Variational Quantum Eigensolver (VQE)

Evan Anderson – 12/09/2020

Outline

- Brief Introduction
- NISQ Recap
- Variational Method
- VQE Outline
- Toy Example
- Quantum Chemistry Considerations
- Experiment

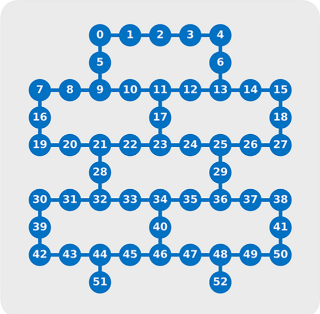
Variational Quantum Eigensolver (VQE)

- Often called hybrid-classical algorithm(s)
- Uses the variational method
  - Other algorithms include factoring, data generation, deflation
- Find the lowest possible eigenvalue of a Hamiltonian
- Can approximate classical optimization problems
  - QAOA implementation used to solve MaxCut/Ising problems
- Mind blowing applications for quantum chemistry

Noisy Intermediate Scale-Quantum (NISQ) Computing Recap

- Scaling qubits is hard. State of the art is ~50-100 noisy qubits vs millions required for fully error corrected algorithms like Shor's factoring
- Error correcting codes use up too many physical qubits
- Gate operations may introduce error or be limited
- Circuit depth is limited due to error (noise) propagation and short T1/T2 decoherence times relative to gate operations
  - Qubit "connectedness" can also play a role in limiting circuit depth depending on hardware architecture

53 Qubit Rochester Device



https://ibm.com/blogs/research/2019/09/quantum-computation-center/

Variational Method

Provides a way of approximating the lowest energy eigenstate :

Consider a Hamiltonian H with eigenvals and eigenstates given by: $H|\psi_\lambda\rangle = \lambda|\psi_\lambda\rangle$

Then we know, for any given arbitrary state (defined by a parameter θ): $\langle\psi(\theta)|H|\psi(\theta)\rangle \geq E_0$

We can tune or optimize θ such that we are left (hopefully) with a close upper bound to E_0

Variational Method Example

Helium Atom Hamiltonian where $|r_1 - r_2|$ is the repulsion term of the electrons:

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2) - \frac{e^2}{4\pi\varepsilon_0}\left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\right)$$

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For the trial wavefunction we drop the interaction term and the Hamiltonian is just the sum of two hydrogen-like atoms with charge 2e+ and thus the trial wavefunction is just the product of two ground state wavefunctions of the hydrogen like atom:

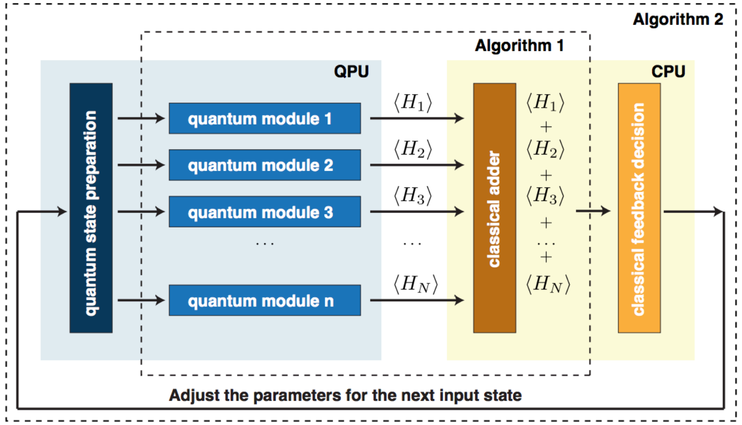
$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{Z^3}{\pi a_0^3} e^{-Z(r_1+r_2)/a_0} .$$

Here, Z is the tunable parameter and starts off as the nuclear charge Z=2. In varying it, a tight upper bound is found for Z=1.69 which is interpreted as a “shielding” from the electrons

The expectation value of this process is found to be within 2% of the true ground state energy

