Add implementations of Variational Quantum Algorithms for excited states to Qiskit

https://github.com/qiskit-advocate/qamp-fall-21/issues/28

The Team

Qiskit

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Variational Quantum Eigensolver

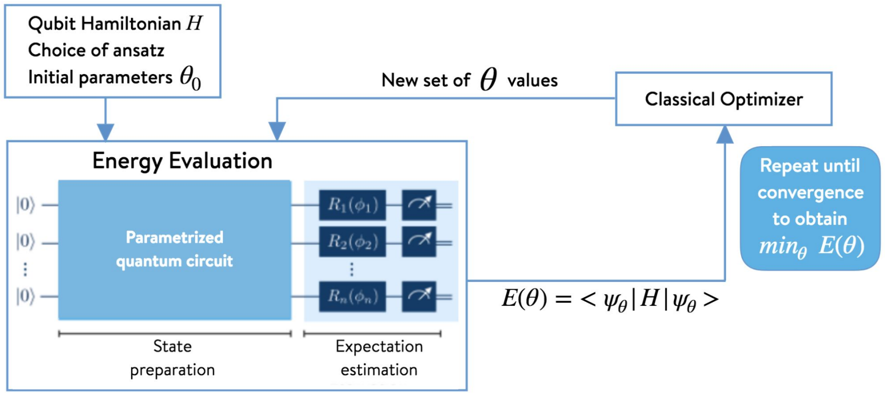
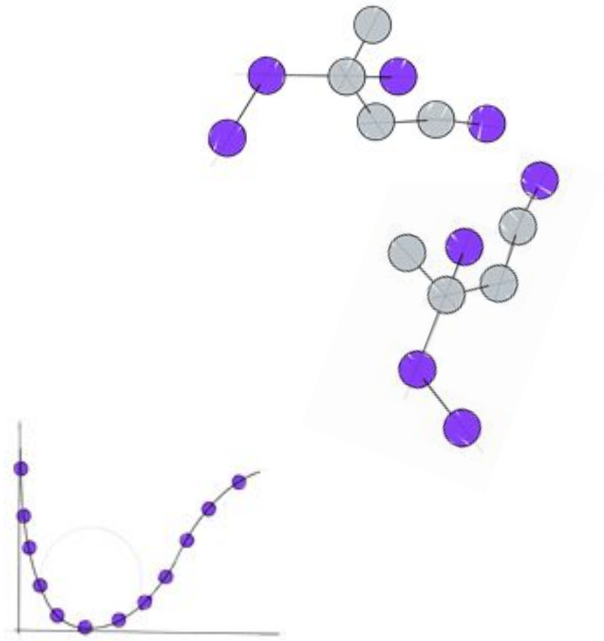


Image source: http://openqemist.1qbit.com/docs/vqe_microsoft_qsharp.html

- VQE is a hybrid quantum/classical algorithm used to determine the eigenvalues of a matrix ***H***, typically the hamiltonian of a system
- A quantum subroutine is run inside of a classical optimization loop
- The subroutine has two fundamental steps: preparation of the ansatz $|\Psi(\theta)\rangle$, and measurement of the expectation value $\langle\Psi(\theta)|H|\Psi(\theta)\rangle$
- We use a classical optimizer to minimize the expectation value by varying the ansatz parameter θ

Need for computing excited states

- Molecules in their excited states exhibit spectroscopic and photodynamic properties which are quite different from their ground state molecules.
- Study of photoinduced molecular processes, which plays an important role in biology, physics and chemistry, such as photostability of DNA, photosynthesis and light-harvesting, photocatalysis, organic photovoltaics, and photo - devices.
- Helps analyze properties of intermediate states of chemical reactions.
- Qiskit currently supports specialised higher state eigensolvers in Qiskit Chemistry (QEOM), but a domain independent method that can be implemented by higher level application still has a lot of scope.



Approach

Variational Quantum Deflation Algorithm (VQD)

Subspace Search Variational Quantum Eigensolver (SSVQE)

Variational Quantum Deflation algorithm (VQD)

- The VQD extends the VQE to calculate the *k*th excited state by optimizing the parameters θ_k for the ansatz state $\langle|\Psi(\theta_k)\rangle$ such that the cost function:

  $$F(\theta_k) := \langle\Psi(\theta_k)|H|\Psi(\theta_k)\rangle + \sum_{i=0}^{k-1}(\beta_i\langle\Psi(\theta_k)|\Psi(\theta_i)\rangle)^2$$

  is minimized.

