Quantum chemistry with SC qubits

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Scalable Quantum Simulation of Molecular Energies

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We report the first electronic structure calculation performed on a quantum computer without exponentially costly precompilation. We use a programmable array of superconducting qubits to compute the energy surface of molecular hydrogen using two distinct quantum algorithms. First, we experimentally execute the unitary coupled cluster method using the variational quantum eigensolver. Our efficient implementation predicts the correct dissociation energy to within chemical accuracy of the numerically exact result. Second, we experimentally demonstrate the canonical quantum algorithm for chemistry, which consists of Trotterization and quantum phase estimation. We compare the experimental performance of these approaches to show clear evidence that the variational quantum eigensolver is robust to certain errors. This error tolerance inspires hope that variational quantum simulations of classically intractable molecules may be viable in the near future.

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Subject Areas: Condensed Matter Physics, Quantum Information

I. INTRODUCTION

Universal and efficient simulation of physical systems [1] is among the most compelling applications of quantum computing. In particular, quantum simulation of molecular energies [2], which enables numerically exact prediction of chemical reaction rates, promises significant advances in our understanding of chemistry and could enable *in silico* design of new catalysts, pharmaceuticals, and materials. As scalable quantum hardware becomes increasingly viable [3–7], chemistry simulation has attracted significant attention [8–28], since classically intractable molecules require a relatively modest number of qubits and because solutions have commercial value associated with their chemical applications [29].

The fundamental challenge in building a quantum computer is realizing high-fidelity operations in a scalable architecture [30]. Superconducting qubits have made rapid progress in recent years [3–6] and can be fabricated in microchip foundries and manufactured at scale [31]. Recent experiments have shown logic gate fidelities at the threshold required for quantum error correction [3] and dynamical suppression of bit-flip errors [4]. Here, we use the device reported in Refs. [4,7,32] to implement and compare two quantum algorithms for chemistry. We have previously characterized our hardware using randomized benchmarking [4] but related metrics (e.g., fidelities) only loosely bound how well our devices can simulate molecular energies. Thus, studying the performance of hardware on small instances of real problems is an important way to measure progress towards viable quantum computing.

Our first experiment demonstrates the recently proposed variational quantum eigensolver (VQE), introduced in Ref. [19]. Our VQE experiment achieves chemical accuracy and is the first scalable quantum simulation of

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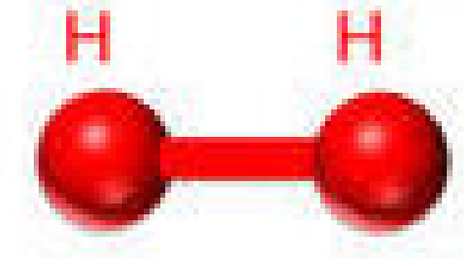
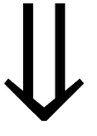




Find E_0 depending on bond lenth R

outline

- **Representation with qubits**:

  Hamiltonian of molecular hydrogen

- **2 algorithms to find ground state energy**:
  - Variational Quantum Eigensolver
  - Phase Estimation Algorithm

- **concrete implementation and outlook**:

  Chip, further experiments

Part I: Representation with qubits

Why quantum computing?

Problem: find ground state energy E_0 of physical system

classical: N spin-$\frac{1}{2}$ particles

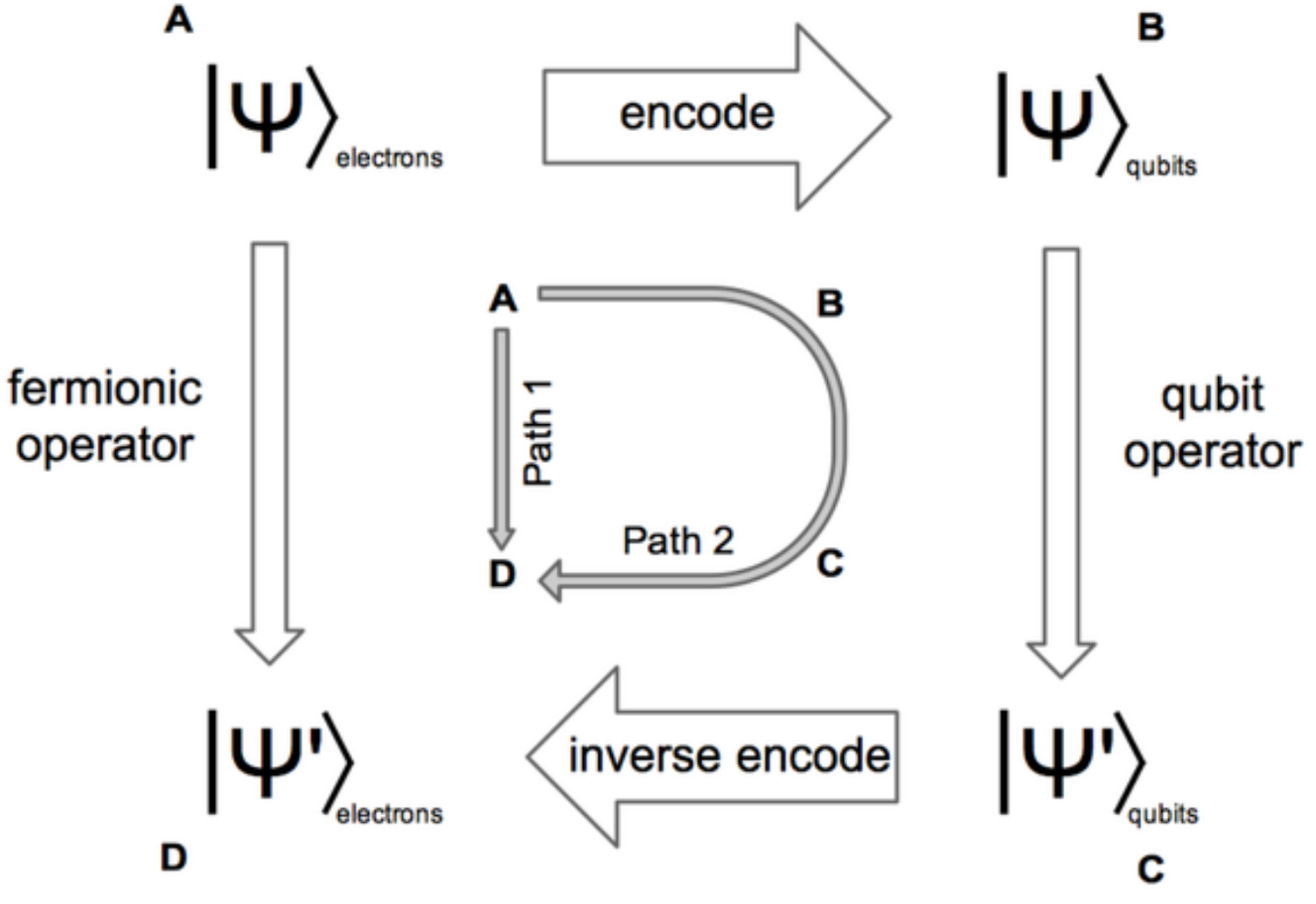
$\rightarrow$ need 2^N basis states $|\phi_k\rangle$ to represent $|\Psi\rangle = \sum_{k=1}^{2^N} c_k |\Phi_k\rangle$

