# Scalable Quantum Simulation of Molecular Energies

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Based on
*Scalable Quantum Simulation of Molecular Energies*
by
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# Introduction

**Goal:** Compute the energy surface of molecular hydrogen

**2 Methods:**

- Variational Quantum Eigensolver
- Quantum Phase Estimation algorithm

**Hamiltonian:**

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

# Hamiltonian (1)

Start:

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

$R_i$: positions of nuclei
$r_i$: positions of electrons
$M_i$: masses of nuclei
$Z_i$: charges of nuclei

Second quantization representation:

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{\text{pqrs}} h_{\text{pqrs}} a_p^\dagger a_q^\dagger a_r a_s, \quad \text{with}$$

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

$$h_{\text{pqrs}} = \int d\sigma_1 d\sigma_2 \frac{\phi_p^*(\sigma_1) \phi_q^*(\sigma_2) \phi_s(\sigma_1) \phi_r(\sigma_2)}{|r_1 - r_2|}$$

# Hamiltonian (2)

Bravyi-Kitaev:

$$
\begin{aligned}
H = {} & f_0 \mathbb{1} + f_1 Z_0 + f_2 Z_1 + f_3 Z_2 + f_1 Z_0 Z_1 \\
& + f_4 Z_0 Z_2 + f_5 Z_1 Z_3 + f_6 \boldsymbol{X_0} Z_1 \boldsymbol{X_2} + f_6 \boldsymbol{Y_0} Z_1 \boldsymbol{Y_2} \\
& + f_7 Z_0 Z_1 Z_2 + f_4 Z_0 Z_2 Z_3 + f_3 Z_1 Z_2 Z_3 \\
& + f_6 \boldsymbol{X_0} Z_1 \boldsymbol{X_2} Z_3 + f_6 \boldsymbol{Y_0} Z_1 \boldsymbol{Y_2} Z_3 + f_7 Z_0 Z_1 Z_2 Z_3
\end{aligned}
$$

Finally:

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

# Variational Quantum Eigensolver

# Variational Principle

For an ansatz wave function $|\varphi(\theta)\rangle$ :

$$E_0 \leq \langle\varphi(\theta)| H |\varphi(\theta)\rangle = E(\theta)$$

From unitary coupled cluster (UCC) theory for $H_2$:

$$|\varphi(\theta)\rangle = e^{-\theta X_0 Y_1} |01\rangle$$

How to get this?

**Algorithm**

Step I

For some θ, prepare ansatz wavefunction

Step II

Compute E(θ)

