Ansatze for Noisy Variational Quantum Eigensolvers

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Outline

- The electronic problem
- Classical variational methods
- Predetermined ansatze for VQE
- Trainability issues
- Dynamic ansatze for VQE
- Noise-resilience of the approaches

The Electronic Problem: Classical Approaches
The Variational Principle

Schrödinger's non-relativistic time-independent equation

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle$$

Goal: understand the stable configurations and the motion of the quantum-mechanical system

The Variational Principle

$$\langle\psi|\,\hat{H}\,|\psi\rangle \geq E_0$$

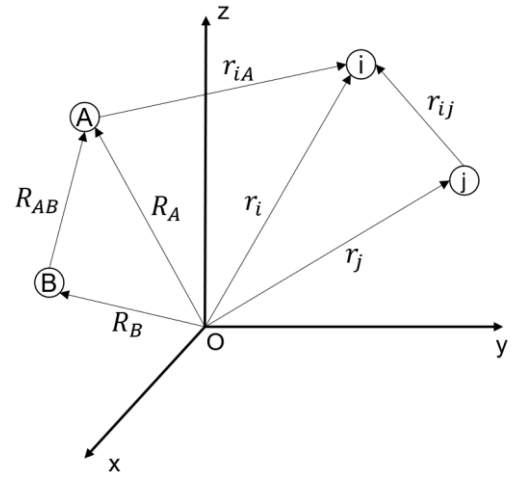
(assuming $\langle\psi|\psi\rangle = 1$)

- Under the variational principle, finding the ground state of the electronic Hamiltonian amounts to a minimization problem
- Excited states can be targeted as well (by e.g. imposing orthogonality constraints)

Molecular Dynamics

Schrödinger's non-relativistic time-independent equation

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle$$



Molecular Hamiltonian

$$\hat{H} = \underbrace{-\sum_{i=1}^{N}\frac{1}{2}\nabla_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M}\frac{Z_a}{r_{iA}} + \sum_{i=1}^{N}\sum_{j>i}^{N}\frac{1}{r_{ij}}}_{\text{Electronic Hamiltonian}} - \sum_{A=1}^{M}\frac{1}{2M_A}\nabla_A^2 + \sum_{A=1}^{M}\sum_{B>A}^{M}\frac{Z_A Z_B}{R_{AB}}$$

A. Szabo and N. S. Ostlund. Modern quantum chemistry: introduction to advanced electronic structure theory. Courier Corporation, 2012

The Electronic Problem: Classical Approaches
The Mean-Field Approximation

Electronic Hamiltonian

$$\hat{H}_e = -\sum_{i=1}^{N} \frac{1}{2}\nabla_i^2 - \sum_{i=1}^{N}\sum_{A=1}^{M} \frac{Z_a}{r_{iA}} + \sum_{i=1}^{N}\sum_{j>i}^{N} \frac{1}{r_{ij}}$$

Schrödinger Equation

$$\hat{H}\,|\psi\rangle = E\,|\psi\rangle$$

Mean-Field Approximation

$$\hat{f}(i) = -\frac{1}{2}\nabla_i^2 - \sum_{A=1}^{M} \frac{Z_a}{r_{iA}} + v(i)$$

$$\hat{f}(i)\chi(\vec{x}_i) = \epsilon\chi(\vec{x}_i)$$

The Electronic Problem: Classical Approaches
Variational Form

Hartree Method: Hartree Product

$$\psi(\vec{x}_1, \vec{x}_2, ..., \vec{x}_{N-1}, \vec{x}_N) = \chi_\alpha(\vec{x}_1)\chi_\beta(\vec{x}_2)...\chi_\pi(\vec{x}_{N-1})\chi_\rho(\vec{x}_N)$$

> Does not respect the antisymmetry principle $\psi(\vec{x}_1, ..., \vec{x}_i, ..., \vec{x}_j, ..., \vec{x}_N) = -\psi(\vec{x}_1, ..., \vec{x}_j, ..., \vec{x}_i, ..., \vec{x}_N)$

Hartree-Fock Method: Slater Determinant

$$\psi(\vec{x}_1, \vec{x}_2, ..., \vec{x}_{N-1}, \vec{x}_N) =$$

$$\begin{vmatrix} \chi_1(\vec{x}_1) & \chi_2(\vec{x}_1) & \cdots & \chi_{N-1}(\vec{x}_1) & \chi_N(\vec{x}_1) \\ \chi_1(\vec{x}_2) & \chi_2(\vec{x}_2) & \cdots & \chi_{N-1}(\vec{x}_2) & \chi_N(\vec{x}_2) \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \chi_1(\vec{x}_{N-1}) & \chi_2(\vec{x}_{N-1}) & \cdots & \chi_{N-1}(\vec{x}_{N-1}) & \chi_N(\vec{x}_{N-1}) \\ \chi_1(\vec{x}_N) & \chi_2(\vec{x}_N) & \cdots & \chi_{N-1}(\vec{x}_N) & \chi_N(\vec{x}_N) \end{vmatrix}$$

