Exploring the LAS-UCC method on a quantum simulator

Ruhee Dcunha[1], Riddhish Pandharkar[1], Matthew Otten[2], Matthew Hermes[1], Yuri Alexeev[3], Stephen K. Gray[3], Laura Gagliardi[1, 4, 5]

1. Department of Chemistry, University of Chicago, Chicago, IL, United States.
2. HRL Laboratories LLC, Malibu, CA, United States.
3. Argonne National Laboratory, Lemont, IL, United States.
4. James Franck Institute, Chicago, IL, United States.
5. Pritzker School of Molecular Engineering, Chicago, IL, United States.

In many extended systems strong correlation is localized in spatially separated subunits. This feature can be leveraged to lower the computational cost of quantum calculations, especially in the emerging field of quantum computation for quantum chemical simulation. Quantum computers have inbuilt advantages over classical computers in their ability to efficiently simulate wave functions as well as their unitary time evolution, but the newness of the field means that efficient algorithms are both necessary and scarce. A recently developed method, LAS-UCC, combines localization of the wave function with quantum phase estimation (QPE) performed only on local fragments and the variational quantum eigensolver (VQE) to add inter-fragment correlation. LAS-UCC is used to compute the energy of large molecules in which strong correlation is localized within subunits. This algorithm provides accuracy above that of both the VQE using the UCCSD ansatz on the whole system, and the classical localized active space self-consistent field (LASSCF) method upon which it builds.

In this work, we explore the limits of the LAS-UCC method in terms of the required number of ancilla qubits and gate depths, as well as the accuracy with respect to an exact diagonalization (FCI). The goal of this study is to analyze errors due to qubit and circuit depth limitations, and apply the method, while minimizing error, to interesting chemical problems. Thus, errors arising due to Trotterization, the scaling of the Hamiltonian for QPE, as well as similar errors for the VQE step, will provide insight into the efficiency of the method. In order to model real systems, keeping the error sources in mind, we then apply the LAS-UCC method as implemented on a quantum simulator using Qiskit to compute the total energies of conjugated organic molecules, and compare it to the classical LASSCF method.