ADAPT-VQE: Quasi-optimally compact wavefunctions for simulating molecules on a quantum computer

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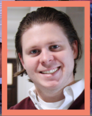
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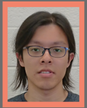
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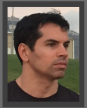
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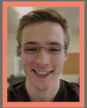
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- For years, Computational Chemistry grew alongside computational resources
- **Moore's Law ending?:** parallelization difficult for quantum many-body problems
- **Quantum computing:** possible path for continuing Moore's law

  Quantum computing is the use of quantum-mechanical phenomena such as **superposition** and **entanglement** to perform computation.

- Recent investments have led to rapid growth of hardware/algorithms
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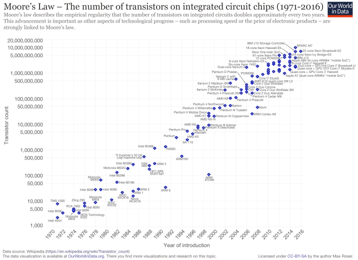

Extending Moore’s Law

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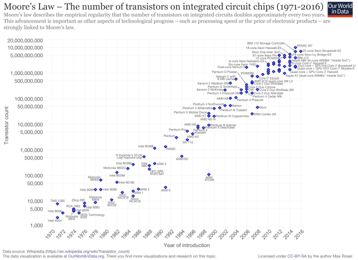

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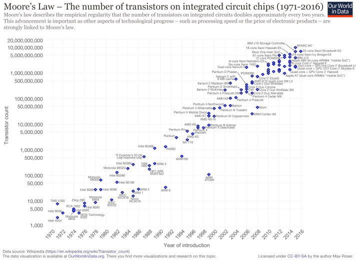

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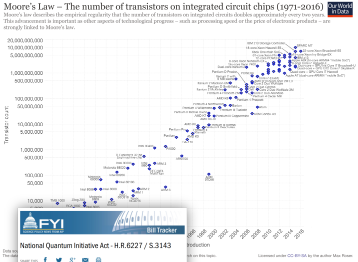

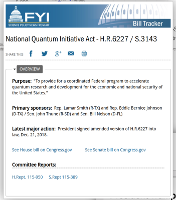

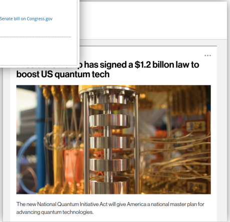

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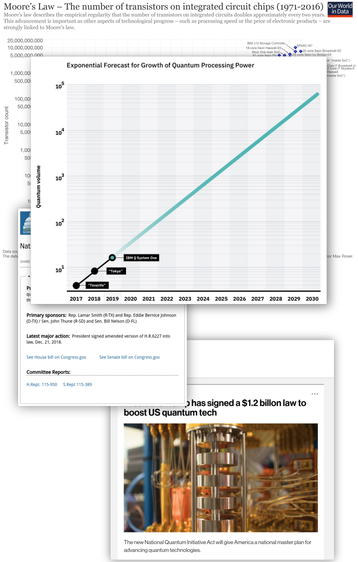
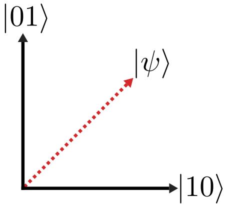


- Natural representation of quantum states $\rightarrow$ Computational speedup
- **Classical Computer**: Only represents "classical" basis vectors
  - Store (manipulate) quantum state as vector of numbers in memory
- **Quantum Computer**: Directly represents arbitrary vector in Hilbert space
  - Create (measure) quantum state on hardware to mimic simulated quantum state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|10\rangle \pm |01\rangle\right)$$



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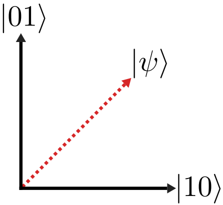

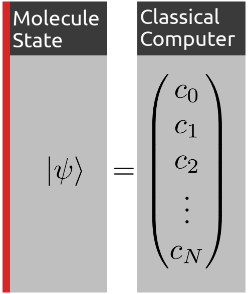

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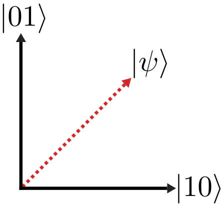
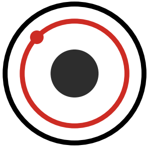


Molecule State		Classical Computer		Quantum Computer
$\vert\psi\rangle$	$=$	$\begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$	$=$	$\vert\phi^{\mathrm{DEVICE}}\rangle$

How to create state on hardware?