The Electronic Problem: Classical Approaches
Post-Hartree-Fock Methods

Full Configuration Interaction

$$|FCI\rangle = (1+T)\,|HF\rangle$$

-> Not tractable

Truncated Configuration Interaction

$$|CI\rangle = (1+T^{(k)})\,|HF\rangle$$

-> Not size-consistent

Truncated Coupled Cluster

$$|CC(k)\rangle = e^{T^{(k)}}\,|HF\rangle$$

-> Not variational

Truncated Unitary Coupled Cluster

$$|UCC(k)\rangle = e^{T^{(k)}-T^{(k)\dagger}}\,|HF\rangle$$

*-> Not **classically** tractable*

Cluster Operator

$$T = \sum_{i=1}^{N} T_i,$$

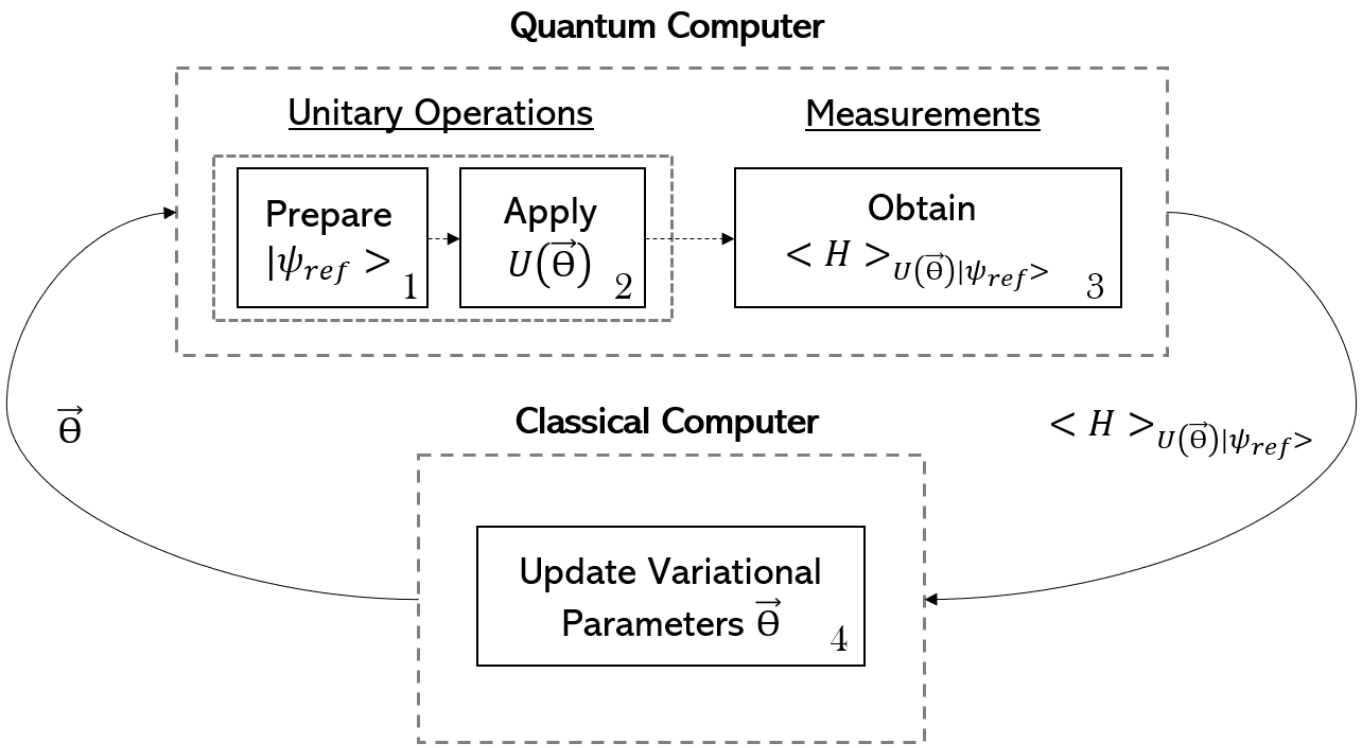
$$T_1 = \sum_{i,a} t_a^i a_a^\dagger a_i$$

$$T_2 = \sum_{i>j,a>b} t_{ab}^{ij} a_a^\dagger a_b^\dagger a_i a_j$$

$$\vdots$$

Truncated Cluster Operator

$$T^{(k)} = \sum_{i=1}^{k} T_i$$



- Measurement of the energy of variational wavefunctions on the quantum computer
- Small-depth circuits and classical feedback for hybrid computation
- Goal: solve quantum chemistry problems using near-term quantum computers

Variational Quantum Eigensolver

PERUZZO ET AL. A VARIATIONAL EIGENVALUE SOLVER ON A PHOTONIC QUANTUM PROCESSOR. NATURE COMMUNICATIONS 5 (1), 4213 (2014).

Predetermined Ansatze for VQE

Problem-Tailored

Example: Unitary Coupled Cluster Singles and Doubles

$$|UCCSD\rangle = e^{(T_1+T_2)-(T_1^\dagger+T_2^\dagger)}\,|HF\rangle$$

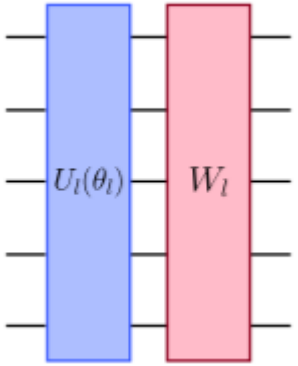
> Less hardware-efficient

Problem-Agnostic

Example: Random Parameterized Quantum Circuits

$$U(\boldsymbol{\theta}) = U(\boldsymbol{\theta}_1.....\boldsymbol{\theta}_L) = \prod_{l=1}^{L} V(\boldsymbol{\theta}_l)W_l$$

