Quantum Computing of the 6Li nuclei via ordered unitary coupled cluster

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Keypoint: We study the ordering of fermionic operators anc compute low energy nuclear eigenstates with the Variational Quantum Eigensolver

Paper: Kiss et al., *Phys. Rev. C* **106**, 034325 (2022)

An overview of the Variational Quantum Eigensolver

Goal: obtain the ground state energy of an Hamiltonian by using the Variaional principle.

$$E_0 \leq \frac{\langle \psi(\theta) | \, H \, | \psi(\theta) \rangle}{\langle \psi(\theta) | \psi(\theta) \rangle}.$$

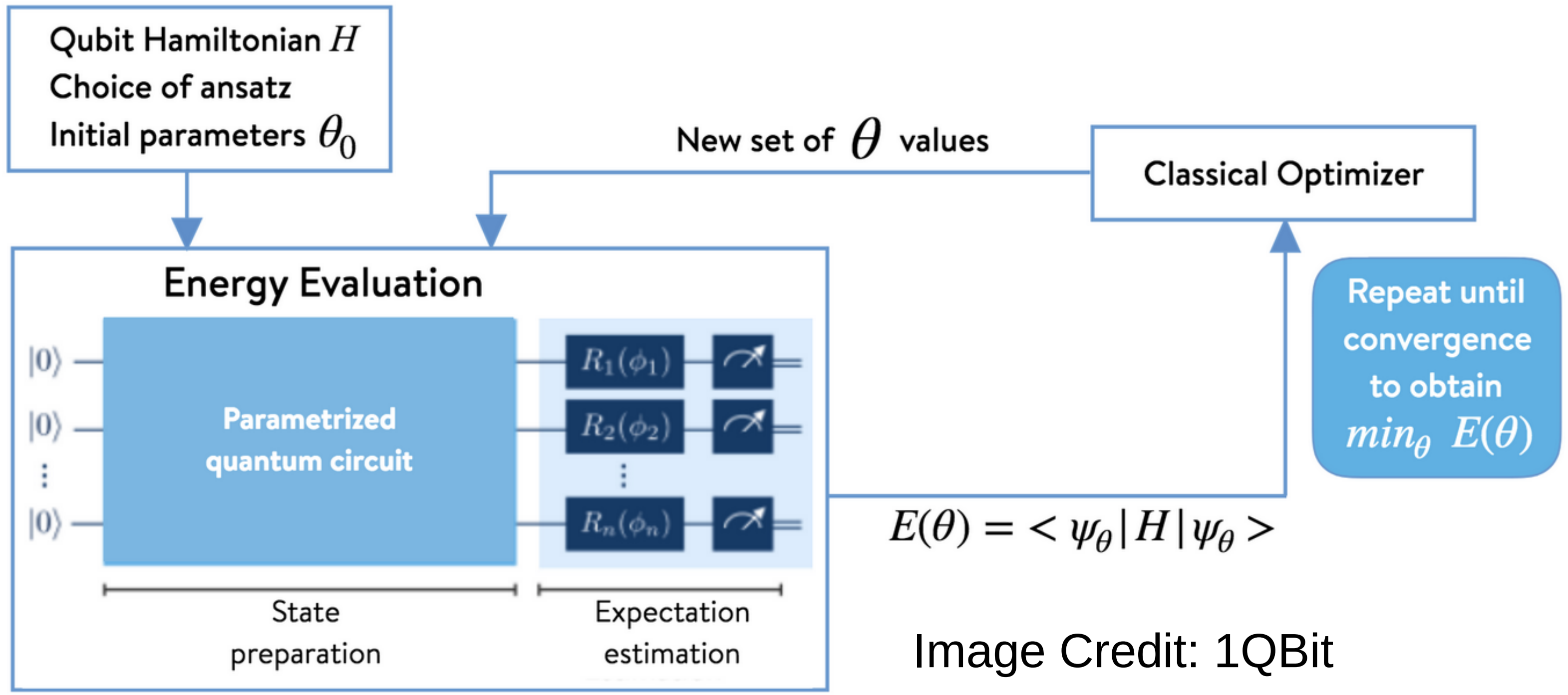


Image Credit: 1QBit

Peruzzo A. et al., Nat. Commun. **5**, 4123 (2014).

