

# **Solving Quantum Chemistry Problems on Quantum Computers**

Nov 14, 2019  
Renke Huang

# Origin of using quantum computer to simulate quantum system



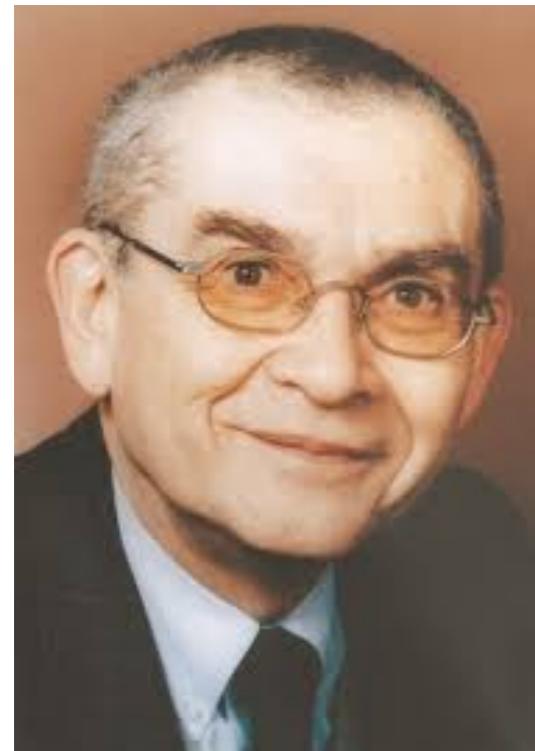
*International Journal of Theoretical Physics, Vol. 21, Nos. 6/7, 1982*

## Simulating Physics with Computers

**Richard P. Feynman**

*Department of Physics, California Institute of Technology, Pasadena, California 91107*

*Received May 7, 1981*



Manin, Y. *Computable and Uncomputable*; Sovetskoye Radio: Moscow, 1980.

- **NP-complete:** Mean-field approximation of the ground state (lowest energy) of a general quantum system
- Strongly correlated molecules and materials are difficult to simulate due to the **exponential scaling of Hilbert space**.

# Background

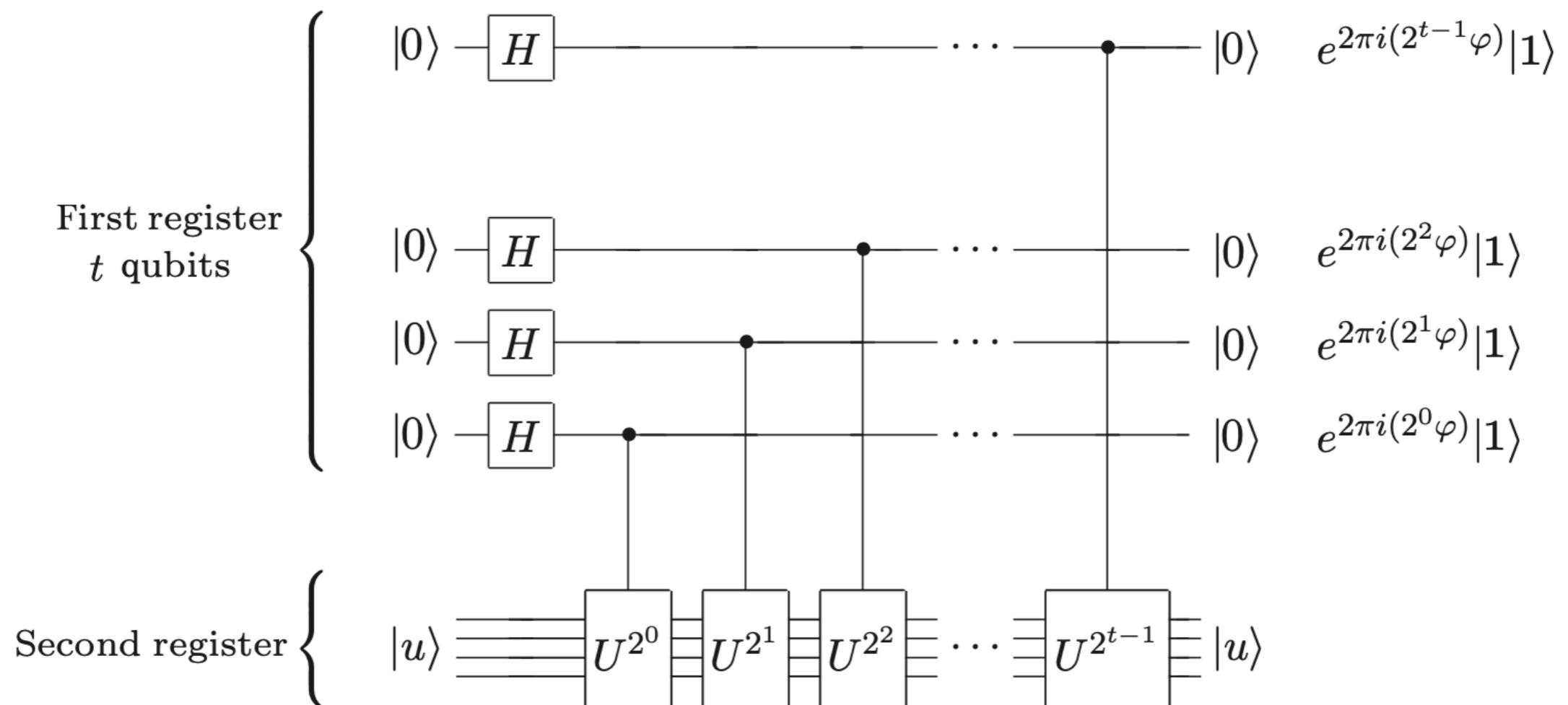
- Problems that quantum chemists care about:
  - ★ static: electronic energies of a molecule
    - > spectrum of Hamiltonian (Hermitian matrix) of the molecule.
    - ground-states
  - ★ dynamical: time evolution of quantum states  $|\psi(t)\rangle = e^{-iHt} |\psi_0\rangle$
- Complexity of problems:
  - ◆ QMA-complete: Solving eigenvalue problem of a general Hamiltonian
  - ◆ BQP: Simulating unitary time evolution of a wavefunction driven by the Hamiltonian; Quantum Phase Estimation (QPE)