$\rightarrow$ $O(e^N)$ bits for coefficients

Quantum: A wavefunction is approximated with a wavefunction

$\rightarrow$ N spin-$\frac{1}{2}$ particles $\rightarrow$ $O(N)$ qubits

Qubit representation of physical systems



We need to:

- ▷ represent the wavefunction Ψ with qubits
- ▷ represent the Hamiltonian as unitary acting on qubits

Qubit representation of physical systems

Second quantization: need to represent $|\Psi\rangle$, $a_i^\dagger$, a_i

simple way to represent $|\Psi\rangle$ (fermionic systems):

- $|\Psi\rangle = |f_{N-1}\ldots f_i\ldots f_0\rangle \quad \rightarrow \quad (f_{N-1}\ldots f_i\ldots f_0)^T, \quad f_i \in \{0,1\}$

  $|\Psi\rangle = |f_{N-1}\ldots f_i\ldots f_0\rangle$: occupation number of i'th state

  $(f_{N-1}\ldots f_i\ldots f_0)^T$: i'th qubit

- $a_i^\dagger = \mathbb{1}^{\otimes n-j-1} \otimes \hat{Q}^+ \otimes [\sigma_z^{\otimes j}]$, $\hat{Q}^\dagger = |1\rangle\langle 0| = \frac{1}{2}(\sigma_x - i\sigma_y)$

$\Rightarrow$ choose matrix A s.t. low number of gates necessary to represent $a_i^\dagger$, a_i $\rightarrow$ **Bravij-Kitaev transformation**

- generalize: $|\Psi\rangle \quad \rightarrow \quad A \cdot (f_{N-1}\ldots f_i\ldots f_0)^T \bmod 2$

  (transformation has to be invertable)

molecular hydrogen

second quantization + Born-Oppenheimer approximation

$$\Longrightarrow \quad \boxed{H = \sum_{ij} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l}$$

Which orbitals do we have?

Use minimal basis (STO-6G) → one orbital for each H-atom ($|\Psi_{H_1}\rangle$, $|\Psi_{H_2}\rangle$)

$$|\Psi_g\rangle = \frac{1}{\sqrt{2}}(|\Psi_{H_1}\rangle + |\Psi_{H_2}\rangle),\ |\Psi_u\rangle = \frac{1}{\sqrt{2}}(|\Psi_{H_1}\rangle - |\Psi_{H_2}\rangle)$$

add spin:

$$|\chi_0\rangle = |\Psi_g\rangle|\alpha\rangle, \quad |\chi_1\rangle = |\Psi_g\rangle|\beta\rangle, \quad |\chi_2\rangle = |\Psi_u\rangle|\alpha\rangle, \quad |\chi_3\rangle = |\Psi_u\rangle|\beta\rangle$$

→ 4 orbitals → **4 qubits**

Bravij-Kitaev transformation

$$H = f_0\mathbb{1} + f_1 Z_1 + f_3 Z_2 + f_1 Z_0 Z_1 + f_4 Z_0 Z_2 + f_5 Z_1 Z_3 + f_6 \mathbf{X_0} Z_1 \mathbf{X_2} + f_6 \mathbf{Y_0} Z_1 \mathbf{Y_2}$$
$$+ f_7 Z_0 Z_1 Z_2 + f_4 Z_0 Z_2 Z_3 + f_3 Z_1 Z_2 Z_3 + f_6 \mathbf{X_0} Z_1 \mathbf{X_2} Z_3$$
$$+ f_6 \mathbf{Y_0} Z_1 \mathbf{Y_2} Z_3 + f_7 Z_0 Z_1 Z_2 Z_3$$

* **initial state**: use Hartree-Fock-state

  $\rightarrow$ qubit 'i' is eigenstate of Z_i

  $\rightarrow$ qubits 1 and 3 remain unchanged by H

  $\rightarrow$ reduce system to only qubits 0 and 2

$$\Longrightarrow H = g_0\mathbb{1} + g_1 Z_0 + g_2 Z_1 + g_3 Z_0 Z_1 + g_4 Y_0 Y_1 + g_5 X_0 X_1$$
$$= \sum_\gamma g_\gamma H_\gamma$$

