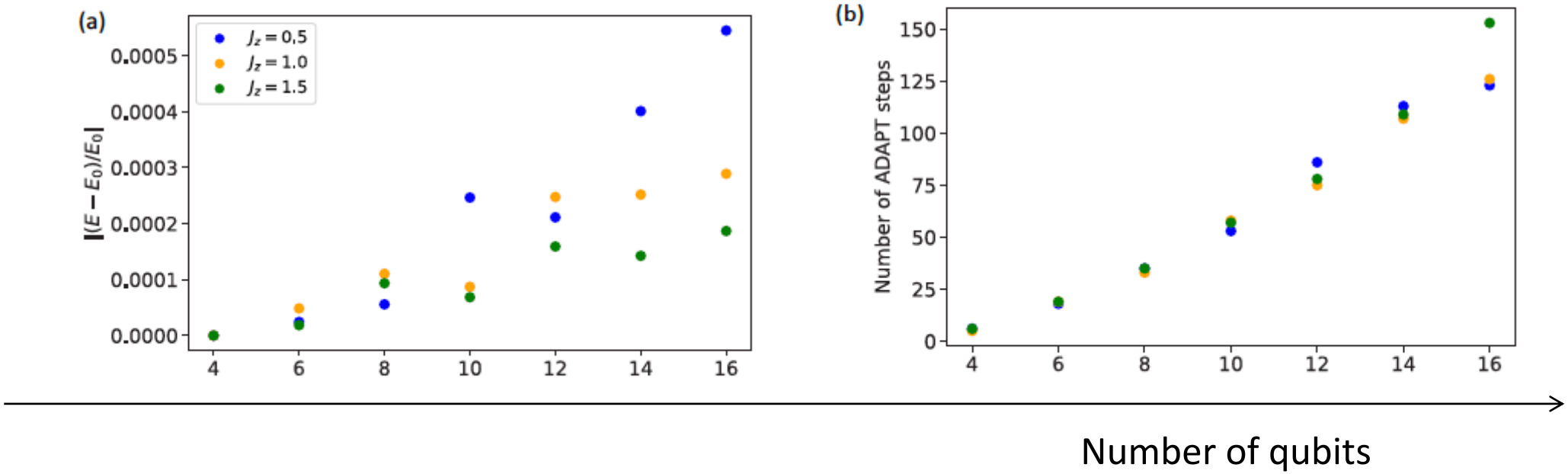
- For a 1x3 tile, ADAPT always converges in three steps
- ADAPT selects operator set *IXY, IYX, XYI, XIY, YXI, YIX, ZXY, YZX, YXZ, XZY, ZYX, XYZ* across several runs

2D case:

- For a 2x2 tile, ADAPT always converges in five steps
- ADAPT selects operator set *IIXY, IIYX, XYII, YXII, XYZI, IZXY, XZIY, ZYIX, YZXI, YIZX, XIYZ, IZYX, IXZY, XYIZ, ZIYX, ZXYI, YXZI, YXIZ, IYXZ, ZIXY, ZZYX, YXZZ, ZZXY, XYZZ*

XXZ model with tiling: results for up to 16 qubits for 1D

$$H = \sum_{j=1}^{L-1} \left(\frac{J_{xy}}{2} (S_{j+1}^{+} S_{j}^{-} + h.c.) + J_z S_{j+1}^{z} S_{j}^{z} \right)$$