# Background

- **Two models of quantum simulation:**
  - ★ **Analogue:** domain-specific, first-quantized encoding (real Hilbert space), e.g. ultracold atoms to simulate electrons (<https://www.nature.com/articles/s41586-019-1614-4>)
  - ★ **Digital: standard circuit model, scalability; second-quantized encoding (fock space)**
- **(Digital) Algorithms for simulating Molecular Hamiltonian:**
  - \* **Fault-tolerant QC:** quantum phase estimation (QPE)
  - \* **NISQ:** Hybrid scheme, e.g. [variational quantum eigensolver \(VQE\)](#), quantum annealing (QAOA), etc.

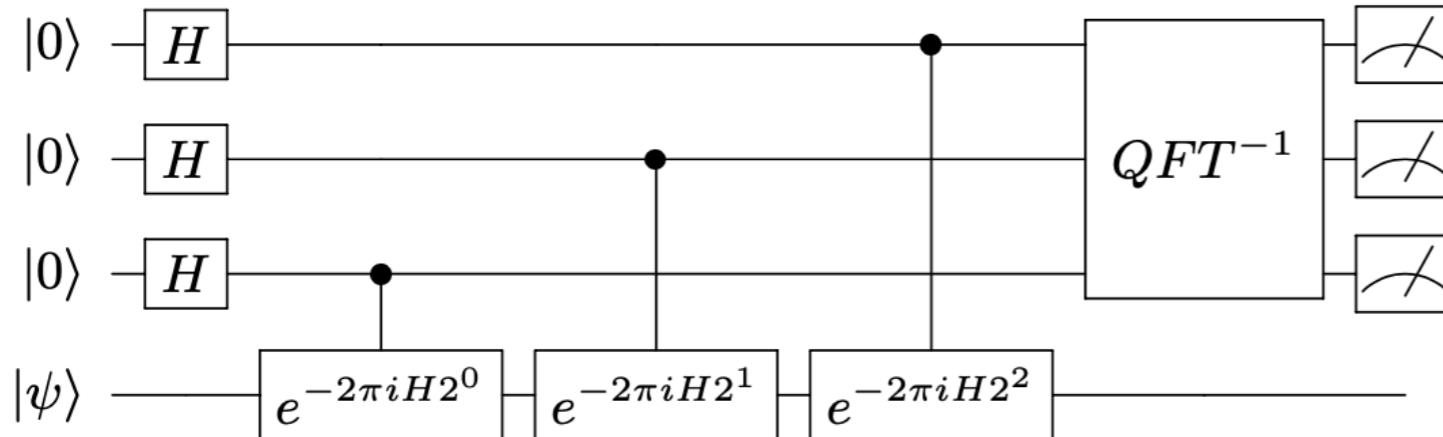
# Quantum Phase Estimation (QPE)

