Problem-tailored variational quantum algorithms

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Outline

- VQEs for quantum simulation
- Choice of ansatz
- Adaptive, problem tailored VQE (ADAPT-VQE)
- Beyond digitized gates: ctrl-VQE

Observable (Hamiltonian) in second quantized form

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

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

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

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

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

Mapping fermions to qubits: Jordan-Wigner

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

- Jordan-Wigner mapping:
- Each orbital is mapped onto a qubit: |0> → unoccupied orbital, |1> → occupied orbital

$$a_3^{\dagger}|1001\rangle = a_3^{\dagger} a_1^{\dagger} a_4^{\dagger}|0000\rangle = -a_1^{\dagger} a_3^{\dagger} a_4^{\dagger}|0000\rangle$$

- Fermions satisfy Pauli exclusion principle but qubits are distinguishable → impose on qubits through Z strings

$$a_i^{\dagger} = \frac{1}{2}(X_i - iY_i) \bigotimes_{j<i} Z_j$$

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

VQE overview

Nat. Comm. **5**, 4213 (2014)
New J. Phys. **18**, 023023 (2016)
arXiv:2012.09265 (2021)

Variationally change $\vec{\theta}$

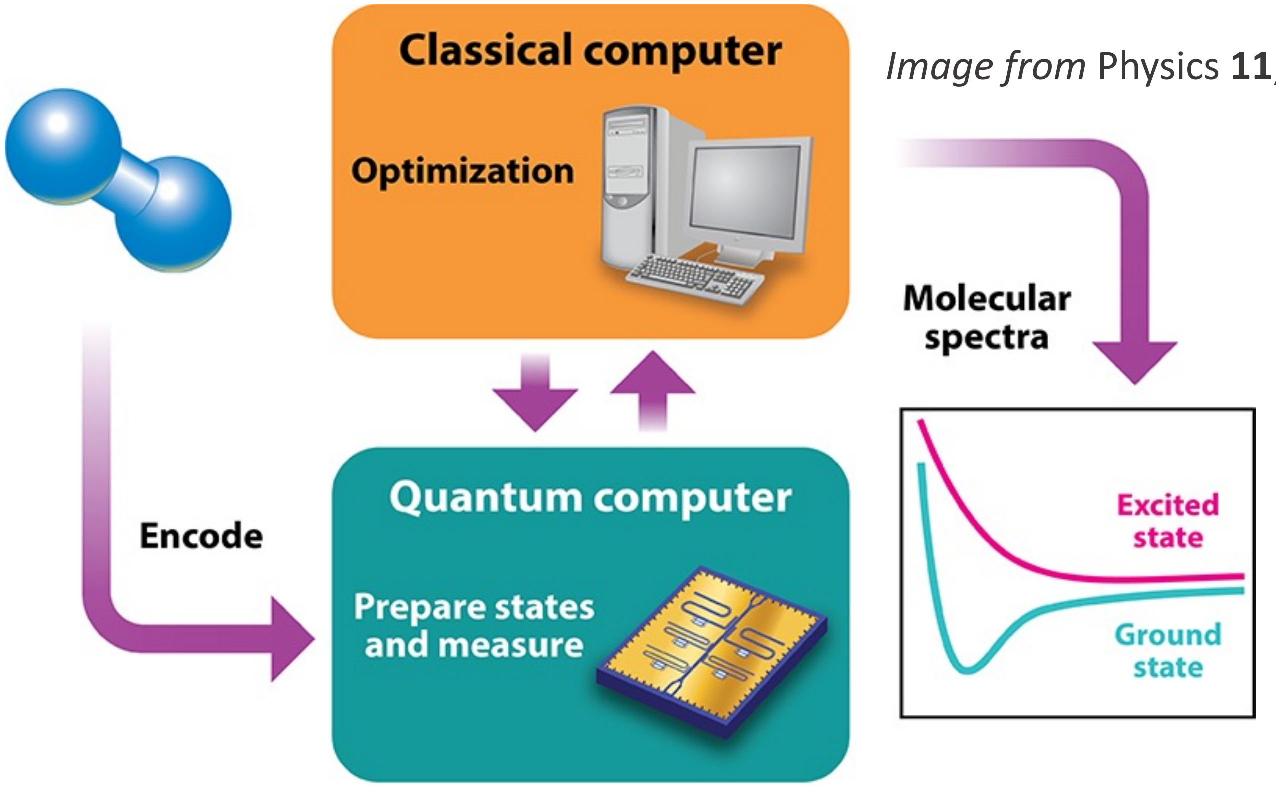


Image from Physics **11**, 14 (2018)

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

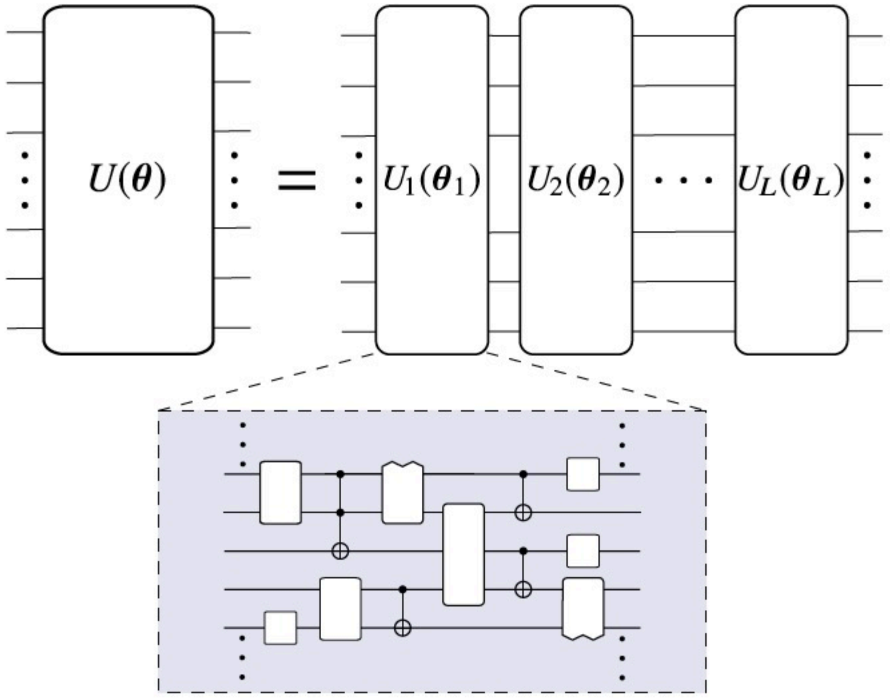
Measured energy $E(\vec{\theta}) = \langle\Psi(\vec{\theta})|H|\Psi(\vec{\theta})\rangle$

Objective function form

$$\langle A(\vec{\theta})\rangle = \langle\Psi(\vec{\theta})|A|\Psi(\vec{\theta})\rangle$$

Depends on:

- Observable measured (e.g., Hamiltonian)
- Ansatz (parameterized wavefunction)
  - Reference state
  - Parameterized circuit