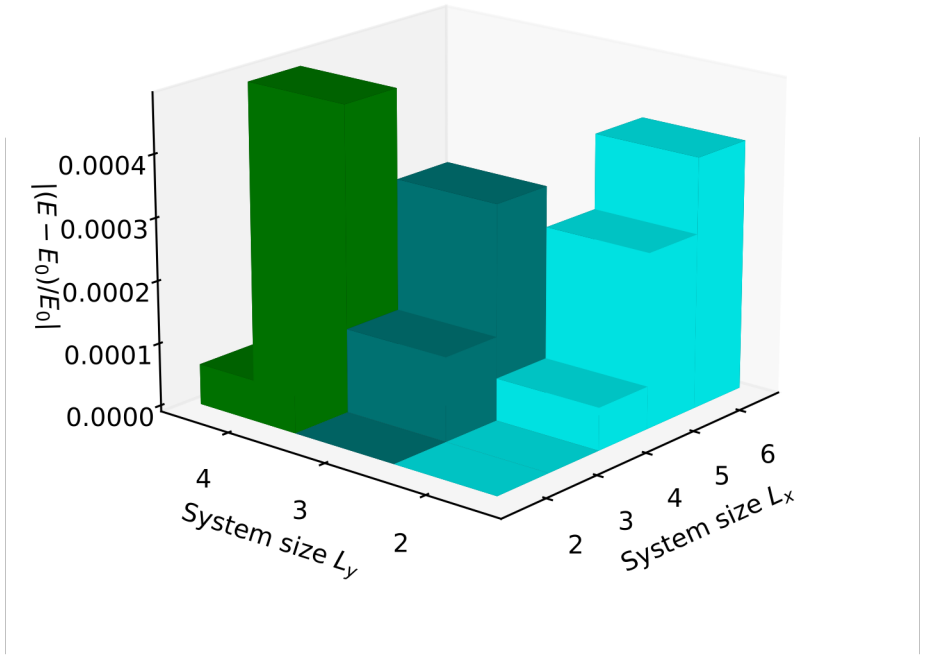


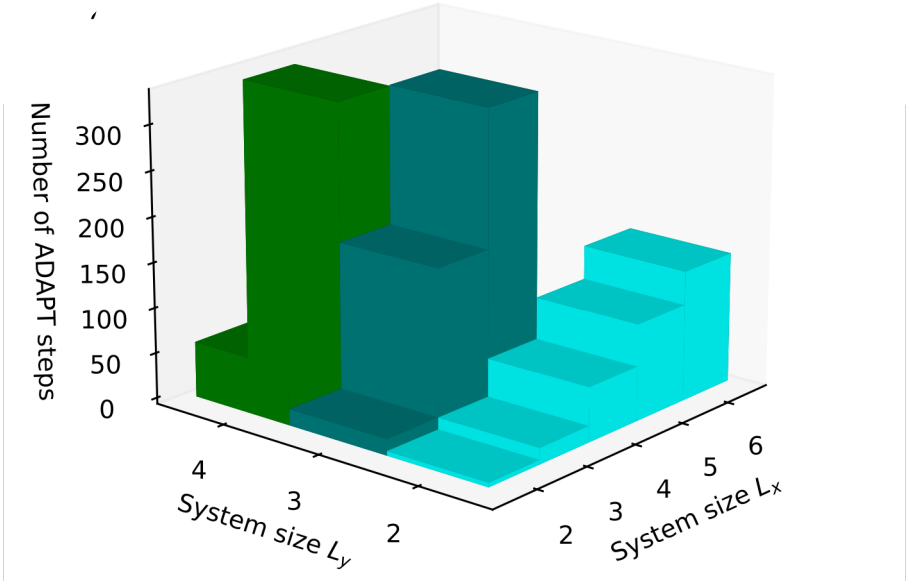
Exponential reduction in pool size

Van Dyke et al, arXiv:2206.14215
(to be updated soon)

XXZ model with tiling: results for up to 12 qubits for 1D

- Computational complexity greater due to increased connectivity of lattice
- Tiling strategy able to achieve good accuracy (error < 0.05%)





Beyond pure states: Gibbs state preparation

- Given Hamiltonian H acting on data system D with N_D qubits, we wish to prepare mixed thermal states at arbitrary temperature T

$$\rho_G(T) = \frac{e^{-H/T}}{\mathrm{Tr}(e^{-H/T})}$$

- This has useful applications in quantum simulation, quantum machine learning, quantum optimization, etc., but is a hard problem in general

- Need additional ancilla qubits to purify the state on the whole system

- Standard approach: prepare state that minimizes $F\left(\rho(\vec{\theta})\right) = \mathrm{Tr}\left(\rho(\vec{\theta})H + T\rho(\vec{\theta})\ln\rho(\vec{\theta})\right)$

- Challenges:
  - It's hard to know *a priori* what will make an efficient, effective ansatz
  - Measuring the entropy (and gradients) is difficult on hardware

Wu and Hsieh. PRL **123**, 220502 (2019)
Chowdhury, Low, and Wiebe. arXiv:2002:00055 (2020)
Wang, Li, and Wang. PRA **16**, 054035 (2021)