Nuclear shell model (Cohen-Kurath)

$$H = \sum_i \epsilon_i \hat{a}_i^\dagger \hat{a}_i + \frac{1}{2} \sum_{ijkl} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l,$$

Single particle energies

Two body interaction

1. Frozen Helium core
2. 0p1/2 and 0p3/2 harmonic oscillator orbitals for the neutron and proton.
3. 12 orbitals (6 protons and 6 neutrons)

$$|i\rangle = |n = 0, l = 1, j, j_z, t_z\rangle,$$

radial, angular, spin, spin projection, isospin

- Map to qubit Hamiltonian with the **Jordan-Wigner** transformation.

$$\hat{a}_i^\dagger = \frac{1}{2}\left(\prod_{j=0}^{i-1} -Z_j\right)(X_i - iY_i),$$

Additional information about J_z

- Groundstate has total angular momentum projection of -1, 0 or 1.
- First excited state has total angular momentum projection of -3, -2, 2 or 3.

Dumitrescu E. F. et al., Phys. Rev. Let. **120** 210501 (2018).
Stetcu I. et al,, Pjus. Rev. C **105** 064308 (2022).

Quantum Circuit Ansätze

Unitary Coupled Clusters (UCC)

$$|\psi(\boldsymbol{\theta})\rangle = e^{i(\hat{T}(\boldsymbol{\theta})-\hat{T}^\dagger(\boldsymbol{\theta}))}\,|\psi_0\rangle\,.$$

Hartree Fock solution

1 Step Trotterization

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \dots$$

Cluster operators

$$\hat{T}_1 = \sum_{i\in\text{virt};\alpha\in\text{occ}} \theta_i^\alpha \hat{a}_i^\dagger \hat{a}_\alpha$$

Single fermionic excitation terms

$$\hat{T}_2 = \sum_{i,j\in\text{virt};\alpha,\beta\in\text{occ}} \theta_{ij}^{\alpha\beta} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_\alpha \hat{a}_\beta.$$

Double fermionic excitation terms

Maped to qubit via Jordan Wigner

We manually select only the operators that preserve J_z (Important).

Ordering of the excitation operators

- Each fermionic excitation operator is **associated** with a term in the Hamiltonian.
- Single excitation operator $\iff$ single-particle energy ϵ_i.
- Doubles excitation operators $\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_\alpha \hat{a}_\beta \iff$ two-body $V_{ij\beta\alpha}$.
- **Ordering by magnitude** of the corresponding coefficient.
- **Conclusion:** important terms should be placed at the beginning of the circuit.