Cerezo et al, arXiv:2012.09265

Most widely considered ansatze

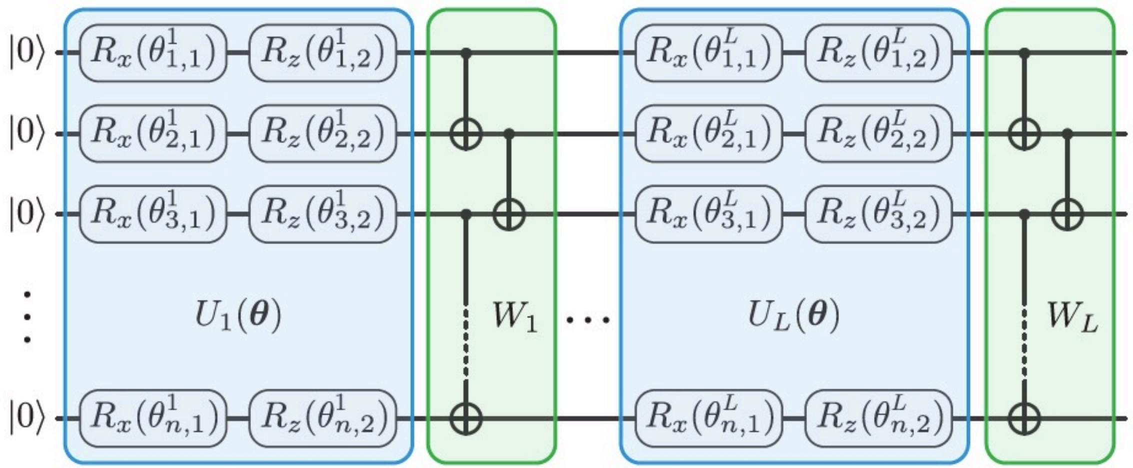
I. Hardware-efficient ansatz

- Natural for hardware

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

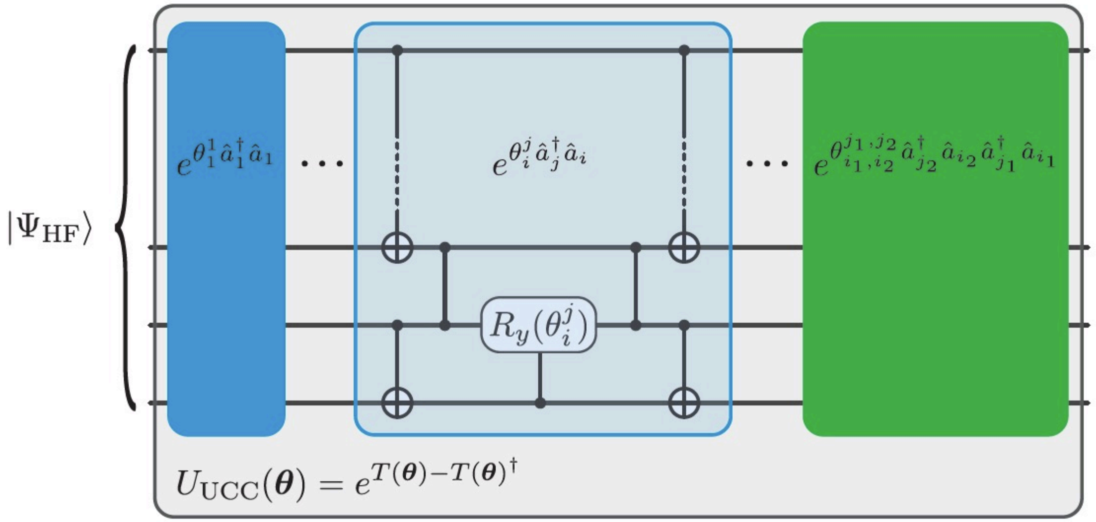
- Inefficient—too much of the Hilbert space sampled
- Difficult to optimize (barren plateaus)

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



II. Chemistry-inspired ansatz (UCC)

- Naturally generalizes classical simulation



Figures from Bharti et al. review on NISQ algorithms, arXiv:2101.08448

UCC is not unique in NISQ devices

$$U_{\mathrm{UCC}}(\boldsymbol{\theta}) = e^{T(\boldsymbol{\theta}) - T(\boldsymbol{\theta})^\dagger}$$

$$T(\boldsymbol{\theta}) = \sum_{ij} \theta_i^j a_j^\dagger a_i + \sum_{i_k, j_l,} \theta_{i_k}^{j_l} a_{j_2}^\dagger a_{i_2} a_{j_1}^\dagger a_{i_1} + \cdots$$

- To implement this on quantum processors, we need to use the terms entering in the *T*'s as separate gates
- These don't generally commute with each other
- Need to trotterize
- Finite-order trotterization not unique

- Different choices of trotterization give qualitatively different results!

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

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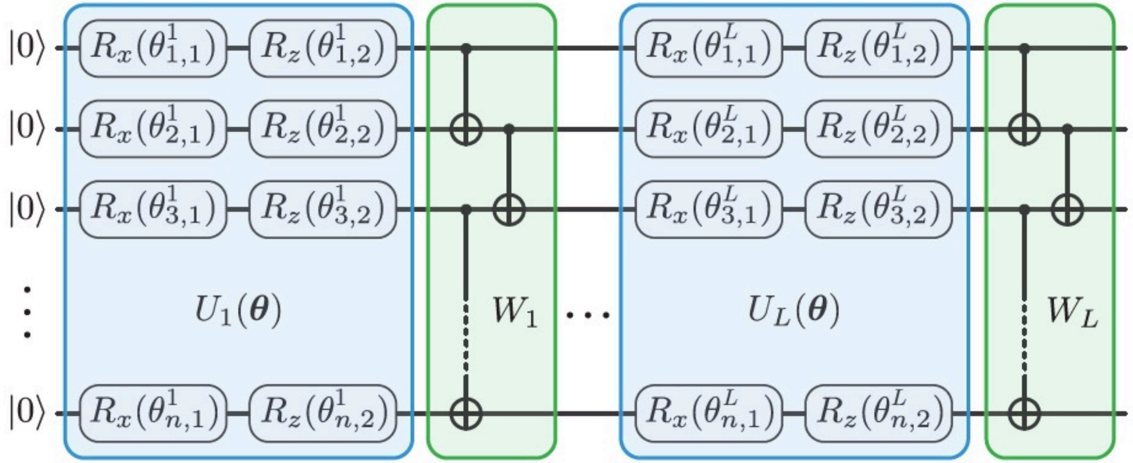
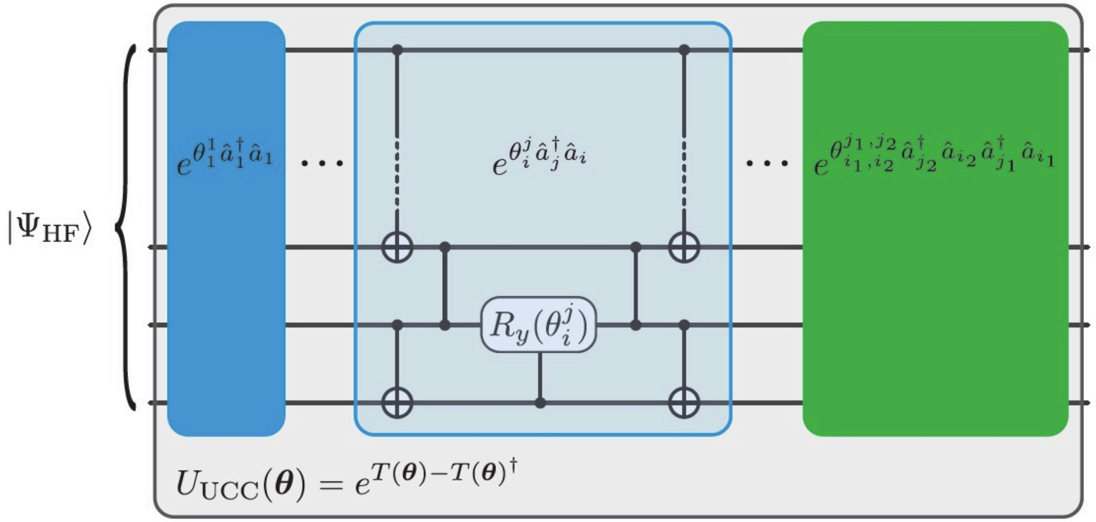


II. Chemistry-inspired ansatz (UCC)

- Naturally generalizes classical simulation
- Impractically long circuits
- Inconsistent under low-order Trotterization

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



Neither are problem-tailored

Figures from Bharti et al. review on NISQ algorithms, arXiv:2101.08448

Properties of a good ansatz

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

- Quantum coherence is very limited → shallow circuit
- Classical optimization is not infinitely powerful→ not too many optimization parameters
- Need to span the space where the solution lives; *it should help to have some input from the Hamiltonian*

Our approach: problem-tailored ansatze

Features:

✓shallow circuits

✓small/minimal number of optimization parameters

✓Exactness

Key idea:

✓Use the quantum computer to help determine the ansatz

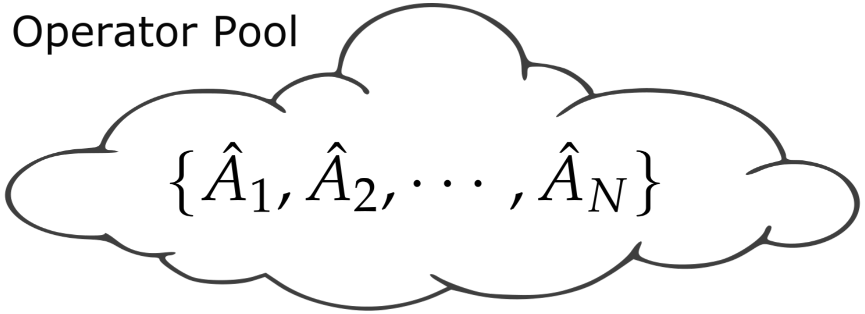
ADAPT-VQE

- Adaptive, Problem tailored (ADAPT)-VQE introduced the first dynamically created ansatz
- Start from a simple/short depth ansatz (e.g., Hartree-Fock)
- Use measurements on the QC to determine how to grow the ansatz further
- The resulting ansatz depends on the Hamiltonian, hence problem-tailored

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 : $U_m = \exp(\theta_{\mathrm{m}} A_{\mathrm{m}})$ to a reference state



ADAPT-VQE ingredients: (ii) update criterion

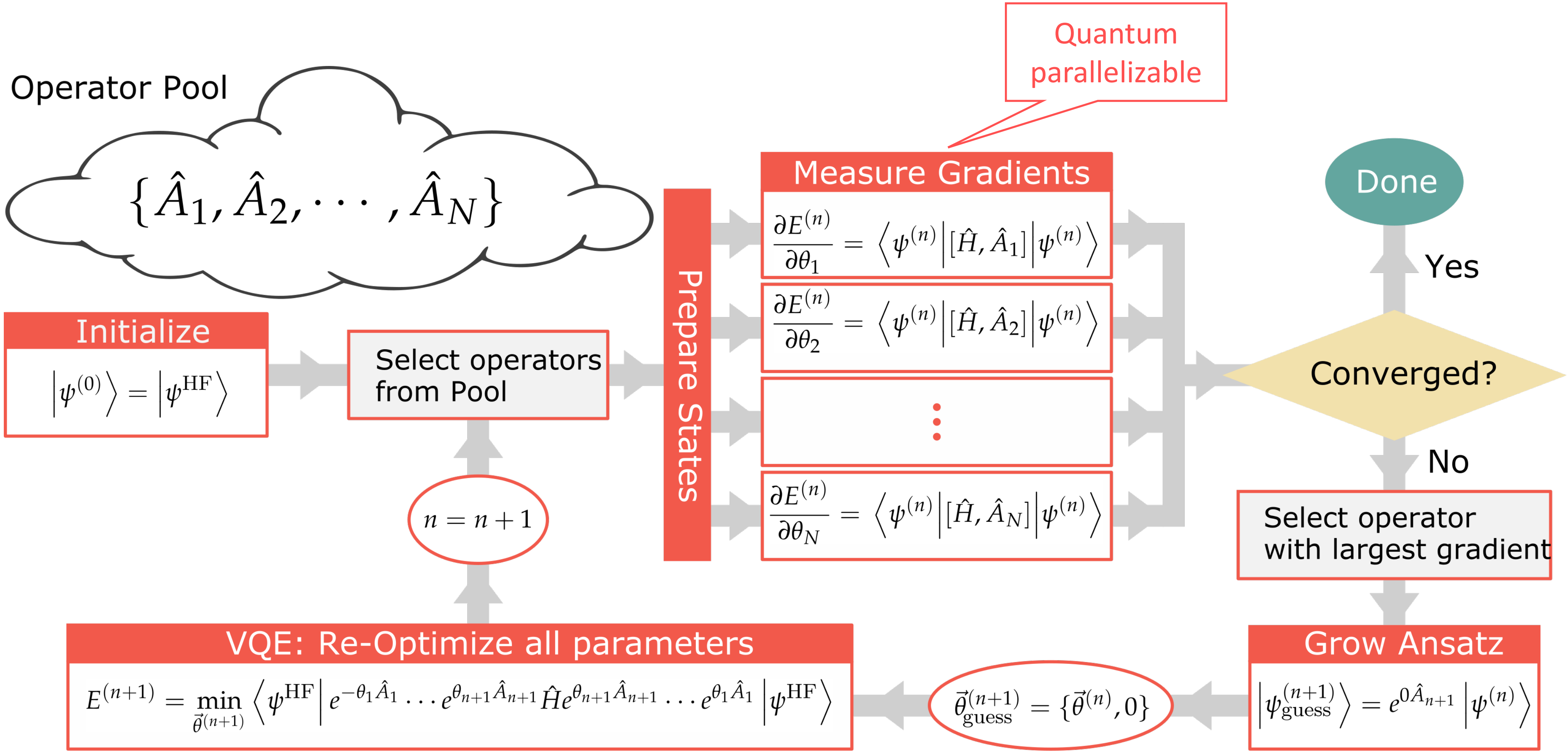
- Identify which $e^{\theta A}$ to apply to reference state $|\Psi_0\rangle$
- Take gradient of mean energy wrt θ

$$\frac{\partial}{\partial\theta}\langle\Psi_0|e^{-\theta A}He^{\theta \mathrm{A}}|\Psi_0\rangle|_{\theta=0} = \langle\Psi_0|\underbrace{[H,A]}|\Psi_0\rangle$$