Some remarks on prior work

- The thermofield double has been considered as a tool
- Create it based on QAOA-like ansatz [1]

$$|\vec{\alpha}_n, \vec{\gamma}_n\rangle = \prod_{k=1}^{n} e^{i\alpha_k H_{AD}} e^{i\gamma_k (H_A + H_D)/2} |\psi_0\rangle$$

Eigenstate of H_{AD}

Problem H

$$H_A + H_D = H \otimes \mathbb{1} + \mathbb{1} \otimes H$$

where

$$H_{AD} = \sum_{k=1}^{N_D} (X_{D_k} X_{A_k} + Y_{D_k} Y_{A_k} + Z_{D_k} Z_{A_k})$$

- Algorithm starts from highly entangled state (fully thermal)
- But interesting/challenging regime is low T (modest/low entanglement)
- Algorithm largely undoes entanglement → wasteful in q resources, deep circuits

[1] Wu and Hsieh. PRL **123**, 220502 (2019)

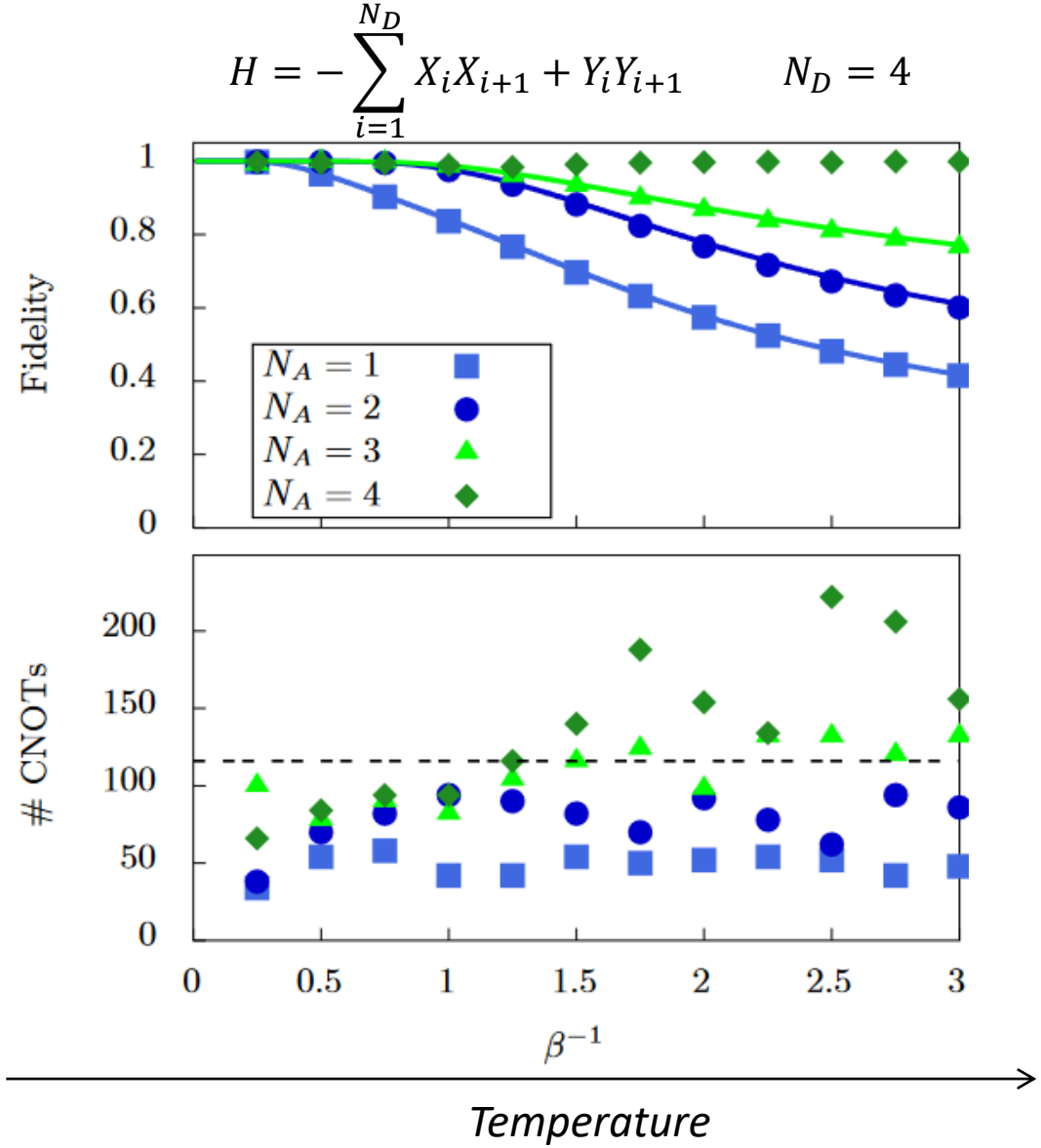
Gibbs-ADAPT-VQE

- Our approach:
  - ✓New objective function that is easier to measure: $C\left(\rho\left(\vec{\theta}\right)\right) = -\mathrm{Tr}\left(\rho_G(T)\rho\left(\vec{\theta}\right)\right) + \frac{1}{2}\mathrm{Tr}\left(\rho\left(\vec{\theta}\right)^2\right)$
  - ✓ADAPT-VQE approach to grow the ansatz
- Two strategies, one good for low T, one for high T
- Low T approach:
  - Start with partially entangled data-ancilla state
  - Operator pool: all 1- and 2-qubit Paulis on combined data/ancilla system