$\Longrightarrow$ **starting point for VQE and PEA**

Part II: Algorithms to find ground state energy

Variational Quantum Eigensolver

goal: find E_0 of H_2 depending on bond length R

- use variational principle: $\frac{\langle \Psi(\vec{\Theta})|H|\Psi(\vec{\Theta})\rangle}{\langle \Psi(\vec{\Theta})|\Psi(\vec{\Theta})\rangle} = E(\vec{\Theta}) \geqslant E_0$
- ground state: $|\Psi(\vec{\Theta}^*)\rangle$, $\vec{\Theta}^* = \text{argmin}(E(\vec{\Theta}))$, $E(\vec{\Theta}^*) = E_0$
- $|\Psi(\vec{\Theta})\rangle = U(\vec{\Theta})\,|\Phi\rangle$, $|\Phi\rangle$: initial state, $U(\vec{\Theta})$: unitary

unitary coupled cluster theory: $|\Psi(\vec{\Theta})\rangle = e^{-i\Theta X_0 Y_1}\,|01\rangle$

initial state $|\Phi\rangle = |01\rangle$, Hartree-Fock state

VQE Algorithm

reminder:

$$H = g_0\mathbb{1} + g_1 Z_0 + g_2 Z_1 + g_3 Z_0 Z_1 + g_4 Y_0 Y_1 + g_5 X_0 X_1 = \sum_\gamma g_\gamma H_\gamma$$

$$|\Psi(\vec{\Theta})\rangle = e^{-i\Theta X_0 Y_1} |01\rangle$$

1. Prepare initial state $|\Phi\rangle = |01\rangle$

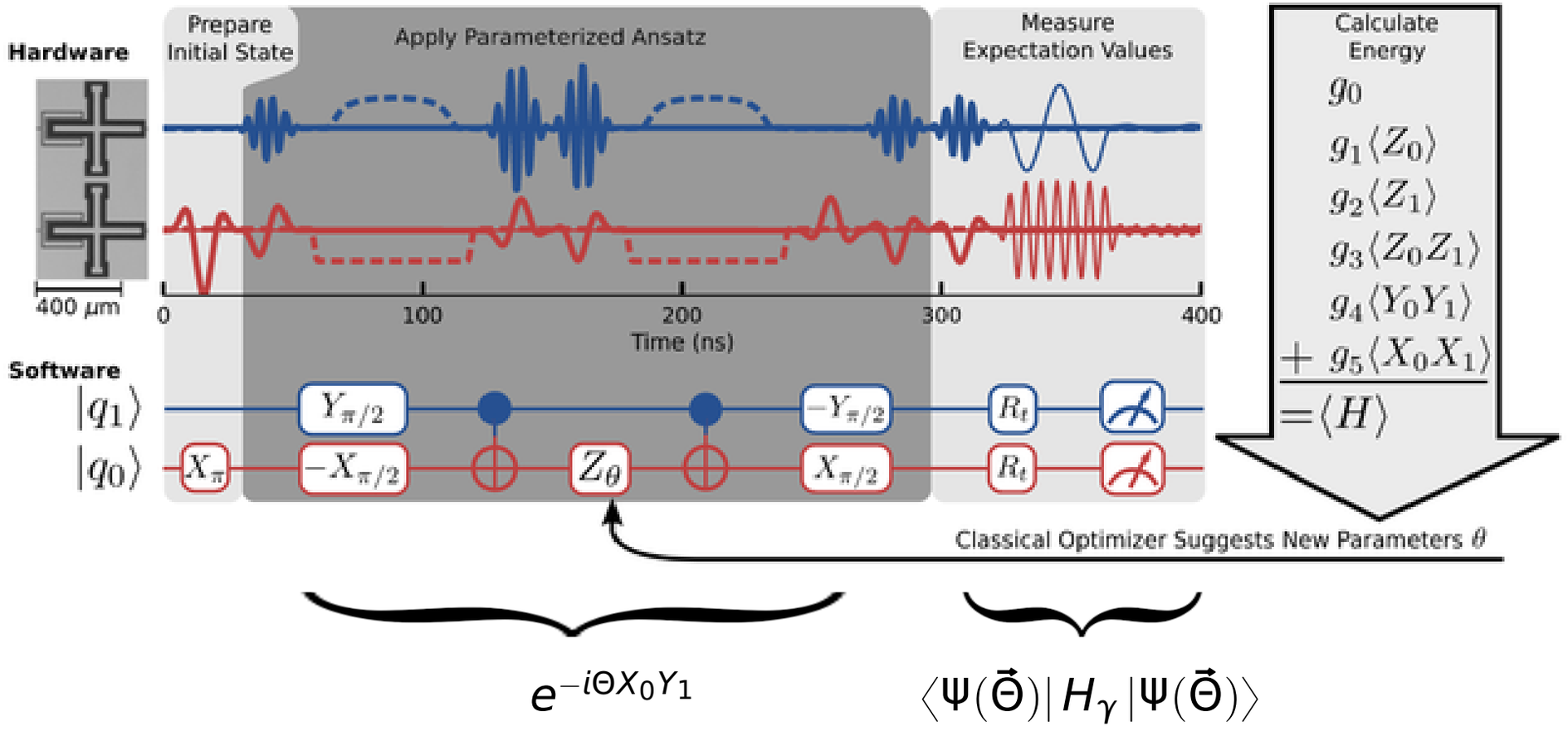
2. Measure $E(\vec{\Theta})$ for ”all” (e.g. 1000) values of $\Theta \in [-\pi, \pi]$ (R given)

$$E(\vec{\Theta}) = \langle\Psi(\vec{\Theta})| H |\Psi(\vec{\Theta})\rangle = \sum_\gamma g_\gamma \langle\Psi(\vec{\Theta})| H_\gamma |\Psi(\vec{\Theta})\rangle$$