New Hermitian operator → measure on hardware

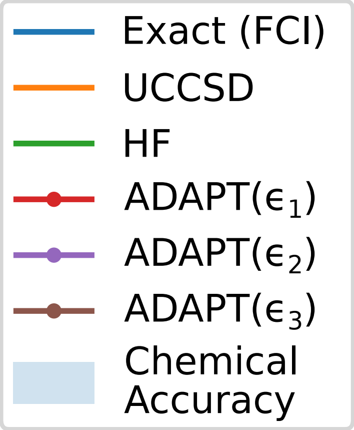
ADAPT-VQE overview

Adaptive **D**erivative **A**ssembled **P**roblem **T**ailored VQE

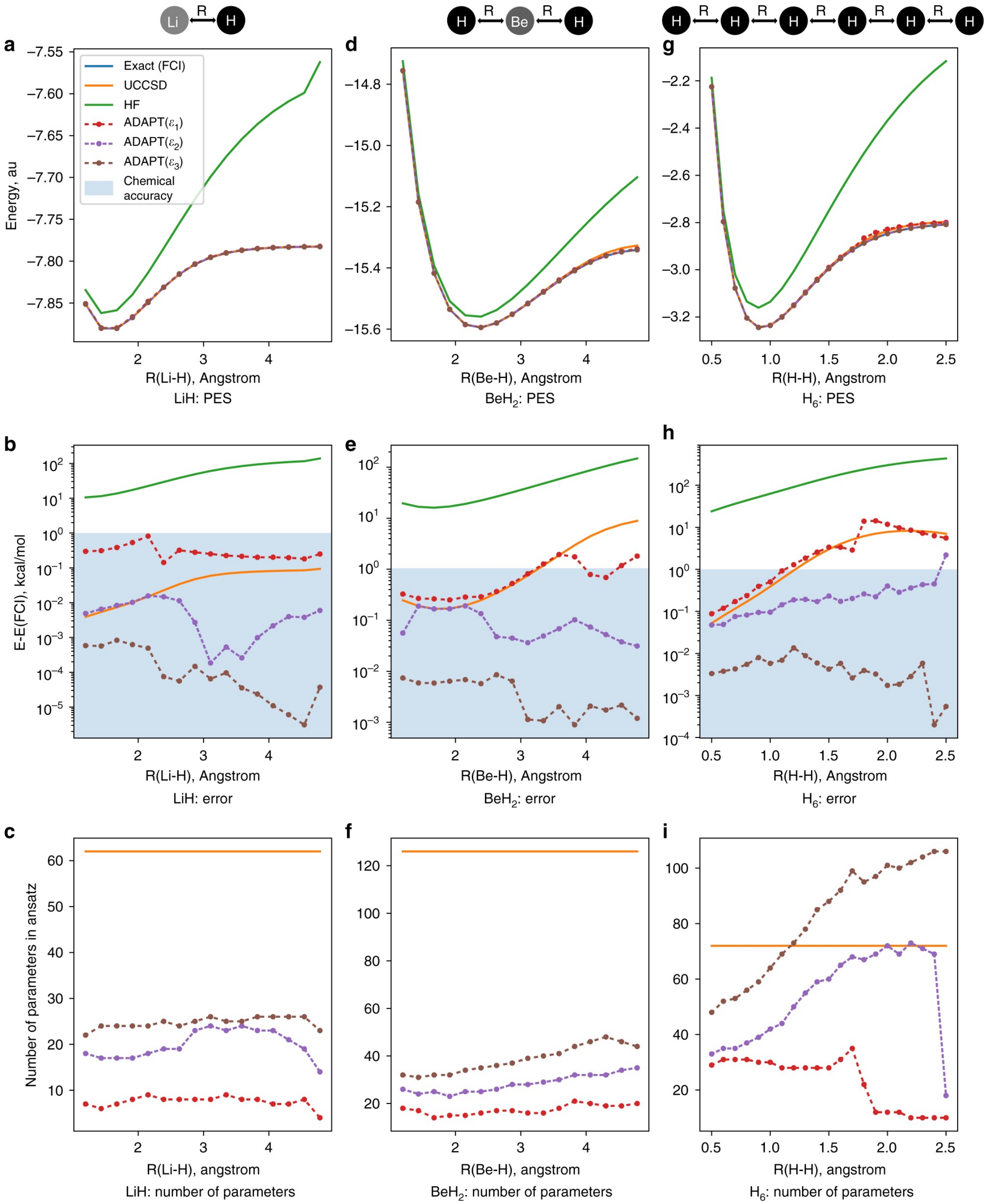


Grimsley, Economou, Barnes, Mayhall, Nature Communications **10**, 3007 (2019)

