Reducing the Resource Requirements of Quantum Computing for Electronic Structure

Robert A. Lang and Artur F. Izmaylov

Department of Chemistry, University of Toronto, ON, Email: robert.lang@mail.utoronto.ca

Application of current and near-term quantum computing platforms to the electronic structure problem is highly limited by qubit counts, coherence times, and gate fidelities. To address these restrictions within the variational quantum eigensolver (VQE) framework, many recent contributions have suggested similarity transforming ("dressing") the electronic Hamiltonian to include a part of electron correlation, leaving the rest to be accounted for by quantum state preparation. We present our developments of a novel dressing scheme that combines preservation of the Hamiltonian hermiticity and an exact quadratic truncation of the Baker-Campbell-Hausdorff expansion. The new transformation is constructed as the exponent of an involutory linear combination of anti-commuting Pauli operator products. It incorporates important strong correlation effects in the dressed Hamiltonian and can be viewed as a classical preprocessing step alleviating the resource requirements of the subsequent VQE application.

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