
# Introduction to Quantum Computing II

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# Algorithms and Applications

- Terminology
- Bernstein-Varizani Algorithm
- Variational Quantum Eigensolver Algorithm



# Working Terminology

- **classical algorithm**: a defined sequence of transformations to solve a specific problem by manipulating a classical logic state
- **quantum algorithm**: a defined sequence of transformations to solve a specific problem by manipulating a quantum state
- **quantum circuit**: a visual schematic to represent a sequence of transformations acting on a quantum state
- **quantum program**: a sequence of ordered instructions for a quantum computer
- **quantum application**: a quantum program to solve a specific problem
- **quantum advantage**: an improvement in performance of a quantum application relative to a classical baseline



Given the black box function

$$f: \{0,1\}^n \rightarrow \{0,1\}$$

with promise that

$$f(x) = s \cdot x \ (\mathrm{mod}\ 2)$$

find the string $s \in \{0,1\}^n$

$$s = 101 = (1,0,1)$$

$$x = 011 = (0,1,1)$$

$$s \cdot x \ (\mathrm{mod}\ 2) = 1 \cdot 0 + 0 \cdot 1 + 1 \cdot 1 (\mathrm{mod}\ 2)$$

$$= 0 + 0 + 1 (\mathrm{mod}\ 2)$$

$$= 1$$



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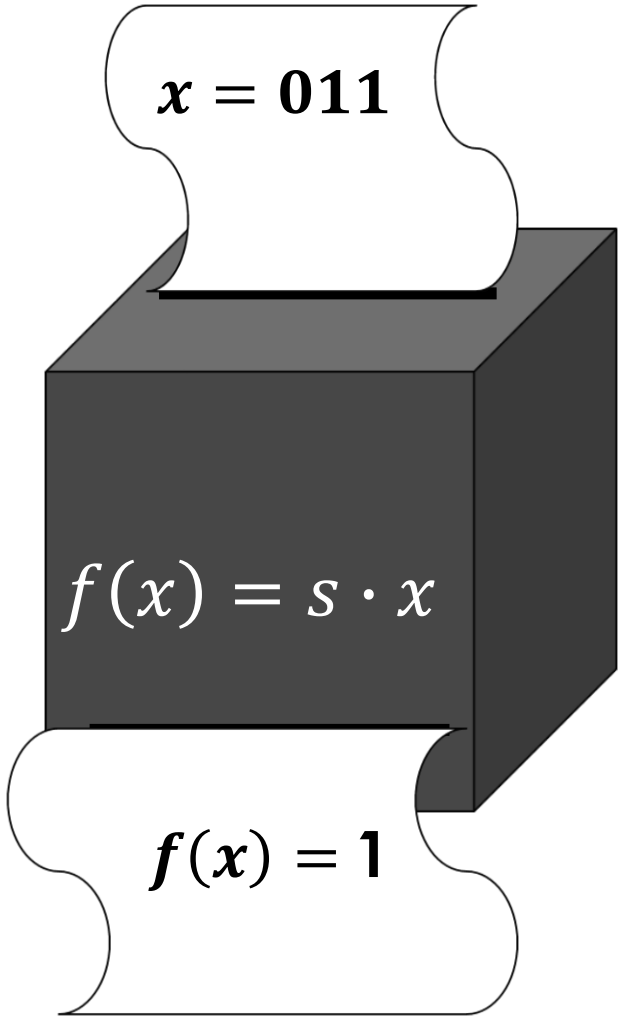

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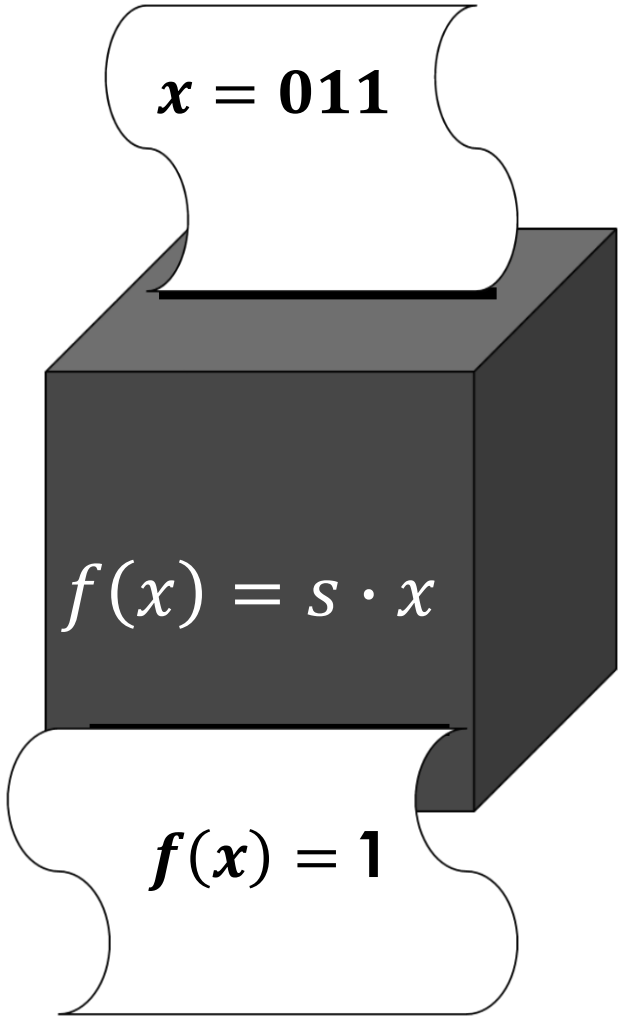

