Equation of motion variational quantum eigensolver (EOM-VQE) method for molecular excitation energy, ionization potential and electron affinity

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Near-term quantum computers are expected to facilitate material and chemical research through accurate molecular simulations. Several developments have already shown that accurate ground-state energies for small molecules can be computed on present-day quantum devices. Although molecular excited states play a vital role in chemical research, the search for a reliable and practical approach for routine excited-state calculations on near-term quantum devices is ongoing. Inspired by excited-state methods developed for unitary coupled-cluster theory in quantum chemistry, we present an equation-of-motion based method to compute excitation energies on top of variational quantum eigensolver algorithms on a quantum computer. We perform numerical simulations on H_2, H_4, H_2O and LiH to test the equation-of-motion variational quantum eigensolver (EOM-VQE) method and compare it to the state of the art methods. EOM-VQE makes use of self-consistent operators to satisfy vacuum annihilation conditions. It provides accurate and size-intensive ionization potential (IP), electron affinity (EA) and excitation energies (EE). We also find that EOM-VQE is more suitable for implementation on NISQ devices as it is resilient to measurement noise and does not require higher than 2-body reduced density matrices (RDMs).