  - Pool requires initial state be only **partially entangled** (use non-optimized random y-rotations and CNOTs)
  - Use ADAPT criterion to minimize Gibbs energy iteratively

Warren et al, arXiv: 2203.12757

Gibbs-ADAPT-VQE: numerical results for XY Hamiltonian

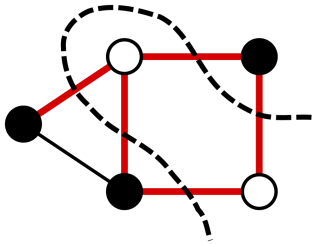
- Pool requires initial state be only **partially entangled** (use non-optimized random y-rotations and CNOTs)
- Ancilla system can be any size, allowing resource savings (though $N_A = N_D$ needed at larger T)
- Improvement (reduction) in number of CNOTs, number of ancilla qubits



Warren et al, arXiv: 2203.12757

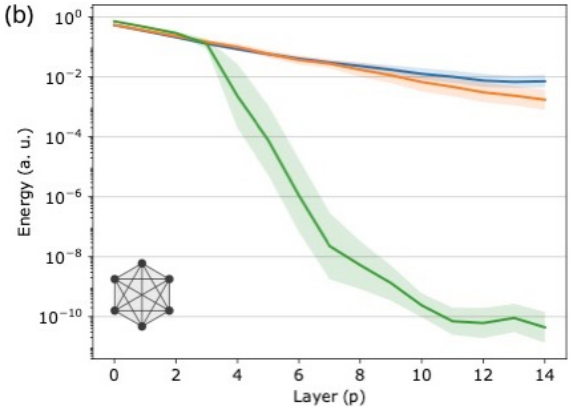
Other applications of ADAPT-VQE

- Optimization: ADAPT-QAOA, where we use ADAPT to determine mixers



Zhu et al, PRR 4, 033029 (2022)
Chen et al, arxiv:2205.12283

See also recent Quantum-inspired classical ADAPT-Clifford-QAOA
arxiv: 2310.15022



- Nuclear physics: LMG ('Lipkin' model), where ADAPT finds g.s. across phase transition
  Romero et al, Phys. Rev. C 105, 064317

- ADAPT + randomness
  Magann, Economou, Arenz, PRR 5, 033227 (2023)

- Time dynamics: ADAPT-VQE for time-evolved state (minimize 'McLachlan distance')
  Yao et al, PRX Quantum 2, 030307 (2021)

Outline

- Typical ansatze & issues
- Our approach: Adaptive quantum simulation
- Control-VQE: optimizing at the pulse level