Suppose a unitary operator  $U$  has an eigenvector  $|u\rangle$  with eigenvalue  $e^{2\pi i\varphi}$ , where  $\varphi$  is unknown.



effect of controlled-U operations: take  $|j\rangle|u\rangle$  to  $|j\rangle U^j |u\rangle$

# Phase Estimation for simulating molecular energies



Canonical Quantum Phase Estimation circuit with **3 ancilla qubits**. When the ancilla qubits are in state  $|x\rangle$ , a control rotation  $e^{-2\pi i H x}$  is applied to the target state  $|\psi\rangle$

- State preparation: Initialize a register in a reference state  $|\psi\rangle$  + register of ancilla qubits in the  $|0\rangle^{\otimes \omega}$   
 $|\psi\rangle = \sum_i c_i |E_i\rangle$ ,  $c_0$  should be **large** (adiabatic state preparation, interpolation)
- Apply Walsh-Hadamard transformation to the ancilla register:  $\frac{1}{\sqrt{2^\omega}} \sum_x |x\rangle$
- Apply controlled-unitary gates:  $\frac{1}{\sqrt{2^\omega}} \sum_i \sum_x |x\rangle c_i |E_i\rangle \rightarrow \frac{1}{\sqrt{2^\omega}} \sum_i \sum_x e^{-2\pi i E_i x} c_i |x\rangle |E_i\rangle$
- Apply inverse Quantum Fourier Transformation to ancilla qubits:  $\rightarrow \sum_i c_i |\text{bin}(E_i)\rangle |E_i\rangle$
- Measure ancilla qubits in standard basis  $\rightarrow$  ground state energy  $|\text{bin}(E_0)\rangle$  as binary bit-string with prob.  
 $p \times |c_0|^2$ , precise to n bits, required ancilla qubits  $\omega = n + \log_2 \left( 2 + \frac{1}{2p} \right)$  ( $p$ : success probability)
- Main register projected to corresponding eigenvector  $|E_0\rangle$

# Variational Quantum Eigensolver (VQE)

**Variational Principle:**

any Hermitian matrices can be expressed as  $H = \sum_{i=1}^N \lambda_i |\psi_i\rangle\langle\psi_i|$ , then

expectation value of  $H$  on an arbitrary quantum state  $|\psi\rangle$  is given by

