HQC2 SDU

Quantum Computing for Quantum Chemists

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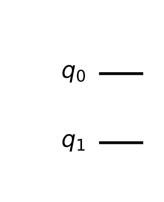
Qubits and orbitals

HQC2

State vector representation - Single qubit

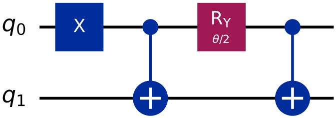
$$|q_0\rangle = |0\rangle = \left| \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right\rangle \tag{1}$$

State vector representation - Multi qubit



$$|q_0 \otimes q_1\rangle = |00\rangle = \left| \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{2}$$

Gates can only be unitary.



$$\text{circ} = \langle 00| \left(X \otimes I\right) \mathrm{cx}(0,1) \left(\mathrm{R_Y}\left(\frac{\theta}{2}\right) \otimes I\right) \mathrm{cx}(0,1) \tag{3}$$

$$= \begin{pmatrix}1\\0\\0\\0\end{pmatrix} \left(\begin{pmatrix}0 & 1\\1 & 0\end{pmatrix} \otimes \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}\right) \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix} \left(\begin{pmatrix}\cos\frac{\theta}{2} & -\sin\frac{\theta}{2}\\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2}\end{pmatrix} \otimes \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}\right) \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0\end{pmatrix} \tag{4}$$

Jordan-Wigner transformation

Fermionic operators are in general not unitary.

$$a = \frac{X + iY}{2}, \quad a^\dagger = \frac{X - iY}{2} \tag{5}$$

Example - 4 spin orbitals

$$\hat{a}_3^\dagger \hat{a}_2 = (Z \otimes Z \otimes Z \otimes a^\dagger)(Z \otimes Z \otimes a \otimes I) \tag{6}$$

$$= \frac{i}{4}(I \otimes I \otimes Y \otimes X) + \frac{1}{4}(I \otimes I \otimes X \otimes X) \tag{7}$$

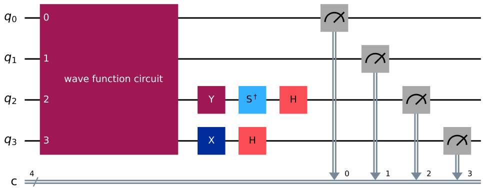
$$+ \frac{1}{4}(I \otimes I \otimes Y \otimes Y) - \frac{i}{4}(I \otimes I \otimes X \otimes Y)$$

In general

$$\left\langle 0 \middle| \hat{O}_{\text{fermionic}} \middle| 0 \right\rangle = \sum_i c_i \left\langle 0 \left| P_i \right| 0 \right\rangle \tag{8}$$

Example - 4 spin orbitals

$$\left\langle 0 \middle| \hat{a}_3^\dagger \hat{a}_1 \middle| 0 \right\rangle = \frac{i}{4} \left\langle 0 \left| IIYX \right| 0 \right\rangle + \frac{1}{4} \left\langle 0 \left| IIXX \right| 0 \right\rangle + \frac{1}{4} \left\langle 0 \left| IIYY \right| 0 \right\rangle - \frac{i}{4} \left\langle 0 \left| IIXY \right| 0 \right\rangle \tag{9}$$



Unitary Coupled Cluster

$$|\mathrm{UCC}\rangle = \exp\left(\sum_{ia}\theta_i^a\left(\hat{T}_i^a - \hat{T}_i^{a\dagger}\right) + \sum_{ijab}\theta_{ij}^{ab}\left(\hat{T}_{ij}^{ab} - \hat{T}_{ij}^{ab\dagger}\right) + \ldots\right)|\mathrm{HF}\rangle \tag{10}$$

$$\hat{T}_i^a = \hat{a}_a^\dagger\hat{a}_i, \quad \hat{T}_{ij}^{ab} = \hat{a}_a^\dagger\hat{a}_b^\dagger\hat{a}_j\hat{a}_i, \quad \ldots \tag{11}$$

