Molecular Energies with Electron Correlation from Linear Depth Quantum Circuits

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Abstract

A promising technological avenue of quantum computing is the computation of molecular energies in quantum chemistry, as qubits can map onto spin orbitals of specific electrons. Taking inspiration from Arute et al's method of orbital optimization for the mean field Hartree-Fock energy on a noisy intermediate-scale quantum (NISQ) device,[1] we seek to adapt a similar orbital optimization approach to include dynamical electron correlation energy from second order Møller-Plesset perturbation theory (OMP2) [2] into the molecular energy cost function to be minimized in a variational quantum algorithm. More rigorous methods to recover correlation energy such as the unitary coupled cluster method involve deep entangling circuit ansätze and are thus limited to small molecules. To improve resource efficiency, our NISQ-OMP2 method uses multiple shallow circuits with a QR decomposition of the orbital optimization U(θ) with O(N) depth,[3] and a basis rotation grouping scheme to reduce the number of Pauli measurements from O(N^4) to O(N),[4] as depicted in Figure 1. This work demonstrates the estimating of OMP2 energies of H_2, H_3^+, and LiH using classical simulations with noise models, and on cloud-accessed NISQ devices.[5] Results for H_2 on NISQ devices are summarized in Figure 2.

References

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[3] Clements, W. R. et al., Optica, 12 (2016) 1460.
[4] Huggins, W. J. et al., npj Quantum Information, 7 (2021) 23.
[5] Chee C. H. et al., arXiv:2207.03949

Figures

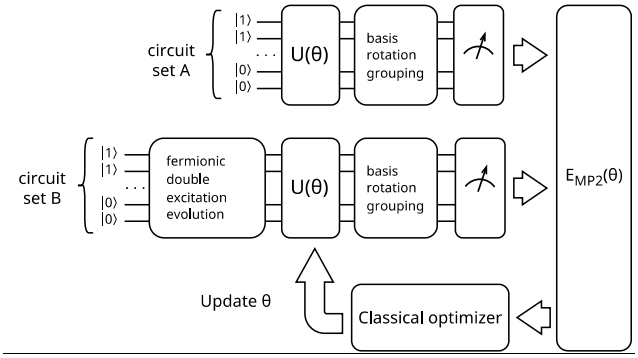

Figure 1: Schematic process diagram showing quantum circuit sets A and B used to estimate orbital-optimized MP2 energies using a variational quantum algorithm.

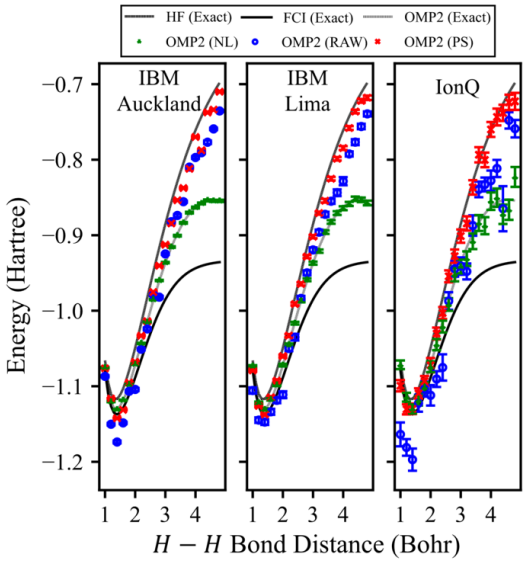

Figure 2: OMP2 Energy of H_2 at various bond distances, estimated using various NISQ devices.