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【572】Can quantum algorithms in chemistry outperform their classical equivalent? Advanced Quantum Unitary Coupled Cluster methods for strongly correlated systems.

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The truncated classical coupled cluster (CC) methods have been known to provide non-variational energies in the systems that present multiconfigurational nature of the ground state. Methods such as paired CC (pCC) and singlet CC (CC0) unreliably correct this failure by eliminating excitations in the cluster operator.
In this work, we show that their unitary implementation (q-pUCC, q-UCC0) on digital quantum computers (QC) using the variational quantum eigensolver algorithm (VQE) with a single Trotter step unconditionally cures the breakdown of their classical counterparts. In addition, the q-UCC0 reproduces the geometric features of the exact energy landscape more accurately than the quantum pCC (q-pUCC) method.
Moreover, we propose a selection criterion that improves on the existing MP2 amplitude-based selection scheme by eliminating the single excitations which enables the optimiser to recover the correlation energy in less iterations. The robustness of these methods is tested on the H4, H2O, N2 molecules and the repulsive Hubbard model, in a QC simulator, Qiskit, using various qubit and circuit depth reduction schemes which are currently necessary for the implementation on the NISQ hardware.

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