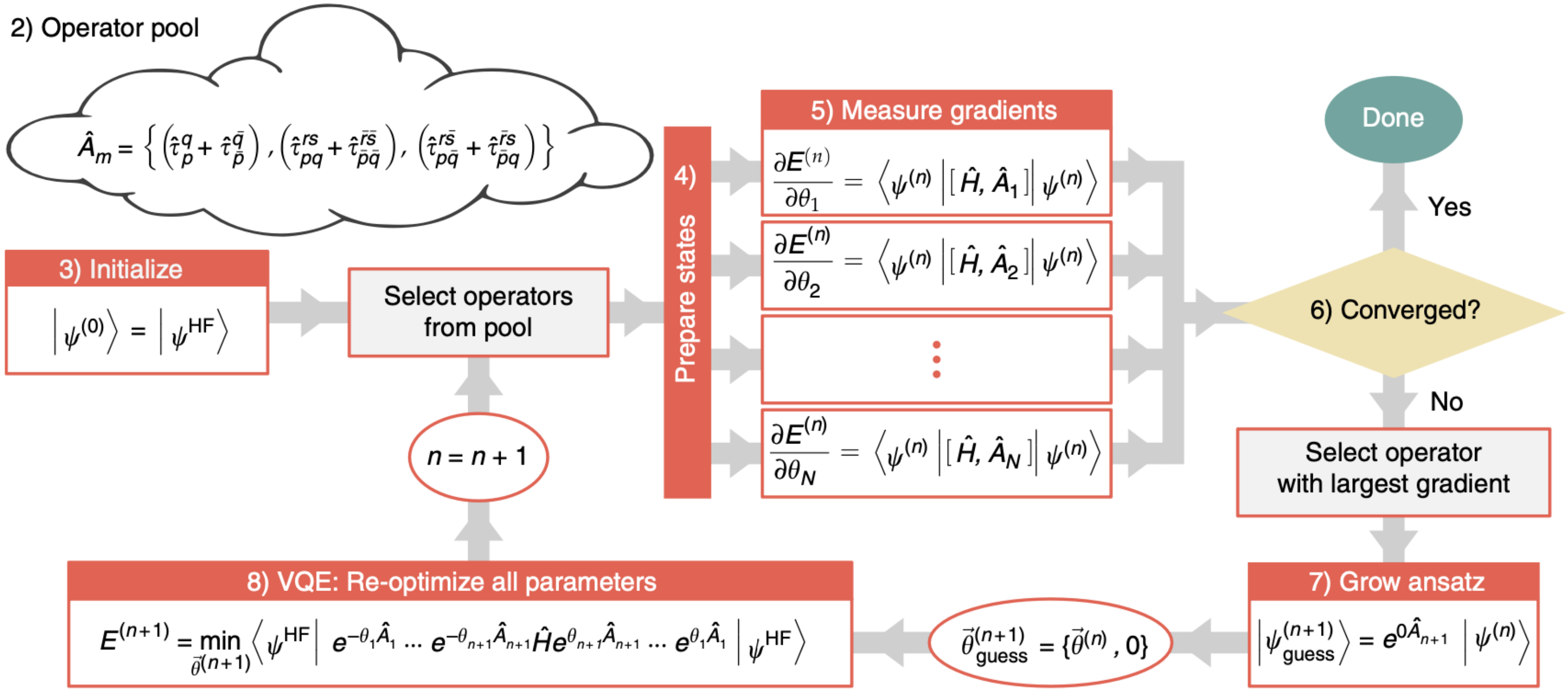
Variante of the UCC Ansätze

[4] Yordanov Y. S. et al., Phys. Rev. A. **102** 062612, (2020).

- **Qubit-Based Excitation (QBE) [4]:** Neglect the internal Z operator in the JW mapping of $\exp\left(i\left(\hat{T}(\theta) - \hat{T}^{\dagger}(\theta)\right)\right) \rightarrow$ less CNOTs and Swaps gates $\rightarrow$ Hardware efficient.

- **Iterative Construction of the Ansatz:** append an operator at each step according to its gradient (ADAPT-VQE) or predefined by an ordering scheme (Layerweise).

Grimsley, H.R., Economou, S.E., Barnes, E. *et al*. *Nat Commun* **10**, 3007 (2019).



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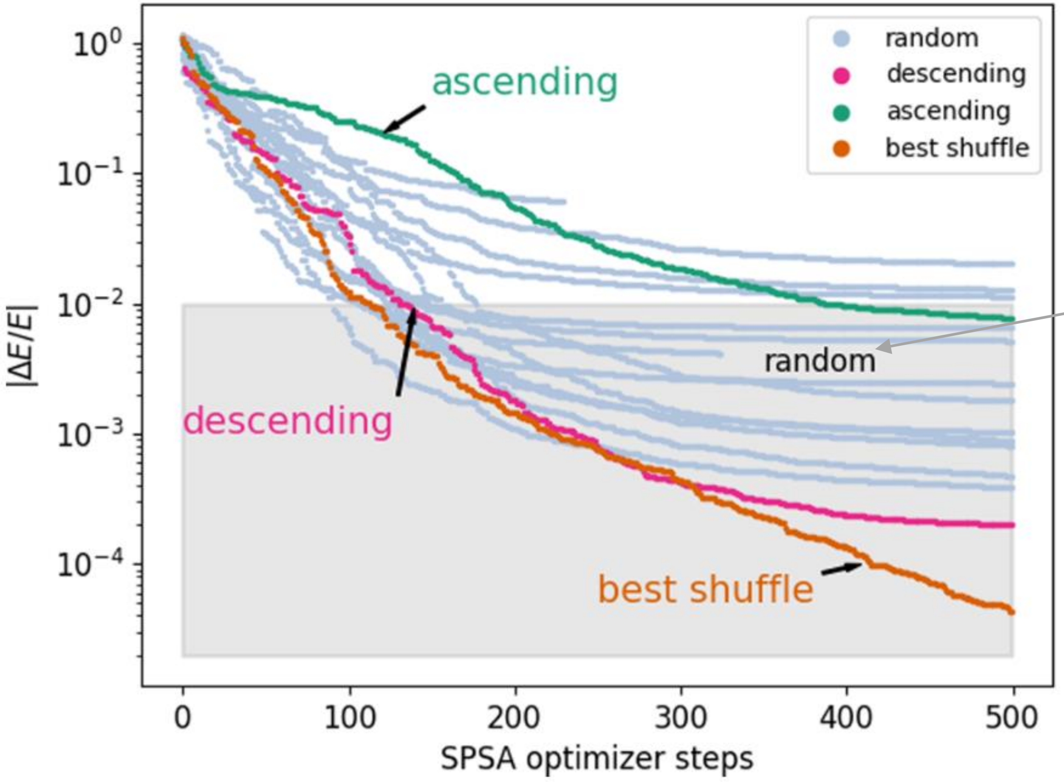
1. Train the first term for k steps.
2. Add a second term according to the ordering.
3. Repeat until all operators have been added.