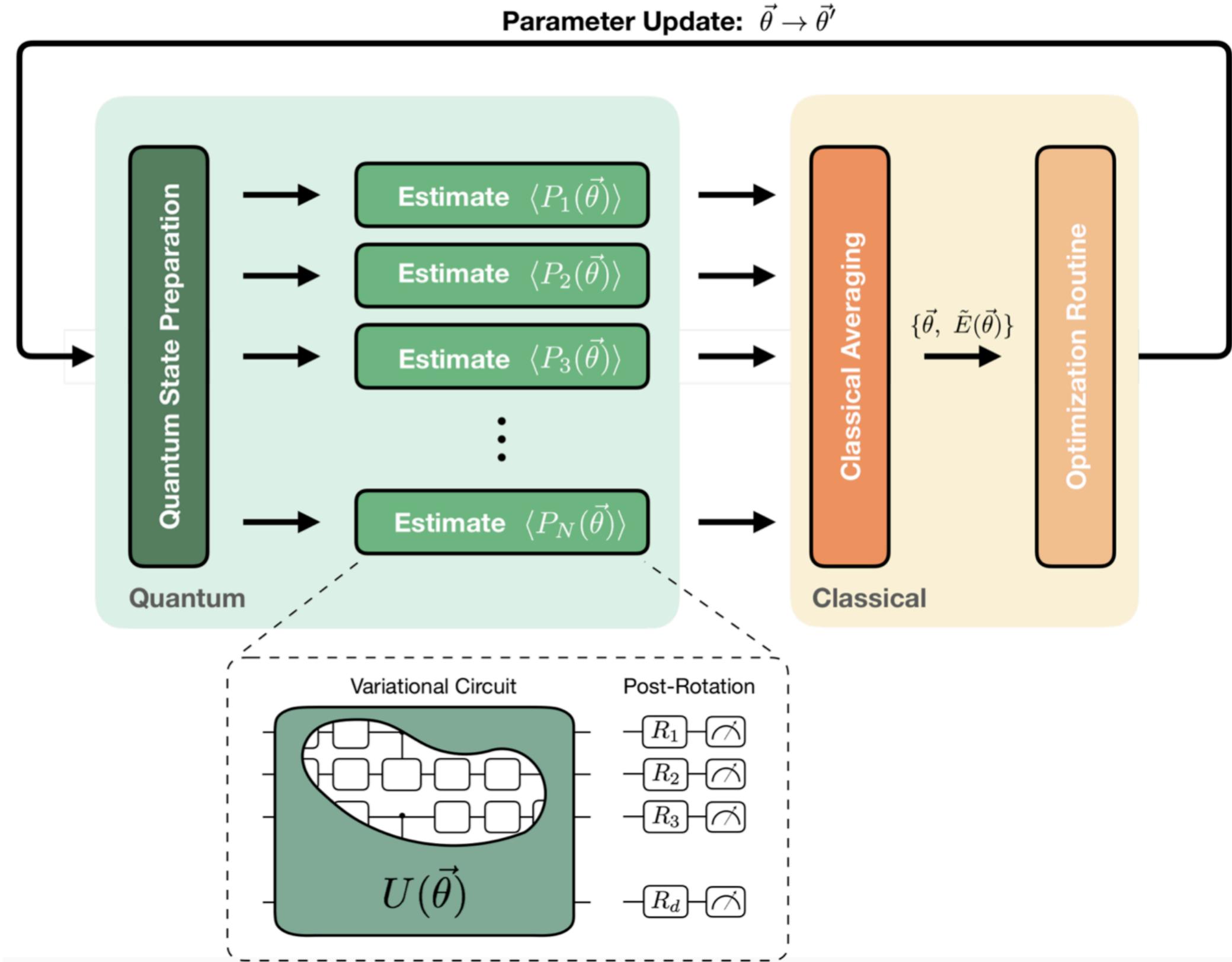
$$\langle H \rangle_\psi \equiv \langle \psi | H | \psi \rangle = \langle \psi | \left( \sum_{i=1}^N \lambda_i |\psi_i\rangle\langle\psi_i| \right) | \psi \rangle = \sum_{i=1}^N \lambda_i \langle \psi | \psi_i \rangle \langle \psi_i | \psi \rangle = \sum_{i=1}^N \lambda_i |\langle \psi_i | \psi \rangle|^2$$

$$\text{where } |\langle \psi_i | \psi \rangle|^2 \geq 0, \text{ thus, } \lambda_{\min} \leq \langle H \rangle_\psi = \langle \psi | H | \psi \rangle = \sum_{i=1}^N \lambda_i |\langle \psi_i | \psi \rangle|^2$$

**Ground state energy bounded:**  $E_{\text{gs}}$  of the system is the smallest eigenvalue of Hamiltonian.

Arbitrarily tight bounds on  $E_{\text{gs}}$  may be obtained by parametrizing a trial wavefunction **ansatz**, computing the expectation value of  $H$ , and iteratively updating parameters of the ansatz.

# Variational Quantum Eigensolver (VQE)



# Variational Quantum Eigensolver (VQE)

## Structure of variational forms (ansatz):

VQE use a parametrized circuit with a fixed form.