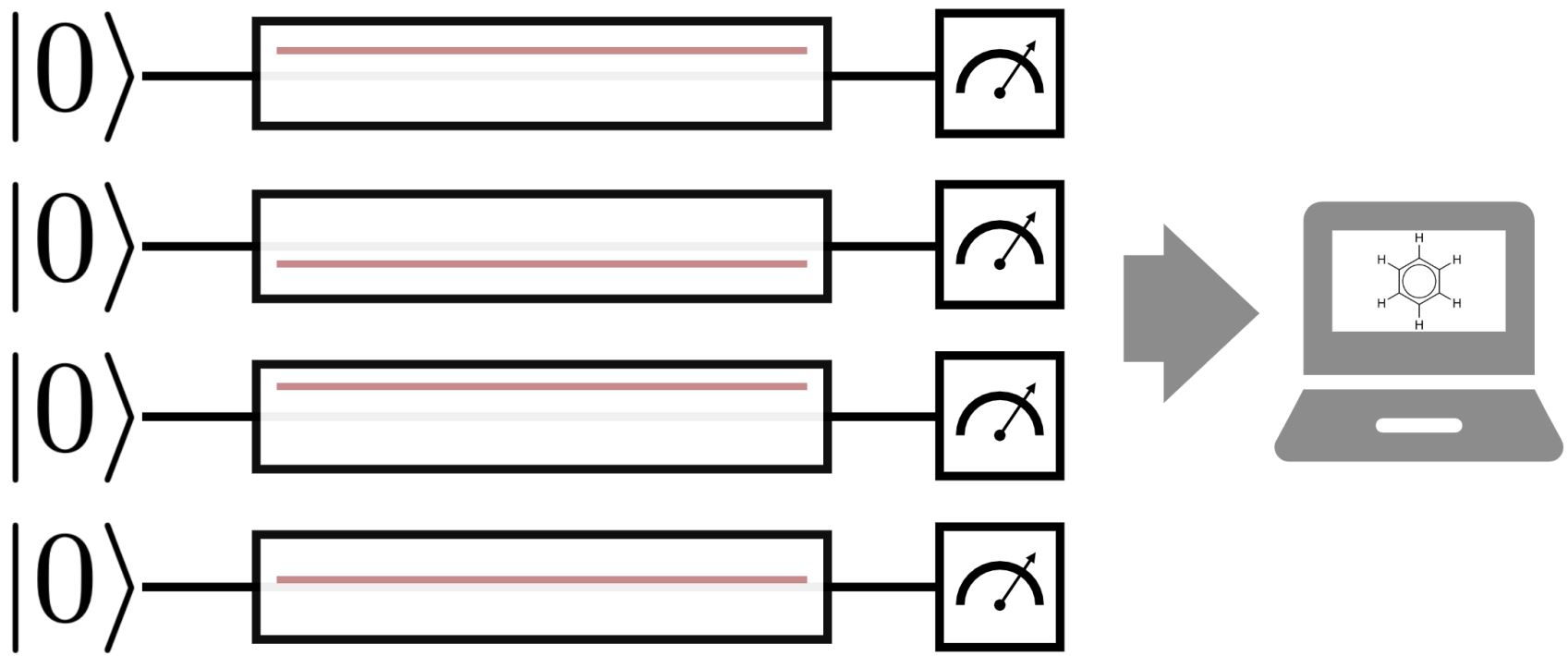
Hardware currently noisy even for VQEs

Pulse-level optimization:

- Throw out the gates, parameterize pulse directly
- Measure <H>
- Classical optimization → update pulse parameters
- Repeat until convergence