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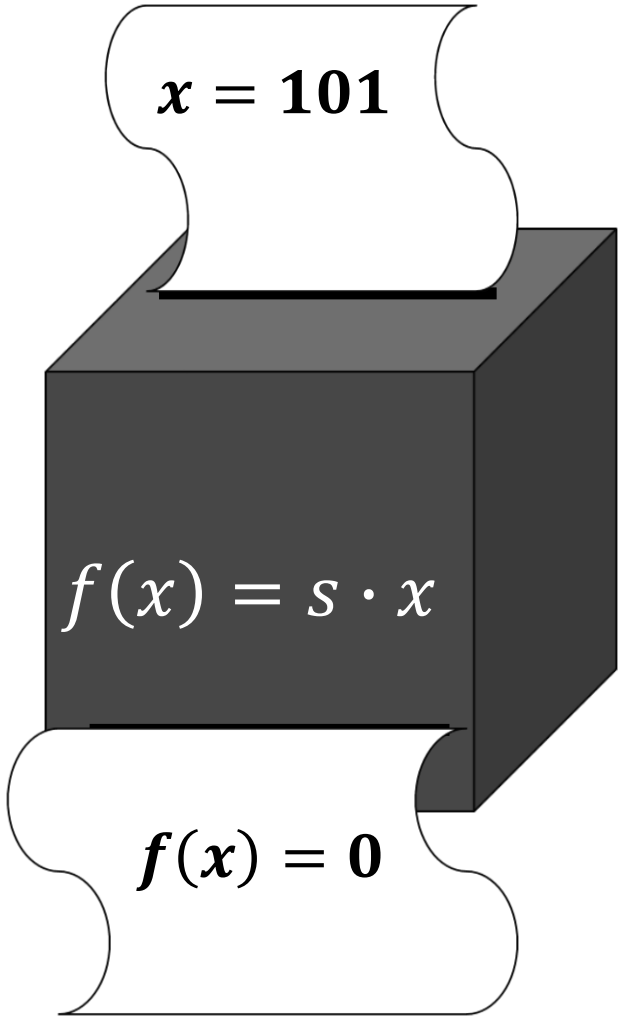

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- What is a **classical algorithm** to solve this problem?

**BestClassicalAlgorithm**$(n, f)$

Require $n \in Z^+, f: \{0,1\}^n \rightarrow \{0,1\}$

1. for $i \in \{0, \ldots, n-1\}$:
2. $\quad x_i = \mathbf{1}_i$
3. $\quad s_i \leftarrow f(x_i)$
4. end for
5. $s = s_0 s_1 \ldots s_{n-1}$

Sample all input strings of Hamming weight 1

Requires $n$ queries

Given the black box function

$$f: \{0,1\}^n \to \{0,1\}$$

with promise that

$$f(x) = s \cdot x \ (\mathrm{mod}\ 2)$$

find the string $s \in \{0,1\}^n$

- What is a **quantum algorithm** to solve this problem?

Recall Hadamard gate/operator

$$H: |0\rangle \to \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle$$

$$H: |1\rangle \to \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = |-\rangle$$

$$H^{\otimes n}|0\rangle^{\otimes n} = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle$$



Given the black box function

$$f: \{0,1\}^n \to \{0,1\}$$

with promise that

$$f(x) = s \cdot x \ (\mathrm{mod}\ 2)$$

find the string $s \in \{0,1\}^n$

- What is a **quantum algorithm** to solve this problem?

Consider unitary operator, "oracle"

$$U_f: |x\rangle|b\rangle \to |x\rangle|b \oplus f(x)\rangle$$

Apply unitary operator to register

$$U_f H^{\otimes n}|0\rangle^{\otimes n}|b\rangle = \frac{1}{\sqrt{2^n}} \sum_{x \in \{0,1\}^n} |x\rangle|b \oplus f(x)\rangle$$



Given the black box function

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with promise that

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find the string $s \in \{0,1\}^n$

- What is a **quantum algorithm** to solve this problem?

Let $|b\rangle = H|1\rangle = |-\rangle$

Phase kick back shifts phase

$$U_f H^{\otimes m}|0\rangle^{\otimes n}|1\rangle = \sum_x (-1)^{f(x)}|x\rangle|-\rangle$$

here $m = n + 1$



Given the black box function

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with promise that

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find the string $s \in \{0,1\}^n$

- What is a **quantum algorithm** to solve this problem?

"Phase kick back" from $|x\rangle|b \oplus f(x)\rangle$

If $f(x) = 0$

$$U_f|x\rangle(|0\rangle - |1\rangle) = |x\rangle|-\rangle$$

else $f(x) = 1$

$$U_f|x\rangle(|0\rangle - |1\rangle) = -|x\rangle|-\rangle$$

Putting these pieces together:

$$U_f|x\rangle|-\rangle = (-1)^{f(x)}|x\rangle|-\rangle$$

Given the black box function

$$f: \{0,1\}^n \to \{0,1\}$$

with promise that

$$f(x) = s \cdot x \ (\mathrm{mod}\ 2)$$

find the string $s \in \{0,1\}^n$

- What is a **quantum algorithm** to solve this problem?

Substitute $f(x) = s \cdot x$

$$U_f H^{\otimes m} |0\rangle^{\otimes n} |1\rangle = \sum_x (-1)^{s \cdot x} |x\rangle |-\rangle$$

Note the equivalent form

$$\sum_{x \in \{0,1\}^n} (-1)^{s \cdot x} |x\rangle = \prod_{i=0}^{n-1} (|0_i\rangle + (-1)^{s_i} |1_i\rangle)$$

If $s_i = 0$ then the *i*-th qubit is in $|+\rangle$

If $s_i = 1$, then the *i*-th qubit is in $|-\rangle$



Given the black box function

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- What is a **quantum algorithm** to solve this problem?

Rotate states to computational basis

$$H^{\otimes m} U_f H^{\otimes m} |0\rangle^{\otimes n} |1\rangle = \prod_{i=0}^{n-1} |s_i\rangle |1\rangle$$

Measure!

$$\mathrm{Prob}(s_i = 0) = |\langle 0|s_i\rangle|^2$$

$$\mathrm{Prob}(s_i = 1) = |\langle 1|s_i\rangle|^2$$



# Bernstein-Vazirani Algorithm

Given the black box function

$$f: \{0,1\}^n \rightarrow \{0,1\}$$

with promise that

$$f(x) = s \cdot x \ (\mathrm{mod}\ 2)$$

find the string $s \in \{0,1\}^n$

**BestQuantumAlgorithm**$(n, f)$

Require $n \in Z^+$, $f: \{0,1\}^n \rightarrow \{0,1\}$

Require x, an $n$-qubit register

Require b, a 1-qubit register

Require $U_f: |x\rangle|b\rangle \rightarrow |x\rangle|b \oplus f(x)\rangle$

1. Initialize register x to $|0\rangle^{\otimes n}$
2. Initialize register b to $|1\rangle$
3. Apply $H$ to $\mathrm{x}_i$ $\forall\ i \in \{0, \dots, n-1\}$:
4. Apply $H$ to $\mathrm{b}_1$
5. Apply $U_f$ to x and b
6. Apply $H$ to $\mathrm{x}_i$ $\forall\ i \in \{0, \dots, n-1\}$:
7. $s \leftarrow$Measure(x)

