Modeling Electronic Systems on Quantum Computers

University of Florida, October

Recap of last time

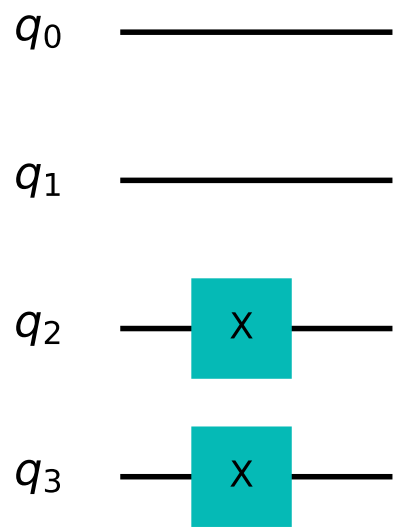
- Jordan-Wigner transformation to map between the fermioinc degrees of freedom and the qubits degrees of freedom.

- Using JW we have,

$$a_i^\dagger a_i = \frac{1}{2}(1 + \sigma_i^z)$$

- In the qubits degrees of freedom the Hamiltonian is a linear combination of polynomial number of Pauli strings. For the Hydrogen molecule case,

$$\hat{H} = \sum_{i,j,k,l=0}^{3} j^{ijkl} \sigma_1^i \sigma_2^j \sigma_3^k \sigma_4^l$$



Outline

1. VQE algorithm circuit design for UCCSD

Unitary coupled-cluser (UCC) expansion

The UCC method uses the following ansatz,

$$|\Psi_0\rangle = e^{T(\boldsymbol{\theta})-T^\dagger(\boldsymbol{\theta})}\,|\Phi_0\rangle$$

$$T(\boldsymbol{\theta}) = T_1(\boldsymbol{\theta}) + T_2(\boldsymbol{\theta}) + \ldots$$

$$T_1(\boldsymbol{\theta}) = \sum_{\substack{m\in\text{emp}\\ i\in\text{occ}}} \theta^{mi} a_m^\dagger a_i$$

$$T_2(\boldsymbol{\theta}) = \frac{1}{2}\sum_{\substack{m,n\in\text{emp}\\ i,j\in\text{occ}}} \theta^{mnij} a_m^\dagger a_n^\dagger a_i a_j$$

$$\vdots$$

$$e^{T(\boldsymbol{\theta})-T^\dagger(\boldsymbol{\theta})} = e^{\sum_i \theta_i(\tau_i-\tau_i^\dagger)},$$

where τ_i include all kinds of excitations.

- For this ansatz to be computationally efficient we need to include only a few excitation operators.
- UCCSD include single and double excitations.
- Next step would be to design a circuit that implement this unitary operation.

Trotterization

Different terms of τ_i don't necessarily commute which make simulating the exponential with quantum circuits not easy. We make use of the following identity,

$$e^{\sum_i \theta_i(\tau_i - \tau_i^\dagger)} = \lim_{N\to\infty} \left(\prod_i e^{\frac{\theta_i(\tau_i - \tau_i^\dagger)}{N}} \right)^N$$

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- Taking N to infinity is not possible for computations. Good results can be achieved by taking just a few trotter steps.

$$e^{\sum_i \theta_i(\tau_i - \tau_i^\dagger)} = \left(\prod_i e^{\frac{\theta_i(\tau_i - \tau_i^\dagger)}{\rho}} \right)^\rho$$

- The smaller the θ_i's are the better the approximation.
- It's better to start with a good initial guess.

Converting to qubits operations

one-body exponentials

One body exponential $e^{\theta(a_m^\dagger a_i - a_i^\dagger a_m)}$. Note: $m > i$.

$$a_m^\dagger a_i - a_i^\dagger a_m = -\sigma_i^- \left(\prod_{s=i+1}^{m-1} \sigma_s^z \right) \sigma_m^+ + \sigma_i^+ \left(\prod_{s=i+1}^{m-1} \sigma_s^z \right) \sigma_m^-$$

$$a_m^\dagger a_i - a_i^\dagger a_m = \frac{i}{2} \left[\sigma_i^y \left(\prod_{s=i+1}^{m-1} \sigma_s^z \right) \sigma_m^x - \sigma_i^x \left(\prod_{s=i+1}^{m-1} \sigma_s^z \right) \sigma_m^y \right]$$

Note that the two terms commute.