3. Find minimum Θ^* of $E(\Theta)$ classically

$\rightarrow$ ground state energy for bond length R: $E(\Theta^*)$

VQE algorithm



2. Algorithm: Phase Estimation Algorithm, How to implement time evolution?

- Implement : $U = \exp(-iHt) = \exp(-\imath \sum_\gamma H_\gamma t) \neq \prod_\gamma \exp(-\imath H_\gamma t)$

- Use : *Theorem 4.3*: (**Trotter formula**) Let A and B be Hermitian operators. Then for any real t,

$$\lim_{n\to\infty} (e^{iAt/n} e^{iBt/n})^n = e^{i(A+B)t} . \qquad (4.98)$$

- Apply : $e^{-iHt} = e^{-it\sum_\gamma g_\gamma H_\gamma} \approx U_{\text{Trot}}(t) \equiv \left(\prod_\gamma e^{-ig_\gamma H_\gamma t/\rho}\right)^\rho$

Phase Estimation Algorithm: Goal.

- General case: $U\left|\Psi\right\rangle = \exp\left(2\pi i\Theta\right)\left|\Psi\right\rangle, \quad \Theta \in [0,1]$
- Our case: $\exp\left(-iHt\right)\left|E_n\right\rangle = \exp\left(-iE_nt\right)\left|E_n\right\rangle$
- Relation between phase & energy: $E_n = \dfrac{2\pi\Theta}{t}$

Writing phase in binary representation:

- With $\Theta \in [0,1]$, $\Theta = \sum_i \frac{\Theta_i}{2^i}$

$$= \Theta_1 \frac{1}{2} + \Theta_2 \frac{1}{4} + \Theta_3 \frac{1}{8} + ...$$

$$= 0.\Theta_1\Theta_2\Theta_3..$$

- Example : $0.75 = 1 * \frac{1}{2} + 1 * \frac{1}{2^2} + 0 * \frac{1}{2^4} + .. = 0.11000...$

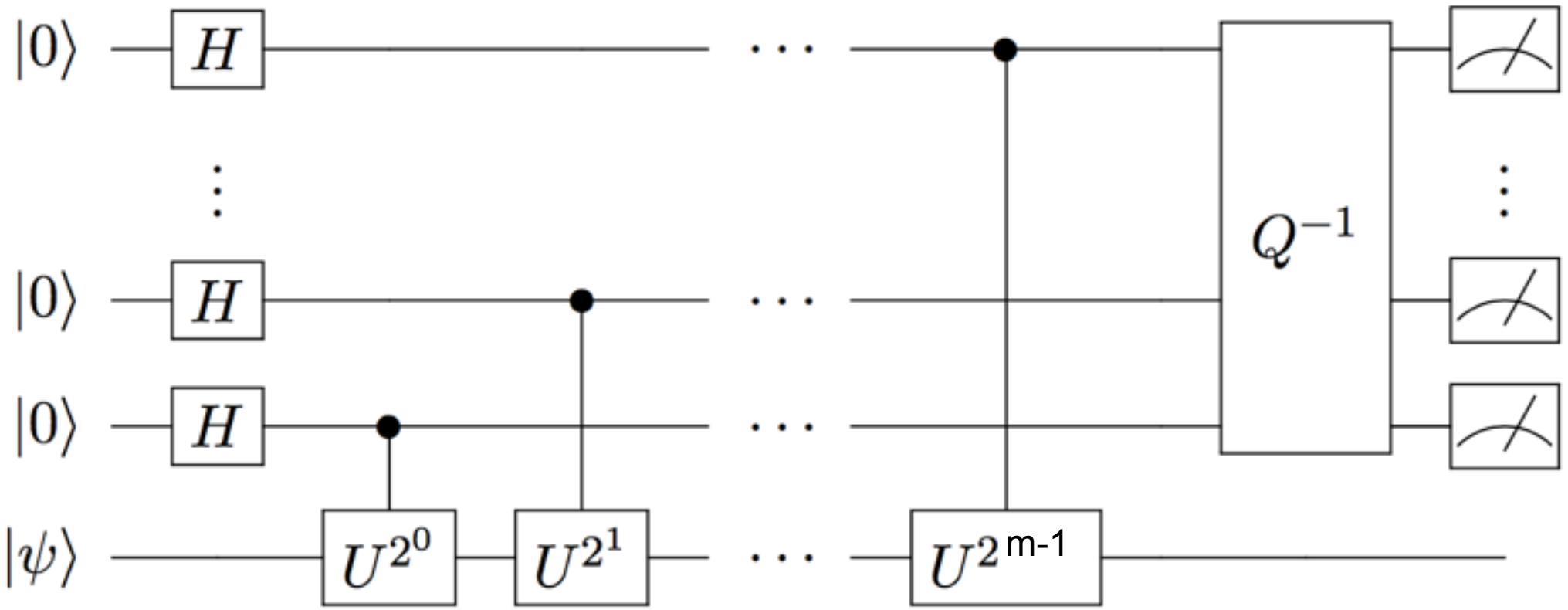
Idea:

$$\begin{pmatrix} |0_1\rangle \\ |0_2\rangle \\ .. \\ .. \\ |0_m\rangle \\ |\Psi\rangle \end{pmatrix} \rightarrow H \rightarrow CU^{2^k} \rightarrow |F\rangle = QFT \begin{pmatrix} |\Theta_1\rangle \\ |\Theta_2\rangle \\ .. \\ .. \\ |\Theta_m\rangle \\ |\Psi\rangle \end{pmatrix}, (\Theta = 0.\Theta_1\Theta_2\Theta_3..\Theta_m).$$

$$E_n = \frac{2\pi\Theta}{t}$$

$$\rightarrow |F\rangle \rightarrow QFT^{-1} \rightarrow \begin{pmatrix} |\Theta_1\rangle \\ |\Theta_2\rangle \\ .. \\ .. \\ |\Theta_m\rangle \\ |\Psi\rangle \end{pmatrix}$$

PEA (1): Circuit.