Very hard problem

$$\exp\left(\sum_{ia}\theta_i^a\left(\hat{T}_i^a - \hat{T}_i^{a\dagger}\right) + \sum_{ijab}\theta_{ij}^{ab}\left(\hat{T}_{ij}^{ab} - \hat{T}_{ij}^{ab\dagger}\right) + \ldots\right) \rightarrow \text{circuit} \tag{12}$$

Factorized Unitary Coupled Cluster

$$|\text{fUCC}\rangle = \ldots \prod_{ijab} \exp\left(\theta_{ij}^{ab}\left(\hat{T}_{ij}^{ab} - \hat{T}_{ij}^{ab\dagger}\right)\right) \prod_{ia} \exp\left(\theta_{i}^{a}\left(\hat{T}_{i}^{a} - \hat{T}_{i}^{a\dagger}\right)\right) |\text{HF}\rangle \tag{13}$$

This is not the same as UCC,

$$|\text{fUCC}\rangle \neq |\text{UCC}\rangle \tag{14}$$

Since in general,

$$\left[\hat{T}_I - \hat{T}_I^\dagger, \hat{T}_J - \hat{T}_J^\dagger\right] \neq 0 \tag{15}$$

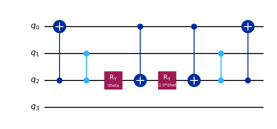
Wave function circuits

Known representation

$$\exp\left(\theta_I\left(\hat{T}_I-\hat{T}_I^{\dagger}\right)\right)\rightarrow \text{circuit} \tag{16}$$

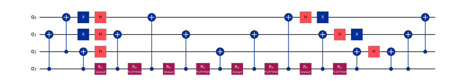
Fermionic singles

$$\exp\left(\theta_i^a\left(\hat{a}_a^{\dagger}\hat{a}_i-\hat{a}_i^{\dagger}\hat{a}_a\right)\right)$$



Fermionic doubles

$$\exp\left(\theta_{ij}^{ab}\left(\hat{a}_a^{\dagger}\hat{a}_b^{\dagger}\hat{a}_j\hat{a}_i-\hat{a}_i^{\dagger}\hat{a}_j^{\dagger}\hat{a}_b\hat{a}_a\right)\right)$$



More general wave function

$$|\text{UPS}\rangle = \prod_I \exp\left(\theta_I \left(\hat{T}_I - \hat{T}_I^\dagger\right)\right)|\text{HF}\rangle \tag{17}$$

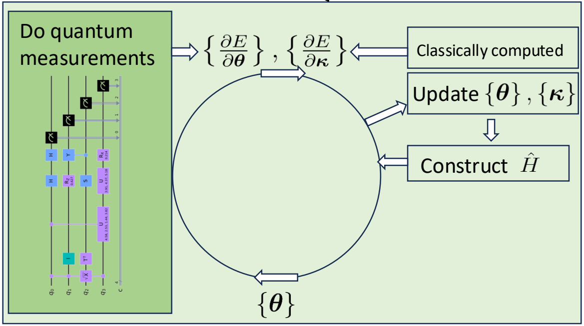
The same $\hat{T}$ operator can be used multiple times without being redundant. In essence we can do matrix product states with some restrictions,

- The matrices has to be unitary.
- We have to know how to represent them as a circuit.