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Note that the two terms commute.

We rotate σ^x and σ^y to σ^z,

$$e^{i\theta\sigma_i^y \left(\prod_{s=i+1}^{m-1} \sigma_s^z\right)\sigma_m^x} = H_m R_i^x(\pi/2) \left(e^{i\theta \left(\prod_{s=i}^{m-1} \sigma_s^z\right)\sigma_m^z} \right) H_m^\dagger R_i^{x\dagger}(\pi/2),$$

using,

$$H\sigma_z H^\dagger = \sigma_x$$

$$R^x(\pi/2)\,\sigma_z R^{x\dagger}(\pi/2) = \sigma_y$$

Converting to qubit operations

one-body exponentials

Need to implement $\exp\left[i\theta\left(\prod_{s=i}^{m-1}\sigma_s^z\right)\sigma_m^z\right]$.

- $\prod_{s=i}^{m-1}\sigma_s^z$ counts the parity of qubits from i to $m-1$.
- $e^{\pm i\theta\sigma_m^z}$ makes a rotation around the z-axis on the m-th qubit accordingly.

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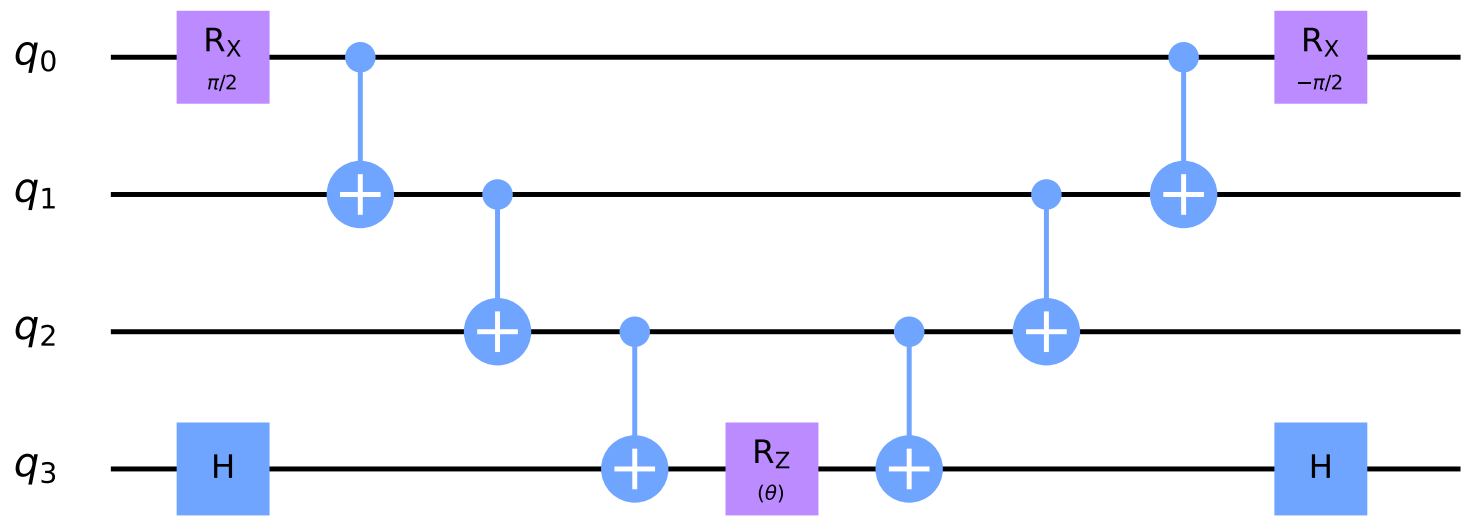
Example: $\exp\left[i\theta\sigma_1^y(\sigma_2^z\sigma_3^z)\sigma_4^x\right]$ for Hydrogen molecule.