Action of this circuit is represented by  $U(\theta)$

$$U(\theta) |\psi\rangle \equiv |\psi(\theta)\rangle$$

Iterative optimization over  $|\psi(\theta)\rangle$  yields  $\langle\psi(\theta)|H|\psi(\theta)\rangle \approx E_{gs} \equiv \lambda_{\min}$

## How to span the target subspace:

hardware efficient ansatz:  $R_y$ ,  $R_y R_z$ , domain-agnostic

chemically inspired ansatz: **unitary coupled cluster** (capable of generating close approximations based on the problem's structure (symmetries of the system))



... Following

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This week, we at the MolSSI threw our Software Fellow Bootcamp. We had such an exciting time in the classroom! Thanks to all that participated!



<http://esciencecommons.blogspot.com/2019/02/a-new-spin-on-computing-chemist-leads-4.html>

Tuesday, February 5, 2019

## A new spin on computing: Chemist leads \$3.9 million DOE quest for quantum software



"Quantum computers are not just exponentially faster, they work in a radically different way from classical computers," says chemist Francesco Evangelista, who is leading a project to develop quantum software.

By Carol Clark

# Quantum Chemistry for Quantum Computers

Francesco A. Evangelista (Emory University), Alán Aspuru-Guzik (University of Toronto), Garnet K.-L. Chan (California Institute of Technology), Gustavo E. Scuseria (Rice University), Toru Shiozaki (Northwestern University), James D. Whitfield (Dartmouth College), Dominika Zgid (University of Michigan)

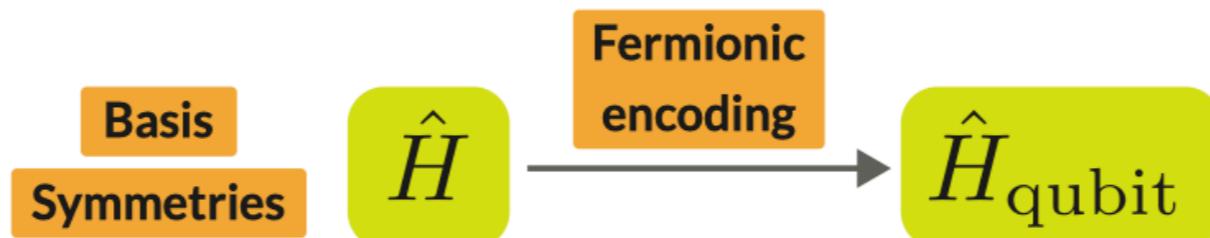
## Thrust III

### Quantum Algorithms for Quantum Chemistry

#### Goals

- Create quantum algorithms based on generalized unitary coupled cluster theory.<sup>1,2</sup>
- Fermionic mappings that incorporate spin and spatial symmetry in quantum algorithms.<sup>3</sup> Combination of relativistic Hamiltonians and quantum algorithms.

#### Opportunities to improve the mapping of the electronic Hamiltonian



#### Generalized unitary coupled cluster (UCC) theory

$$|\Psi_{\text{UCC}}\rangle = e^{\hat{T} - \hat{T}^\dagger} |\Phi\rangle = e^{\hat{\sigma}} |\Phi\rangle$$

**Cluster operator**                                   **Correlated reference**

- (1) A. Peruzzo, J. McClean, P. Shadbolt, M.-H. Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik, and J. L. O'Brien, *Nat Commun.* **5**, 4213 (2014).  
(2) G. Harsha, T. Shiozaki, and G.E. Scuseria, *J. Chem. Phys.* **148**, 044107 (2018).  
(3) K. Setia and J.D. Whitfield, *J. Chem. Phys.* **148**, 164104 (2018).

# A Multireference Quantum Krylov Algorithm for Strongly Correlated Electrons

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## Abstract

We introduce a multireference selected quantum Krylov (MRSQK) algorithm suitable for quantum simulation of many-body problems. MRSQK is a low-cost alternative to the quantum phase estimation algorithm that generates a target state as a linear combination of non-orthogonal Krylov basis states. This basis is constructed from a set of reference states via real-time evolution avoiding the numerical optimization of parameters. An efficient algorithm for the evaluation of the off-diagonal matrix elements of the overlap and Hamiltonian matrices is discussed and a selection procedure is introduced to identify a basis of orthogonal references that ameliorates the linear dependency problem. Preliminary benchmarks on linear  $H_6$ ,  $H_8$ , and  $\text{BeH}_2$  indicate that MRSQK can predict the energy of these systems accurately using very compact Krylov bases.