# Bernstein-Vazirani Algorithm

Notes:

- Developed by Ethan Bernstein and Umesh Vazirani in 1990‘s
- Requires only 1 query of the function $f$, i.e., the oracle $U_f$
- Returns the answer exactly
- Special case of Deutsch-Josza algorithm

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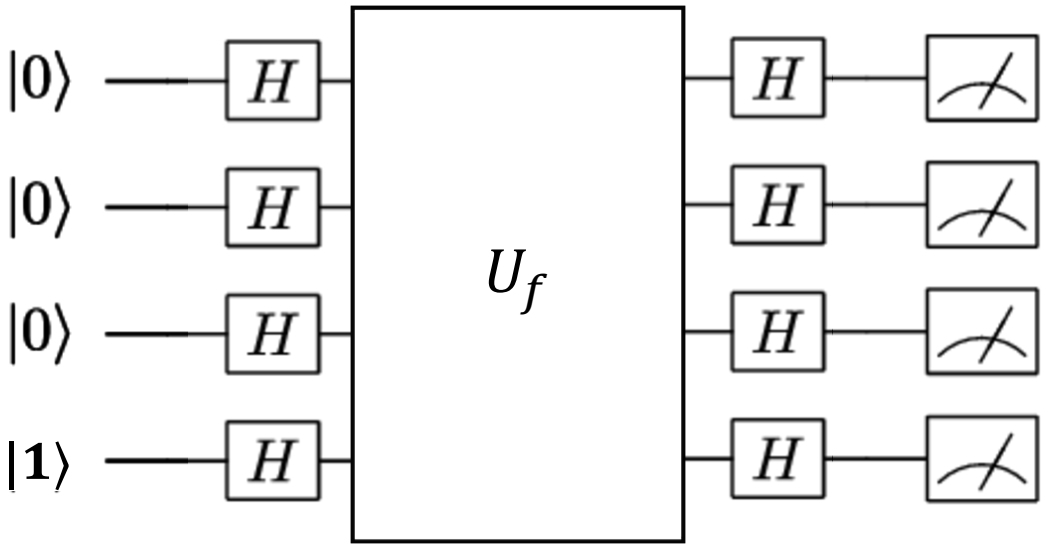
# Bernstein-Vazirani Algorithm

Quantum circuit for BV algorithm with n = 3

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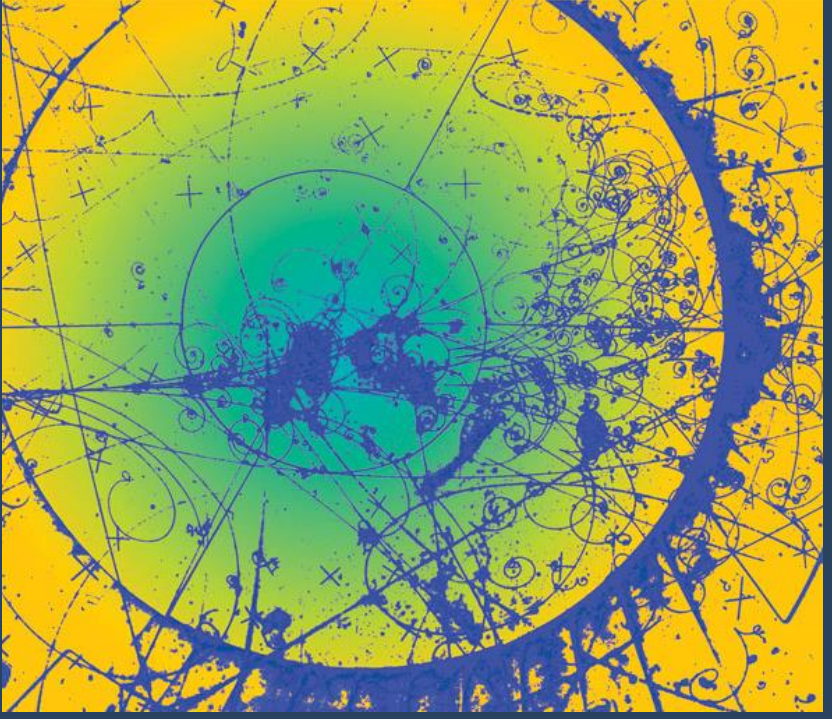
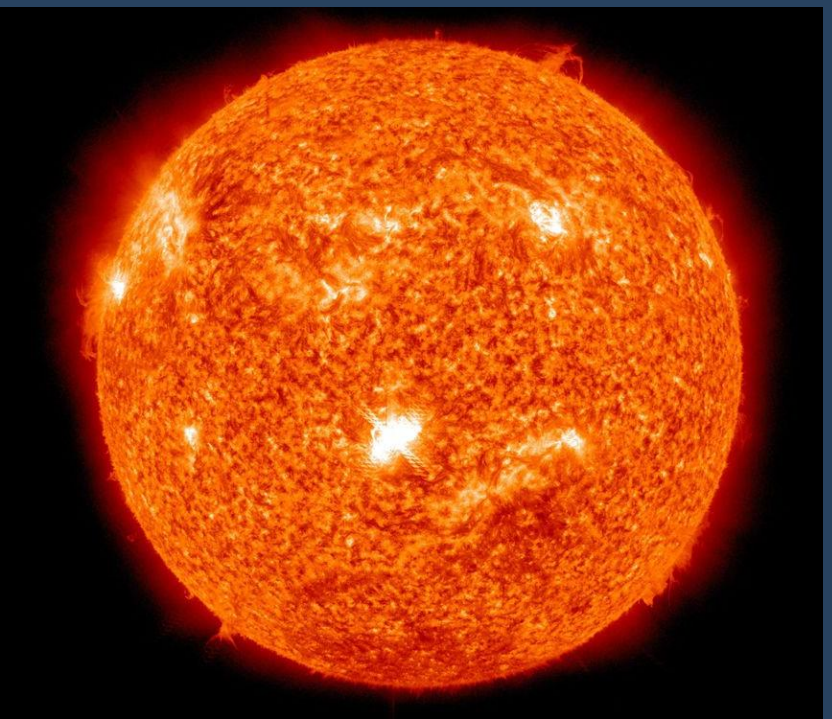
# Questions?

