Improved implementation of the Quantum Self-Consistent Equation-of-Motion (Q-SC-EOM) method in INQUANTO

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Abstract

The Quantum Self-Consistent Equation-of-Motion (Q-SC-EOM) method for the calculation of excitation energies has been recently published by Asthana, Kumar *et al*. [1] We have now built upon the original method with an implementation in INQUANTO[2] that employs an alternative state preparation procedure for the linear combination of states, by using the method based on Givens rotations.[3] We benchmark our implementation against classical calculations for small systems such as H_2, LiH and H_3^+, and discuss the required circuit depths for different parts of the implementation. In addition, we further improve our implementation by using symmetry filtering, in order to avoid the calculation of redundant elements, which facilitates the study of larger systems. We show here the results for H_4, H_2O, as well as a challenging case of scanning the potential energy surface of ethylene (using minimum active space) along its torsion angle rotation coordinate.

References

[1] Asthana, A.; Kumar, A.; Abraham, V.; *et al*. *Chem. Sci.* 14 (2023) 2405
[2] https://www.quantinuum.com/computationalchemistry/inquanto
[3] Arrazola, J. M.; Di Matteo, O.; Quesada, N; *et al*. *6 Quantum* (2022) 742

Figures

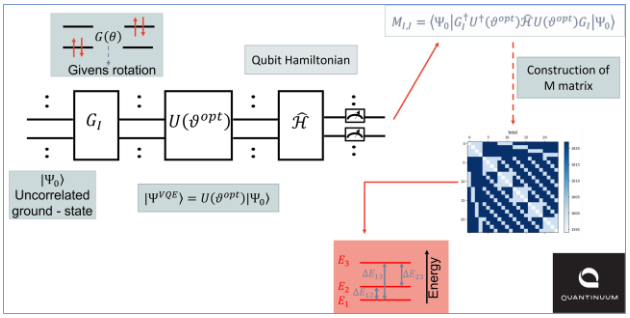

Figure 1: Schematic picture of the implementation of the Q-SC-EOM method in INQUANTO