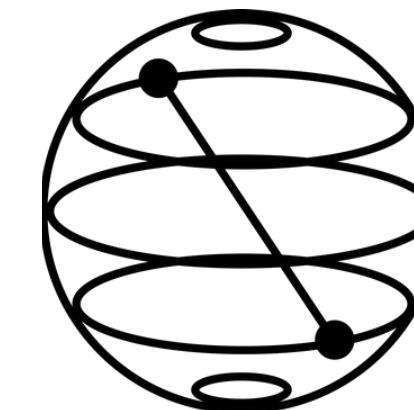


Quantum Computing for Quantum Chemistry



QISKit MEETUP, BY PABLO MORENO (QISKit ADVOCATE)



WHO AM I?

- BSc in Physics, Universidad de Extremadura
- MSc in Mathematical and Theoretical Physics, University of Oxford
- PhD in Quantum Algorithms, Universidad Complutense de Madrid



Effective Altruism

**"Effective altruism is about answering:
how can we use our resources to help others
the most?"**

QFold: Quantum Walks and Deep Learning to Solve Protein Folding

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(Dated: January 26, 2021)

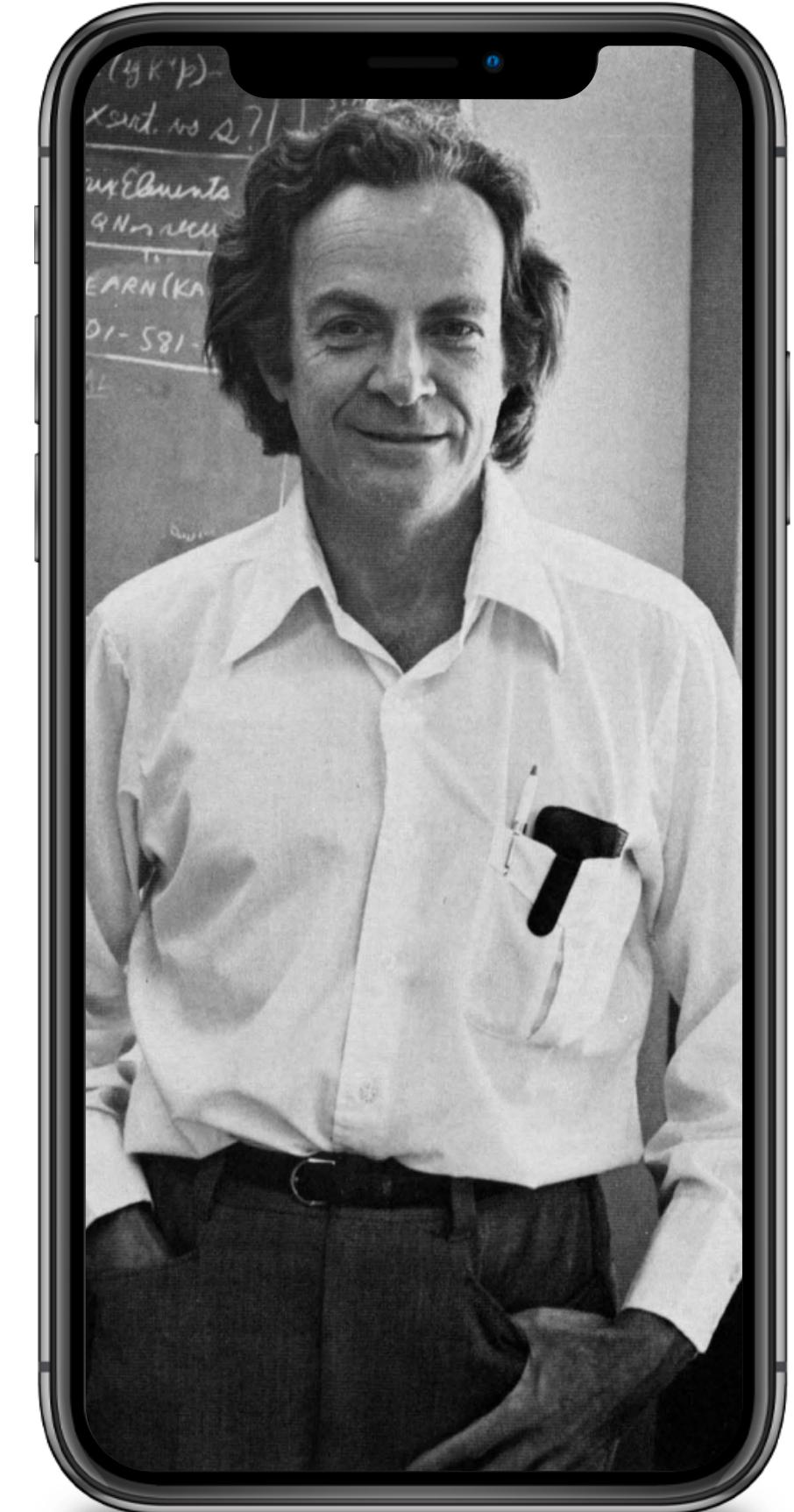
We develop quantum computational tools to predict how proteins fold in 3D, one of the most important problems in current biochemical research. We explain how to combine recent deep learning advances with the well known technique of quantum walks applied to a Metropolis algorithm. The result, QFold, is a fully scalable hybrid quantum algorithm that in contrast to previous quantum approaches does not require a lattice model simplification and instead relies on the much more realistic assumption of parameterization in terms of torsion angles of the amino acids. We compare it with its classical analog for different annealing schedules and find a polynomial quantum advantage, and validate a proof-of-concept realization of the quantum Metropolis in IBMQ Casablanca quantum processor.