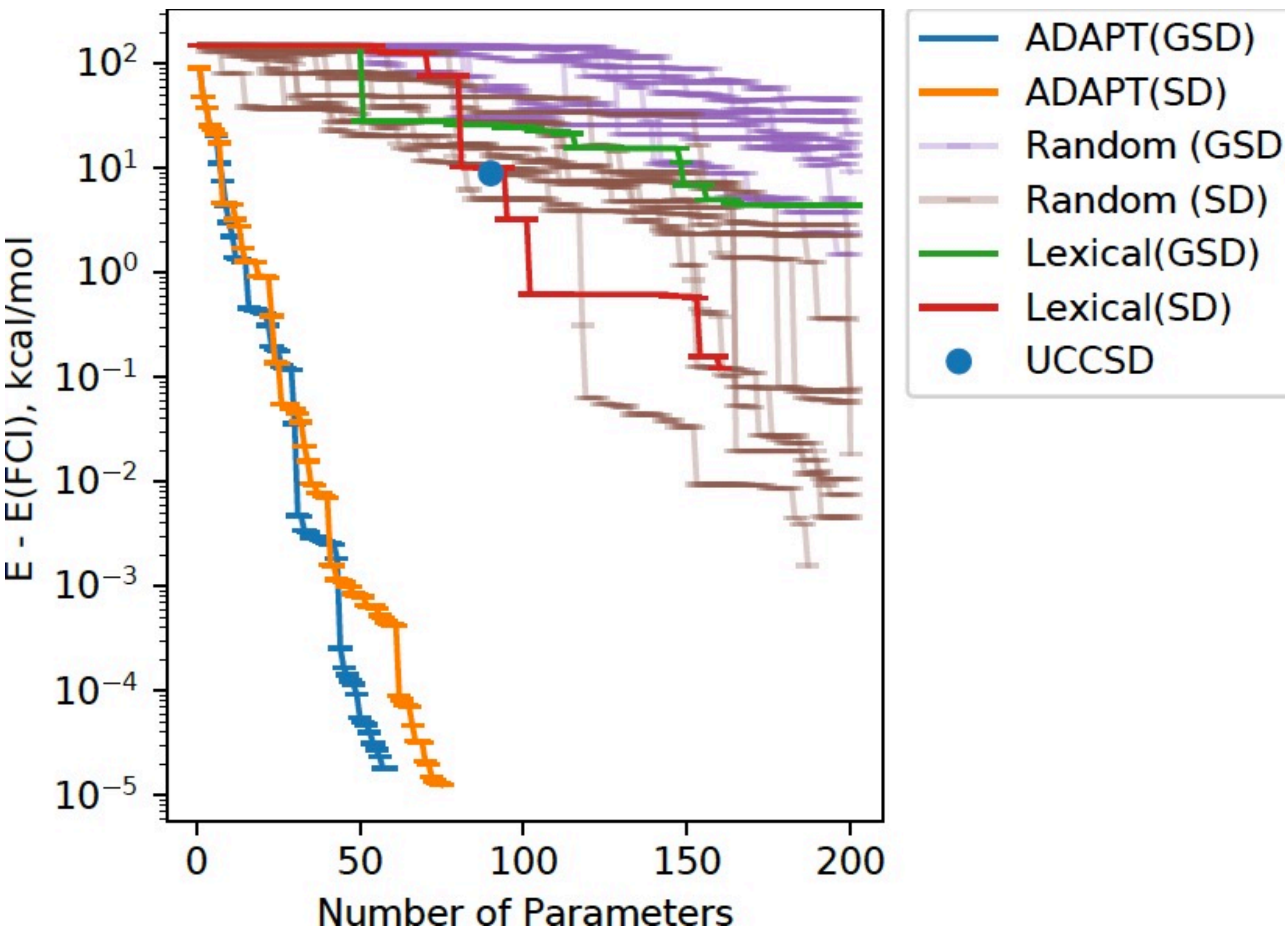
Results



$$\epsilon_1 = 0.1$$
$$\epsilon_2 = 0.01$$
$$\epsilon_3 = 0.001$$



Comparing ADAPT to other pseudo-Trotter orderings

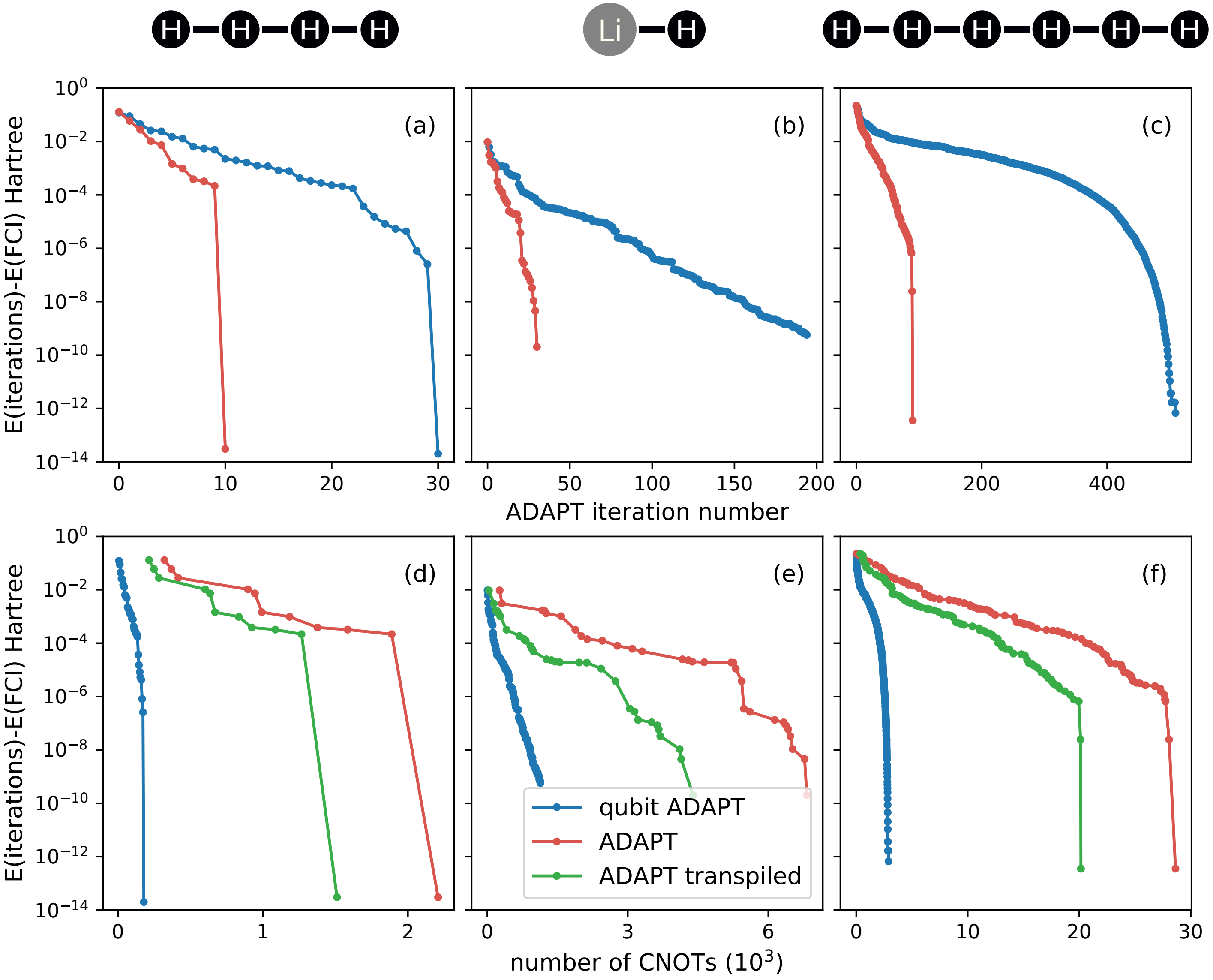


BeH_2
bond distance 2.39 Å

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

Qubit ADAPT-VQE—results

Hardware-efficient pool $\{e^{i\theta_j P_j}\}$, where P_j is a Pauli string with up to 4 Paulis



- 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?

Operator Pool

$$\{\hat{A}_1, \hat{A}_2, \cdots, \hat{A}_N\}$$

- We can choose it according to hardware constraints
- However, 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 $\{B_i\} = \{A_1, A_2, ..., [A_1, A_2], ..., [A_1, [A_2, A_3]], ...\}$

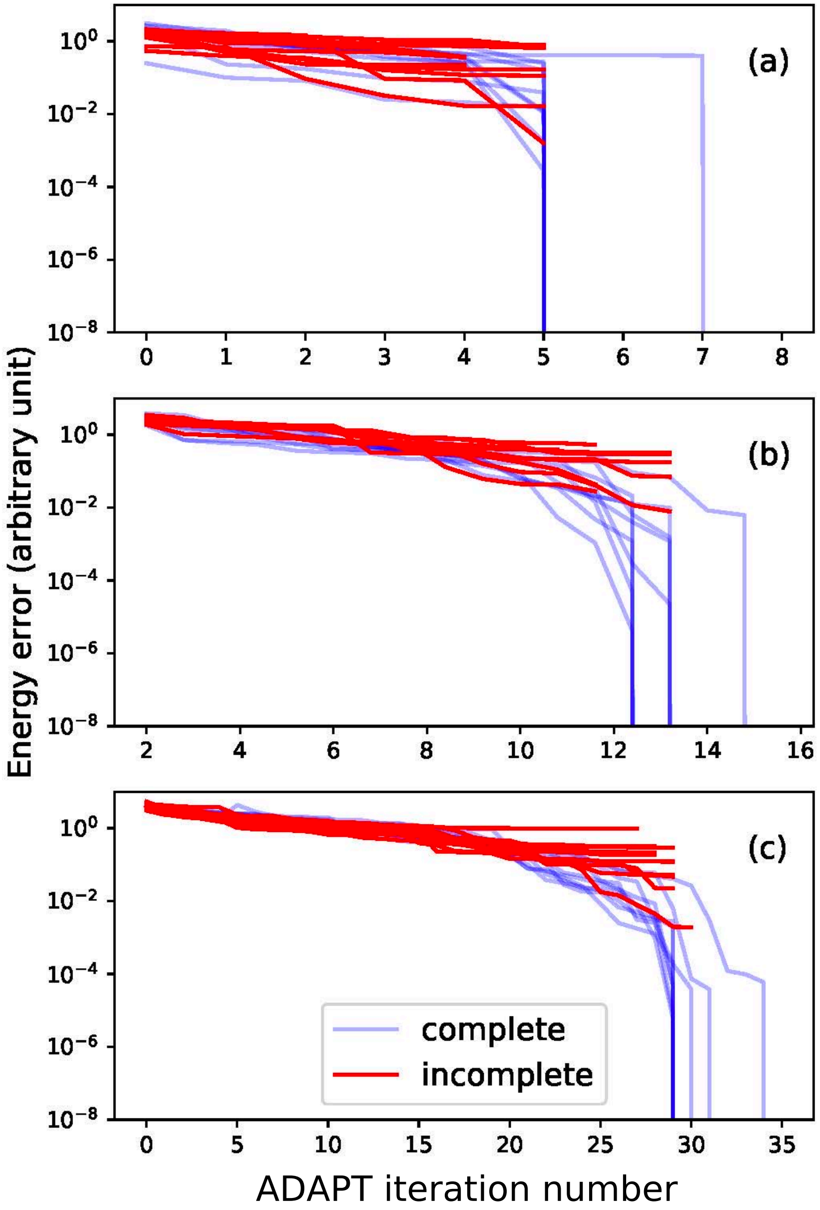
We have a complete pool and qubit-ADAPT is capable of converging to the exact ground state* when states $B_i|\psi\rangle$ form a complete basis (where $|\psi\rangle$ is an arbitrary *real* state)

*We are assuming throughout that we have time reversal symmetry → all eigenstates are real

Complete vs incomplete pool convergence

Test complete vs incomplete pools for random Hamiltonians for (a) 3 qubits, (b) 4 qubits, (c) 5 qubits

For pools that satisfy completeness criterion ADAPT always converges



Minimal complete pools (MCPs)

Minimal complete pool: smallest sized complete pool

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

Example of min complete pool
"*G* pool"

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

Shkolnikov, Mayhall, Economou, Barnes, arXiv:2109.05340

Proof of *G* pool completeness—outline

Show that any real state can be transformed into |000…> with *G* operators

- Define alternate pool *V*, which is comprised of products of *G* operators:

$$V_1 = ZZ\ldots ZY, \quad V_2 = ZZ\ldots ZYI,$$
$$V_3 = ZZ\ldots ZYII, \quad \ldots, \quad V_{n-1} = ZYII\ldots I, \quad V_n = YII\ldots I,$$
$$V_{n+1} = ZZ\ldots ZIYI, \quad V_{n+2} = ZZ\ldots ZIYII,$$
$$\ldots, \quad V_{2n-3} = ZIYII\ldots I, \quad V_{2n-2} = IYII\ldots I.$$

- Prove that any 3-qubit real state can be transformed to |000> using only *V* operators

- Inductive proof: assume it holds for *n* qubits and prove it holds for *n*+1 qubits