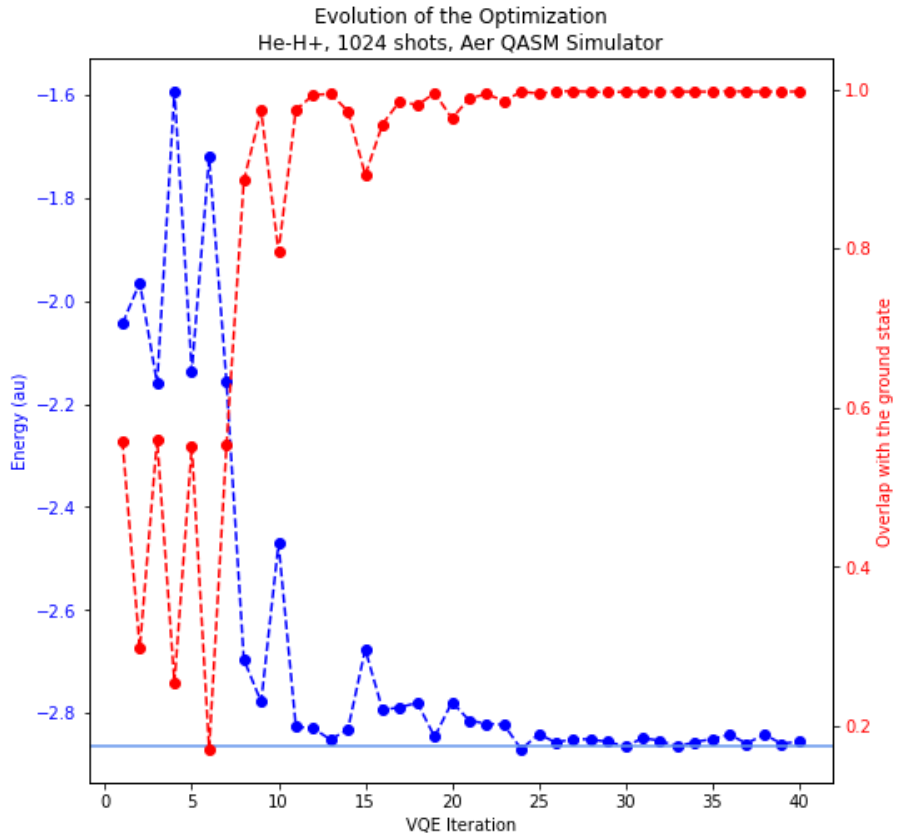
$$V(\boldsymbol{\theta}_l) = \bigotimes_{j=1}^{Q} R_{lj}(\theta_{lj})$$



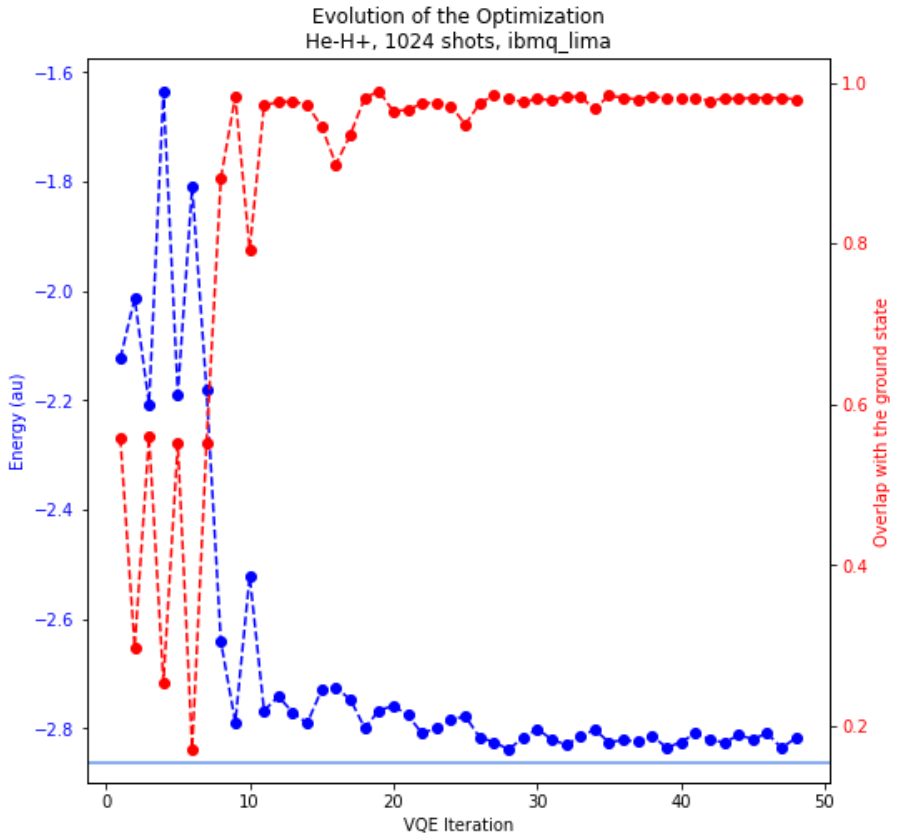
> More trainability issues

J. R. McClean et al. “Barren plateaus in quantum neural network training landscapes”. Nature Communications, 9(1), Nov 2018

VQE Optimization (He-H+)