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WHAT ARE QUANTUM COMPUTERS GOOD FOR?

Kinds of algorithms

- Shor-like algorithms, for some theoretical problems with a lot of structure.
- Grover-like algorithms, that give moderate quadratic speedups for combinatorial problems.
- Heuristic algorithms like Variational parametrized circuits.
- Simulating quantum systems -> Quantum Chemistry



WHY CHEMISTRY?

- The wave function of a quantum system has exponentially many terms, but can be stored in a quantum computer state.
- The evolution of quantum systems is unitary, precisely like in quantum computers!



QUANTUM PHASE ESTIMATION

Evolution in a quantum computer is generated by

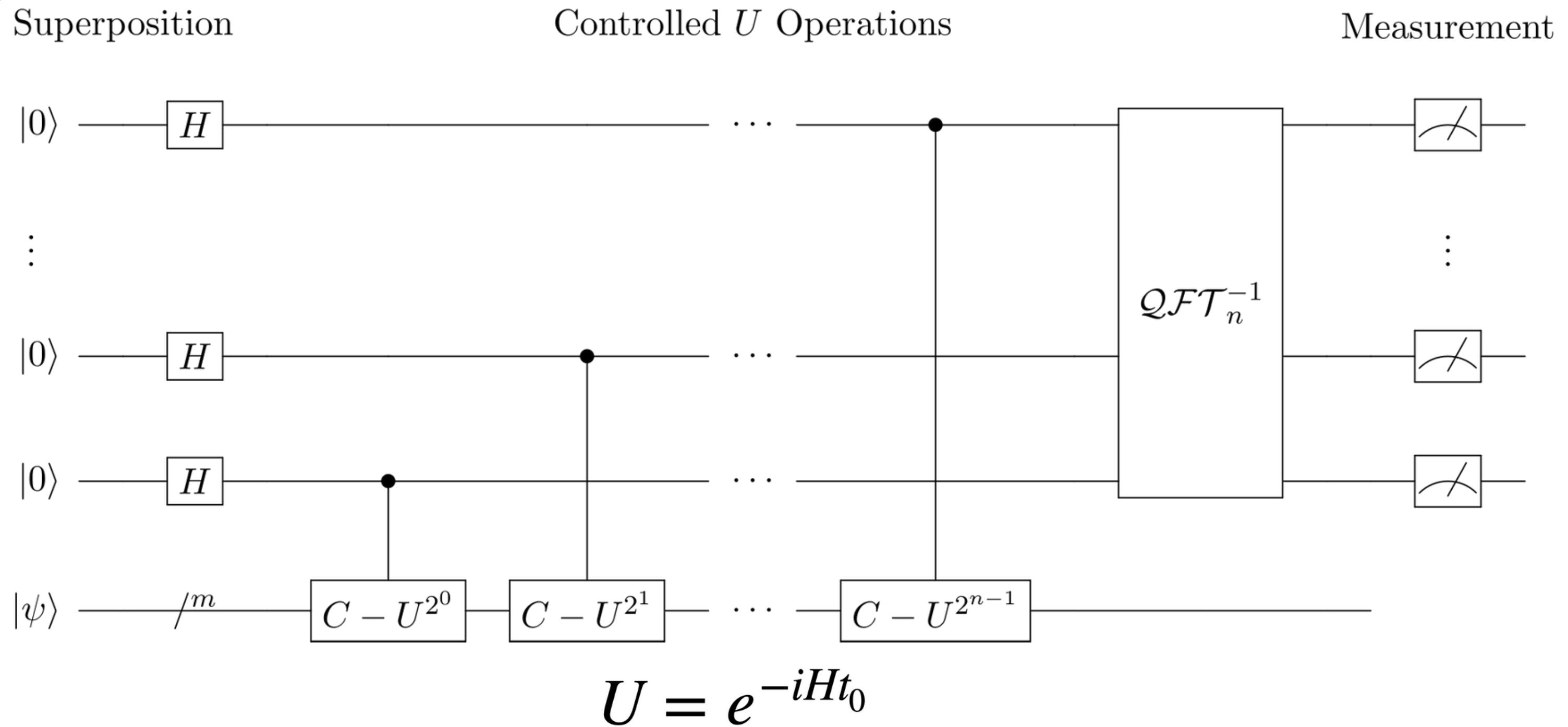
$$|\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle$$