Step III

Propose new θ and start over

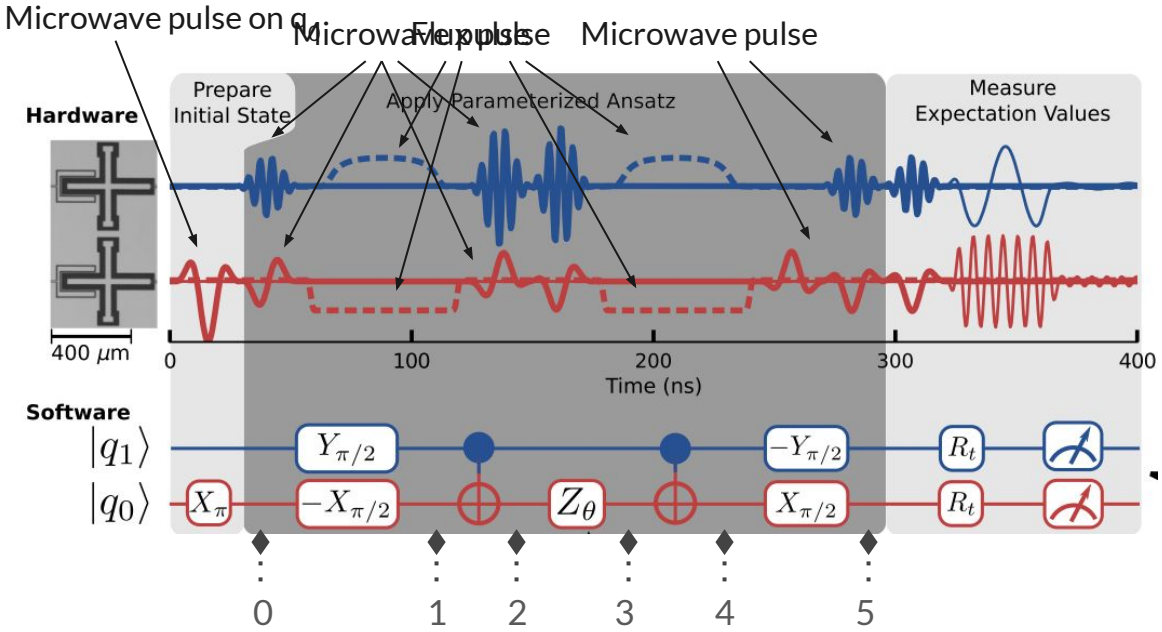
Stop if E(θ) is minimised

Quantum

Classically

$$
\begin{aligned}
e^{-i\theta X_0 Y_1}\,|01\rangle &= \cos\theta\,|01\rangle - i\sin\theta\; Y_1\,|0\rangle\; X_0\,|1\rangle \\
&= \cos\theta\,|01\rangle - i\sin\theta\; i\,|1\rangle\,|0\rangle \\
&= \cos\theta\,|01\rangle + \sin\theta\,|10\rangle
\end{aligned}
$$

# The quantum circuit



# Runtime

Execution time for one θ:

$$(\text{circuit runtime}) \times (\text{expectation value computation}) \times (\#\ \text{expectation values})$$

The hamiltonian consists of 5 summands, hence:

$$400\text{ns} \times 100 \text{ to } 1000 \times 5 = 20 \text{ to } 200\mu\text{s}$$

**But** we still need to minimise over θ...
→ Scan 1000 possible values and select minimum:

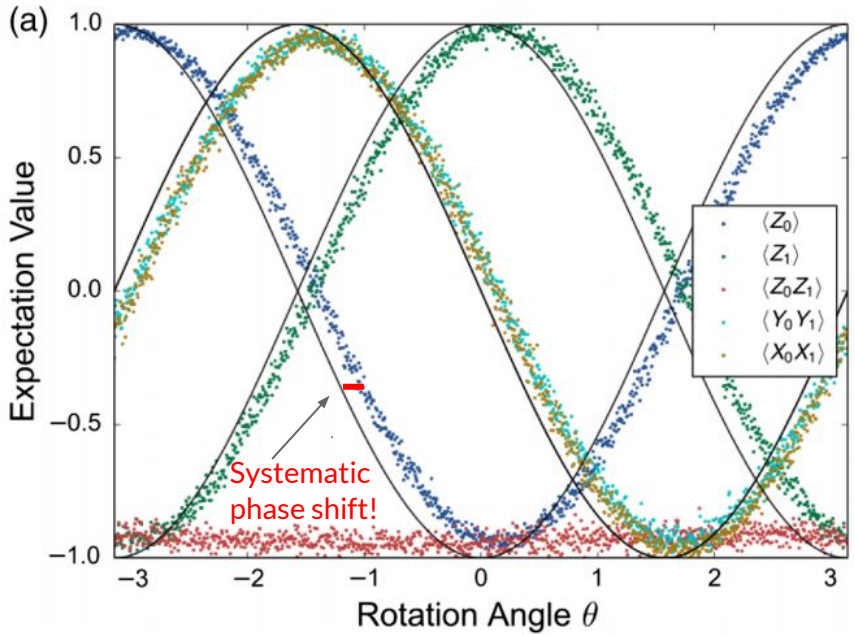
$$(20 \text{ to } 200\mu\text{s}) \times \#(\theta \text{ evals}) = 20 \text{ to } 200\text{ms}$$

# What about accuracy?

$$\langle H \rangle = g_0 + g_1 \langle Z_0 \rangle + g_2 \langle Z_1 \rangle + g_3 \langle Z_0 Z_1 \rangle + g_4 \langle X_0 X_1 \rangle + g_5 \langle Y_0 Y_1 \rangle$$

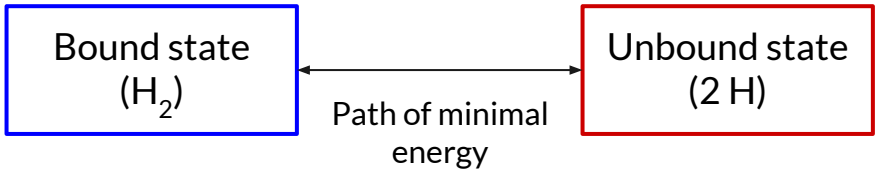
- Systematic phase shift
  → **BUT** algorithm is very robust
- Error in dissociation energy of $H_2$:
  $(8 \pm 5) \times 10^{-4}$ hartree