- This can be seen as minimizing $E(\theta_k)$ subject to the constraint $|\Psi(\theta_k)\rangle$ is orthogonal to the states $|\Psi(\theta_0)\rangle, |\Psi(\theta_1)\rangle, \ldots, |\Psi(\theta_{k-1})\rangle$.

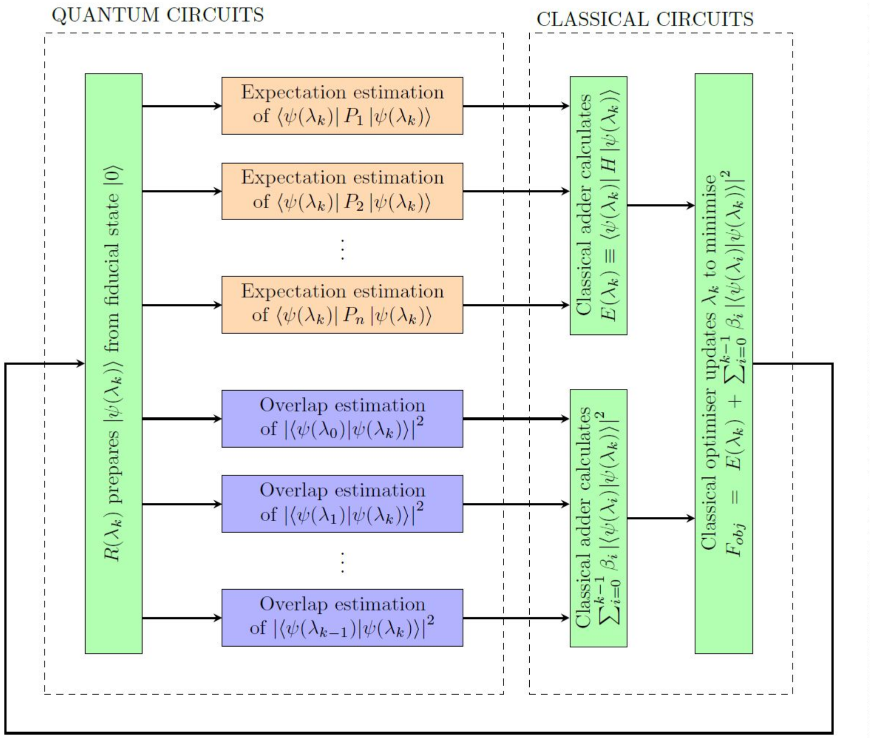


Image source: https://quantum-journal.org/papers/q-2019-07-01-156/

Subspace Search Variational Quantum Eigensolver (SSVQE)

- This algorithm searches a low-energy subspace by supplying orthogonal input states to the variational ansatz and relies on the unitarity of transformations to ensure the orthogonality of the output states.

- The kth excited state is obtained as the highest-energy state in the low-energy subspace.

- It allows for finding of the kth excited state with only one optimization procedure by finding the global optimum of the function,

$$L_w(\theta) = w\langle\varphi_k |U^\dagger(\theta)HU(\theta)|\varphi_k\rangle + \sum_{j=0}^{k-1} \langle\varphi_j|U^\dagger(\theta)HU(\theta)|\varphi_j\rangle$$

Expected Outcome

- Add the kstateVQE() algorithm to qiskit terra that implements the EigenSolver() interface.
- Write a tutorial explaining use of the kstateVQE and add it to the Qiskit tutorials

References

- Hans Lischka, Dana Nachtigallová, Adélia J. A. Aquino, Péter G. Szalay, Felix Plasser, Francisco B. C. Machado, and Mario Barbatti, *“ Multireference Approaches for Excited States of Molecules”,* Chemical Reviews 2018 118 (15), 7293-7361, DOI: 10.1021/acs.chemrev.8b00244
- Nakanishi, Ken M., Kosuke Mitarai, and Keisuke Fujii. "*Subspace-search variational quantum eigensolver for excited states.*" Physical Review Research 1.3 (2019): 033062
- Higgott, Oscar, Daochen Wang, and Stephen Brierley. "*Variational quantum computation of excited states.*" Quantum 3 (2019): 156.