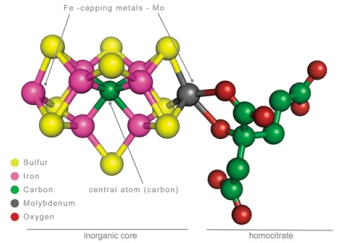


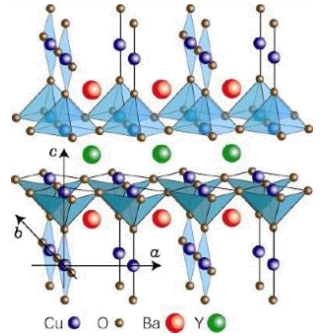


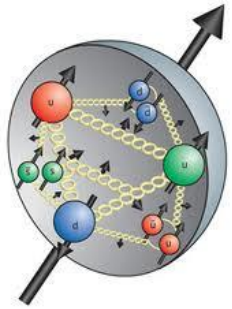


# Quantum Algorithms for Scientific Computing

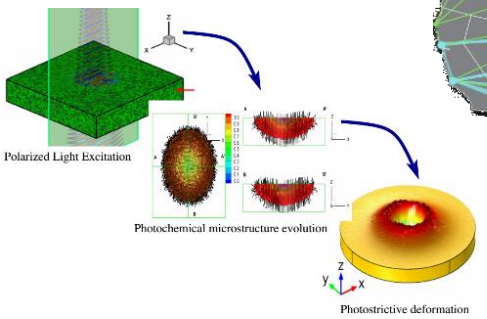
- Algorithms in the quantum computing model have been found to take fewer steps to solve problems
  - **Quantum Simulation**
  - Partition Functions
  - Discrete Optimization
  - Machine Learning
  - Factoring
  - Unstructured Search
  - Eigensystems
  - Linear Systems

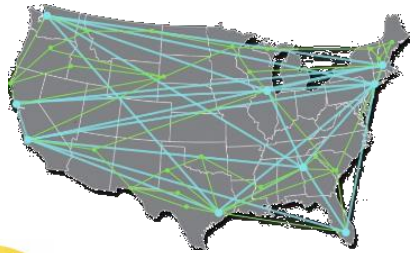


- Several physical domains motivate quantum computing as a paradigm for scientific computing
  - High-energy Physics
  - Materials Science
  - Chemistry
  - Biological Systems
  - Artificial Intelligence
  - Data Analytics
  - Planning and Routing
  - Verification and Validation



## Time-dependent Schrodinger Equation

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = H(t)|\Psi(t)\rangle$$

## Time-independent Schrodinger Equation

$$H|\Phi_n\rangle = E_n|\Phi_n\rangle$$

- The eigenspectrum of the Hamiltonian is ordered with a lowest energy state
- The eigenvectors of the Hamiltonian form a complete basis for representing the state