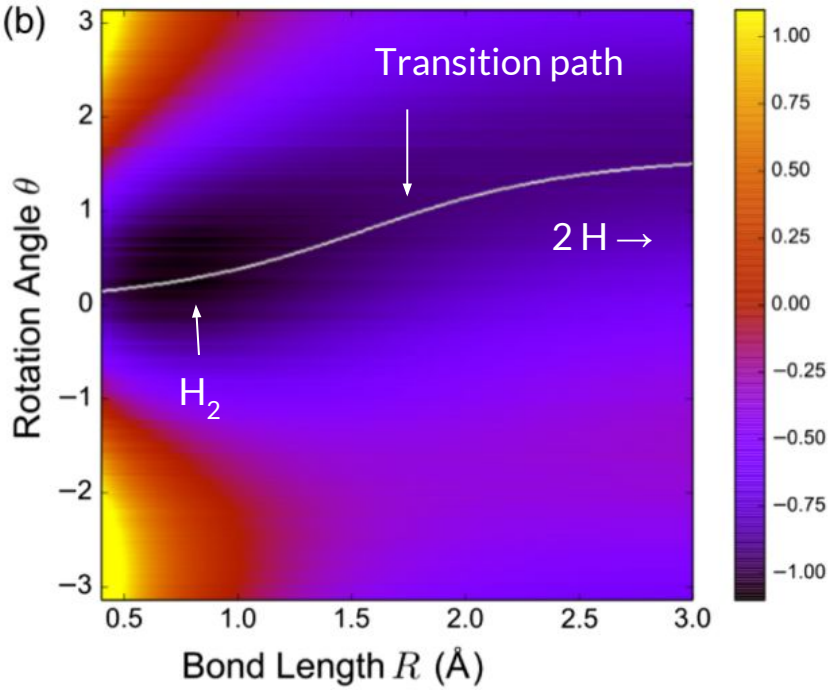
Very good :)



# Energy Surface for VQE

- Compute energy for different parameters
  → Potential energy surface
- Bound state: Minimal energy
  → R = 0.75 and θ = 0



# Quantum Phase Estimation

# Trotterization and Phase Estimation

Time evolution operation :

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

Leading to $E_n$-dependent phase shifts
in the occupation basis states:

$$e^{-iHt}\left|\phi\right\rangle = \left(\sum_n e^{-iE_n t}\left|n\right\rangle\left\langle n\right|\right)\left|\phi\right\rangle = \sum_n a_n e^{-iE_n t}\left|n\right\rangle$$

**Algorithm**

Step I

Prepare ancilla superposition state

Step II

Apply Trotter gate sequence with ancilla as a control bit

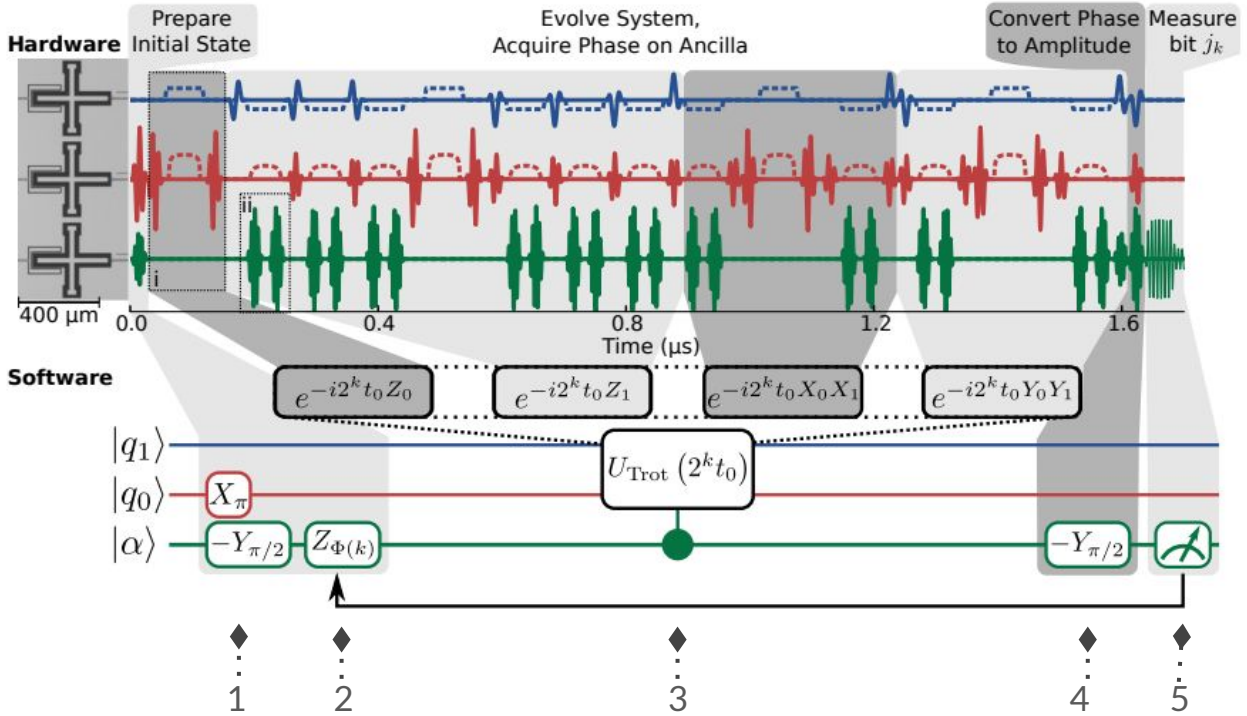
Step III

Measure phase shift on ancilla qubit and repeat with “phase kickback”