PEA (2): Action of one specific power of CU gate.

$$(|0\rangle + |1\rangle) \bigotimes |\Psi\rangle \rightarrow_{CU^{2^k}} |0\rangle |\Psi\rangle + |1\rangle U^{2k} |\Psi\rangle$$

$$= |0\rangle |\Psi\rangle + \exp(2\pi i 2^k \theta) |1\rangle |\Psi\rangle$$

$$= (|0\rangle + \exp(2\pi i 2^k \theta) |1\rangle) \bigotimes |\Psi\rangle$$

PEA (3): Circuit.

$$\begin{pmatrix} |0\rangle \\ |0\rangle \\ .. \\ .. \\ |0\rangle \end{pmatrix} \rightarrow_{H} \begin{pmatrix} |0\rangle + |1\rangle \\ |0\rangle + |1\rangle \\ .. \\ .. \\ |0\rangle + |1\rangle \end{pmatrix} \rightarrow_{Controlled-U^{2^k}} \begin{pmatrix} |0\rangle + \exp 2\pi\imath 2^0\theta\,|1\rangle \\ .. \\ |0\rangle + \exp 2\pi\imath 2^k\theta\,|1\rangle \\ .. \\ |0\rangle + \exp 2\pi\imath 2^{m-1}\theta\,|1\rangle \end{pmatrix}$$

PEA (4).

- Write phase in binary representation:

$$\begin{pmatrix} |0\rangle + \exp\left(2\pi i 2^0 \theta\right)|1\rangle \\ .. \\ |0\rangle + \exp\left(2\pi i 2^k \theta\right)|1\rangle \\ .. \\ |0\rangle + \exp\left(2\pi i 2^{m-1} \theta\right)|1\rangle \end{pmatrix} = \begin{pmatrix} |0\rangle + \exp\left(2\pi i 2^0 0.\Theta_1..\Theta_{m-1}\Theta_m\right)|1\rangle \\ .. \\ |0\rangle + \exp\left(2\pi i 2^k 0.\Theta_1..\Theta_{m-1}\Theta_m\right)|1\rangle \\ .. \\ |0\rangle + \exp\left(2\pi i 2^{m-1} 0.\Theta_1..\Theta_{m-1}\Theta_m\right)|1\rangle \end{pmatrix}$$

- Example: $2^3\Theta = 2^3 0.\Theta_1\Theta_2\Theta_3..\Theta_m = 8(\Theta_1\frac{1}{2} + \Theta_2\frac{1}{4} + \Theta_3\frac{1}{8} + \Theta_4\frac{1}{16} + ..)$

$$= 4\Theta_1 + 2\Theta_2 + 1\Theta_3 + \Theta_4\frac{1}{2} + ..$$

- One gets: $\exp\left(2\pi i 2^3 0.\Theta_1\Theta_2\Theta_3..\Theta_m\right) = \exp\left(2\pi i(4\Theta_1 + 2\Theta_2 + 1\Theta_3 + \Theta_4\frac{1}{2} + ..)\right)$

$$= \exp\left(2\pi i 0.\Theta_4\Theta_5\Theta_6..\Theta_m\right)$$

PEA(5).

$$\begin{pmatrix} |0\rangle + \exp\left(2\pi i 2^0 0.\Theta_1..\Theta_{m-1}\Theta_m\right)|1\rangle \\ .. \\ |0\rangle + \exp\left(2\pi i 2^k 0.\Theta_1..\Theta_{m-1}\Theta_m\right)|1\rangle \\ .. \\ |0\rangle + \exp\left(2\pi i 2^{m-1} 0.\Theta_1..\Theta_{m-1}\Theta_m\right)|1\rangle \end{pmatrix} = \begin{pmatrix} |0\rangle + \exp\left(2\pi i 0.\Theta_1..\Theta_{m-1}\Theta_m\right)|1\rangle \\ .. \\ |0\rangle + \exp\left(2\pi i 0.\Theta_{k+1}..\Theta_{m-1}\Theta_m\right)|1\rangle \\ .. \\ |0\rangle + \exp\left(2\pi i 0.\Theta_m\right)|1\rangle \end{pmatrix} = |F\rangle$$

