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Efficient Symmetry-Preserving State Preparation Circuits for the Variational Quantum Eigensolver Algorithm[1]

BRYAN GARD, Virginia Tech University

The variational quantum eigensolver is one of the most promising approaches for performing chemistry simulations using noisy intermediate-scale quantum (NISQ) processors. The efficiency of this algorithm depends crucially on the ability to prepare multi-qubit trial states on the quantum processor that either include, or at least closely approximate, the actual energy eigenstates of the problem being simulated while avoiding states that have little overlap with them. Symmetries play a central role in determining the best trial states. Here, we present efficient state preparation circuits that respect particle number, total spin, spin projection, and time-reversal symmetries. These circuits contain the minimal number of variational parameters needed to fully span the appropriate symmetry subspace dictated by the chemistry problem while avoiding all irrelevant sectors of Hilbert space. We show how to construct these circuits for arbitrary numbers of orbitals, electrons, and spin quantum numbers, and we provide explicit decompositions and gate counts in terms of standard gate sets in each case. We test our circuits in quantum simulations of the H_2 and LiH molecules and find that they outperform standard state preparation methods in terms of both accuracy and circuit depth.

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