Sketch of proof for three qubits

Three-qubit V pool: $\{V_i\}_{n=3} = \{iZ_3Z_2Y_1, iZ_3Y_2, iY_3, iY_2\}$

Arbitrary 3-qubit state $\xrightarrow{Y_3}$ $|0\rangle|\psi_0\rangle + |1\rangle|\psi_1\rangle$ such that $\langle\psi_0|\psi_0\rangle = \langle\psi_1|\psi_1\rangle$

$$\xrightarrow{(I\pm Z_3)Y_2} |00\rangle\,|y_0\rangle + |01\rangle\,|y_1\rangle + |10\rangle\,|\chi_0\rangle + |11\rangle\,|\chi_1\rangle$$

such that $\langle y_0|y_0\rangle = \langle y_1|y_1\rangle = \langle\chi_0|\chi_0\rangle = \langle\chi_1|\chi_1\rangle$

$$\xrightarrow{Z_3Z_2Y_1,\,(I+Z_3)Y_2} \sqrt{2}|00\rangle\,|y'\rangle + |1\rangle\,(|0\rangle|\chi_0'\rangle + |1\rangle|\chi_1'\rangle)$$

$$\xrightarrow{Z_3Z_2Y_1,\,(I-Z_3)Y_2} |0\rangle|0\rangle|y\rangle + |1\rangle|0\rangle|\chi\rangle$$

$$\xrightarrow{Z_3Z_2Y_1, Y_3,\,Z_3Z_2Y_1} |0\rangle|0\rangle|0\rangle$$

Inductive proof

Define *n*-qubit pool $\{V_i\}_n = \{Z_n\{V_i\}_{n-1}, iY_n, iY_{n-1}\}$

Assume that V_n is complete

Using this assumption, prove that V_{n+1} is complete

The proof follows the same logic of the one for n=3

Shkolnikov, Mayhall, Economou, Barnes, arXiv:2109.05340

So far

- There exist complete pools of size $2n - 2$
- We have explicit examples of such pools, including a local (nearest-neighbor) one

→Pools that are complete and scale linearly with the number of qubits are available to ADAPT-VQE

Can we have even smaller complete pools?

Size of minimal complete pools—proof

- Need operators with odd number of Y Paulis (“odd Paulis”) to transform between arbitrary real states
- Algebra should contain odd operators that flip all possible 2^n combinations of qubits; e.g., YIIIZIZ, YYZIYXZ etc
- Instead of working with the algebra, we will work with the product group
- Can generate all possible flippings with product group generators: $\{Y_1, Y_2, \dots, \underbrace{Y_{n-1}, Z_{n-1}Y_n, Z_1, Z_2, \dots, Z_k}_{\text{Need to determine } k \text{ such that we can generate all odd flippings}}\}$

Need to determine k such that we can generate all odd flippings

$\boxed{\text{Must have } k \geq n-2 \Rightarrow 2n-2 \text{ is MCP size}}$

- This generator set can yield a pool through products that give odd Paulis O
- The algebra generated by this pool is contained in the product group

$[A,B]=0$	$\{A,B\}=0$
$O \cdot O = E$	$O \cdot O = O$
$E \cdot E = E$	$E \cdot E = O$
$O \cdot E = O$	$O \cdot E = E$

Criteria for MCPs

- Given a $2n - 2$ odd pool operators, how can we check for completeness?
- For an MCP, the following statements are equivalent*:

- *(a) The pool O_1, O_2, ..., O_{2n-2} is complete.*
- *(b) The pool O_1, O_2, ..., O_{2n-2} cannot be split into two mutually commuting sets.*
- *(c) The algebra generated by O_1, O_2, ..., O_{2n-2} spans all odd strings from the group G.*

where G is the product group

**We proved that (b) is necessary but not that it is sufficient; it is attractive because it takes polynomial time*

Shkolnikov, Mayhall, Economou, Barnes, arXiv:2109.05340

The role of symmetries

- Physical Hamiltonians typically have structure due to symmetries

- In this case, common issues with a random MCP are:
  - Qubit-ADAPT won't start
  - Qubit-ADAPT won't converge to g.s.

- This is because generically the pool operators do not respect symmetries
- Then the gradient criterion may not allow exiting a symmetry subspace

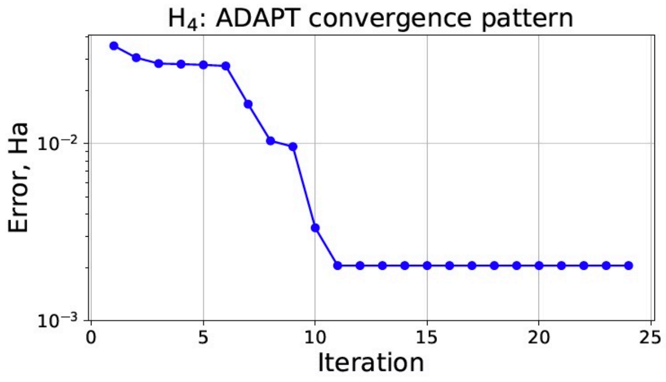
qubit-ADAPT won't find the path from HF to the g.s.

$$\langle\psi_{HF}|[\hat{P},\hat{H}]|\psi_{HF}\rangle = \\ = \langle(\hat{P}\psi_{HF})|\hat{H}|\psi_{HF}\rangle - \langle\psi_{HF}|\hat{H}|(\hat{P}\psi_{HF})\rangle = 0$$

P = Pauli string that violates particle number or spin

$$\langle +,+|[\hat{H},\hat{P}]|+,+\rangle = \\ 2\mathrm{Im}\,\langle +,+|\hat{H}|+,-\rangle = 0$$

P = Pauli string that violates parity (inversion or particle nr)



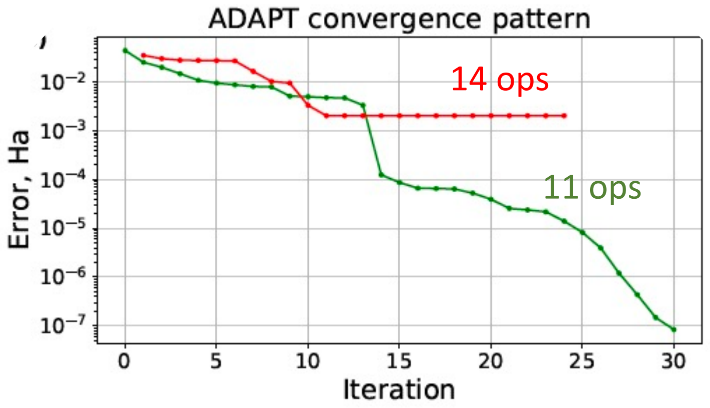
Incorporating symmetries

- These issues 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 uncorrelated state

