ABSTRACT

The application of the variational quantum eigensolver (VQE) on near-term quantum hardware to solve the Kohn-Sham Hamiltonian remains relatively underexplored. In this work, the weighted subspace-search variational quantum eigensolver (weighted SSVQE) is employed to compute the occupied Kohn-Sham orbitals, their associated energies, and the total electronic energy. The influence of entanglement unitary blocks, circuit depth, and optimization strategies on algorithmic performance is systematically investigated. Although the choice of optimization algorithm has a limited effect on the final total energy, it significantly affects convergence behavior, numerical stability, and computational cost. An optimal weight configuration is identified that simultaneously accelerates convergence and improves energy accuracy. Furthermore, the results demonstrate that circuit depth and the structure of entanglement unitary blocks play a critical role in determining total energy accuracy across different molecular geometries. The most effective circuit design is found to begin with a low-expressibility, weakly entangling ansatz-such as linear entanglement unitary blocks-which is repeated until a sufficient number of layers is achieved. Using homoatomic and heteroatomic molecules as benchmark systems, the proposed approach is shown to remain robust and effective across systems exhibiting different types of electron correlation. Overall, this method enables shallow, convergence-friendly quantum circuits that closely reproduce standard density functional theory results, providing a practical design strategy for efficient VQE implementations.

Keywords : Variational quantum eigensolver; weighted subspace-search VQE; Kohn-Sham Hamiltonian; density functional theory; shallow quantum circuits; entanglement unitary blocks; circuit depth optimization; near-term quantum computing