$$E_0 \leq E_1 \leq \cdots \leq E_N$$

$$|\Psi\rangle = \sum_n c_n |\Phi_n\rangle$$

$$E_0 \leq \langle \Psi|H|\Psi\rangle$$

# Variational Quantum Eigensolver (VQE) algorithm

- Construct a candidate quantum state

$$|\Psi(\theta)\rangle = \sum_n c_n(\theta)|\Phi_n\rangle$$

- Compute the energy

$$E(\theta) = \langle \Psi(\theta)|H|\Psi(\theta)\rangle$$

- Compare with actual energy

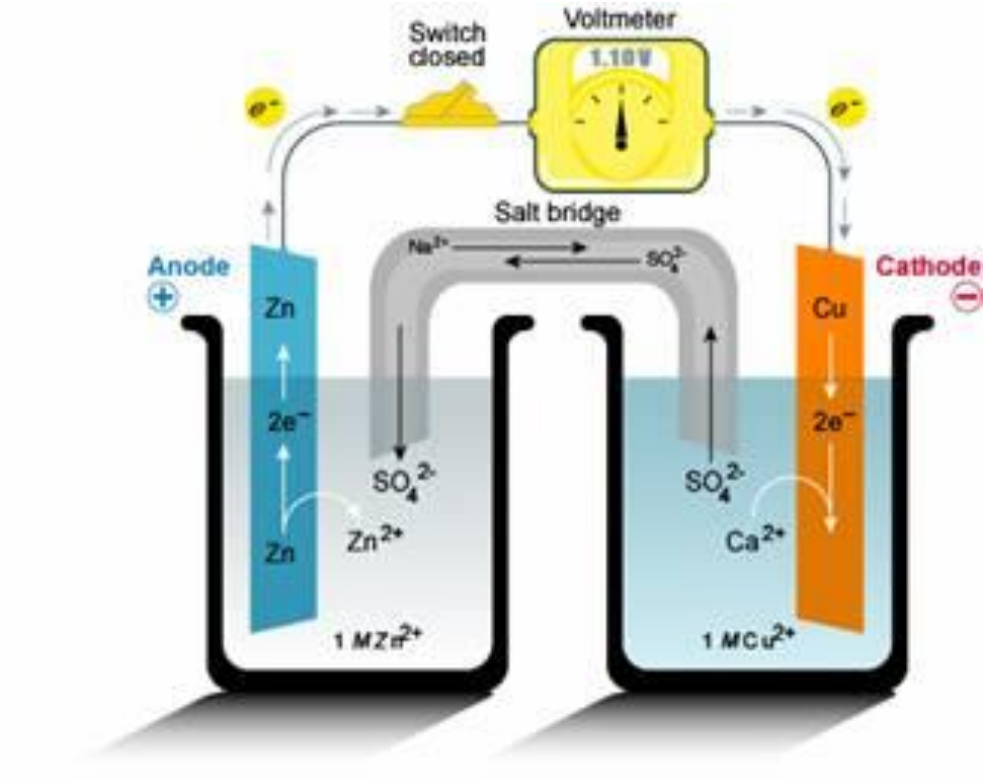
$$E(\theta) = E_0?$$

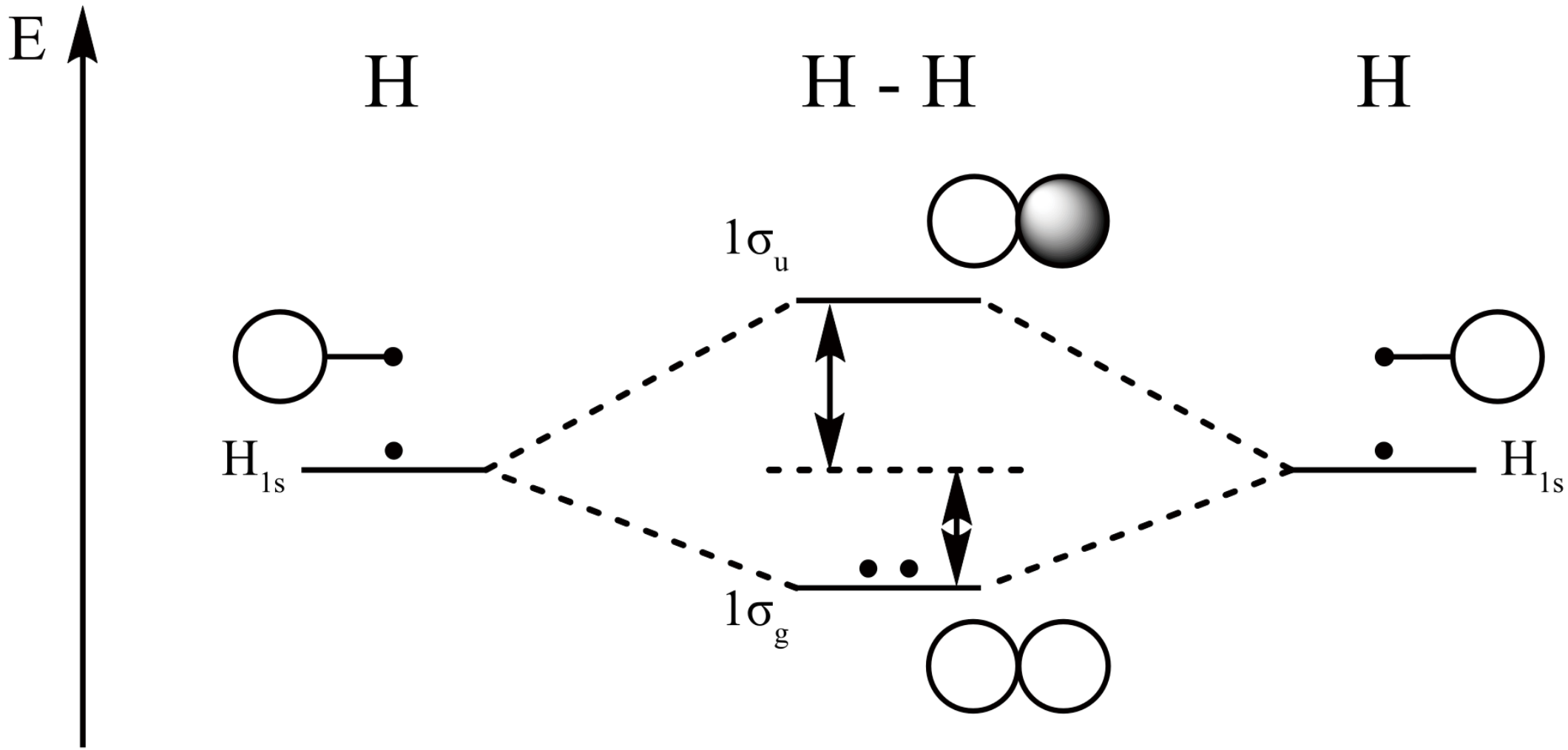
No? Try again!

- The Variational Quantum Eigensolver (VQE) algorithm uses the bound on an operator to construct a quantum state that minimizes the observable.
- VQE was created in 2013 to combine quantum state preparation and measurement with classical search algorithms.



| Group → / Period ↓ | 1 | 2 | | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 H | | | | | | | | | | | | | | | | | | 2 He |
| 2 | 3 Li | 4 Be | | | | | | | | | | | | 5 B | 6 C | 7 N | 8 O | 9 F | 10 Ne |
| 3 | 11 Na | 12 Mg | | | | | | | | | | | | 13 Al | 14 Si | 15 P | 16 S | 17 Cl | 18 Ar |
| 4 | 19 K | 20 Ca | | 21 Sc | 22 Ti | 23 V | 24 Cr | 25 Mn | 26 Fe | 27 Co | 28 Ni | 29 Cu | 30 Zn | 31 Ga | 32 Ge | 33 As | 34 Se | 35 Br | 36 Kr |
| 5 | 37 Rb | 38 Sr | | 39 Y | 40 Zr | 41 Nb | 42 Mo | 43 Tc | 44 Ru | 45 Rh | 46 Pd | 47 Ag | 48 Cd | 49 In | 50 Sn | 51 Sb | 52 Te | 53 I | 54 Xe |
| 6 | 55 Cs | 56 Ba | * | 71 Lu | 72 Hf | 73 Ta | 74 W | 75 Re | 76 Os | 77 Ir | 78 Pt | 79 Au | 80 Hg | 81 Tl | 82 Pb | 83 Bi | 84 Po | 85 At | 86 Rn |
| 7 | 87 Fr | 88 Ra | ** | 103 Lr | 104 Rf | 105 Db | 106 Sg | 107 Bh | 108 Hs | 109 Mt | 110 Ds | 111 Rg | 112 Cn | 113 Nh | 114 Fl | 115 Mc | 116 Lv | 117 Ts | 118 Og |
| | | | * | 57 La | 58 Ce | 59 Pr | 60 Nd | 61 Pm | 62 Sm | 63 Eu | 64 Gd | 65 Tb | 66 Dy | 67 Ho | 68 Er | 69 Tm | 70 Yb | | |
| | | | ** | 89 Ac | 90 Th | 91 Pa | 92 U | 93 Np | 94 Pu | 95 Am | 96 Cm | 97 Bk | 98 Cf | 99 Es | 100 Fm | 101 Md | 102 No | | |