- Think of a “trapped-ion” in it’s ground state
- Excite to it’s first excited state (these two states will define the qubit)
- Now “associate” a single qubit to a molecular orbital
- $|0\rangle$ means MO is unoccupied. $|1\rangle$ means MO is occupied.

$|0\rangle$



Atom in Ground State

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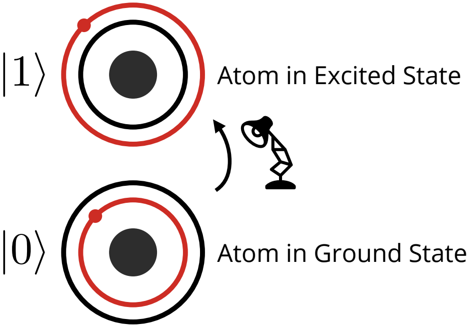

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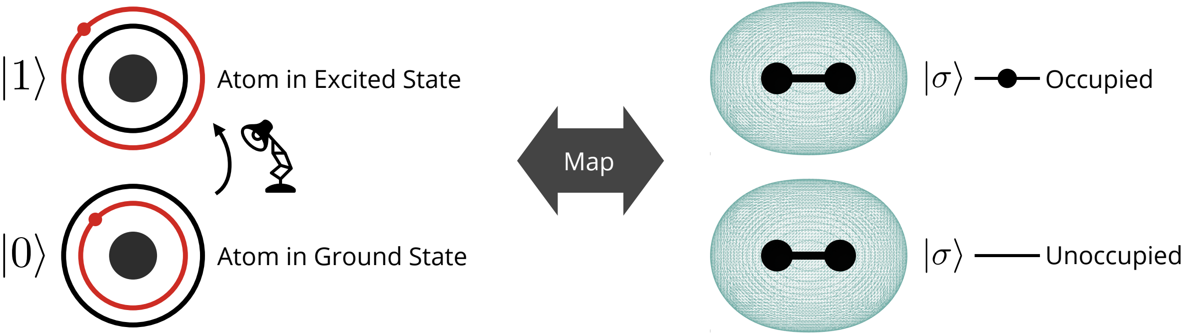
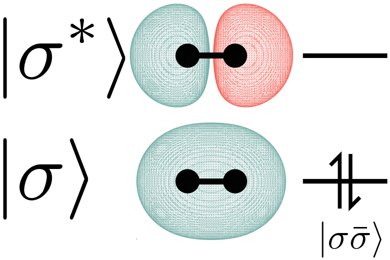


Create many electron configuration to QPU



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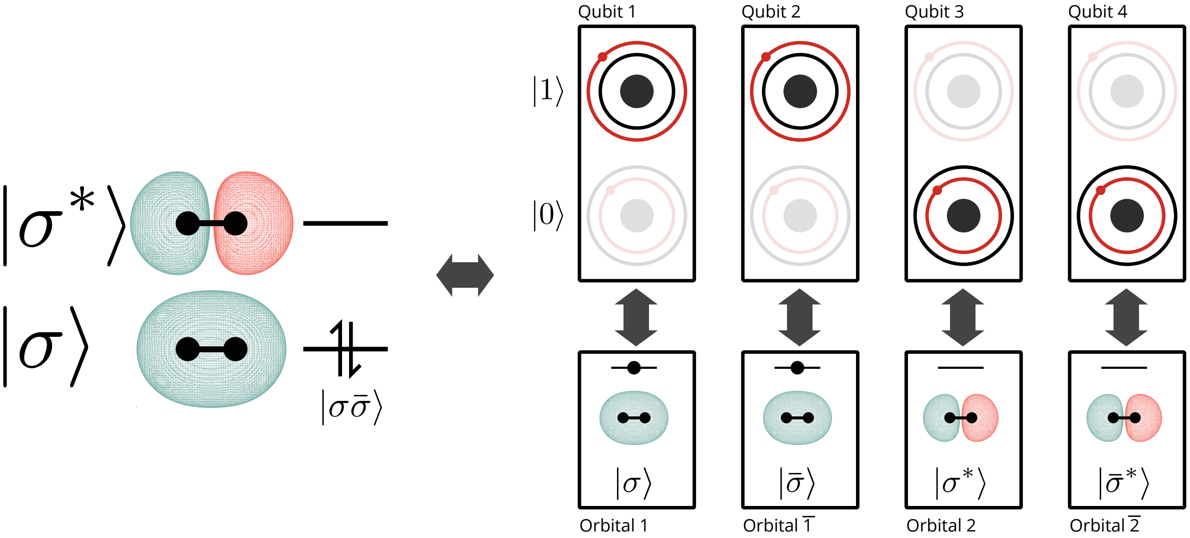


How to create a more complicated state on a QPU?

