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Quantum chemistry on NISQ devices beyond variational quantum algorithms

Keita Kanno

QunaSys

Abstract

Quantum chemistry has been one of the most promising applications of quantum computing, motivated by the natural correspondence between the quantum states on quantum computers and the electronic states in chemical systems. The quantum phase estimation algorithm enables one to exploit this correspondence to calculate ground- and excited-state energies of complex molecules accurately and efficiently, but its demanding gate complexity requires fault-tolerance for a successful execution. Variational quantum algorithms such as the variational quantum eigensolver (VQE) has been proposed to exploit noisy, non-fault-tolerant quantum computers by using them repeatedly in combination with classical computers, but they have problems such as the large number of quantum circuit executions for optimization and for suppressing the sampling error, in addition to its insufficient noise resilience. Developing a noise-resilient algorithm with a practical runtime is a fundamental challenge to take advantage of noisy quantum computers in quantum chemistry.

In this talk, as a potential solution to this challenge, I will introduce the Quantum-Selected Configuration Interaction (QSCI) algorithm. QSCI uses more of classical computing than a simple VQE, thereby resulting in a more accurate and reliable result. I will also touch on the subsequent studies and future directions that further develops QSCI.