Results (Simulations)

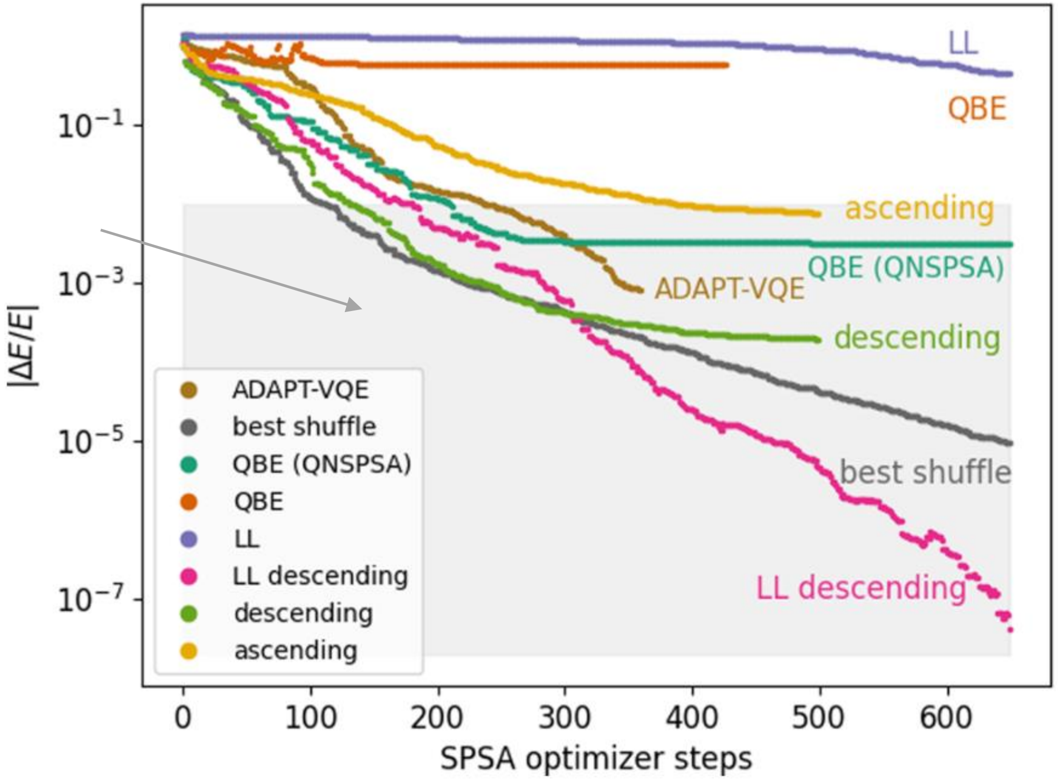
Kiss et al., *Phys. Rev. C* **106**, 034325 (2022)

- The effect of shuffling the fermionic excitations operators.
- We should order them in descending order.
- Optimizer: gradient free SPSA

- Best approach: train the ansatz recursvily in descending order.
- Qubit Based Excitation UCC: adapted to NISQ devices



1% barrier needed for most applications



Hardware results (IBMQ)

Error mitigation

- Start from the classical solution (warm start).
- Qubit Based Excitation descending UCC Ansatz.
- 10 runs on the 27 qubits IBMQ mumbai chip.