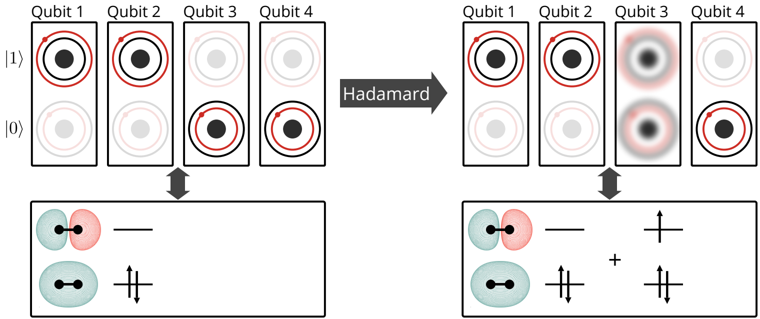
1. Create **superposition** on qubit 3: HADAMARD $= (\hat{x} + \hat{y})/\sqrt{2}$

   $|1\rangle\,|1\rangle\,|0\rangle\,|0\rangle \xrightarrow{\text{H}} |1\rangle\,|1\rangle\,|1+0\rangle\,|0\rangle$

2. Create **entanglement** between qubits 1 and 3: CNOT $= \hat{P}_0 \otimes \hat{I} + \hat{P}_1 \otimes \hat{x}$

   $|1\rangle\,|1\rangle\,|1+0\rangle\,|0\rangle \xrightarrow{\text{CNOT}} |1\rangle\,|1\rangle\,|0\rangle\,|0\rangle + |1\rangle\,|0\rangle\,|1\rangle\,|0\rangle$

3. Continue to entangle other qubits



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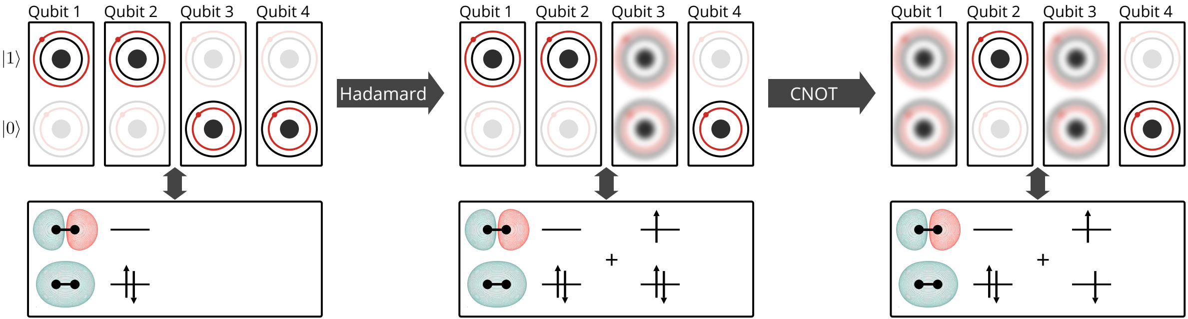

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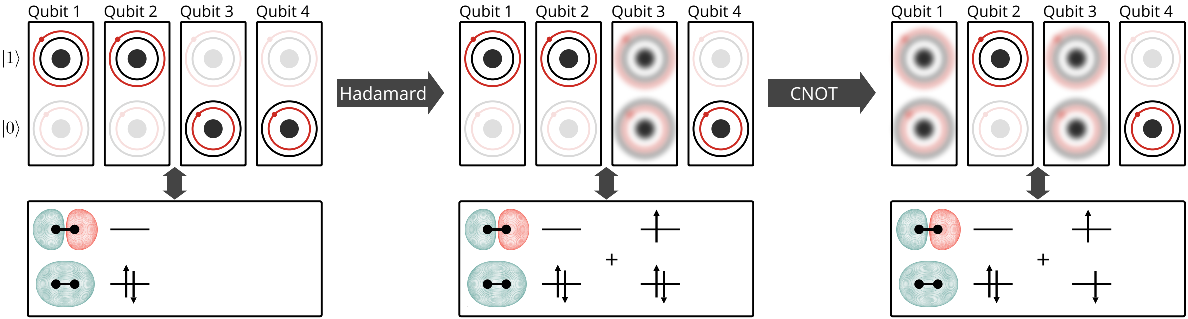