VQE Algorithm and Setup

1. Encode the Hamiltonian into a qubit Hamiltonian (sum of Pauli operators and their tensor products).
2. Choose/update an ansatz for state preparation on the quantum computer and build the quantum circuit
3. Measure in the basis of your qubit Hamiltonian to get expectation values for the state
4. Send the results to a classical optimizer to update the gate/wave parameters and repeat steps 2-4 until convergence



https://arxiv.org/pdf/1304.3061.pdf

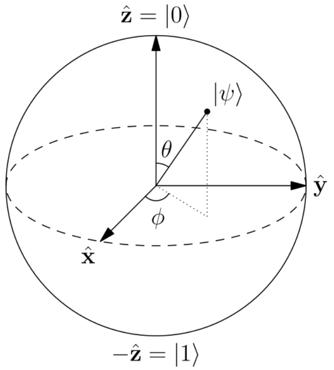
Simple Toy Example

$$x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$y = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix},$$

$$z = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- Start with a single qubit Hamiltonian that looks like
  - $H = 2Z + X + I = \begin{bmatrix} 3 & 1 \\ 1 & 0 \end{bmatrix}$
- Next we choose an ansatz, or set of gates that will explore states in a given subspace. Lets choose rotation about the y-axis: $Ry(\theta)$.
  - This allows states given by: $\cos(\theta)\,|0\rangle + \sin(\theta)\,|1\rangle = \begin{bmatrix} \cos(\theta) \\ \sin(\theta) \end{bmatrix}$



- Measurement typically occurs in the computational basis (along z) so for X we would need to also rotate into that basis $Ry(-\pi/2)$.
  - Z circuit: 

  - X circuit: 

  - $\theta = 0 \Rightarrow \langle H \rangle = 2 + 0 + 1 = 3$
  - $\theta = \pi \Rightarrow \langle H \rangle = -2 + 0 + 1 - 1$

Comments on Classical Optimizers

- Gradient Descent
  - Commonly chosen in classical optimization problems
  - Update parameter(s) based on largest energy change
  - Requires many circuit evaluations
  - Easy to get stuck in local minima
- Simultaneous Perturbation Stochastic Approximation (SPSA) optimizer
  - Ideal for “noisy” cost functions
  - Perturbs all parameters at once
  - Runs circuit twice, takes set of parameters that minimizes energy

Quantum Chemistry

Fermionic Hamiltonians can be generalized to the form $H_F = \sum_{ij} t_{ij} a_i^\dagger a_j + \sum_{ijkl} u_{ijkl}\ a_i^\dagger a_k^\dagger a_l a_j$

a_i and $a_i^\dagger$ are the usual creation/anhiliation operators for electrons in the ith orbital

t_{ij} and u_{ijkl} are the one and two electron interaction strengths which can be classically computed

Run into a problem mapping this Hamiltonian onto Pauli operators, considering the commutation rules of a_i and $a_i^\dagger$ do not match that of the Pauli operators.

$\{a_i, a_j\} = 0,\ \{a_i^\dagger, a_j^\dagger\} = 0,\ \{a_i, a_j^\dagger\} = \delta_{ij}$ vs $\{\sigma_a, \sigma_b\} = 2\delta_{ab}\, I.$

A number of mappings exist and an area of open research. Most common are **Jordan-Wigner** and Bravyi-Kitaev transformations

$$x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$y = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix},$$

$$z = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Jordan-Wigner Mapping (1928)

Naively, one might just map $a_i \Rightarrow \sigma_i^+ = \frac{1}{2}(\sigma^x + i\sigma^y)$ and $a_i^\dagger \Rightarrow \sigma_i^- = \frac{1}{2}(\sigma^x - i\sigma^y)$ as they preserve anticommutator relations for same-site occupancy $\{\sigma_i^+, \sigma_i^-\} = 1$

Unfortunately, $[\sigma_i^+, \sigma_j^-] = 0, i \neq j$ implies spins on different sites commute

The Jordan-Wigner mapping gets around this by considering a string of N qubit operations:

$$a_i \Rightarrow I^{\otimes i-1} \otimes \sigma^+ \otimes \sigma^{z \otimes N-i}$$