Variational "quantum" eigensolver

$$E_0 = \min_{\boldsymbol{\theta}} \frac{\left\langle \mathrm{HF} \left| \boldsymbol{U}^\dagger(\boldsymbol{\theta}) \hat{H} \boldsymbol{U}(\boldsymbol{\theta}) \right| \mathrm{HF} \right\rangle}{\left\langle \mathrm{HF} \left| \boldsymbol{U}^\dagger(\boldsymbol{\theta}) \boldsymbol{U}(\boldsymbol{\theta}) \right| \mathrm{HF} \right\rangle} = \left\langle \mathrm{HF} \left| \boldsymbol{U}^\dagger(\boldsymbol{\theta}) \hat{H} \boldsymbol{U}(\boldsymbol{\theta}) \right| \mathrm{HF} \right\rangle \quad (18)$$

oo-VQE



Probabilistic calculation of expectation values

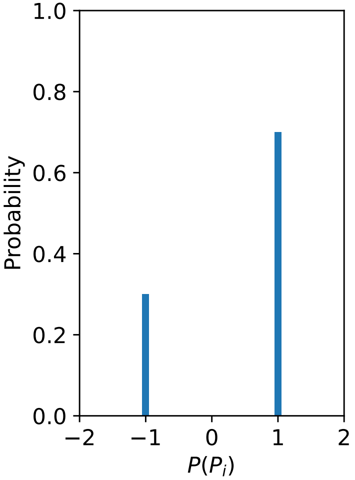
From a measurement, we get a state as a bit-string.

$$b \in \{00, \quad 01, \quad 10, \quad 11\}$$

A Pauli expectation value is a distribution,

$$\langle b \,| P_i |\, b \rangle \in \{-1, \quad 1\}$$

$$\left\langle 0 \middle| \hat{O}_{\text{fermionic}} \middle| 0 \right\rangle = \sum_i c_i \langle 0 \,| P_i |\, 0 \rangle$$



SlowQuant

In-house developed software for unitary wave functions.

https://github.com/erikkjellgren/SlowQuant

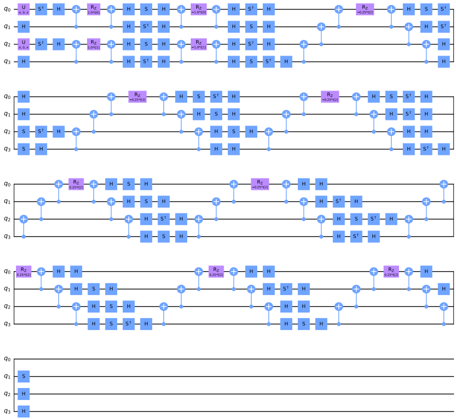
SlowQuant → Qiskit interface mainly made by Karl Michael Ziems