Quantum Simulation: Two key algorithms

- Main limitation of quantum algorithms currently: # of gates

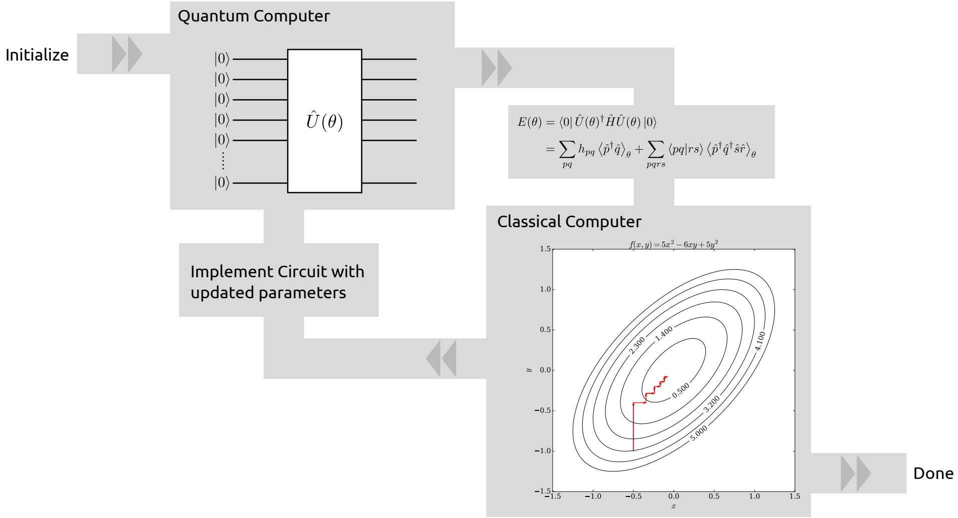
- Phase Estimation (Lloyd '97, Aspuru-Guzik '05)
  - Hamiltonian Evolution $\rightarrow$ Deep circuits - limited by coherence/gate time
  - Provides exact eigenvalues within chosen precision

- Variational Quantum Eigensolver (Peruzzo '14)
  1. Define Ansatz: $\hat{T}(\theta)\left|\right\rangle = \left|\psi(\theta)\right\rangle$
  2. Implement $\hat{T}(\theta)$ as circuit on QPU
  3. Use variational principle to minimize $\left\langle\psi(\theta)\right|\hat{H}\left|\psi(\theta)\right\rangle$

  - Optimize "parameterized circuit"
  - Decrease circuit depth by increasing number of measurements
  - Provides approximate expectation values (e.g., energy)

Abrams & Lloyd, PRL, 79, 2586 (1997)
Aspuru-Guzik, Dutoi, Love, & Head-Gordon, Science, 309, 5741 (2005)
Peruzzo, McClean, Shadbolt, Yung, Zhou, Love, Aspuru-Guzik, O'Brien, Nat Com, 4213 (2014)

VQE: Hybrid Quantum/Classical algorithm



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VQE: How to choose an ansatz?

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  - Familiar to chemists [Bartlett, Kucharski, & Noga, *CPL*, 155, 133 (1989)]

$$|\psi\rangle = e^{\hat{T}-\hat{T}^\dagger}|0\rangle = \hat{U}(\vec{\theta})|0\rangle$$

where,

$$\hat{T} = \sum_{ia} \theta_i^a \hat{t}_i^a + \sum_{ijab} \theta_{ij}^{ab} \hat{t}_{ij}^{ab}$$

- Hardware-efficient ansatz [Kandala et. al, *Nature*, 549, 242 (2017)]
  - Drive one qubit at frequency of neighbor to create entanglement - optimize single qubit rotation angles
- Recent ansatze
  - k-UpCCGSD [Lee, et al., *JCTC*, 15, 311 (2018)]
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- **Exactness:** UCC $\rightarrow$ UCCSD
- **Complexity:** Number of parameters fixed by UCCSD definition
  - Finite coherence times: limits number of gates applied
- **Definition:** only 1 or 2 qubit rotations generally available – Trotterization:

$$e^{\theta_1 \hat{\tau}_1 + \theta_2 \hat{\tau}_2 + \cdots + \theta_N \hat{\tau}_N} |0\rangle \rightarrow \prod_i e^{\theta_i \hat{\tau}_i} |0\rangle$$

  - Trotterized-UCCSD not well defined (*paper out soon*)

$$\ldots e^{\theta_1 \hat{\tau}_1} e^{\theta_2 \hat{\tau}_2} |0\rangle \neq \ldots e^{\theta_2 \hat{\tau}_2} e^{\theta_1 \hat{\tau}_1} |0\rangle$$