Converting to qubit operations

two-body exponentials

Two-body exponential $e^{\theta(a_m^\dagger a_n^\dagger a_j a_i - a_i^\dagger a_j^\dagger a_n a_m)}$, and assume $j > i$, and $m > n$

$$\begin{aligned} a_m^\dagger a_n^\dagger a_i a_j - a_i^\dagger a_j^\dagger a_n a_m =& \sigma_i^- \left(\prod \sigma^z\right) \sigma_j^- \; \sigma_n^+ \left(\prod \sigma^z\right) \sigma_m^+ \\ & -\sigma_i^+ \left(\prod \sigma^z\right) \sigma_j^+ \; \sigma_n^- \left(\prod \sigma^z\right) \sigma_m^- \\ =& \frac{i}{4} \sigma_i^x \left(\prod \sigma^z\right) \sigma_j^x \; \sigma_n^x \left(\prod \sigma^z\right) \sigma_m^y \\ & + \text{terms with odd } \sigma^y \end{aligned}$$

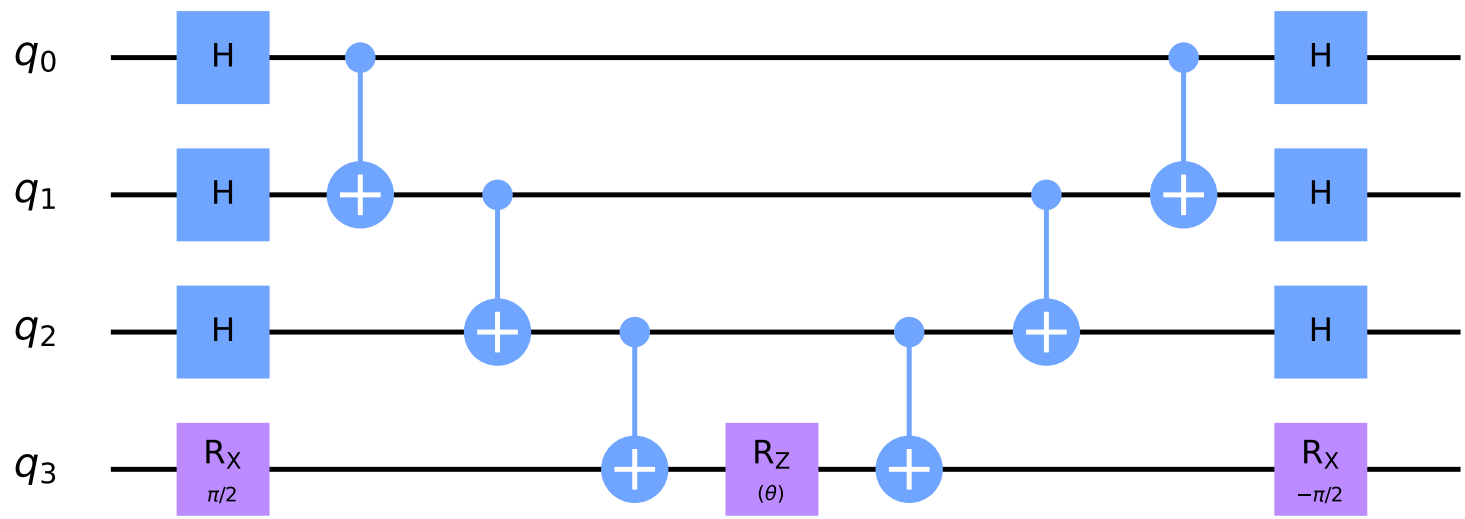
This generate 8 terms, all of which will commute. As before we rotate σ^x and σ^y to σ^z,

$$H_i H_i H_n R_m^x(\pi/2) e^{\frac{i\theta}{4}\left(\left(\prod_i^j \sigma^z\right) \; \left(\prod_n^{m-1} \sigma^z\right)\sigma_m^z\right)} H_i^\dagger H_i^\dagger H_n^\dagger R_m^x(-\pi/2)$$

Converting to qubit operations

two-body exponentials

Note we only add parity from m to n and from j to $i+1$ then perform the rotation on the i-th qubit.
Example: $\exp\{[i\theta\sigma_1^x\sigma_2^x\sigma_3^x\sigma_4^y\ ]\}$ for the Hydrogen molecule,