E
H
H - H
H
1σu
1σg
H1s
H1s

## Molecular Hamiltonian

$$\hat{H}_{\text{mol}} = -\sum_i \frac{\nabla_{R_i}^2}{2M_i} - \sum_i \frac{\nabla_{r_i}^2}{2m_i} - \sum_{i,j} \frac{Z_i}{|R_i - r_j|} + \sum_{i,j>i} \frac{Z_i Z_j}{|R_i - R_j|} + \sum_{i,j>i} \frac{1}{|r_i - r_j|}$$

- Electronic Hamiltonian $H(R)$ depends on the nuclei coordinates $R$ and the interaction of the electrons with the nuclei
- Born-Oppenheimer approximation assumes the electrons equilibrate while the nuclei move
- Second quantization describes electrons as fermionic fields that are created and destroyed by operators

$$a_p^\dagger |\text{vac}\rangle = |1_p\rangle \quad a_p |1_p\rangle = |\text{vac}\rangle$$

$$H(R) = \sum_{pq} h_{pq}(R) a_p^\dagger a_q + \frac{1}{2} \sum_{pqst} h_{pqst}(R) a_p^\dagger a_q^\dagger a_s a_t$$

$$h_{pq}(R) = \int d\sigma \varphi_p^*(\sigma) \left( \frac{\nabla_r^2}{2} - \sum_i \frac{Z_i}{|R_i - r|} \right) \varphi_q(\sigma)$$

$$h_{pqst} = \int d\sigma_1 d\sigma_2 \frac{\varphi_p^*(\sigma_1) \varphi_q^*(\sigma_2) \varphi_s(\sigma_1) \varphi_t(\sigma_2)}{|r_1 - r_2|}$$

The electron spin-orbitals $\{\varphi_p\}$ determine how to represent the electronic state, "coordinate system"

## Fermionic Representation

$$H(R) = \sum_{pq} h_{pq}(R) a_p^\dagger a_q + \frac{1}{2} \sum_{pqst} h_{pqst}(R) a_p^\dagger a_q^\dagger a_s a_t$$

$$\{a_p^\dagger, a_q\} = \delta_{p,q} \qquad \text{and} \qquad \{a_p, a_q\} = 0$$

## Spin Representation

$$H(R) = \sum_j c_j(R) P_j$$

$$P_j \in \{X, Y, Z, I\}^n \qquad [X, Y] = -2iZ$$

Jordan-Wigner transform represents the fermionic operators using spin operators and ensures the correct commutation relations are satisfied. These transformations are widely used when developing quantum applications for solving fermionic field problems, "qubitize"

$$a_p^\dagger = \bigotimes_{i<p} Z_i \otimes \sigma_p^- \qquad a_p = \bigotimes_{i<p} Z_i \otimes \sigma_p^+ \qquad \sigma_p^\pm = (X_p \pm iY_p)/\sqrt{2}$$

- Spin Hamiltonian for $H_2$ transforms to a sum of 15 multi-qubit Pauli operator
- The orbital basis for hydrogen atom is 2 spin orbitals for 2 molecular orbitals
- The molecular spin orbitals are encoded by four qubits

$1_\alpha 1_\beta = |1,1,0,0\rangle \quad 1_\alpha 2_\alpha = |1,0,1,0\rangle$

$2_\alpha 1_\beta = |0,1,1,0\rangle \quad 2_\alpha 2_\beta = |0,0,1,1\rangle$

$$H(R) = c_0 IIII + c_1 ZIII + c_2 IZII + c_3 IIZI + c_4 IIIZ$$

$$+c_5 ZIZI + c_6 IZIZ + c_7 ZZII + c_8 IZZI + c_9 ZIIZ$$

$$+c_{10} IIZZ + c_{11} YYXX + c_{12} XXYY + c_{13} YXXY$$

$$+c_{14} XYYX$$

- Quantum applications build on domain theory to be efficient
- State preparation ansatz derived from unitary coupled cluster (UCC) theory
- UCC Singles-Doubles (UCCSD) is sufficient for two-electron model
- Again, need to transform to spin representation

$$U(\theta) = \exp\left(T(\theta) - T^{\dagger}(\theta)\right) \qquad U(\theta) \approx \prod_{m=1}^{M} e^{\tau_m(\theta)}$$

$$U_{\mathrm{SD}}(\theta) = e^{\tau_1(\theta)} e^{\tau_2(\theta)} \qquad \tau_m(\theta) = T_m(\theta) - T_m^{\dagger}(\theta)$$

$$T_1(\theta) = \sum_{\substack{i \in \mathrm{occ} \\ a \in \mathrm{virt}}} \theta_i^a \hat{t}_i^a \qquad T_2(\theta) = \sum_{\substack{i,j \in \mathrm{occ} \\ a,b \in \mathrm{virt}}} \theta_{i,j}^{a,b} \hat{t}_{i,j}^{a,b}$$