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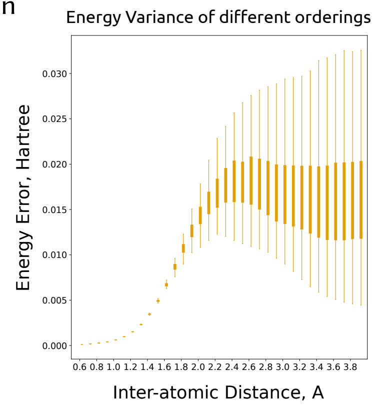

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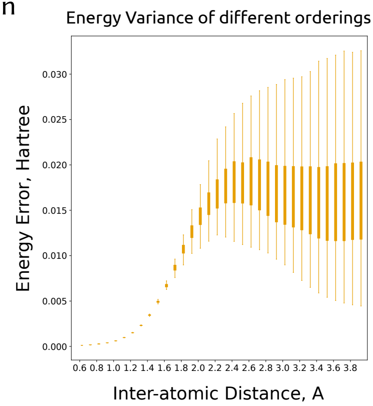

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New Ansatz: ADAPT-VQE

- **Dynamic Ansatz**: Instead of predefining the ansatz, allow the algorithm to *grow* a customized ansatz for each system
  - ✗ $\prod_{ia} e^{\theta_{ia}\hat{\tau}_i^a} \prod_{ijab} e^{\theta_{ijab}\hat{\tau}_{ij}^{ab}} |0\rangle$
  - ✓ $|0\rangle \xrightarrow{grow} e^{\theta_1 \tau_1} |0\rangle \xrightarrow{grow} e^{\theta_2 \tau_2} e^{\theta_1 \tau_1} |0\rangle \xrightarrow{grow} \cdots$
- Grow the ansatz by sequentially choosing the rotation with the largest energy derivative at each iteration (i)

$$\frac{\partial E^{(i)}}{\partial \theta_m} = \langle \psi^{(i)} | [H, \hat{A}_m] | \psi^{(i)} \rangle.$$

- Adaptive Derivative-Assembled Pseudo-Trotter ansatz: (ADAPT-VQE)
  - ✓ Converges to exact solution: FCI
  - ✓ Highly compact: minimizes number of operators
  - ✗ Requires many more measurements

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

New Ansatz: ADAPT-VQE

- **Dynamic Ansatz**: Instead of predefining the ansatz, allow the algorithm to *grow* a customized ansatz for each system
  - ✗ $\prod_{ia} e^{\theta_{ia}\hat{\tau}_i^a} \prod_{ijab} e^{\theta_{ijab}\hat{\tau}_{ij}^{ab}} \left|0\right\rangle$
  - ✓ $\left|0\right\rangle \xrightarrow{grow} e^{\theta_1\tau_1}\left|0\right\rangle \xrightarrow{grow} e^{\theta_2\tau_2}e^{\theta_1\tau_1}\left|0\right\rangle \xrightarrow{grow} \cdots$
- Grow the ansatz by sequentially choosing the rotation with the largest energy derivative at each iteration (i)

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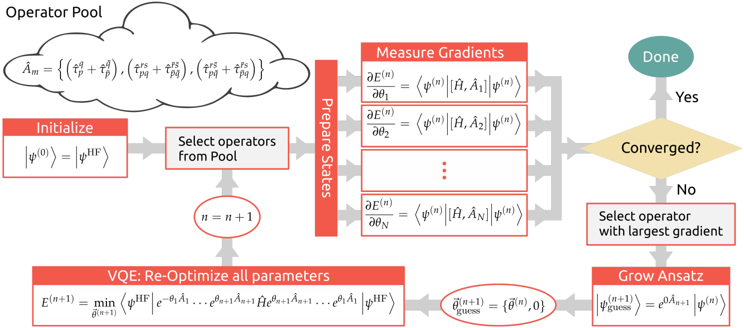
ADAPT-VQE: Algorithm



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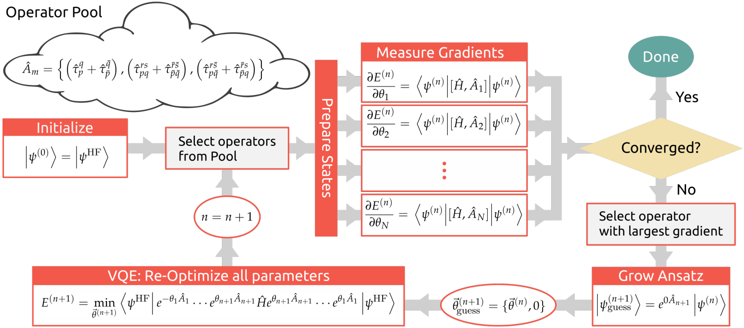