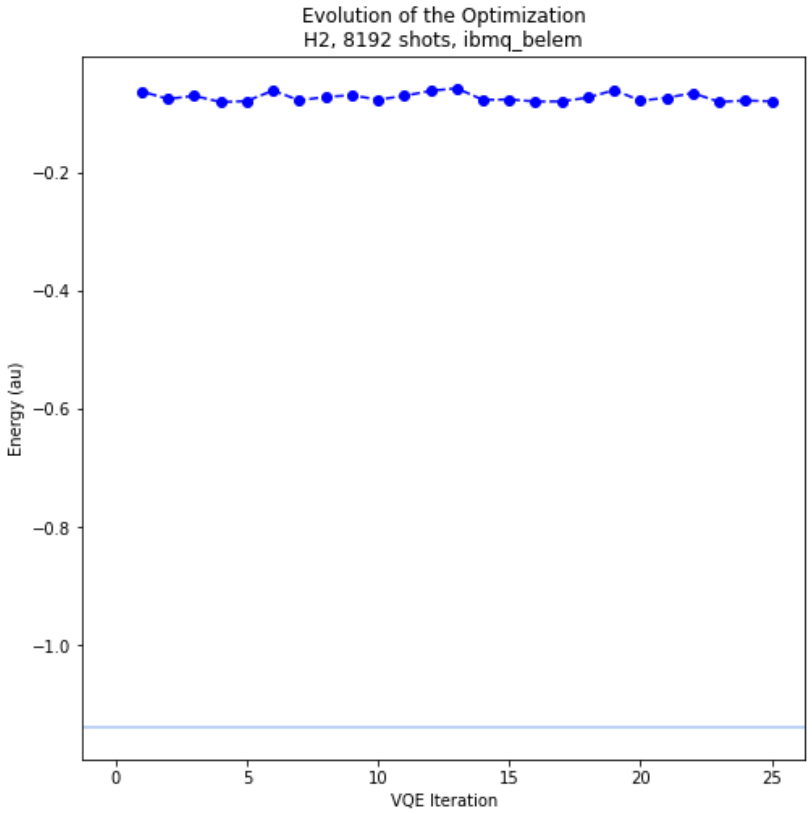


Simulator, 1024 shots



ibmq_lima, 1024 shots

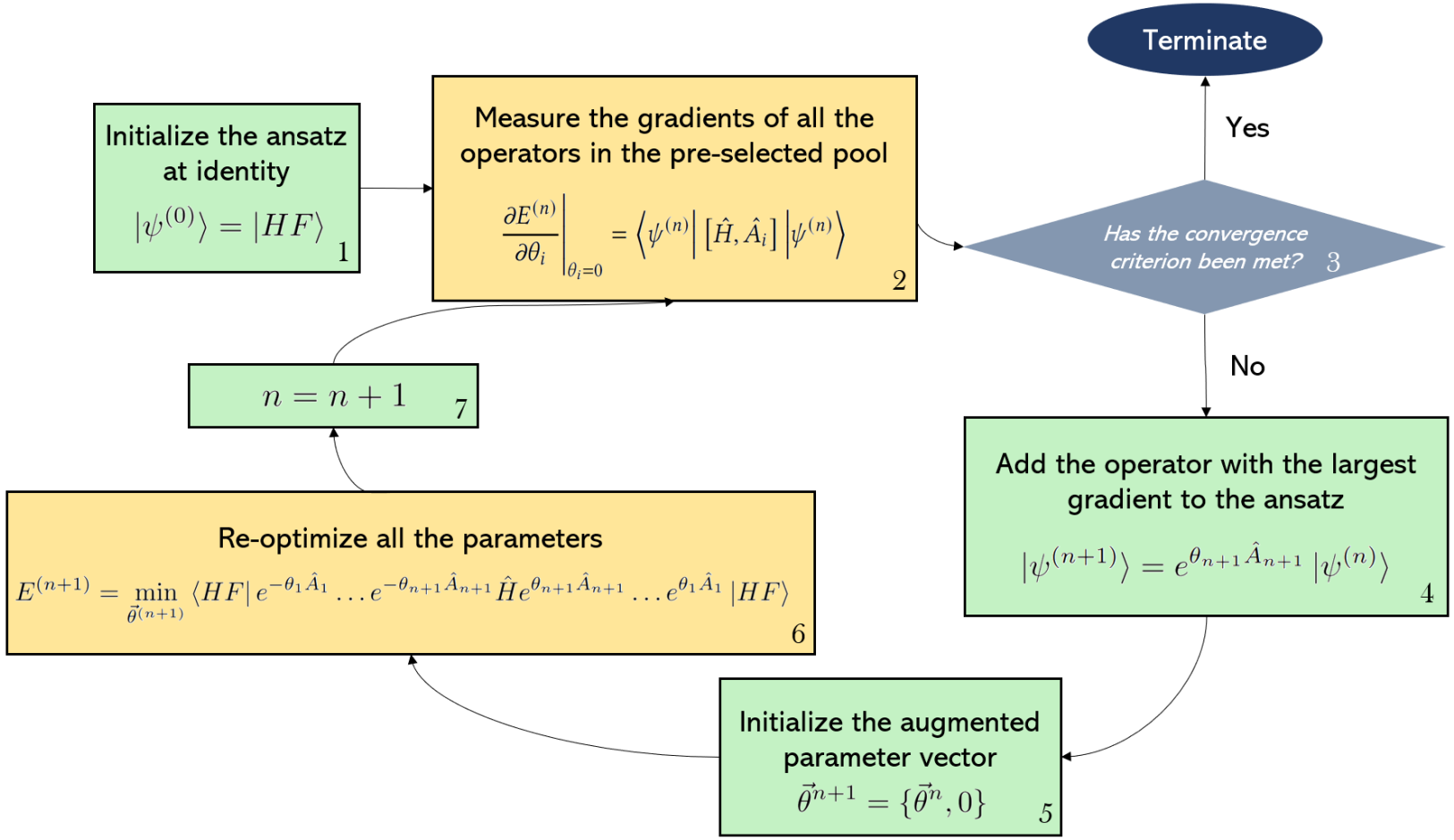
Noise-Induced Barren Plateaus



UCCSD-VQE for H2 in ibmq_belem

In addition to preventing proper evaluation of the cost function, incoherent noise may lead to an exponential decay of the gradients with the size of the system.