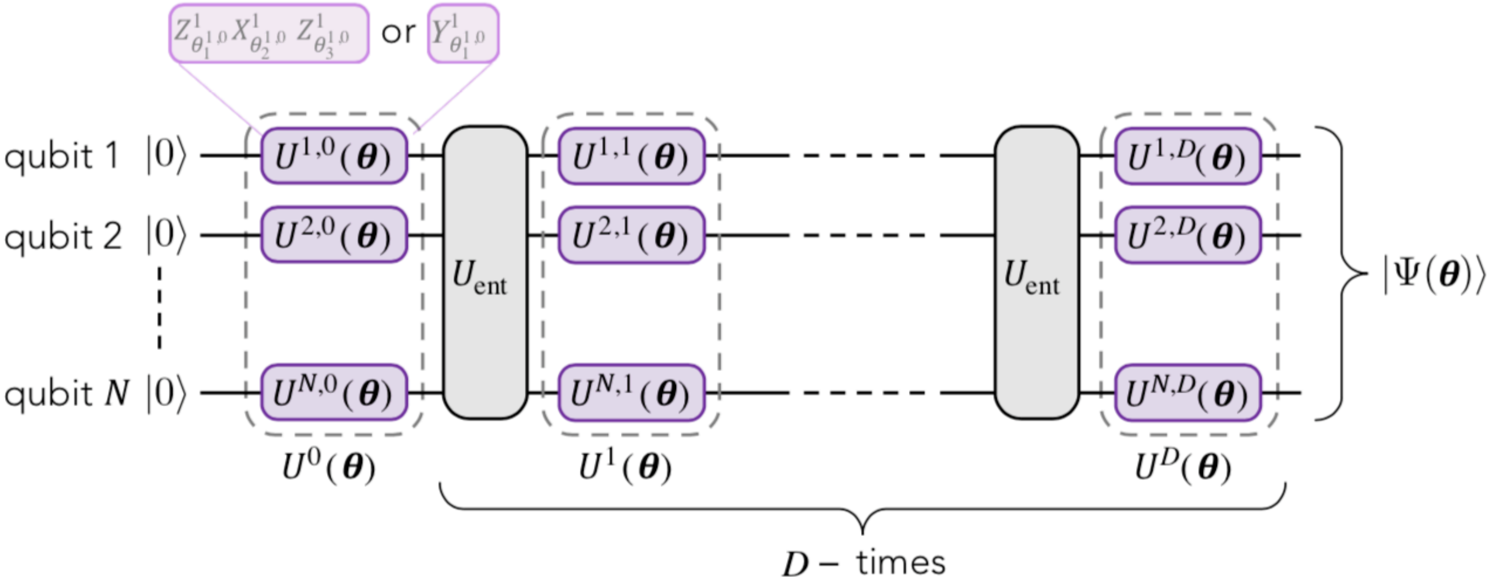
$$a_i^\dagger \Rightarrow I^{\otimes i-1} \otimes \sigma^- \otimes \sigma^{z \otimes N-i}$$

Requires knowledge of the occupancy of the $N - i$ state occupations of those orbitals

Wave function is spread out across all N qubits.

Trial State Preparation

Heuristic Approach



Moll et. al., 2018

Trial State Preparation

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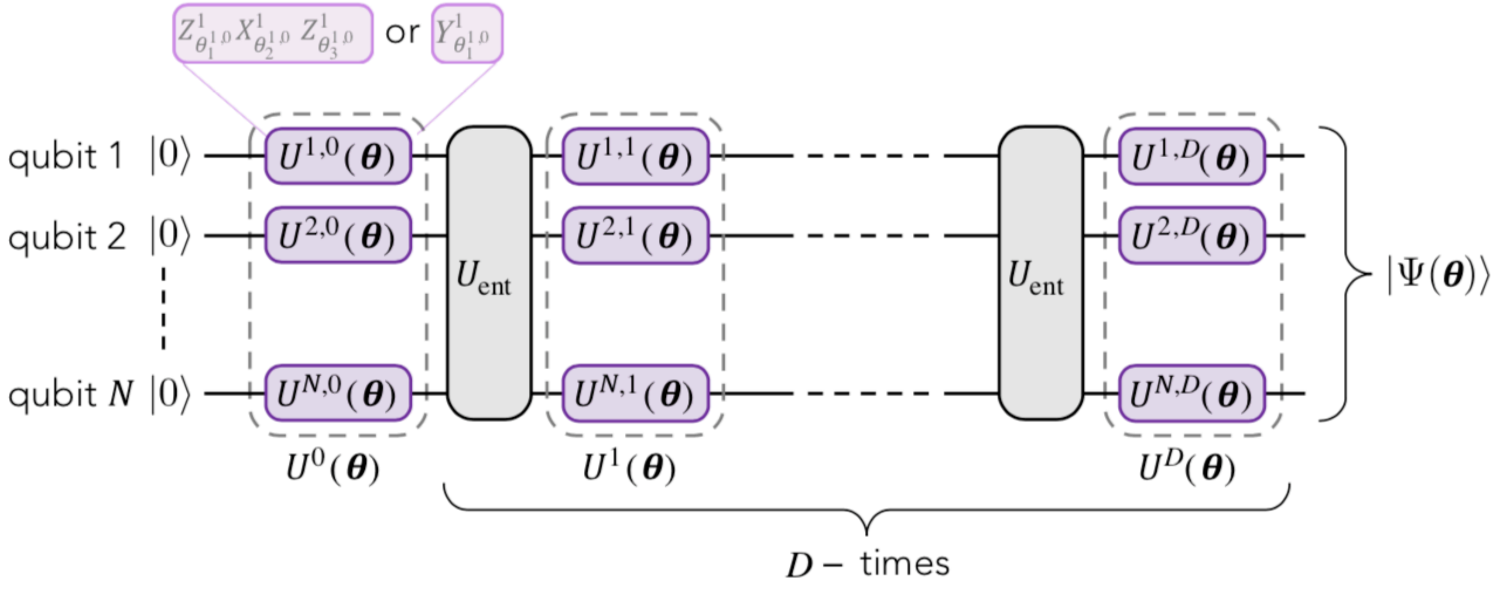