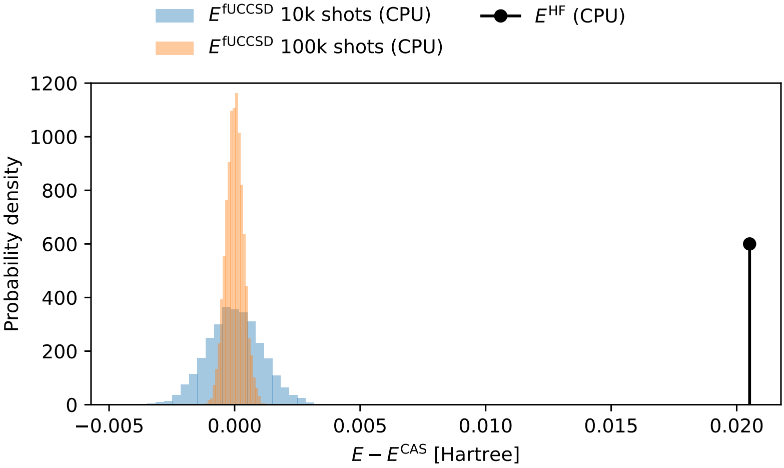
Art by Rachel Thompson

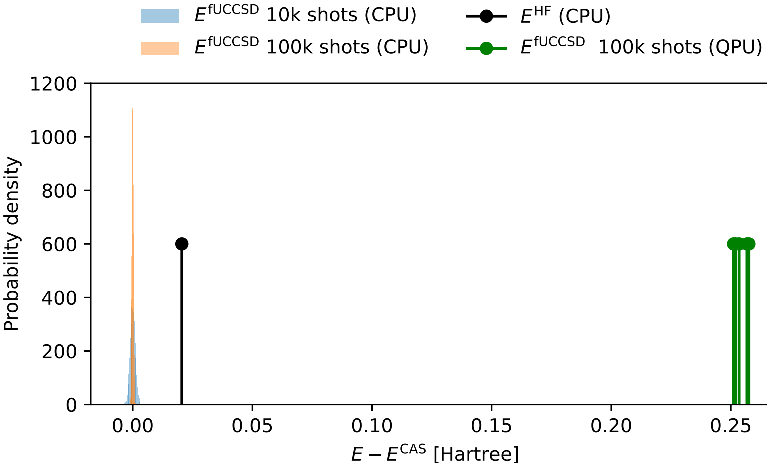
Running on QPU

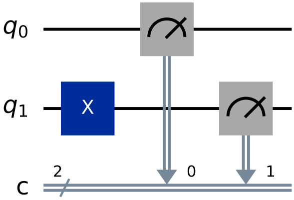
System

- LiH
- (2,2) space
- STO-3G
- fUCCSD: 'cx': 56, 'rz': 50, 'sx': 31 (transpiled).
- IBM Mumbai (retired device)




E^{fUCCSD} 10k shots (CPU)
E^{fUCCSD} 100k shots (CPU)
E^{HF} (CPU)
Probability density
1200
1000
800
600
400
200
0
−0.005
0.000
0.005
0.010
0.015
0.020
$E - E^{\mathrm{CAS}}$ [Hartree]


E^{fUCCSD} 10k shots (CPU)
E^{fUCCSD} 100k shots (CPU)
E^{HF} (CPU)
E^{fUCCSD} 100k shots (QPU)
Probability density
0
200
400
600
800
1000
1200
0.00
0.05
0.10
0.15
0.20
0.25
$E - E^{\mathrm{CAS}}$ [Hartree]



$$P(00|01)$$
$$P(10|01)$$
$$P(01|01)$$
$$P(11|01)$$

M standard - 2 qubit example

$$\boldsymbol{M} = \begin{pmatrix} P(00|00) & P(00|10) & P(00|01) & P(00|11) \\ P(10|00) & P(10|10) & P(10|01) & P(10|11) \\ P(01|00) & P(01|10) & P(01|01) & P(01|11) \\ P(11|00) & P(11|10) & P(11|01) & P(11|11) \end{pmatrix} \tag{19}$$

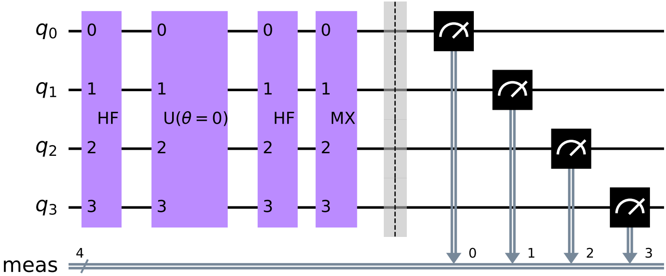
$$\boldsymbol{C} = \begin{pmatrix} P(00) \\ P(10) \\ P(01) \\ P(11) \end{pmatrix} \tag{20}$$