S. Wang et al. Noise-Induced Barren Plateaus in Variational Quantum Algorithms. 2021. arXiv:2007.14384 [quant-ph].



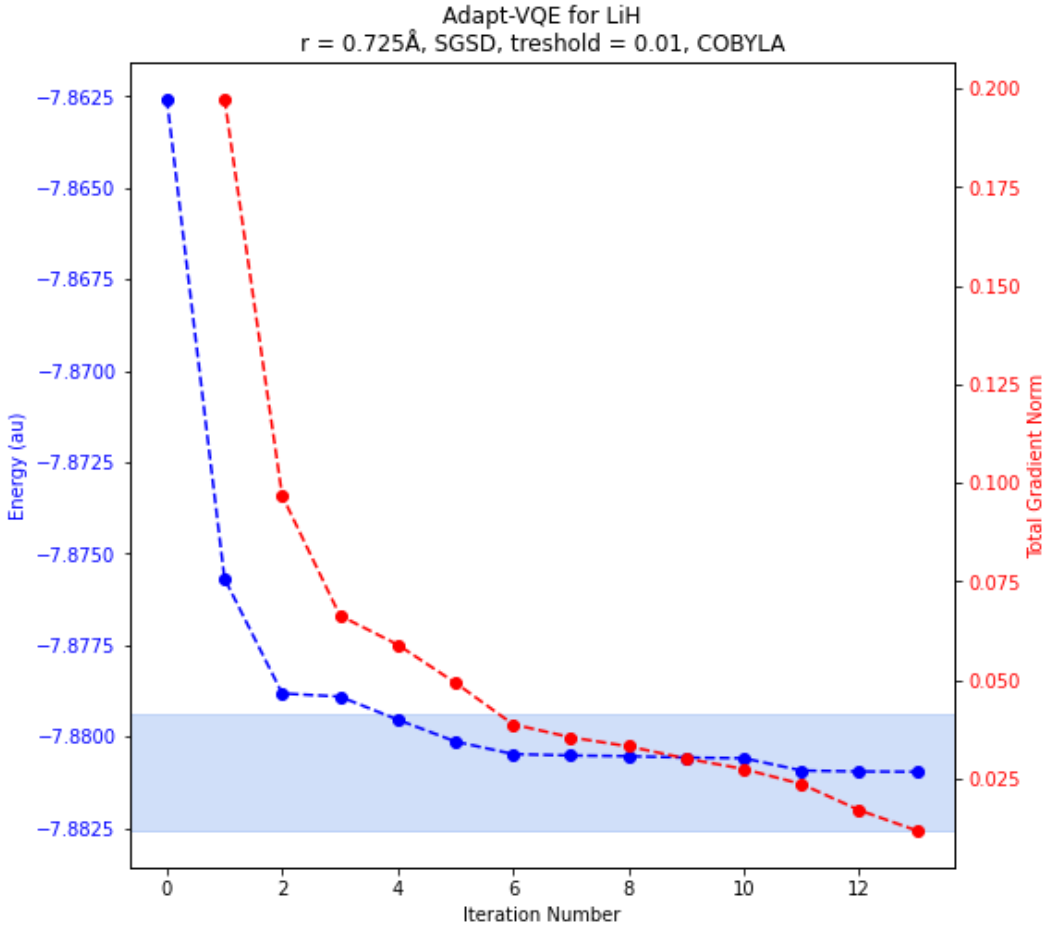
ADAPT-VQE

- Problem tailored, dynamically created ansatz
- Decrease circuit depth at the expense of more measurements and optimizations
- Shallow, NISQ-friendly circuits capable of high accuracy

TANG ET AL. QUBIT-ADAPT-VQE: AN ADAPTIVE ALGORITHM FOR CONSTRUCTING HARDWARE-EFFICIENT ANSATZES ON A QUANTUM PROCESSOR. PREPRINT ARXIV ARXIV:1911.10205 [QUANT-PH].

GRIMSLEY ET AL. AN ADAPTIVE VARIATIONAL ALGORITHM FOR EXACT MOLECULAR SIMULATIONS ON A QUANTUM COMPUTER. NATURE COMMUNICATIONS, 10(1), 3007 (2019).

ADAPT-VQE for LiH



Chemical accuracy achieved with 4 variational parameters, an over 10-fold decrease as compared to UCCSD

Fermionic-ADAPT-VQE

- *Operators are proper ferminic excitations*
- *Pool size grows like $O(N^4)$ on the number of orbitals*
- *Each operator is a linear combination of Pauli strings*
- *Average string length grows like $O(N)$*

Jordan-Wigner Transform

$$a_i^\dagger \rightarrow \frac{1}{2}\prod_{k=1}^{i-1} Z_k \cdot (X_i - iY_i)$$

$$a_i \rightarrow \frac{1}{2}\prod_{k=1}^{i-1} Z_k \cdot (X_i + iY_i)$$

→ *Anticommutation strings*

Example: Triplet Operator (Spin-Adapted Pool)

$$\hat{\tau}_{2,A} = \frac{1}{\sqrt{12}}\Big(2a_r^\dagger a_p a_s^\dagger a_q + 2a_{\bar{r}}^\dagger a_{\bar{p}} a_{\bar{s}}^\dagger a_{\bar{q}} + a_r^\dagger a_p a_{\bar{s}}^\dagger a_{\bar{q}} + a_{\bar{r}}^\dagger a_{\bar{p}} a_s^\dagger a_q + a_r^\dagger a_{\bar{p}} a_{\bar{s}}^\dagger a_q + a_{\bar{r}}^\dagger a_p a_s^\dagger a_{\bar{q}}\Big) - h.c.$$

→ *48 Pauli strings*

GRIMSLEY ET AL. AN ADAPTIVE VARIATIONAL ALGORITHM FOR EXACT MOLECULAR SIMULATIONS ON A QUANTUM COMPUTER. NATURE COMMUNICATIONS, 10(1), 3007 (2019).

Qubit-ADAPT-VQE

- Decompose fermionic operators into the individual Pauli strings and dispose of the Jordan-Wigner string
- Decrease circuit depth per operator at the expense of a higher measurement overhead
- Pool size still grows like $O(N^4)$ (with a worse prefactor)
- Average string length grows like $O(1)$