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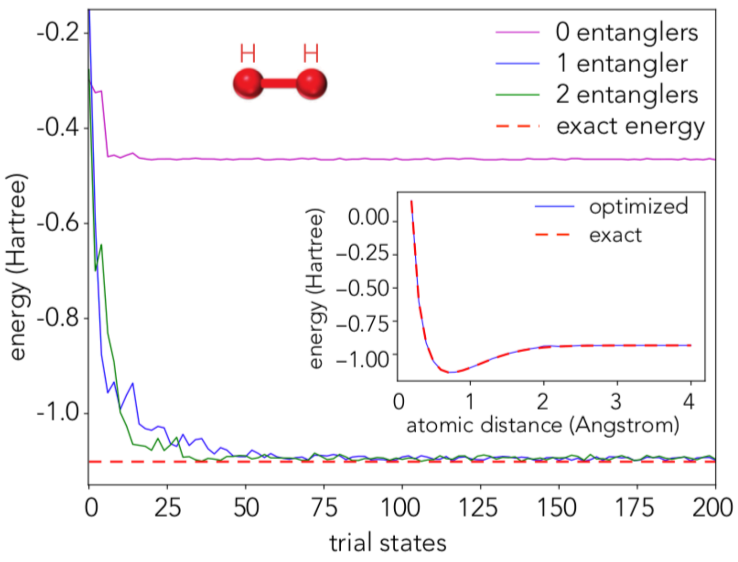
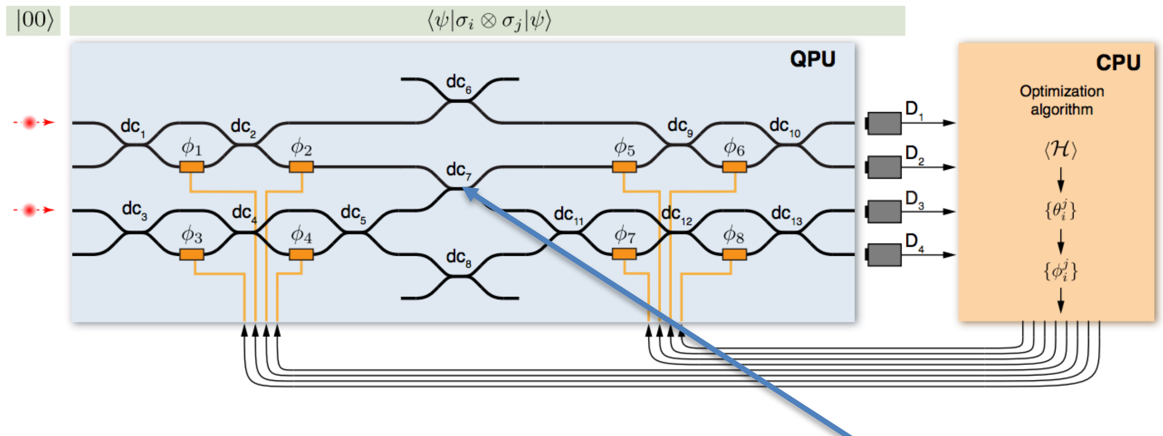