- For convergence, ensure pool operators respect parity symmetries

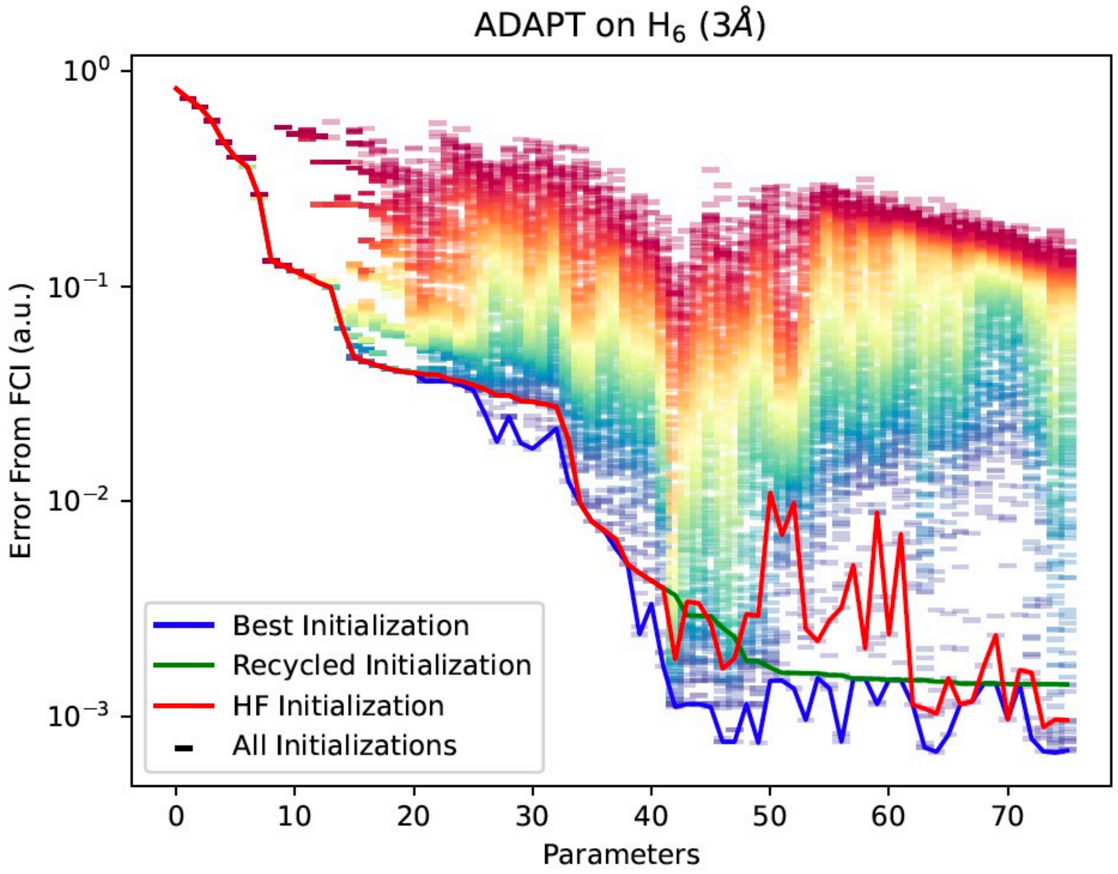
- Symmetry-preserving MCPs have fewer than $2n - 2$ operators
- This is because we do not need to span the full Hilbert space



Shkolnikov, Mayhall, Economou, Barnes, arXiv:2109.05340

Trainability of ADAPT

- ADAPT produces compact, problem tailored ansatze
- We numerically found that ADAPT converges before BPs set in
- Shallow circuit → the landscape is generally too rugged
- Trainability?
- ADAPT avoids the issues associated with trainability



Grimsley et al, in preparation

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Hardware currently noisy even for VQEs

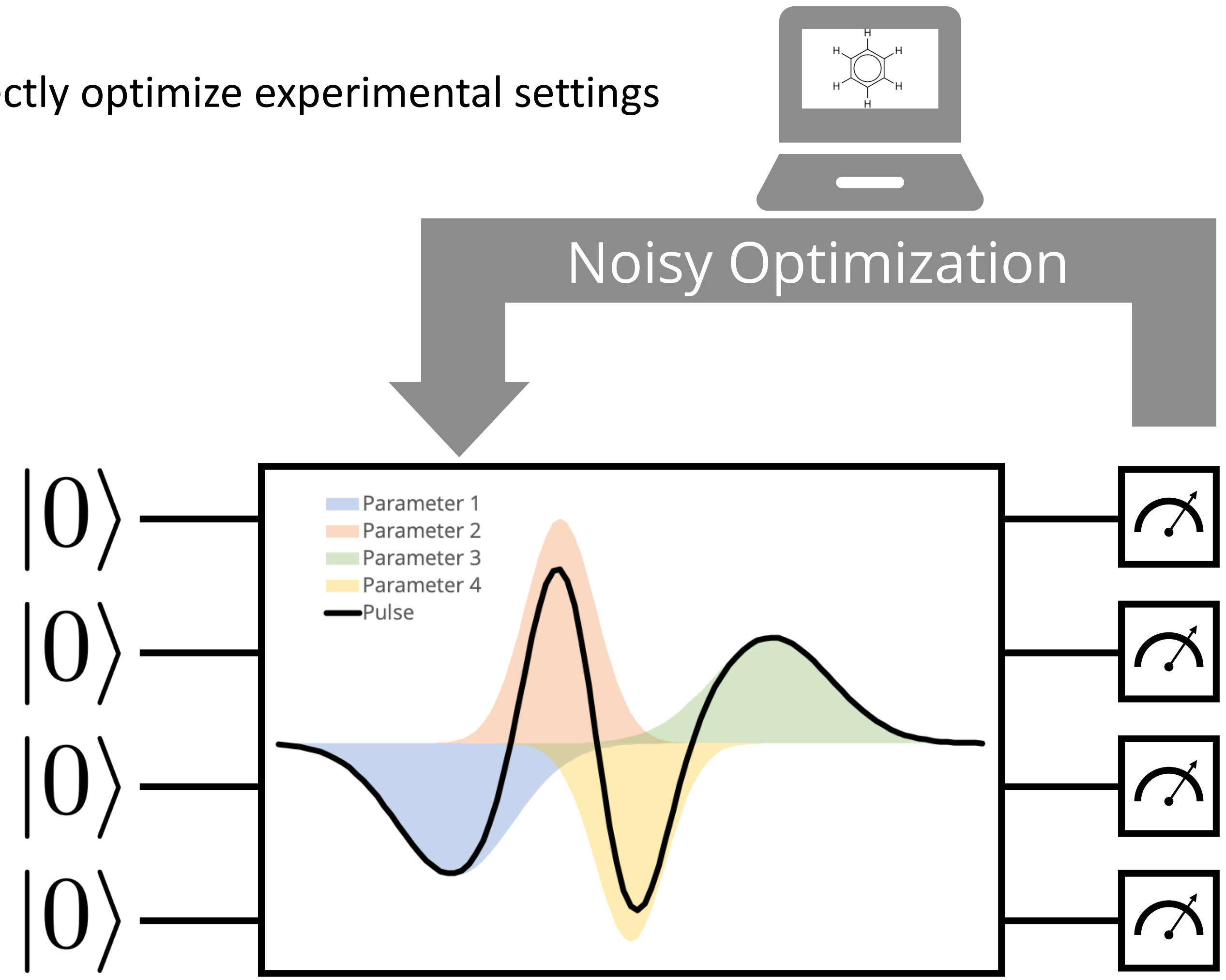
Pulse-level optimization:

- Instead of circuit, parameterize pulse directly
- Measure <H>
- Classical optimization → update pulse parameters
- Repeat until convergence

Meitei et al, npj Quantum Information 7, 155 (2021)
Yang et al, Phys. Rev. X **7**, 021027 (2017)
Magann et al, PRX Quantum 2, 010101 (2021)

ctrl-VQE

- Throw away circuit altogether - directly optimize experimental settings



Classical Simulation:

1. Pick a hardware Hamiltonian
2. Pick controls: 1 qubit microwave drives
3. Compute time evolution
4. Numerically optimize time-domain drives

Device Hamiltonian: Transmons

$$\hat{H}_D = \sum_{k=1}^{N} \left(\omega_k \hat{a}_k^\dagger \hat{a}_k - \frac{\delta_k}{2} \hat{a}_k^\dagger \hat{a}_k^\dagger \hat{a}_k \hat{a}_k \right) + \sum_{\langle kl \rangle} g(\hat{a}_k^\dagger \hat{a}_l + \hat{a}_l^\dagger \hat{a}_k)$$

Control Hamiltonian: RWA

$$\hat{H}_C = \sum_{k=1}^{N} \Omega_k(t)(e^{i\nu_k t}\hat{a}_k + e^{-i\nu_k t}\hat{a}_k^\dagger)$$