Quantum

Classically

# The Quantum Circuit

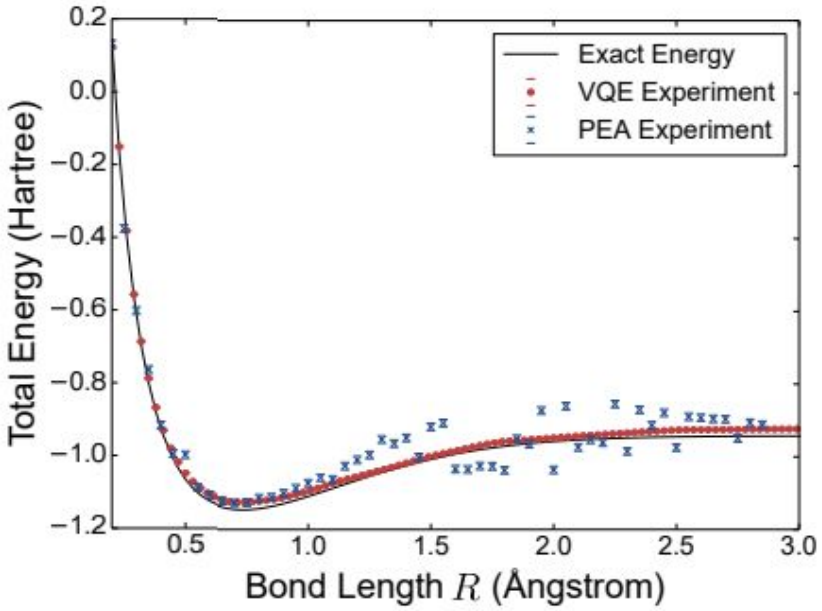


# Data Extraction and Experimental Results

The ground state energy is given by binary expansion of the measured qubits:

$$E_0^b = -\frac{\pi}{t_0} \sum_{k=0}^{b-1} \frac{j_k}{2^{k+1}}$$

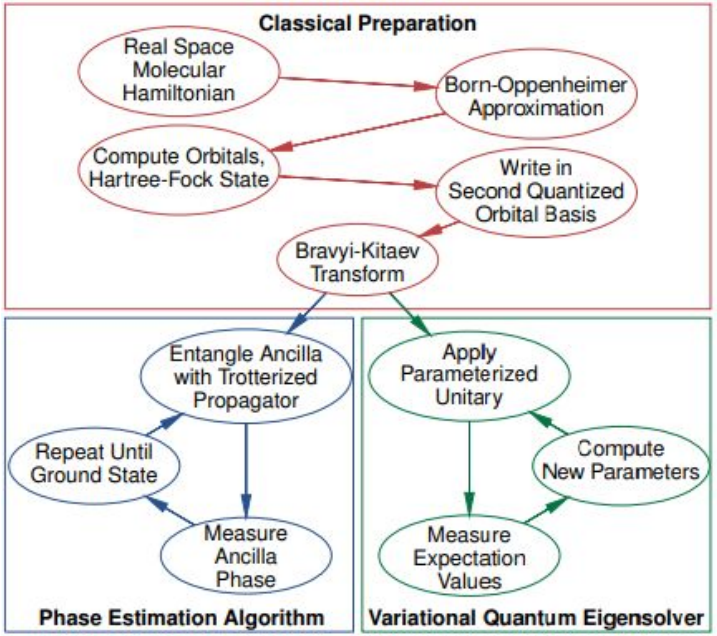
The results differ from the exact values due to the Trotterization being performed with only a *single* step.



# Challenges and Shortcomings

In order to minimize errors the **number of steps** used to simulate the time evolution operation must be increased.
In addition, the quantum *Phase Estimation algorithm* requires extensive classical computation to determine the optimal **Trotter gate sequence.**

Therefore, the *PEA* procedure is less efficient and less accurate compared to the variational approach.



# Conclusion

**Variational Quantum Eigensolver**

Classical outer loop with quantum algorithm that calculates $E(\theta)$

→ robust against errors/phase shifts due to variational parameters
→ chemical accuracy

**Quantum Phase Estimation**

Ancilla superposition state that evolves via Trotter gate sequence

→ requires long coherent evolution
→ no chemical accuracy

# Thank you for your attention!

# No more to see here. Go back.