Example: simple double excitation

Fermionic Pool

$$a_p^\dagger a_q^\dagger a_r a_s - a_r^\dagger a_s^\dagger a_p a_q$$

1 operator in pool, linear combination of 8 Pauli strings of length $O(N)$

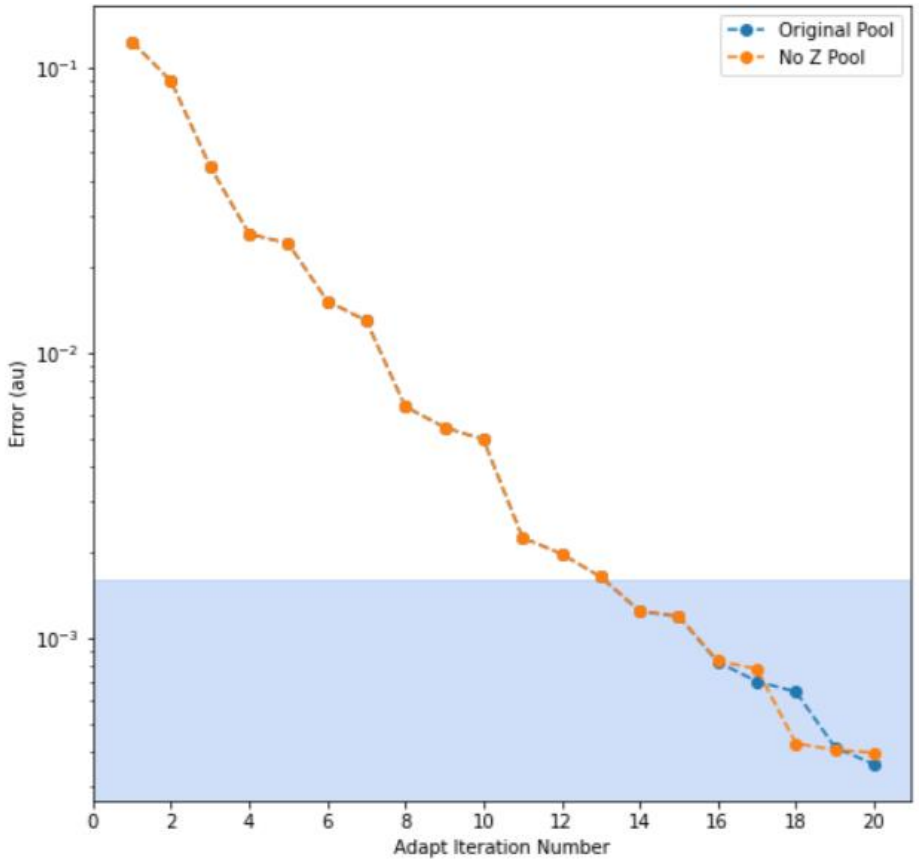
Qubit Pool

$$i \cdot Y_q X_p X_s X_r \quad i \cdot X_q Y_p X_s X_r \quad i \cdot X_q X_p Y_s X_r \quad i \cdot X_q X_p X_s Y_r$$
$$i \cdot X_q Y_p Y_s Y_r \quad i \cdot Y_q X_p Y_s Y_r \quad i \cdot Y_q Y_p X_s Y_r \quad i \cdot Y_q Y_p Y_s X_r$$

8 operators in pool, single Pauli strings of length 4 regardless of system size

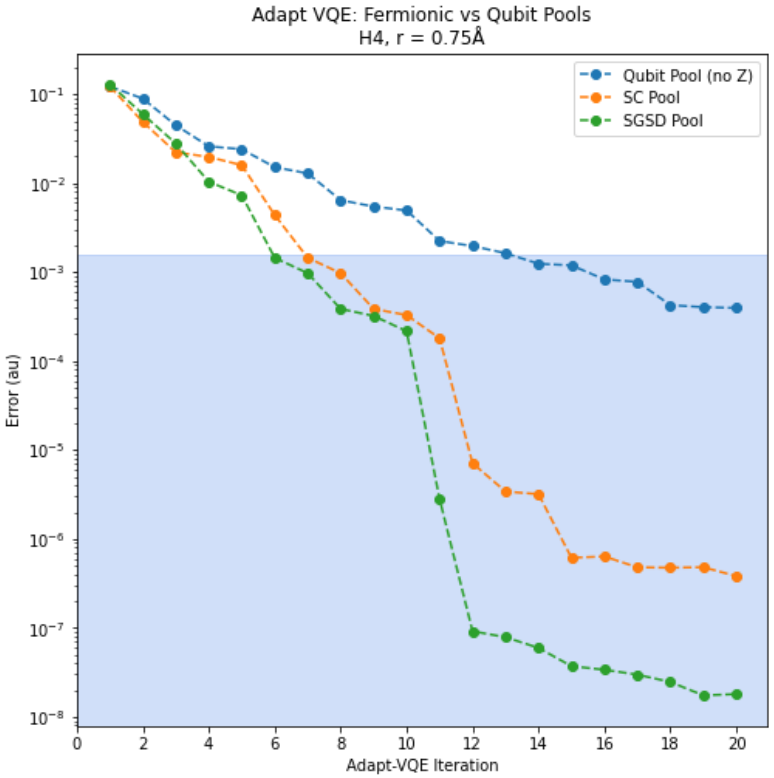
TANG ET AL. QUBIT-ADAPT-VQE: AN ADAPTIVE ALGORITHM FOR CONSTRUCTING HARDWARE-EFFICIENT ANSATZES ON A QUANTUM PROCESSOR. PREPRINT ARXIV ARXIV:1911.10205 [QUANT-PH].

Qubit Pool: Effect of the Jordan-Wigner String (H4)