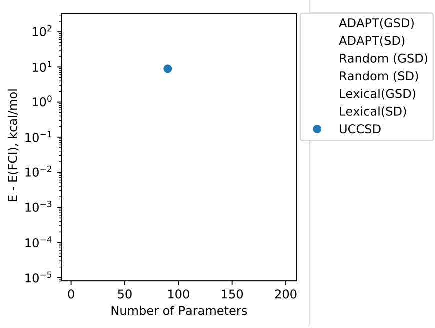

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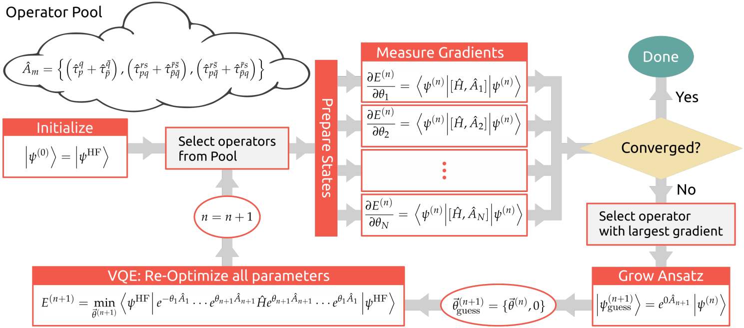

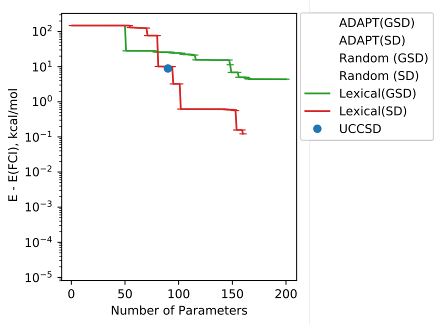

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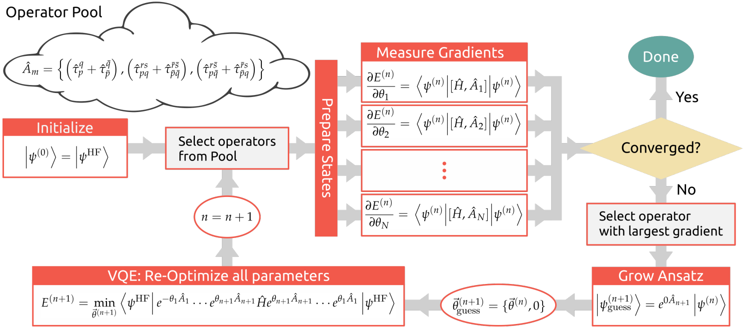

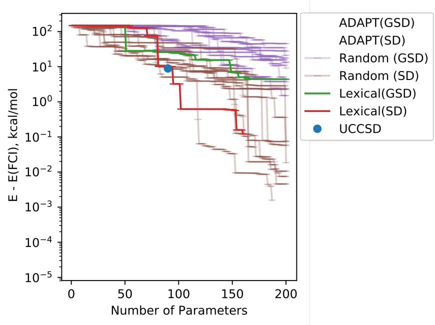

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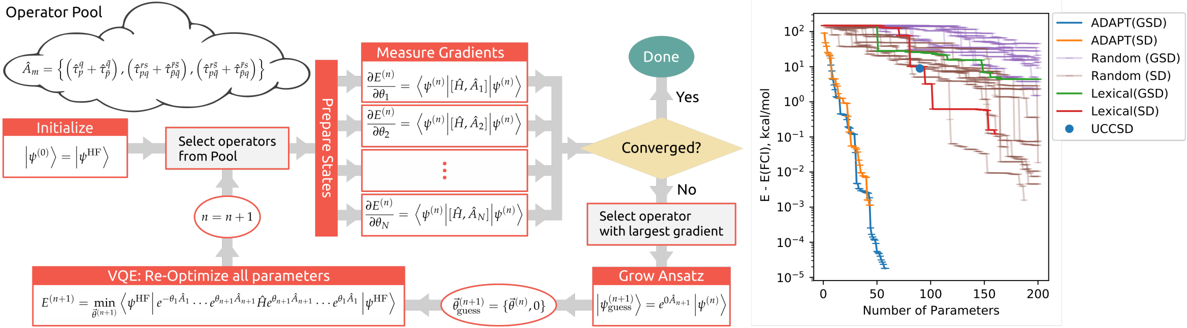