2013

A variational eigenvalue solver on a quantum processor

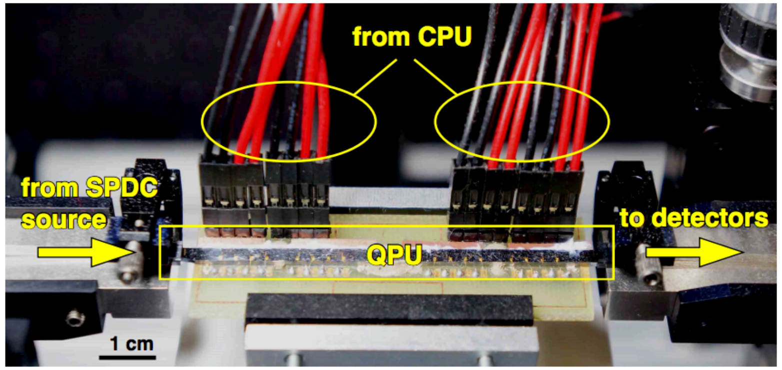
Alberto Peruzzo,[1,*] Jarrod McClean,[2,*] Peter Shadbolt,[1] Man-Hong Yung,[2,3] Xiao-Qi Zhou,[1] Peter J. Love,[4] Alán Aspuru-Guzik,[2] and Jeremy L. O'Brien[1]

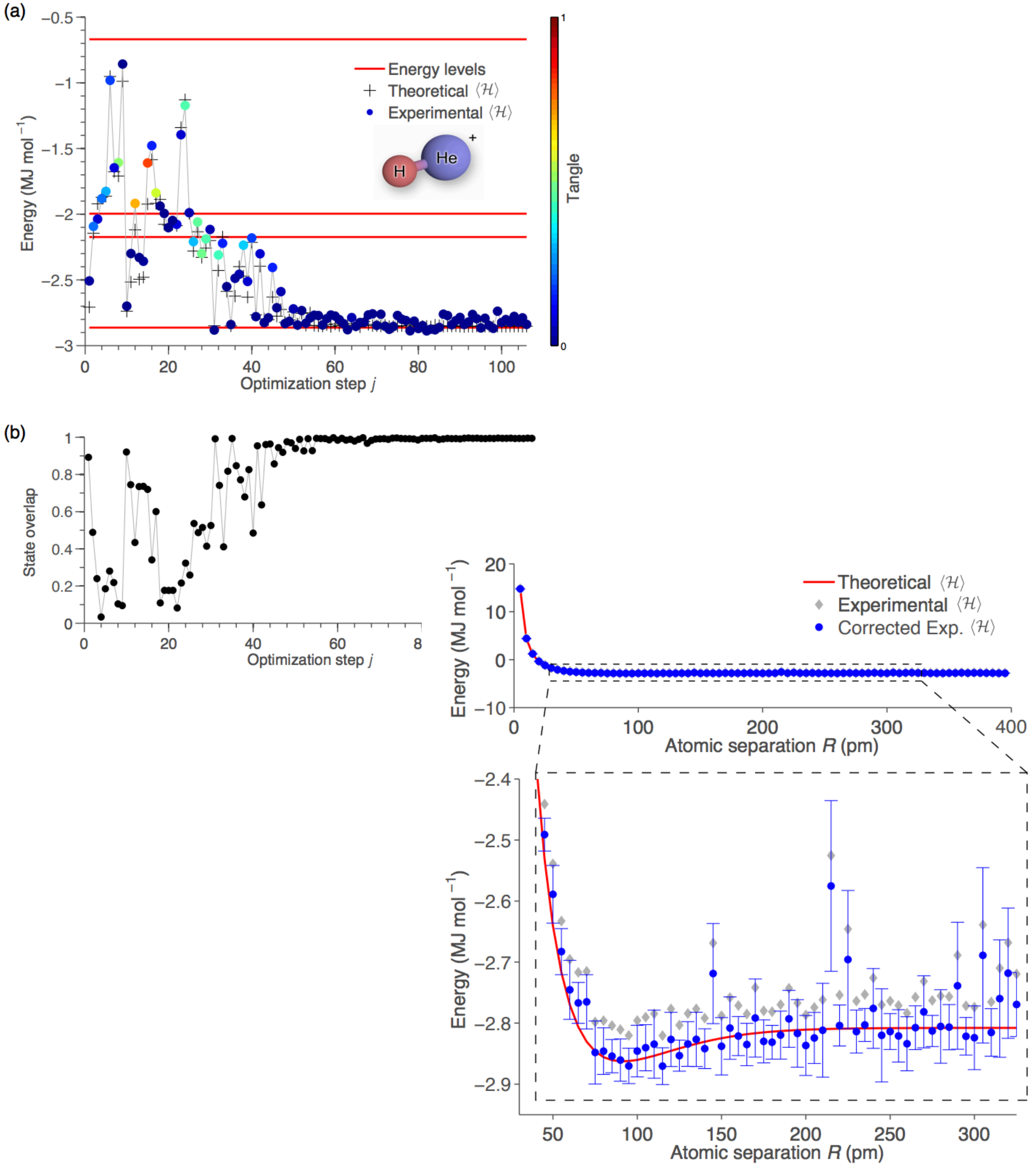
(a)