- **Readout:** individually inverse the error matrices

$$S_k = \begin{pmatrix} P^{(k)}_{0,0} & P^{(k)}_{0,1} \\ P^{(k)}_{1,0} & P^{(k)}_{1,1} \end{pmatrix}.$$

- Here, $P^{(k)}_{i,j}$ is the probability of the k-th qubit to be in state $j \in \{0,1\}$ while measured in state $i \in \{0,1\}$.

hardware	No. parameters	No. CNOT	mean	st. deviation	exact	error ratio
ibmq_mumbai raw (g.s.)	9	209	-6.27	0.269	-5.529	13.36%
ibmq_mumbai mitigated (g.s.)	9	209	-5.319	0.24	-5.529	3.81%
ibmq_mumbai raw (1st es)	3	41	-2.907	0.87	-3.420	14.97%
ibmq_mumbai mitigated (1st es)	3	41	-3.424	0.08	-3.420	0.12%

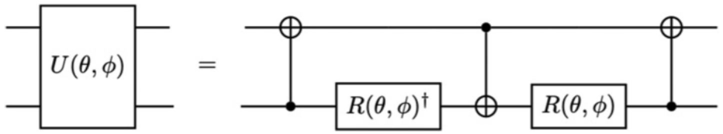
Alternative Ansätze
Excitation Preserving Hardware Efficient Ansatz

Two-qubit gate which maps

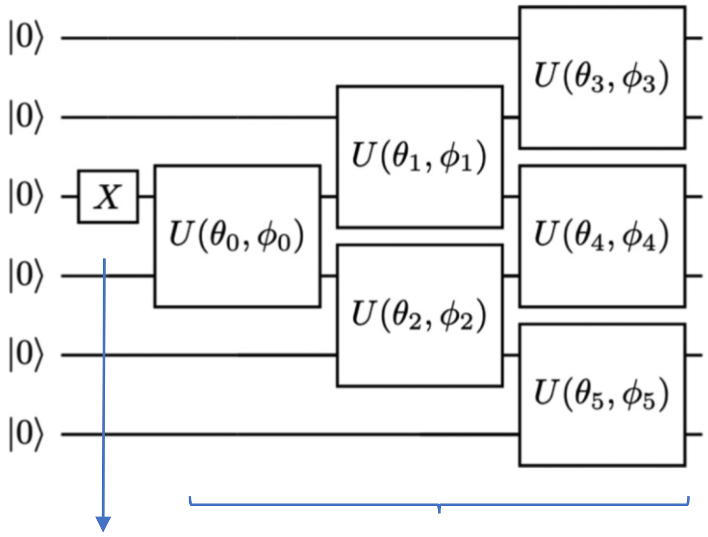
$$
\begin{aligned}
|00\rangle &\mapsto |00\rangle, \\
|01\rangle &\mapsto \cos(\theta)|01\rangle + e^{i\phi}\sin(\theta)|10\rangle, \\
|10\rangle &\mapsto e^{-i\phi}\sin(\theta)|01\rangle - \cos(\theta)|10\rangle, \\
|11\rangle &\mapsto |11\rangle.
\end{aligned}
$$

$$
U(\theta,\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta) & e^{i\phi}\sin(\theta) & 0 \\ 0 & e^{-i\phi}\sin(\theta) & -\cos(\theta) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.
$$

Gate Decomposition



Circuit Construction



Initial state

Preserve excitations

Problems:

- Does not know about the total angular momentum.
- Non trainable, barren plateaus.

Conclusions

- Compute the ground and first excited state of the 6Li nucleus with a quantum computer.
- Studied the ordering of the fermionic operators in the UCC ansatz.
- Operators associated with large coefficients should be placced first.
- Layerweise learning can improve the convergence.
- Error mitigation is vital for NISQ devices.

Thanks for your attention!
Questions?

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