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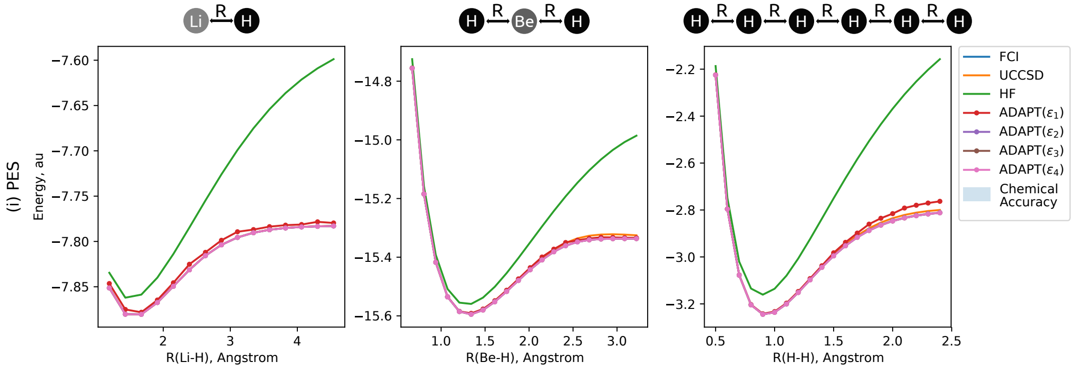
ADAPT-VQE: Potential Energy Curves

- Beyond ϵ_1 indistinguishable (at this scale)
- Chemical accuracy by ϵ_2
- Much more compact than UCCSD - grows beyond UCCSD when needed



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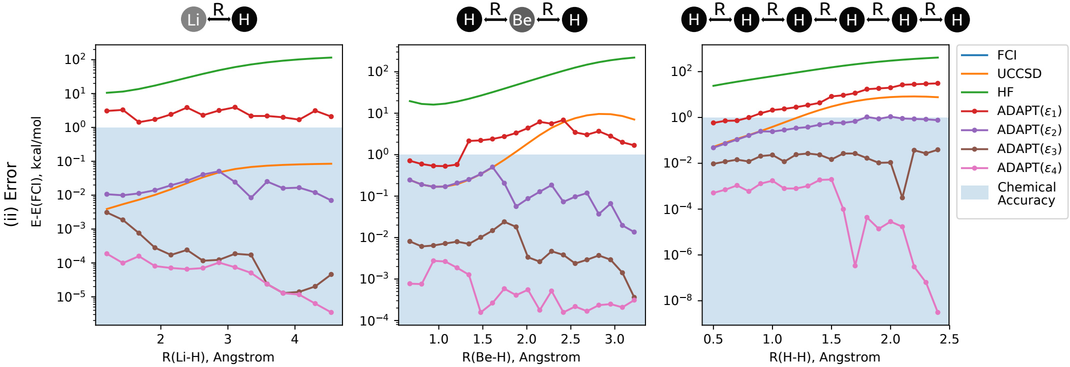

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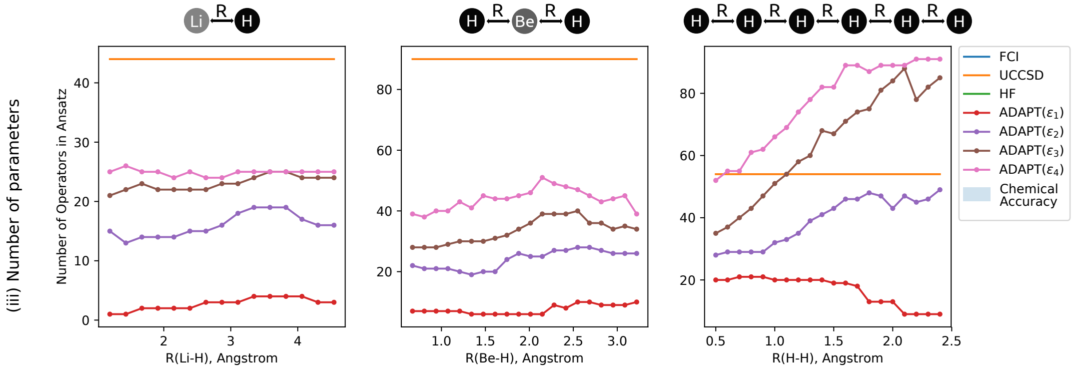

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qubit-ADAPT-VQE: Reduce Circuit Depth

- # parameters $\propto$ # CNOTs - but variability between operators exists
- Fermion $\longrightarrow$ Qubit mapping carries circuit overhead - are there better operator pools?
- New direction: Work directly with qubit operators: $\hat{t}_{ij}^{ab} \xrightarrow{\text{replace}} \hat{\sigma}_i^x \hat{\sigma}_j^x \hat{\sigma}_a^y \hat{\sigma}_b^x$

