New Variational Quantum Algorithms for Quantum Chemistry

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Solving the electronic many-body Schrödinger equation for strongly correlated systems is a significant challenge in physics, materials science, and chemistry. Classical numerical simulations of these systems are severely limited by the exponential scaling of the many-body basis. Quantum computers can represent and manipulate quantum states efficiently, and therefore, could offer an alternative way to simulate many-body problems. In the past few years, advances in quantum hardware engineering have played a critical role in reinvigorating interest in the development of quantum simulation algorithms. Recent work has centered on the development of quantum phase estimation (QPE) and the variational quantum eigensolver (VQE). These two techniques have been successfully applied to solve small molecular problems using quantum simulators and real hardware experiments. Of these two approaches, VQE is seen as the most promising for near-term noisy quantum computers. This talk will discuss several contributions from our group to the development of VQE methods, specifically a recent characterization of exact trials states based on factorized unitary coupled-cluster for VQE, and a new formulation and hardware implementation of an alternative to VQE based on a projective formalism.