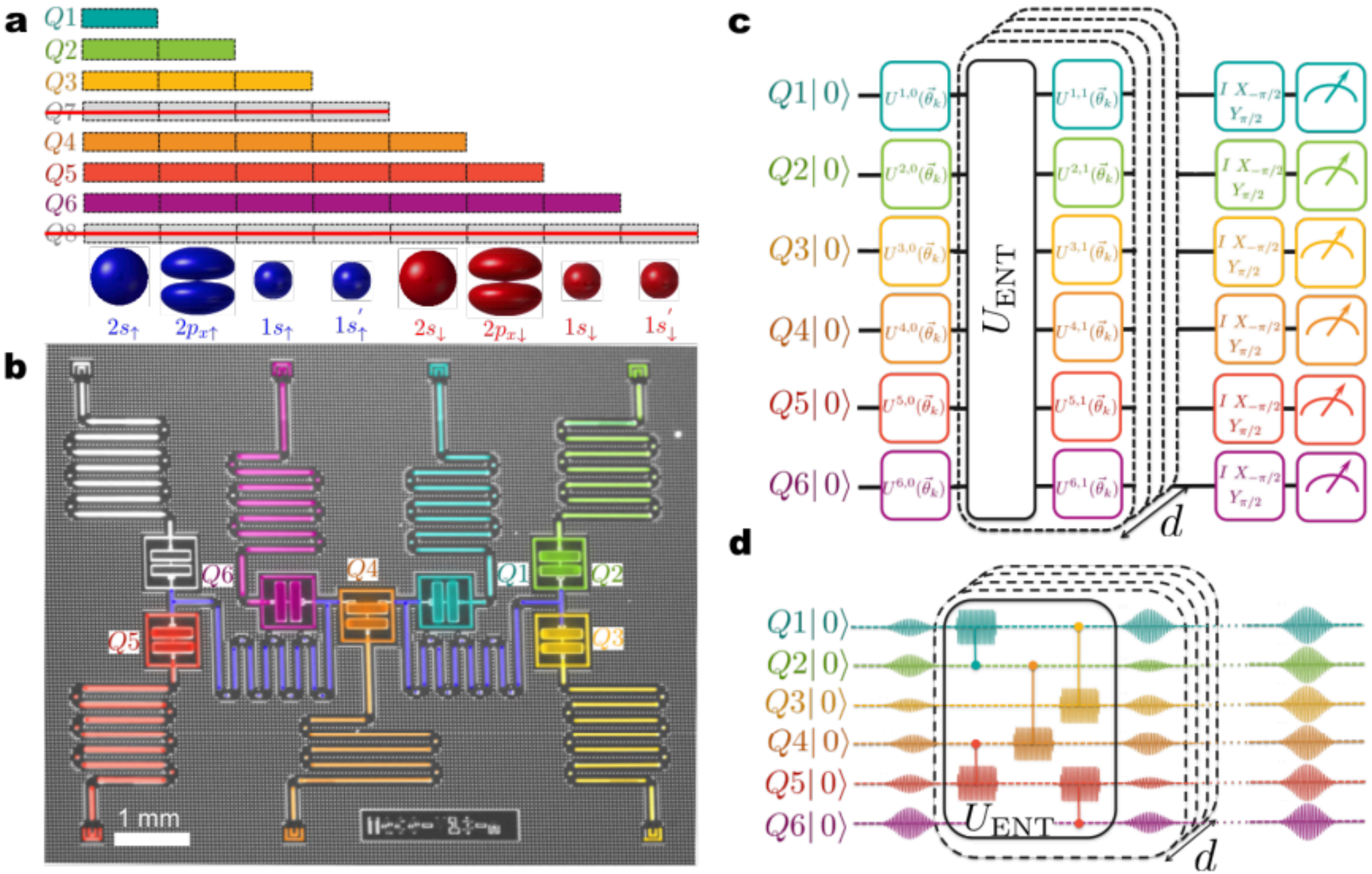
Entanglement

(b)



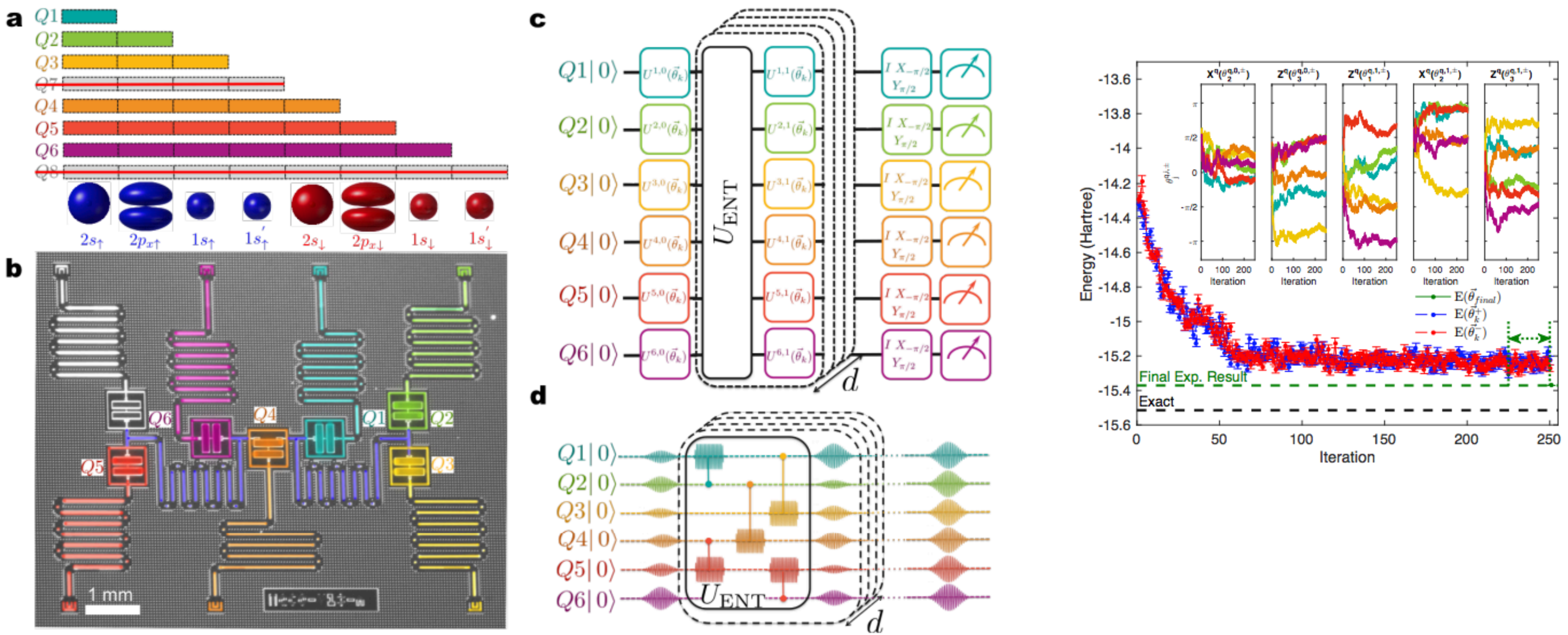


Superconducting Implementation



Kandala et. Al. 2018

Superconducting Implementation



Kandala et. al. 2017

You can do this right now

- Many companies have QC simulators (or build your own)
- Run this on real hardware
  - IBM (superconducting)
  - Riggeti (superconducting)
  - Xanadu (Continuous Variable)

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