Quantum Entanglement Implementation in Energy Gaps Computation for Open-shell Molecules

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Quantum computers can efficiently perform full configuration interaction (FCI) calculations of atoms and molecules using the quantum phase estimation (QPE) algorithm. Also, most chemistry problems discuss energy differences between two electronic states rather than total energies. Thus, direct calculations of energy gaps are promising for future applications of quantum computers to real chemistry problems. In the race to find efficient quantum algorithms to solve quantum chemistry problems, this project will study and test a Bayesian phase difference estimation (BPDE) algorithm, which is based on the time evolution of the wave functions in the superposition of two electronic states and the state preparation is carried out conditionally on the ancillary qubit [1]. This work will use that quantum algorithm to map wavefunctions for open-shell molecules to calculate the difference between two eigenphases of unitary operator's energy gaps between two electronic states into the quantum computing approach. The quantum algorithm will be used to calculate ionization energies, singlet-triplet energy gaps and vertical excitation energies. Possible applications of this current quantum algorithm are presented, which has many advantages over other existing methods. The quantum algorithm implementation will be simulated mainly in Python. Finally, the project will analyze if there are any spatial trends in the properties of the materials through Mathematica, dftb++ with spectroscopy techniques.

REFERENCES

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