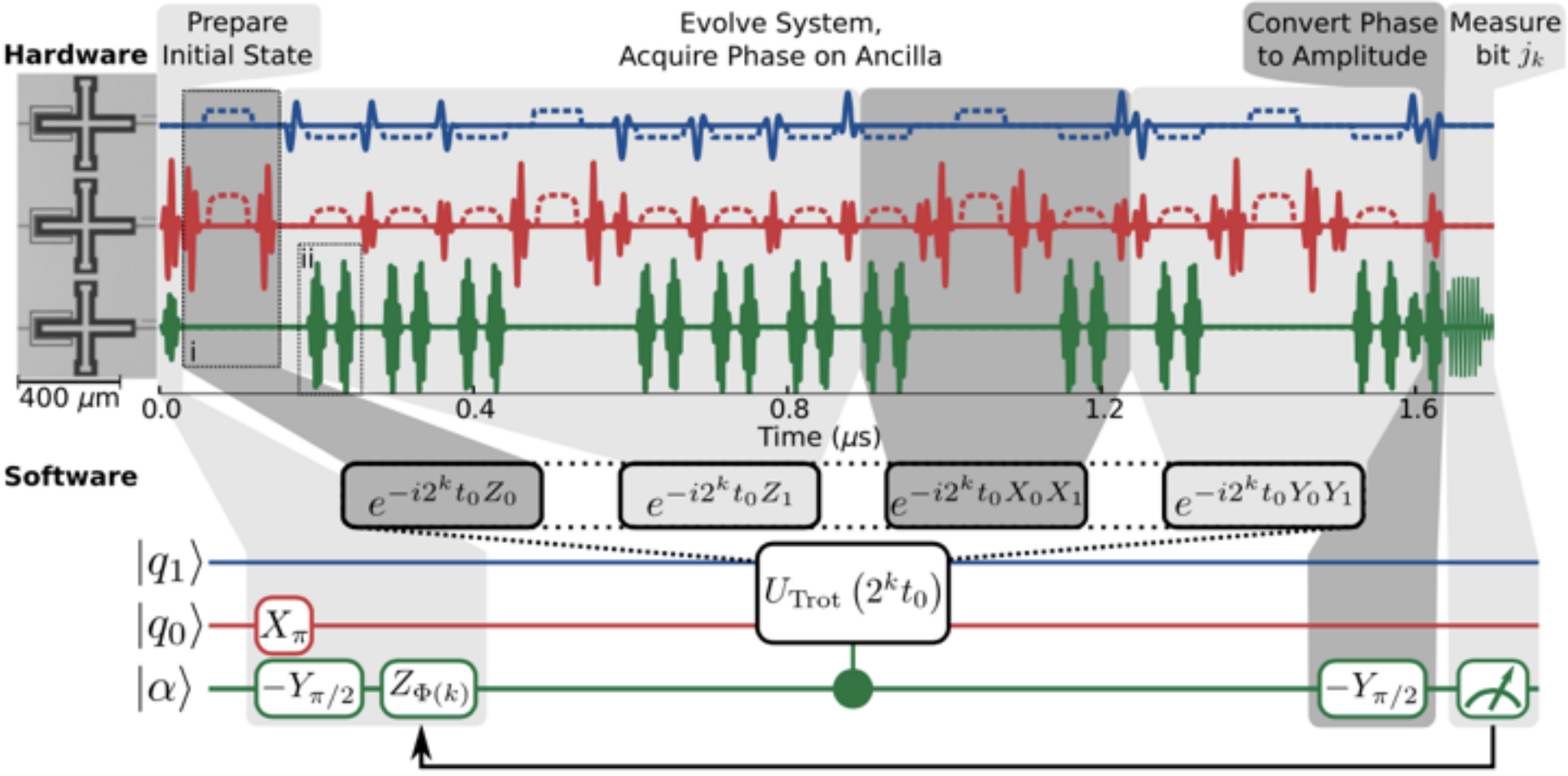
$$\begin{pmatrix} |0_1\rangle \\ |0_2\rangle \\ .. \\ .. \\ |0_m\rangle \\ |\Psi\rangle \end{pmatrix} \rightarrow H \rightarrow CU^{2^k} \rightarrow |F\rangle = QFT \begin{pmatrix} |\Theta_1\rangle \\ |\Theta_2\rangle \\ .. \\ .. \\ |\Theta_m\rangle \\ |\Psi\rangle \end{pmatrix}$$

Fourier Transformation:

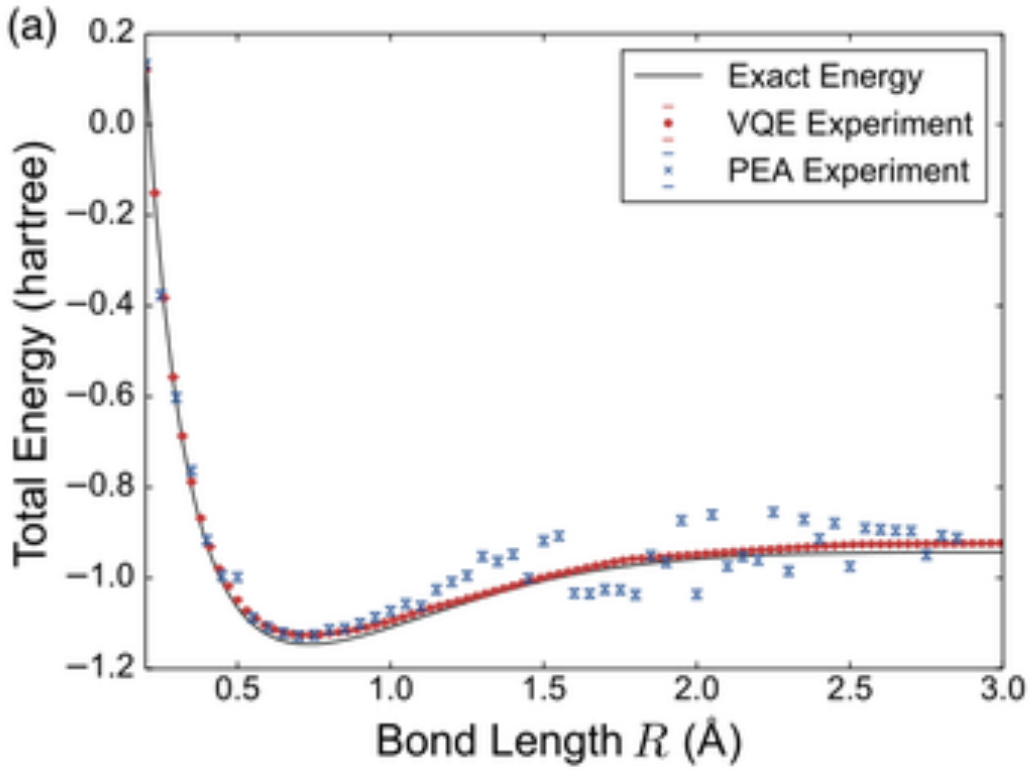
$$|j_1, \ldots, j_n\rangle \rightarrow \frac{\left(|0\rangle + e^{2\pi i 0.j_n}|1\rangle\right)\left(|0\rangle + e^{2\pi i 0.j_{n-1}j_n}|1\rangle\right)\cdots\left(|0\rangle + e^{2\pi i 0.j_1 j_2 \cdots j_n}|1\rangle\right)}{2^{n/2}}.$$