If the state is an eigenvalue of the Hamiltonian

$$e^{-iHt} |\phi_0\rangle = e^{-iE_0 t} |\phi_0\rangle$$

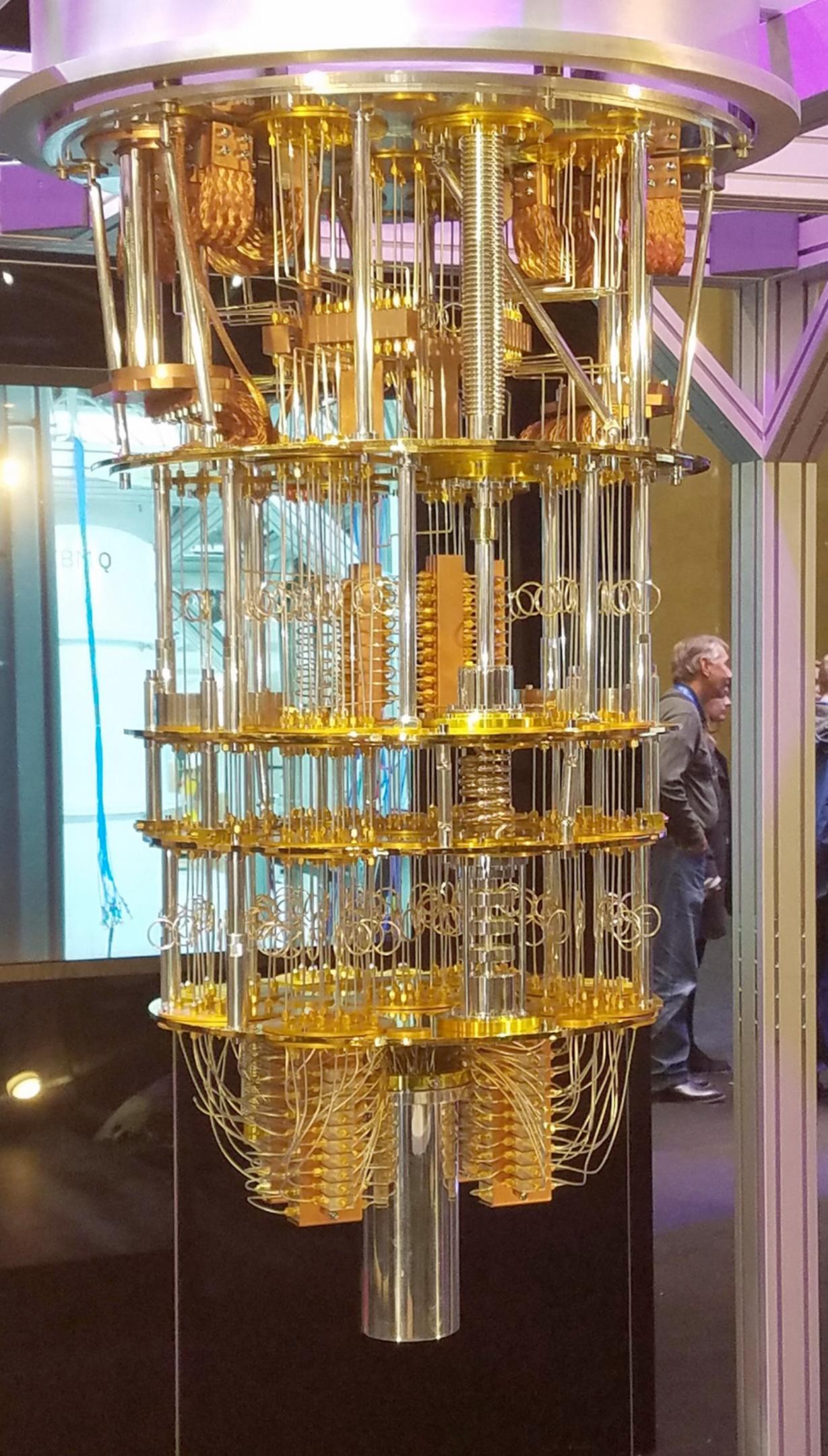
Calculating the Phase, we get the energy

Quantum Phase Estimation circuit



Variational Quantum Eigensolver

What happens if we only have NISQ devices available?



UNITARY COUPLED CLUSTER

To initialize the state

$$|\Psi\rangle = e^{T - T^\dagger} |\Phi\rangle_{\text{ref.}}$$

With T parametrized

$$T = T_1 + T_2 + T_3 + \dots + T_N$$

$$T_1 = \sum_{pr} t_p^r \hat{a}_p^\dagger \hat{a}_r$$

$$T_2 = \sum_{pqrs} t_{pq}^{rs} \hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_r \hat{a}_s$$

Variational parameters

Hartree Fock state

Creation and annihilation operators

QUANTUM EXPECTATION ESTIMATION

The Chemical Hamiltonian is composed of two body interactions:

$$\mathcal{H} = \sum_{i\alpha} h_\alpha^i \sigma_\alpha^i + \sum_{ij\alpha\beta} h_{\alpha\beta}^{ij} \sigma_\alpha^i \sigma_\beta^j + \dots$$

We can calculate the expected value of each term instead and then sum them

$$\langle \mathcal{H} \rangle = \sum_{i\alpha} h_\alpha^i \langle \sigma_\alpha^i \rangle + \sum_{ij\alpha\beta} h_{\alpha\beta}^{ij} \langle \sigma_\alpha^i \sigma_\beta^j \rangle + \dots$$

VARIATIONAL QUANTUM EIGENSOLVER

