Exploring Effective Hamiltonians for Near-term Quantum Computer

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With the advent of real quantum devices, researchers are striving to demonstrate quantum supremacy, which entails finding a problem that is sufficiently interesting and exceedingly challenging on classical devices [1]. Quantum chemistry is a field where one can find complex chemical problems, which can be used to show quantum devices are superior to their classical counterparts. Research efforts have focused on designing efficient quantum algorithms to reliably perform chemistry problems on current noisy and small quantum devices [2]. While it is exciting to see the algorithmic improvement and many experiments have demonstrated the successful use of quantum devices in computing molecular properties, the problem size is still limited to small molecules, which are still simple to solve using a classical computer. This study aims at answering these questions by employing a coarse-grained representation of many-electron systems called effective Hamiltonian obtained from equation-of-motion coupled-cluster (EOM-CC) method. The coarse-grained approach leads to the reduction of molecular complexity into only a few qubits problem. In this study, we demonstrate Hubbard's Hamiltonians can be extracted from the effective Hamiltonian. We also provide an application of obtained Hubbard's model to the macroscopic solid-state property of several open-shell systems using current near-term quantum devices with the help of classical *ab initio* calculations.

References

[1] Arute, F., Arya, K., Babbush, R. *et al.* Quantum superamacy using a programmable superconducting processor. *Nature* **2019**, *574*, 505-510.

[2] Cerezo, M., Arrasmith, A., Babbush, R. *et al.* Variational quantum algorithms. *Nat. Rev. Phys.* **2021**, *3*, 625-644.