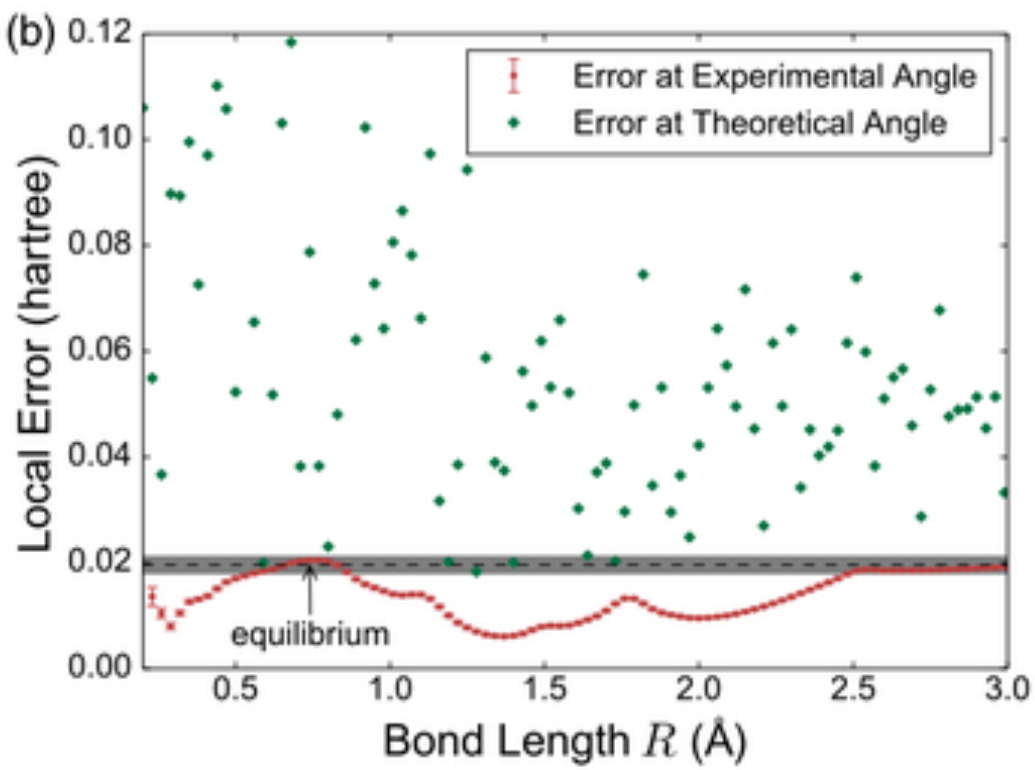
$$|\Theta\rangle = \begin{pmatrix} |\Theta_1\rangle \\ |\Theta_1\rangle \\ .. \\ .. \\ |\Theta_m\rangle \end{pmatrix} \rightarrow_{QFT} \begin{pmatrix} |0\rangle + \exp 2\pi i 0.\Theta_m |1\rangle \\ |0\rangle + \exp 2\pi i 0.\Theta_{m-1}\Theta_m |1\rangle \\ .. \\ |0\rangle + \exp 2\pi i 0.\Theta_2..\Theta_{m-1}\Theta_m |1\rangle \\ |0\rangle + \exp 2\pi i 0.\Theta_1..\Theta_{m-1}\Theta_m |1\rangle \end{pmatrix}$$

Circuit of actual experiment:

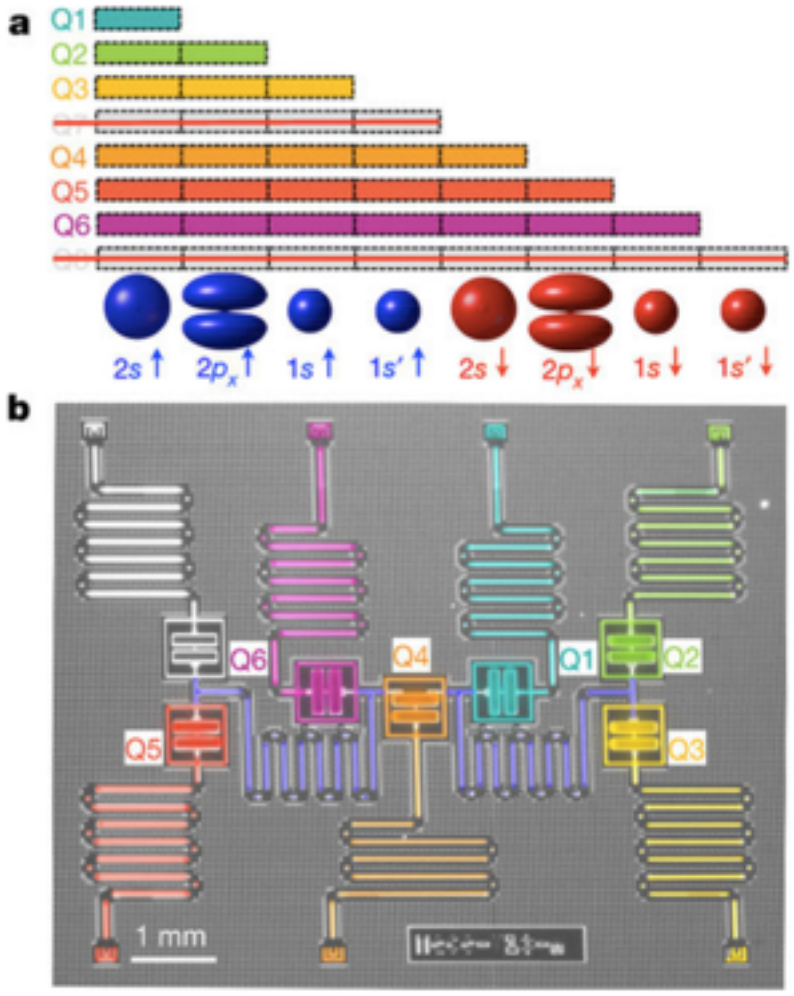


Measurement results for VQE & PEA.





Part 3: Concrete Implementation and outlook (1).



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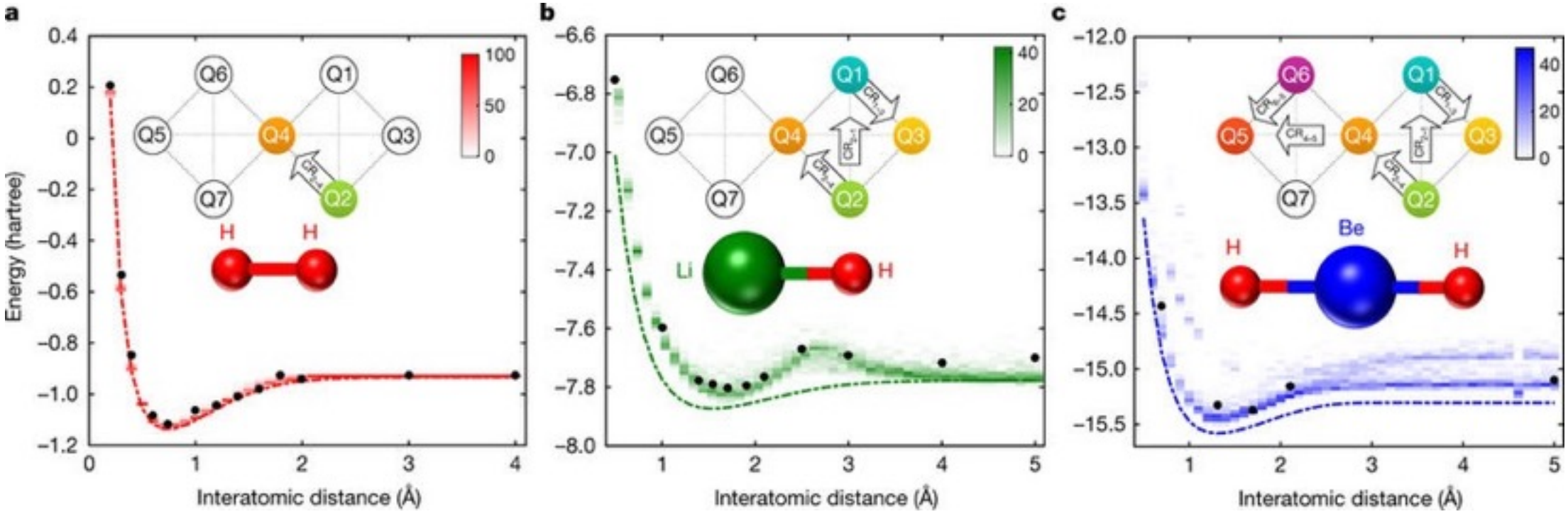
Part 3: Concrete Implementation and outlook (2).



https://www.nature.com/articles/nature23879#f3

Different representations of QFT.

$$
\begin{aligned}
|j\rangle \rightarrow & \frac{1}{2^{n/2}} \sum_{k=0}^{2^n-1} e^{2\pi i j k/2^n} |k\rangle \\
= & \frac{1}{2^{n/2}} \sum_{k_1=0}^{1} \cdots \sum_{k_n=0}^{1} e^{2\pi i j \left(\sum_{l=1}^{n} k_l 2^{-l}\right)} |k_1 \ldots k_n\rangle \\
= & \frac{1}{2^{n/2}} \sum_{k_1=0}^{1} \cdots \sum_{k_n=0}^{1} \bigotimes_{l=1}^{n} e^{2\pi i j k_l 2^{-l}} |k_l\rangle \\
= & \frac{1}{2^{n/2}} \bigotimes_{l=1}^{n} \left[\sum_{k_l=0}^{1} e^{2\pi i j k_l 2^{-l}} |k_l\rangle \right] \\
= & \frac{1}{2^{n/2}} \bigotimes_{l=1}^{n} \left[|0\rangle + e^{2\pi i j 2^{-l}} |1\rangle \right] \\
= & \frac{\left(|0\rangle + e^{2\pi i 0.j_n} |1\rangle\right) \left(|0\rangle + e^{2\pi i 0.j_{n-1} j_n} |1\rangle\right) \cdots \left(|0\rangle + e^{2\pi i 0.j_1 j_2 \cdots j_n} |1\rangle\right)}{2^{n/2}}
\end{aligned}
$$