Fermionic to spin transformation

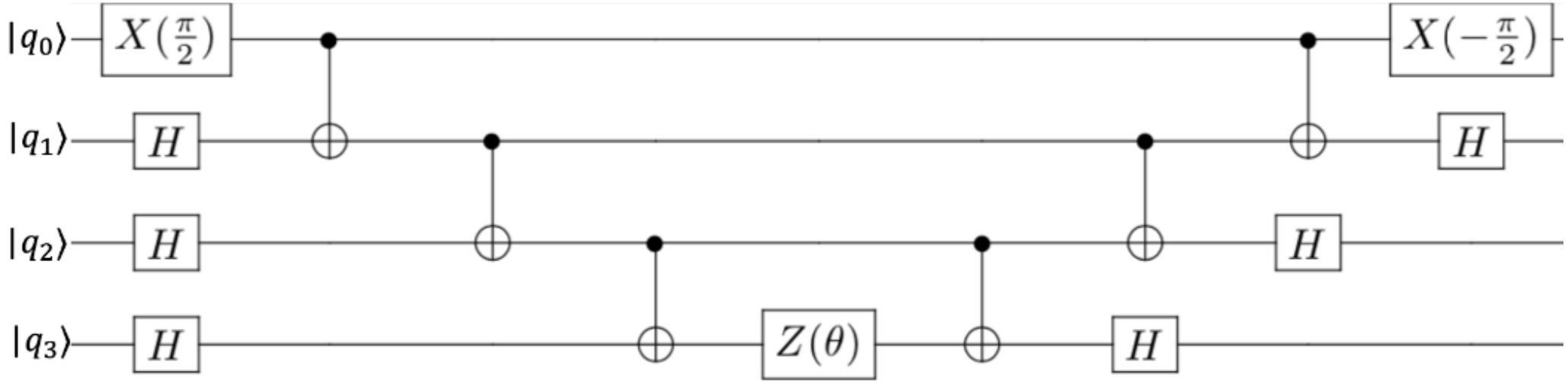
$$U(\theta) = e^{i\theta Y_0 X_1 X_2 X_3}$$



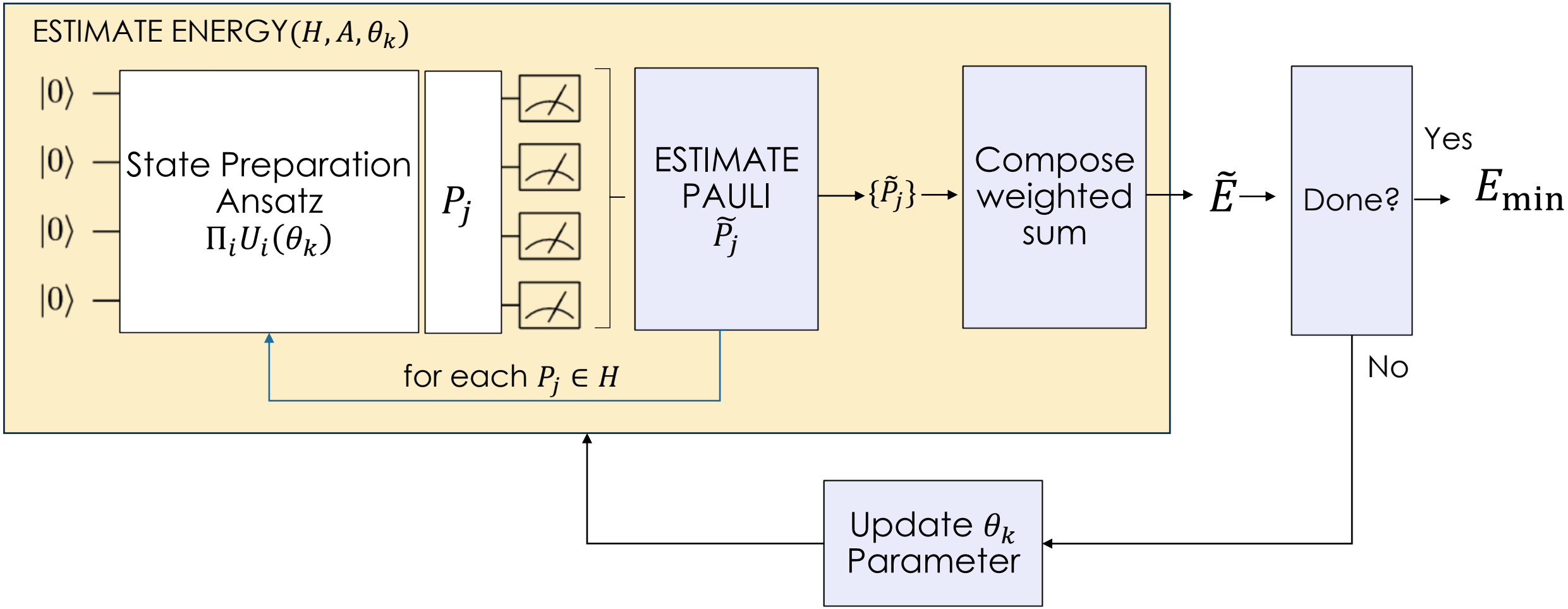
J. Wright, M. Gowrishankar, et al., "Numerical Simulations of Noisy Quantum Circuits for Computational Chemistry," Materials Theory 8, 1 (2022)

UCC-Single-Doubles (UCCSD) one-parameter ansatz using a four-qubit encoding of two spin-orbitals $\{\varphi_p\}$