Meitei et al, npj Quantum Information 7, 155 (2021); arXiv:2008.04302

See also Yang et al, Phys. Rev. X **7**, 021027 (2017) for pulse-based QAOA


|0⟩
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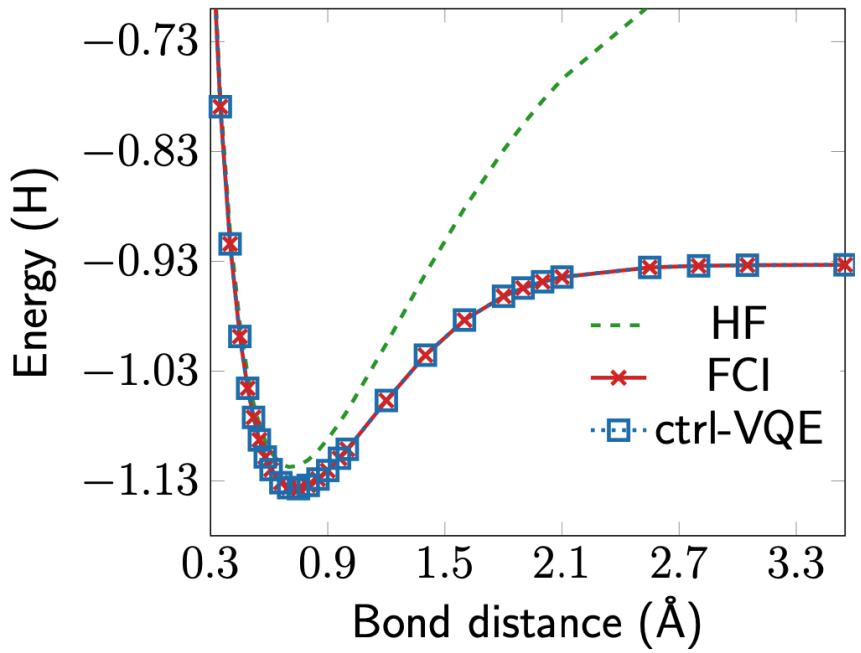
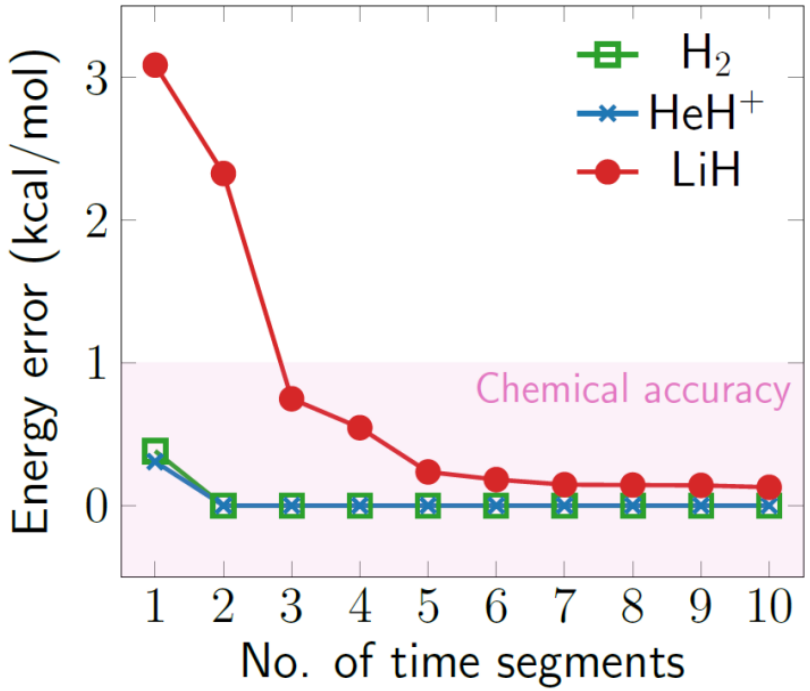
Dissociation curve for H2
(Indistinguishable from FCI)