Measuerment

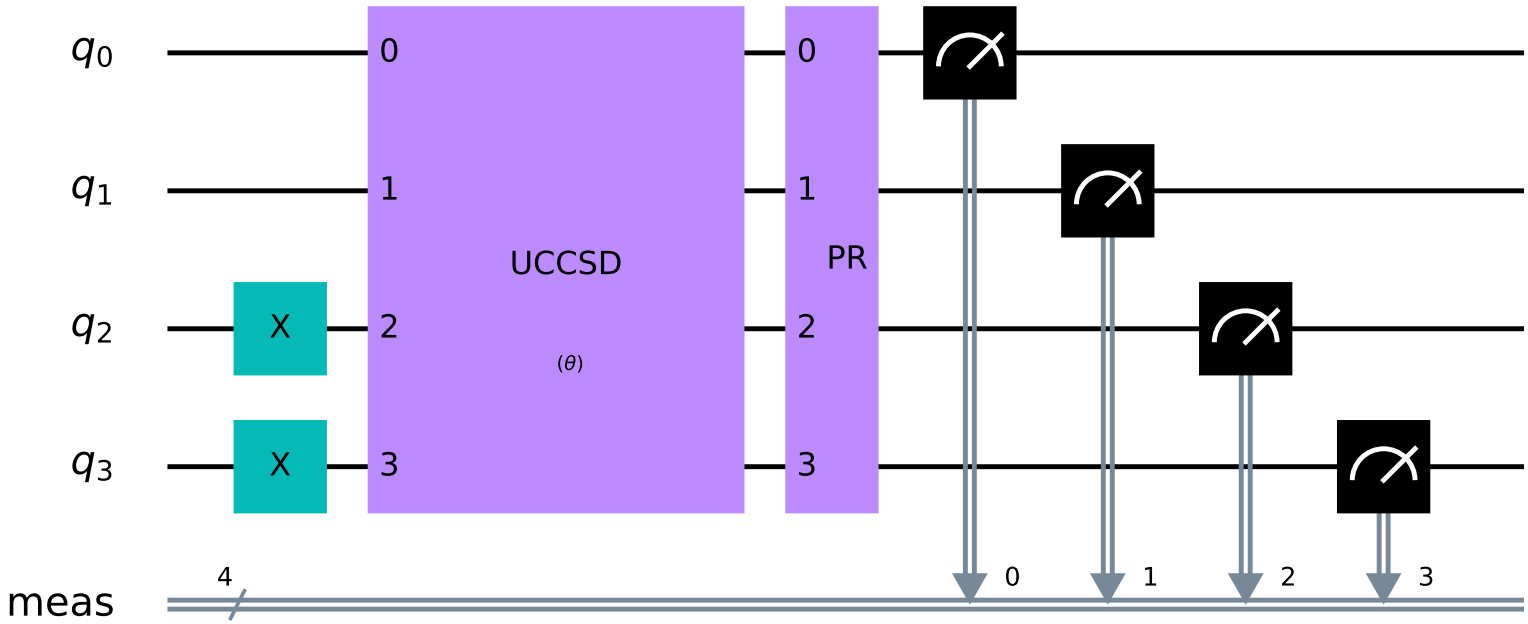
The Hamiltonian expectation value is written as,

$$\langle \hat{H} \rangle = \sum_{i,j,k,l=0}^{3} j^{ijkl} \langle \sigma_1^i \sigma_2^j \sigma_3^k \sigma_4^l \rangle$$

The computational basis is the z-axis. To measure the expectation value a general string of Pauli operators, we need a post-rotation circuit.

- Measuring the qubits gives a string of 0's and 1's, $\{s_i\}$.
- $P(\{s_i\}) = |\langle \{s_i\} | \Psi_0 \rangle|^2$
- To measure the i-th qubit with respect to the x or y-axes we need to rotate our basis for the i-th qubit using H_i or $R_i^x(\pi/2)$ respectively.
- Any Pauli string has eigenvalues of either ± 1.
- $\langle \sigma_1^i \sigma_2^j \sigma_3^k \sigma_4^l \rangle = P(1) - P(-1)$

The end result look something like this:



1. Initialize the qubits
2. Apply the UCCSD gate with parameters $\boldsymbol{\theta}$.
3. Apply post-rotations.
4. Measure the qubits.

Comparison:

$E_{\mathsf{HF}} = -1.116$

$E_{\mathsf{UCCSD}} = -1.137$

$E_{exact} = -1.166$

Summary

The VQE method can be summarized as follows:

1. A classical computer calculate the Hamiltonian and come up with an initial state.
2. A quantum computer samples the Hilber space and measure the energy.
3. A classical computer will run an optimization routine to minimize the energy expectation value.