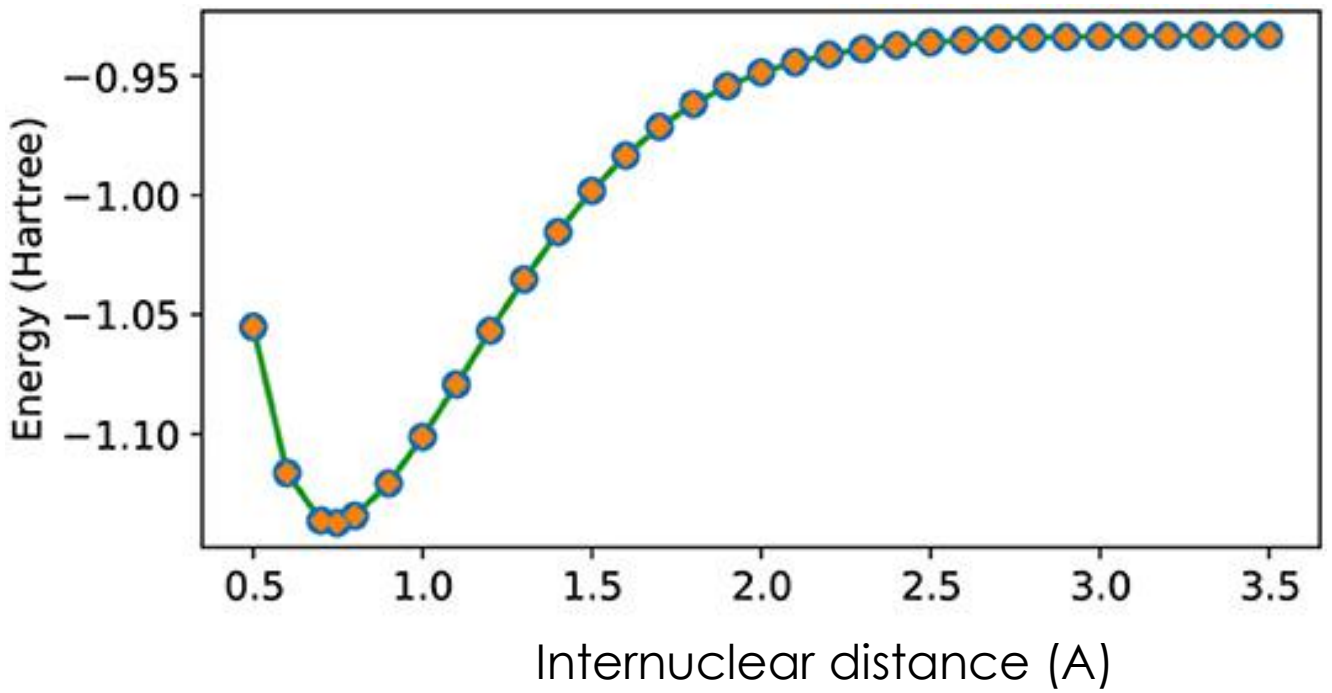
$$U_{\mathrm{SD}}(\theta) = e^{\tau_1(\theta)} e^{\tau_2(\theta)} \longrightarrow e^{i\theta Y_0 X_1 X_2 X_3}$$



$$|\Psi(\theta_k)\rangle = \prod_i U_i(\theta_k)|0\rangle \qquad H(R) = \sum_j c_j(R)P_j$$

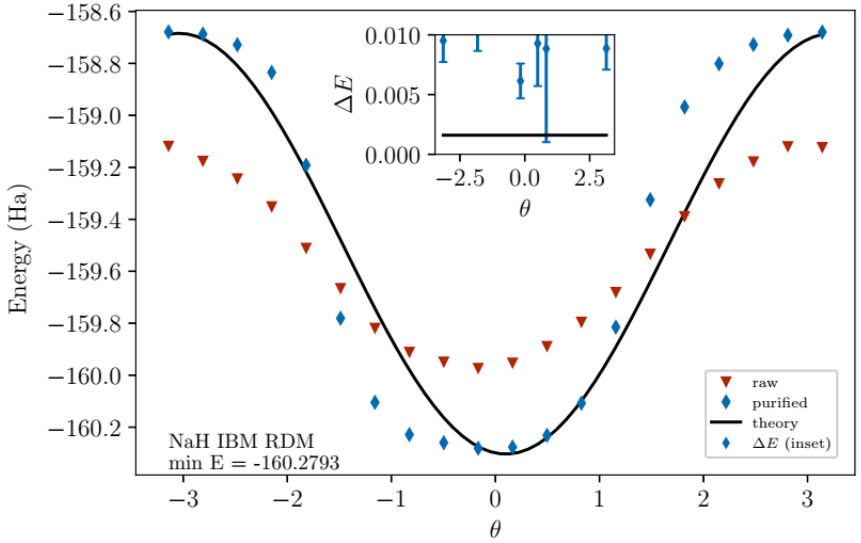


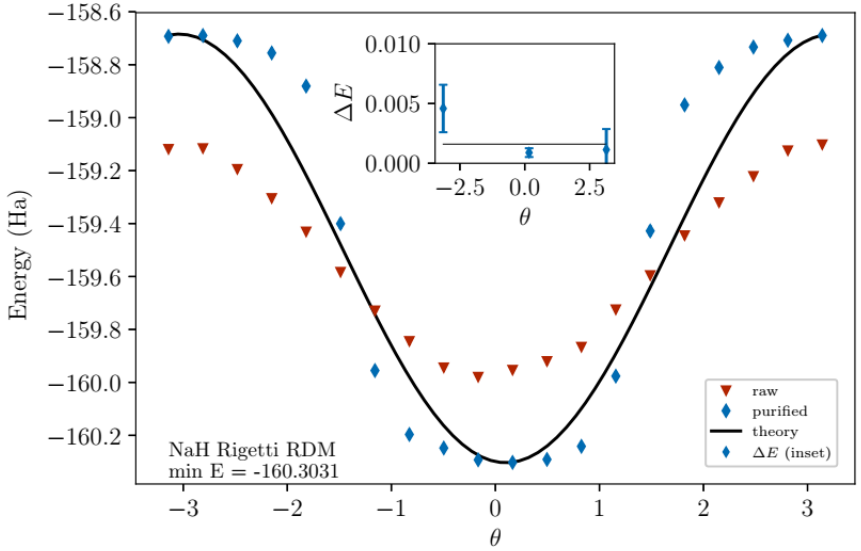
- Potential energy curves of $H_2$ computed with the STO-3G basis set for FCI (green solid line) and VQE (blue circles)
- Search method used the COBYLA optimizer
- Numerical simulation used state-vector calculations of the Pauli estimates.






D. Claudino et al., "Benchmarking Adaptive Variational Quantum Eigensolvers," Front. Chem. 606863 (2020)


- Experimental estimates of Pauli terms introduce noise in state preparation and energy calculation
- Methods for mitigating noise and errors can improve results

FCI energies with 4-qubit frozen-core basis
NaH: −160.3034597
RbH: −2908.125112
KH: −593:5747682

This work supported by DOE ASCR program office



A. J. McCaskey et al., "Quantum Chemistry as a Benchmark for Near-Term Quantum Computers," npj Quantum Information 5, 99 (2019; cf. arXiv:1905.01534 (2019)

# Algorithms and Applications

- Terminology
  - Quantum algorithms, quantum circuits, quantum applications
- Bernstein-Varizani Algorithm
  - Oracle operators, phase kick back, quantum advantage
- Variational Quantum Eigensolver Algorithm
  - Quantum chemistry, quantum application
  - Fermionic and Spin Hamiltonians
  - Unitary Coupled Cluster theory



# Questions?