Quantum Computing in Estimating Ground State Energies of Atoms and Molecules

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Abstract

Knowing the ground state energies of molecules and atoms give scientists critical insight on the behavior of said particles in reactions, thermodynamic and molecular properties, and excitation energies. However, due to the quantum mechanical nature of particles, the ground state energy can not be measured or solved mathematically.

To estimate the ground state energies, computers are utilized. As we are approaching the limits of classical computers, quantum computers present a bright future for computational chemistry.

In this paper, I give a brief summary of classical and quantum algorithms/methods for computational chemistry and discuss upon the current limitations of quantum computers in computational chemistry by analyzing the performance of a Variational Quantum Eigensolver (VQE) with different methods on IBM's noisy quantum computer simulator, `QasmSimulator`.

Keywords: *Quantum Computing, Chemistry, Quantum Chemistry, Quantum Computational Chemistry, Computational Chemistry, Variational Quantum Eigensolver*

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