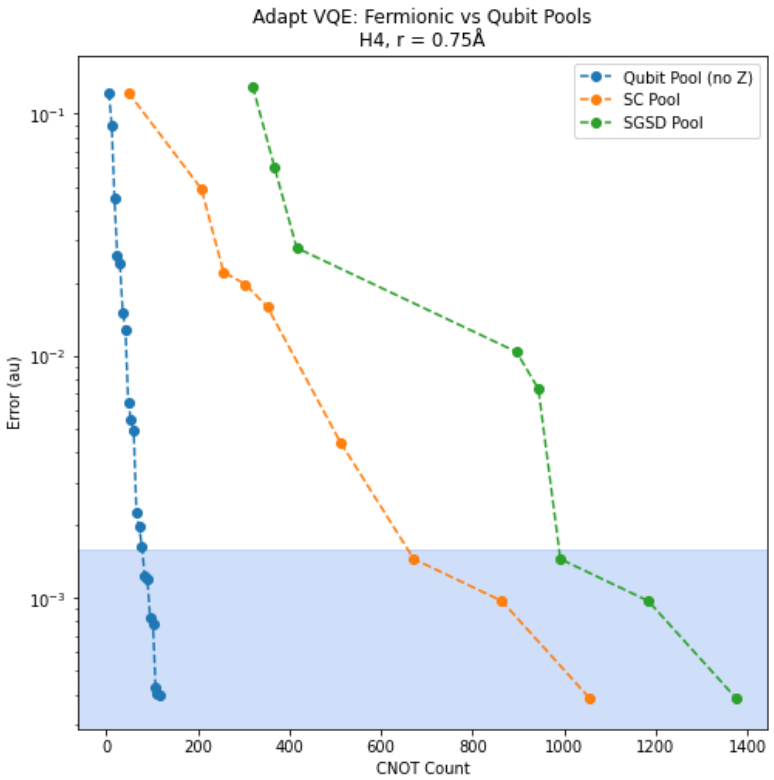


Despite worsening the scaling of the circuit depth per operator, respecting fermionic anticommutation does not seem to contribute to convergence

Fermionic vs Qubit Pools (H4)