Number of segments required for
convergence



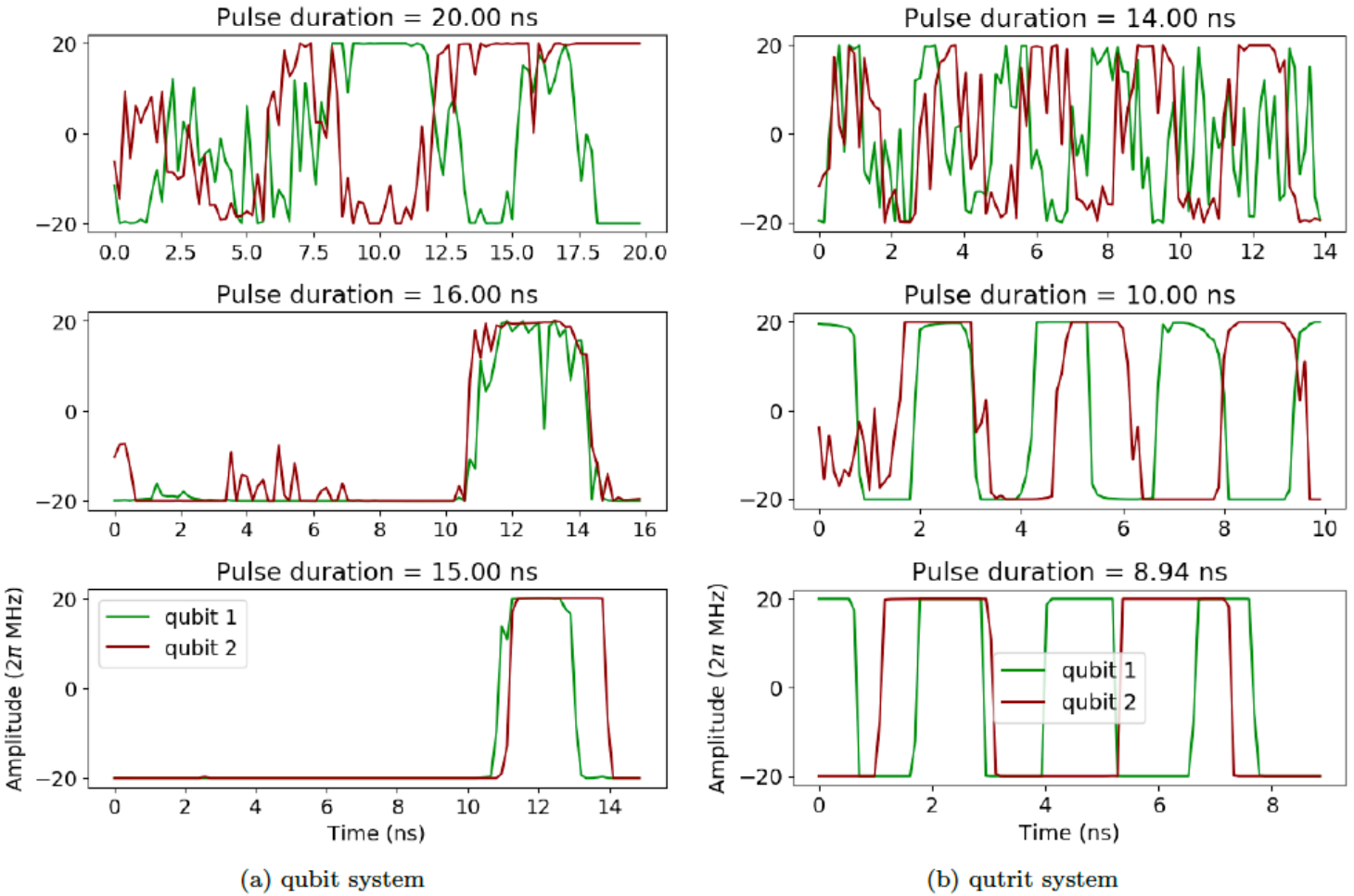
Orders of magnitude improvement:
E.g., for LiH: 80,000ns (gate-based UCCSD) vs. 50ns (ctrl-VQE)

Meitei et al, npj Quantum Information 7, 155 (2021)

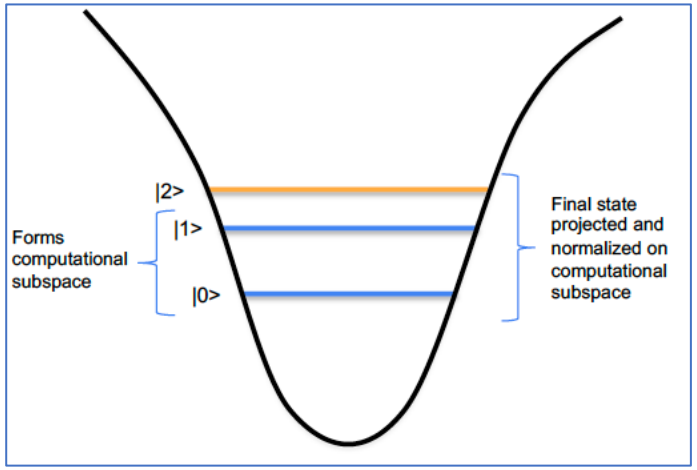
Ctrl-VQE: minimal evolution time

In more recent work we showed:

- Using excited states outside qubit space ***speeds up evolution***
- Shortening the total pulse time leads to ‘bang-bang’ control
- Below a certain evolution time there is no solution



