Measurement Optimization in the Variational Quantum Eigensolver Method of Quantum Computing

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Solving the time-independent Schrödinger equation for molecules requires exploring the Hilbert spaces that grow exponentially with the number of electrons in the systems. This becomes increasingly challenging for classical computers, but recently emerged quantum computers provide a new hope in addressing this problem. One of the promising algorithms, the Variational Quantum Eigensolver (VQE) utilizes a digital quantum computer to parameterize an entangled trial state and variationally minimize the expectation value of the Hamiltonian to find its ground state energy.

One major problem hindering the effectiveness of VQE is necessity to measure the expectation value of the electronic Hamiltonian. Unfortunately, due to limited capabilities of current quantum hardware the entire electronic Hamiltonian cannot be measured. Instead, one needs to partition the Hamiltonian into simpler parts and measures each part individually with identically prepared trial states. This redundancy necessitates efficient methods for dividing Hamiltonian into a sum of few simple fragments that collectively require fewer copies of the trial state. In our works, we proposed several measurement schemes that address this problem [1-3].

[1] T. C. Yen, and A. F. Izmaylov. Cartan sub-algebra approach to efficient measurements of quantum observables, arXiv:2007.01234 (2020).
[2] T. C. Yen, V. Verteletskyi, and A. F. Izmaylov. Measuring all compatible operators in one series of single-qubit measurements using unitary transformations. *Journal of Chemical Theory and Computation* **16**, 2400–2409 (2020).
[3] V. Verteletskyi, T. C. Yen, and A. F. Izmaylov. Measurement optimization in the variational quantum eigensolver using a minimum clique cover. *Journal of Chemical Physics* **152**, 124114 (2020).