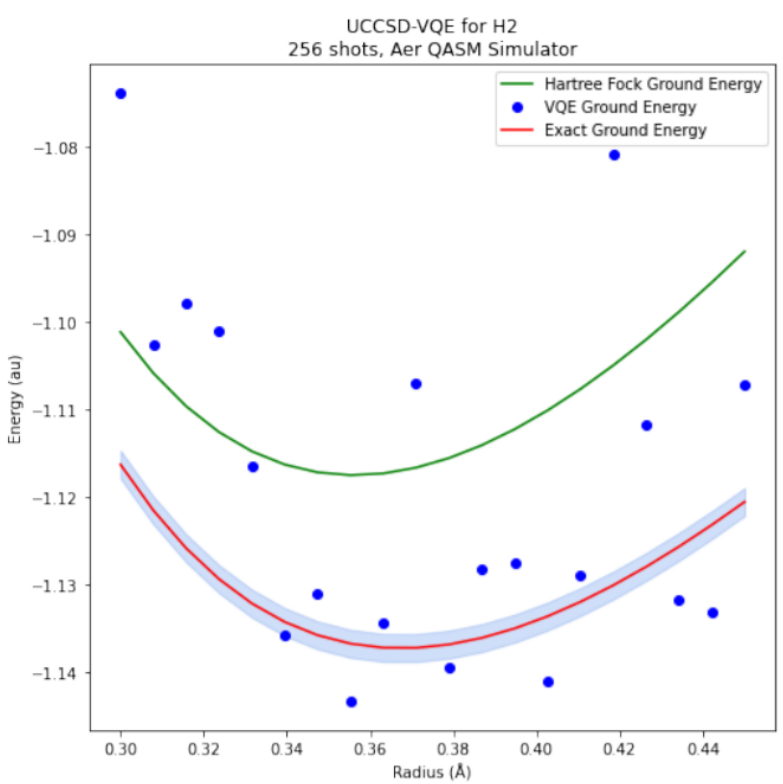
Error vs Iteration



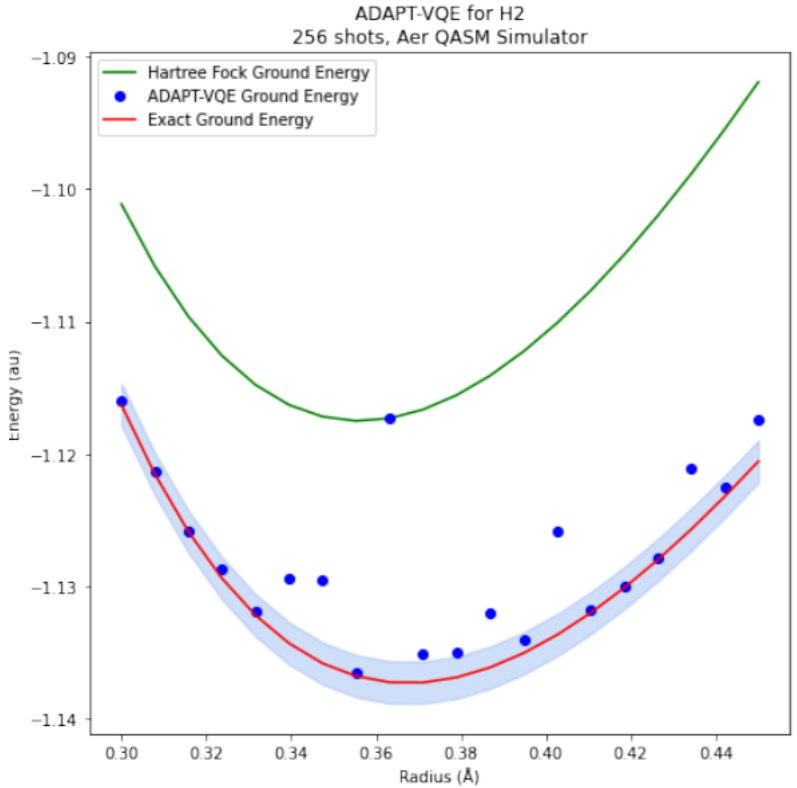
Error vs CNOT Count

UCCSD vs ADAPT (H2): Noise-Resilience

Simulator, 256 shots



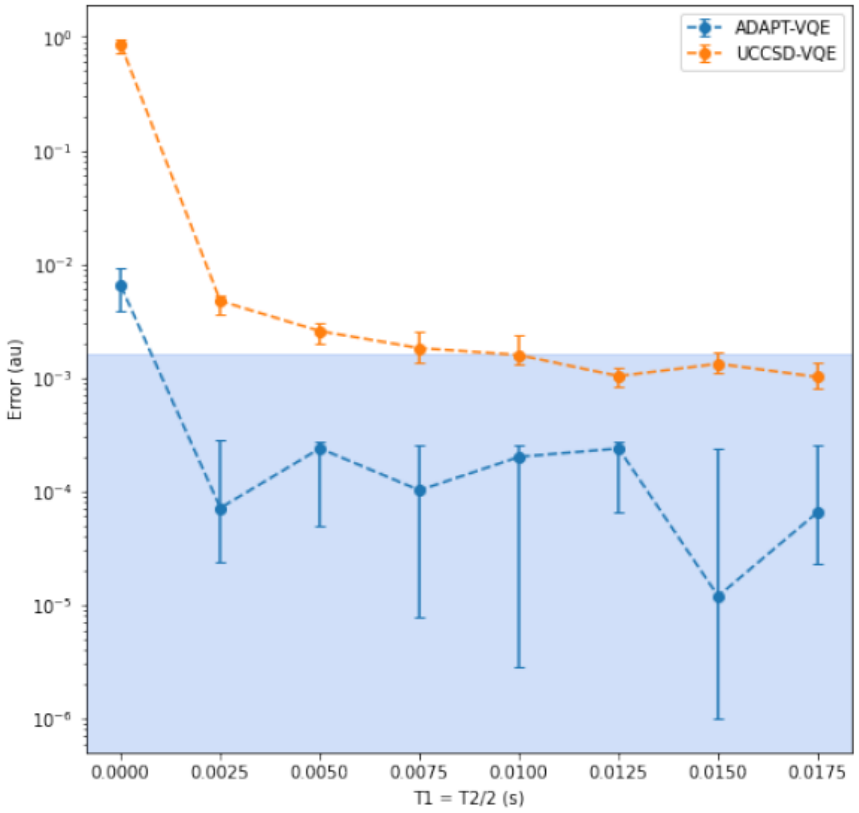
UCCSD-VQE



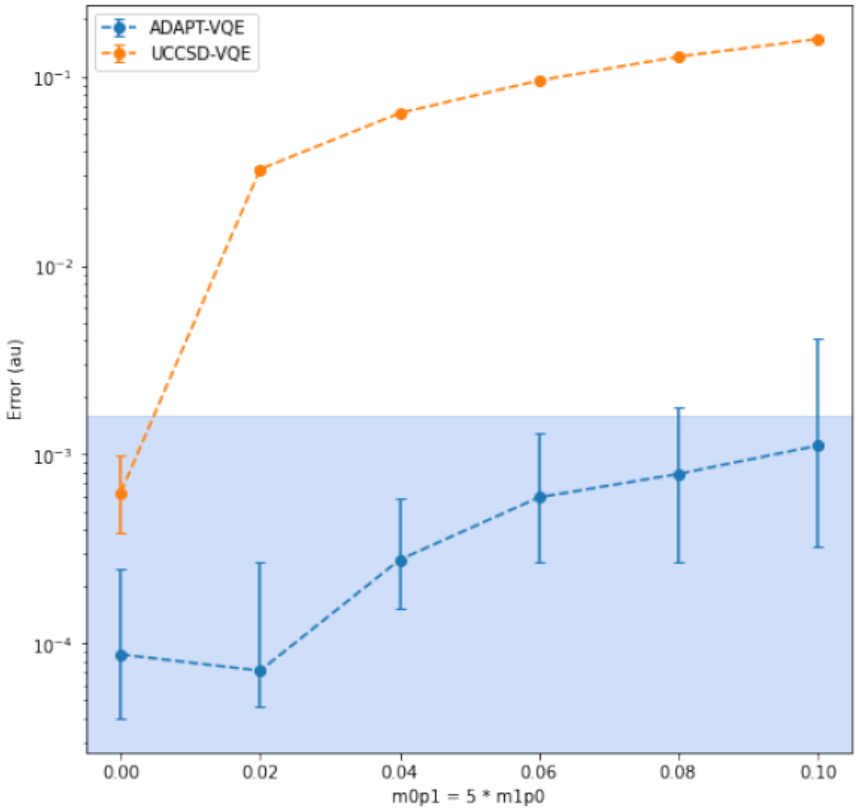
Qubit-ADAPT-VQE

UCCSD vs ADAPT (H2): Noise-Resilience

Thermal Relaxation



SPAM Errors



ADAPT-VQE: Minimal Pools

- It is possible to use symmetry-adapted minimal complete pools whose size grows like $O(N)$ without precluding convergence
- Measurements per iterations go down from $O(N^8)$ to $O(N^5)$ as compared to both fermionic- and qubit-ADAPT-VQE ($O(N^4)$ in tradicional VQE)

Example: Minimal Symmetry-Adapted Pool for LiH
(10-qubits under a frozen-core approximation)

XYYZIIZIZY, XYYYIZZZII, YYIZZZIZXY, XXZXZIIIYI, XYZYIZZIYI, XXXZIIZZZY, XXIIYXZZII,

XYXZXXXYZY, XXIYIIXYZY, IIZIZZYYXY, ZZXZXXIIZY, YZZZXYZZZY, YXZZIZYYII,IXIZXXZZYI

ZHU ET AL. AVOIDING SYMMETRY ROADBLOCKS AND MINIMIZING THE MEASUREMENT OVERHEAD OF ADAPTIVE VARIATIONAL QUANTUM EIGENSOLVERS. PREPRINT ARXIV ARXIV:2109.05340 [QUANT-PH].

Conclusions and Overview

- Since the quantum-mechanical description of chemical systems requires an exponential number of bits but a linear number of qubits, quantum chemistry is a promising area of application for quantum computing.

- The variational quantum eigensolver was proposed in the context of the NISQ era. The noise-resilience and hybrid nature of VQE bring hope that it may allow solving relevant quantum chemistry problems in near-term quantum computers.

- An improper choice of ansatz may lead to trainability issues that obstruct the path to quantum advantage.

- Because they are problem- and system-tailored, dynamic ansatze (as the one from ADAPT-VQE) may help reach high-accuracy solutions with shallower circuits than predetermined options.

Thank you for your attention!