A quantum algorithm for state-averaged, adaptive ansatz construction

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Classical approaches struggle to describe large systems of strongly correlated electrons. Quantum computation is a promising alternative, using controlled evolution of entangled qubits to model correlated electrons. Unfortunately, existing hardware implementations are plagued by various practical issues, such as short coherence times of qubits and low fidelity of quantum gates. Resource-efficient strategies for obtaining electronic ground states have been heavily investigated. Excited states, however, remain relatively unexplored, despite their importance in applications like spectroscopy and photochemistry. To this end, we have generalized the Adaptive, Problem-Tailored (ADAPT-) Variational Quantum Eigensolver (VQE) to simultaneously prepare multiple eigenstates of the Hamiltonian. Our method, the Multistate-Objective Ritz-Eigenspectral (MORE-) ADAPT-VQE, constructs a unitary based on the weighted average of the energies of multiple states. After these states have been identified, the Hamiltonian is diagonalized in their subspace to yield approximate eigenstates of the true Hamiltonian. In addition to energies, important electronic properties can be measured in this eigenbasis. We report on attractive theoretical features of the algorithm and compare MORE-ADAPT-VQE results to those of existing state-specific strategies. As prototypical problems, we consider energy curves with regions of strongly correlated ground and excited states, such as the D_{2h} dissociation of rectangular H_4 and the C_{2v} insertion of Be into H_2. Our results demonstrate the importance of democratic treatment of multiple references in ansatz construction.