Quantum simulation of molecular response properties using the equation of motion formalism

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Modelling the response of the molecular systems to an external electromagnetic field is quite computationally challenging for classical quantum chemistry methods, especially in the regime of strong correlation. We attempt to solve this problem with the help of a quantum computer by making use of the equation of motion (EOM) formalism on top of the ground state calculation using the unitary coupled cluster singles and doubles (UCCSD) ansatz in conjunction with the variational quantum eigensolver (VQE) algorithm. The results obtained are of better quality than the ones obtained using the classical CCSD method and we are also able to obtain the “quantum advantage” by doing measurements of the matrix elements in the EOM procedure. In order to account for the basis set effects which can be quite significant for these properties, we make use of our recently developed transcorrelatted Hamiltonian procedure[1] to obtain quantitative results with minimal quantum resources.

References

1. A. Kumar, A. Asthana, C. Masteran, E. F. Valeev, Y. Zhang, L. Cincio, S. Tretiak, and P. A. Dub, Accurate quantum simulation of molecular ground and excited states with a transcorrelated hamiltonian, arXiv preprint arXiv:2201.09852 (2022)