Read-out mitigation

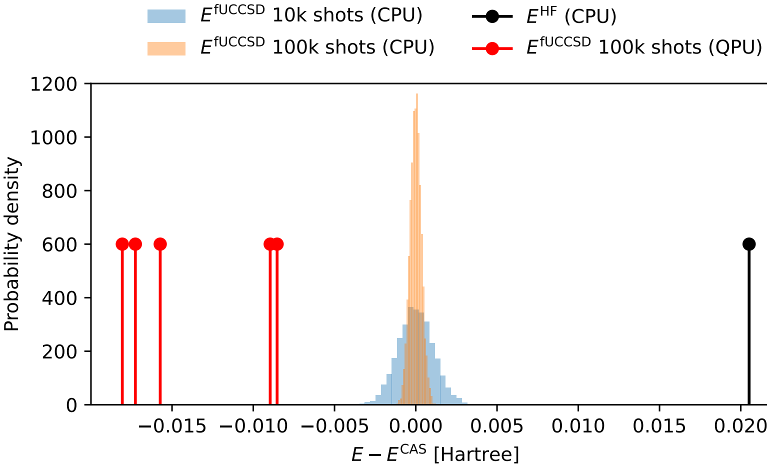
$$\boldsymbol{C}_{\text{mitigated}} = \boldsymbol{M}^{-1}\boldsymbol{C}_{\text{measured}} \tag{21}$$

Read-out and gate-error mitigation

$$C_{\text{mitigated}} = M_{\theta=0}^{-1} C_{\text{measured}} \tag{22}$$



20 min QPU per red line



Qubit-wise commutativity

$$[P, I] = 0, \quad [I, P] = 0, \quad [P, P] = 0 \tag{23}$$

As an example,

$$II, IZ, ZI, ZZ, XX \tag{24}$$

Becomes only two Pauli measurements,

$$ZZ \rightarrow II, IZ, ZI, ZZ \tag{25}$$

$$XX \rightarrow XX \tag{26}$$

Post-selection

For Pauli strings in the computational basis, only Z and I.

$$\sum_i b_i = N_e \tag{27}$$

F.x.:

$$1100 \rightarrow 2 \text{ electrons}$$

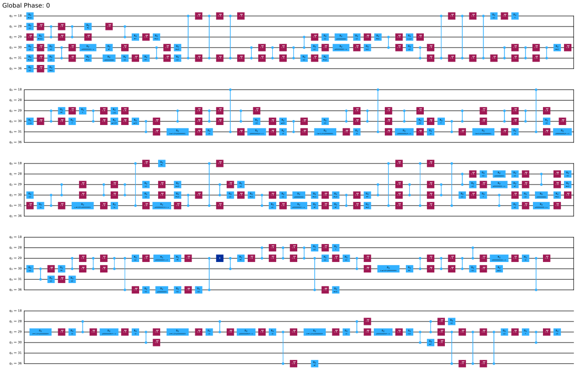
Waiting

- Hardware becomes better
- Hardware vendors become more experienced in calibration

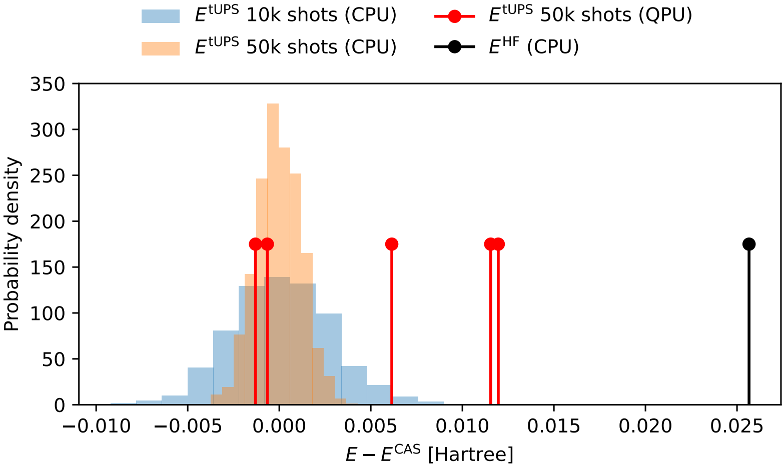
Running on real QPU

System

- H_2
- (2,3) space
- aug-cc-pVTZ
- tUPS: 'sx': 178, 'rz': 137, 'cz': 84, 'x': 1 (transpiled).
- IBM Torino (still active device)



21 min QPU per red line



The end

Website: https://hqc2.github.io/

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