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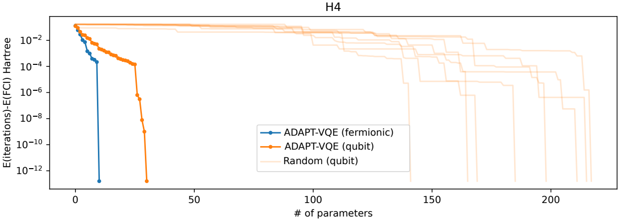

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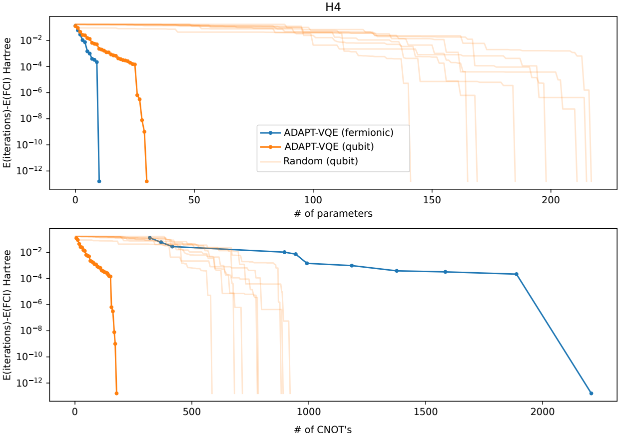

Direct Ansatz: How to construct minimal-parameter circuits?

- Goals
  - Hardware-efficient state preparation
  - Prepare states that span the relevant subspace of the Hilbert space
  - Avoid irrelevant parts of the Hilbert space
  - Avoid 'barren plateaus' [McClean, et. al., *Nature Communications* 9, 4812 (2018)]

- Approach
  - Interested in creating $|\psi\rangle$, not $\hat{U}$
  - Count and parameterize relevant states with given symmetry
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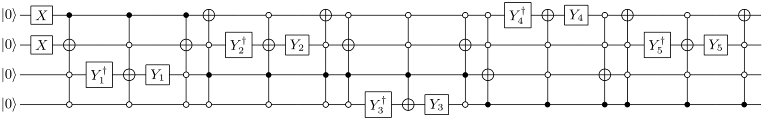
Direct Ansatz: How to construct minimal-parameter circuits?

- $\hat{N}$ Symmetry: Exchange Gate [Barkoutsos et al, PRA 98, 022322 (2018)]

$$A(\theta,\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & e^{i\phi}\sin\theta & 0 \\ 0 & e^{-i\phi}\sin\theta & -\cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

- $\hat{S}_z$ Symmetry: Order qubits: $\alpha, \alpha, \ldots, \beta, \beta, \ldots,$ then remove bridging gates
- Time-Reversal Symmetry: Remove ϕ
- $\hat{S}^2$ Symmetry:

$$\begin{aligned} E_4 \left|0000\right\rangle = &\sin u_1 \sin u_2 \sin u_3 \sin u_4 \sin u_5 \left|0101\right\rangle \\ &+ \sin u_1 \sin u_2 \sin u_3 \sin u_4 \cos u_5 \left|1001\right\rangle \\ &+ \sin u_1 \sin u_2 \sin u_3 \cos u_4 \left|0011\right\rangle \\ &+ \sin u_1 \sin u_2 \cos u_3 \left|0110\right\rangle \\ &+ \sin u_1 \cos u_2 \left|1010\right\rangle \\ &+ \cos u_1 \left|1100\right\rangle . \end{aligned}$$



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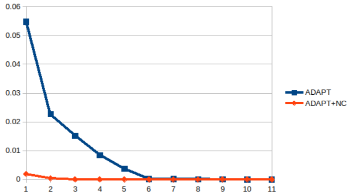
Outlook

- Dependency on reference state
  - Broken symmetry
  - Orbital optimization
- Even more accuracy (and even more measurements) from same state-preparation circuit using a Newton-step

$$H_{i,j} = \frac{\partial^2}{\partial\theta_i\partial\theta_j} = \langle\psi| \, [[\hat{H}, \hat{A}_i], \hat{B}_j] \, |\psi\rangle \tag{1}$$

$$E^{(2)} = E^{(0)} - \tfrac{1}{2} g_i H_{ij}^{-1} g_j \tag{2}$$

- Implementation on hardware (currently being worked on)



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Mayhall Group


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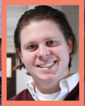
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Nick Mayhall

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VT


Sophia Economou


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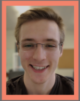
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