PH044

Modelling the Hydrogen Molecule (H_2) with Quantum Circuits

1 Abstract

Quantum devices offers a much more efficient way to simulate molecular interaction as qubits share fundamental similarities with atoms. This leads to more efficient solvers compared to classical methods, especially when atomic number increases. In this report, we offer a simulation that finds the minimum ground state energy (MGSE) of the Hydrogen molecule (H_2) using a Variational Quantum Eigensolver which includes an ansatz prepared by the Unified Coupled Cluster method (VQE-UCC).

We will provide a short introduction regarding quantum computing, quantum chemistry, as well as the two aforementioned methods, namely VQE and UCC. We will explain how VQE-UCC solves for the MGSE by going through the Hamiltonian of the H_2 system and the ansatz preparation. In addition, we will apply artificial noise to make the results more applicable to real quantum computers. Then, we will analyse the experimental results such as the energy landscape obtained from running our quantum circuit with and without noise. Some of the collected data reveal interesting trends about quantum computers which if confirmed, have the potential to cause significant changes in the quantum computing landscape.