(a) qubit system (b) qutrit system

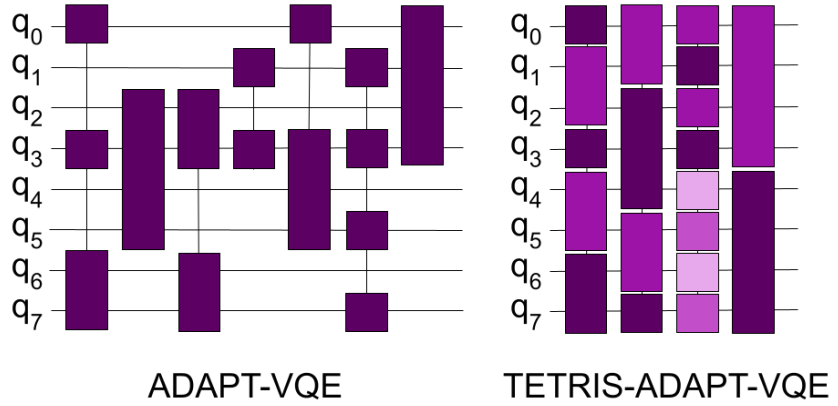


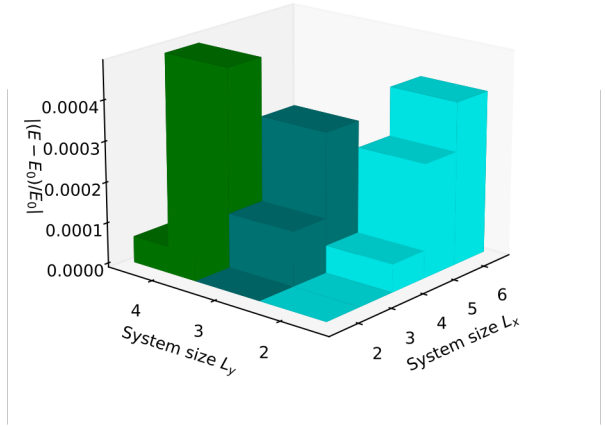
Simulations for H2 at bond distance 1.5 A

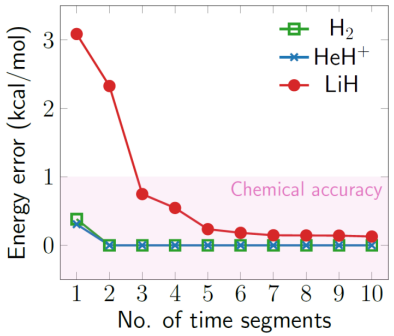
Asthana, Liu, et al,
Phys. Rev. Applied **19**, 064071 (2023)

Summary

- Adaptive variational quantum eigensolver (ADAPT-VQE)
- TETRIS-ADAPT-VQE
- Efficient measurement of gradients
- Algorithms for periodic (pure and thermal) systems
- Control-VQE







Acknowledgements

Student/postdocs:


Peter Anastasiou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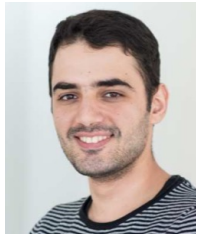
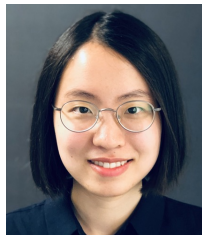

Vlad Shkolnikov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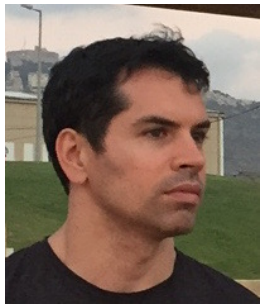
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Co-design Center for
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Postdoc positions open

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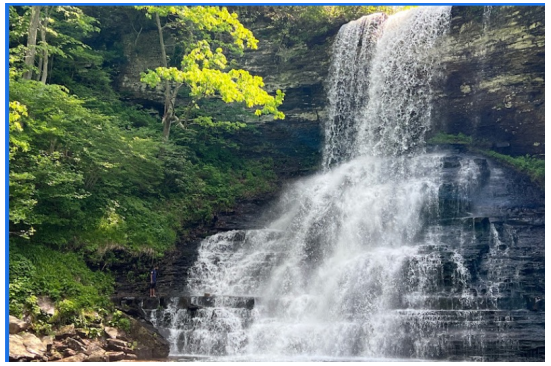

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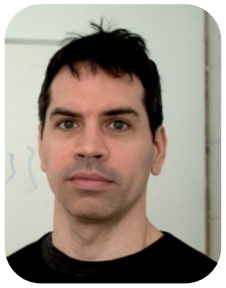

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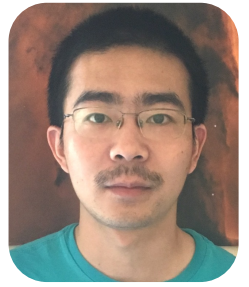

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