Abstract:

The variational quantum eigenvalue solver is a powerful hybrid quantum-classical approach that has been suggested as a candidate method to run on near-term quantum hardware for computing ground state electronic energies of molecular systems. However, even for small molecules, the number of variational parameters and qubits required to minimize the electronic energy is beyond the reach of current quantum computers except for small basis sets. We explore a new paradigm for state preparation where we test how much of the optimization can be approximately prepared with classical computers to reduce the number of optimization steps performed using a quantum device. By adapting a recent algorithm for the factorized form of the UCC ansatz, we can study molecular electronic structure problems with up to 64 qubits. In addition, we also test a related approach of using tensor networks to optimize quantum circuits in order to benchmark various lattice models. We present results using these approaches and discuss strategies for incorporating these ideas into variational algorithms involving near-term quantum computers. Our results help demonstrate the strength of the UCC ansatz and address pressing questions about optimal initial parameterizations and circuit construction.