VQE Ansatz: Time evolution operator

$$\left|\psi^{\text{trial}}(\Omega_n(t), \nu_n)\right\rangle = \mathcal{T} e^{-i\int_0^T dt \hat{\tilde{H}}_C(t, \Omega_n(t), \nu_n)} \left|\psi_0\right\rangle$$

where:

$$\hat{\tilde{H}}(t)_C = e^{i\hat{H}_D t} \hat{H}_C(t) e^{-i\hat{H}_D t}$$

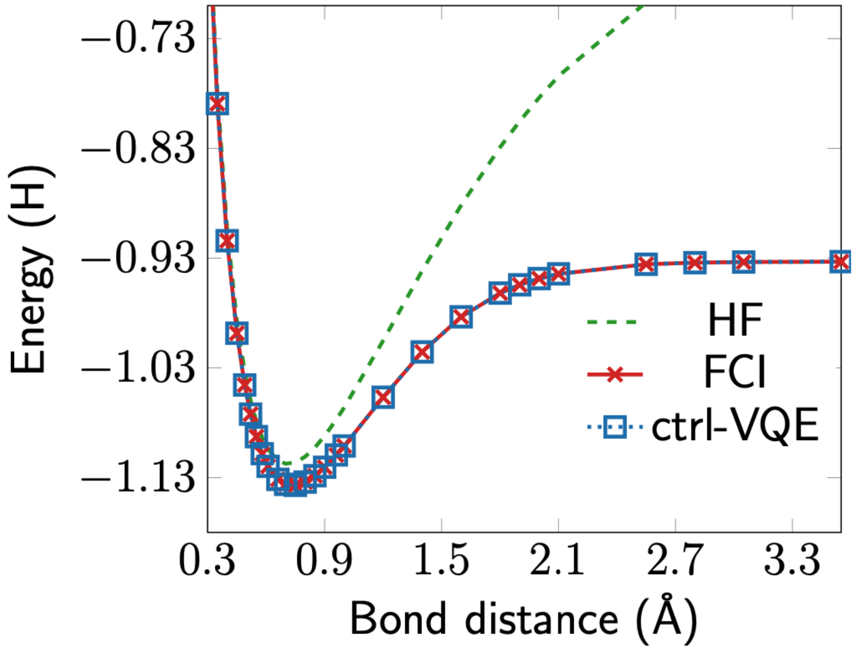
Objective Function: Molecular Energy

$$E(\Omega_n(t), \nu_n) = \left\langle \psi^{\text{trial'}} \right| \hat{H}^{\text{molecule}} \left| \psi^{\text{trial'}} \right\rangle$$

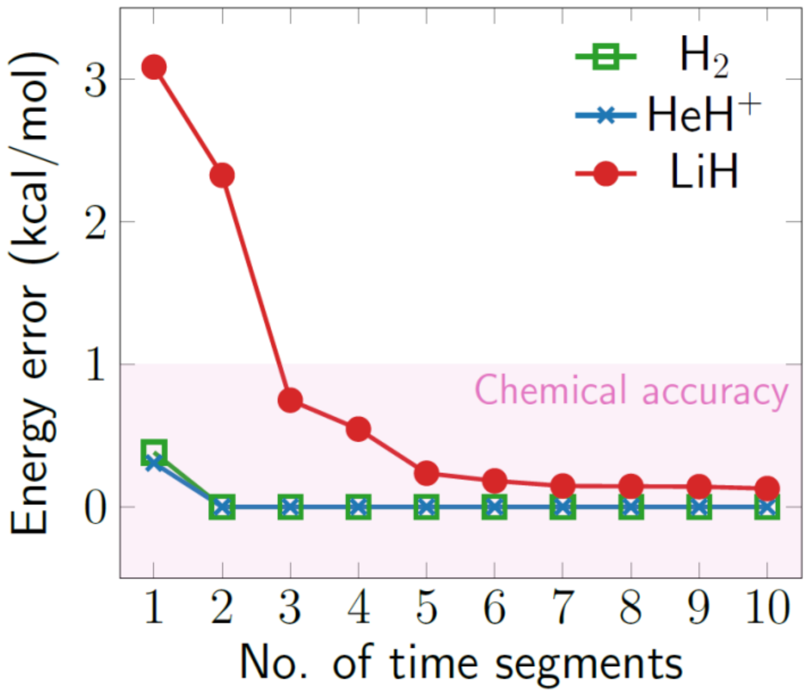
- *Fix pulse duration*
- Only optimize amplitude and frequency (frequency fixed throughout evolution)
- *Numerically,* we can optimize arbitrarily complex pulse shapes using analytic gradients
- *Experimentally*, this is difficult as finite differentiation is used
- To avoid this we propose the following adaptive parameterization to minimize the number of experimental gradients needed (split into n segments):

Nr of parameters: (n+1) per qubit

Dissociation curve for H2
(Indistinguishable from FCI)



Number of segments required for
convergence

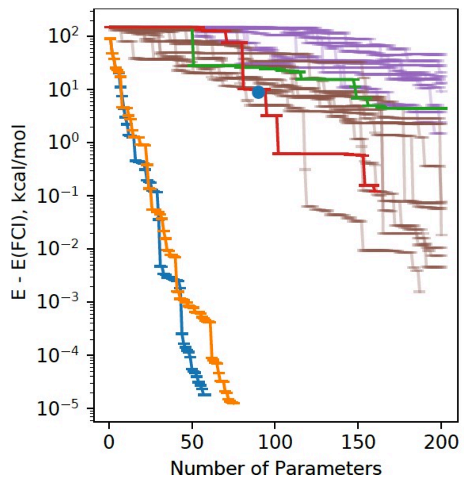


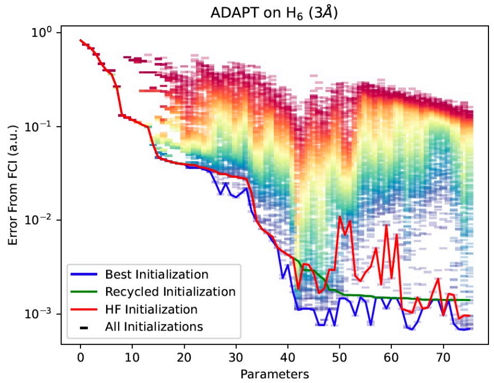
Rough comparison of coherence requirements for gate-based vs ctrl-VQE for LiH:
80,000ns (gate-based UCCSD) vs. 50ns (ctrl-VQE)

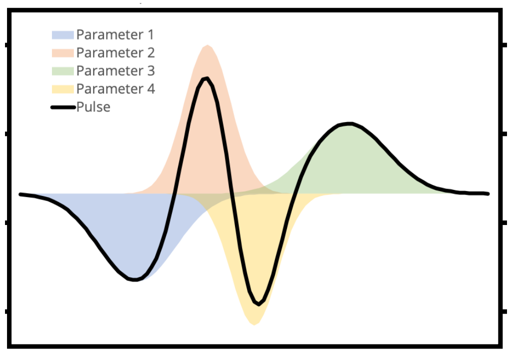
Meitei et al, npj Quantum Information 7, 155 (2021)

Conclusions

- Adaptive, problem tailored (ADAPT) VQE leverages the quantum computer to create an ansatz that is ideally suited to a given Hamiltonian
- Minimal complete pools scale linearly (2n-2) with the nr of qubits
- ADAPT-VQE burrows into the minimum, is immune to rugged landscape
- Even more near term: pulse-level instead of gate-level optimization



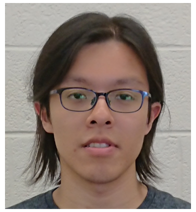




Grimsley, Economou, Barnes, Mayhall, Nature Commun. **10**, 3007 (2019)
Tang, Shkolnikov, Barron, et al, PRX Quantum **2**, 020310 (2021)
Shkolnikov, Mayhall, Economou, Barnes, arXiv:2109.05340
Meitei et al, npj Quantum Information **7**, 155 (2021)

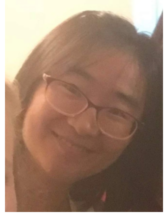
Collaborators

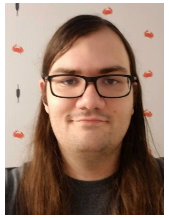
Group:


Ho Lun Tang


Sam Barron


Eva Takou


Fei Zhuang


Ada Warren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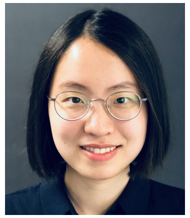
Chenxu Liu


Zahra Raissi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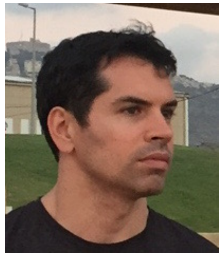
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