Mapping renormalized coupled cluster methods to quantum computers through a compact unitary representation of nonunitary operators

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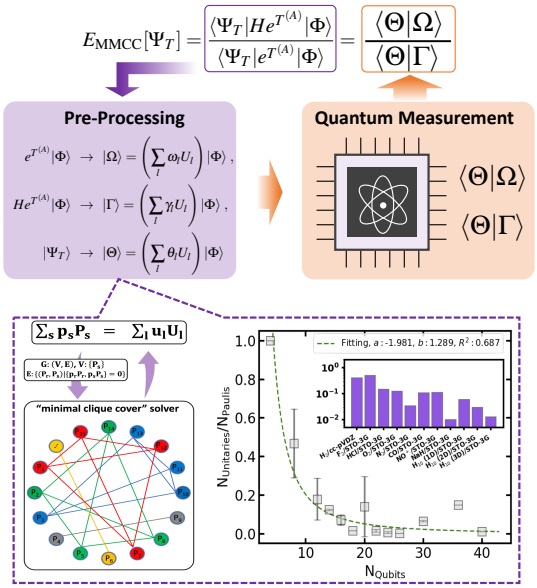
Nonunitary theories are commonly seen in the classical simulations of quantum systems. Among these theories, the method of moments of coupled cluster equations (MMCCs) and the ensuing classes of the renormalized coupled cluster (CC) approaches have evolved into one of the most accurate approaches to describe correlation effects in various quantum systems. The MMCC formalism provides an effective way for correcting the energies of approximate CC formulations (parent theories) using moments, or CC equations, that are not used to determine approximate cluster amplitudes. In this paper, we propose a quantum algorithm for computing MMCC ground-state energies that provides two main advantages over classical computing or other quantum algorithms: (i) the possibility of forming superpositions of CC moments of arbitrary ranks in the entire Hilbert space and using an arbitrary form of the parent cluster operator for MMCC expansion, and (ii) significant reduction in the number of measurements in quantum simulation through a compact unitary representation for a generally nonunitary operator. We illustrate the robustness of our approach over a broad class of test cases, including ~40 molecular systems with varying basis sets encoded using 4–40 qubits, and we exhibit the detailed MMCC analysis for the 8-qubit half-filled, four-site, single impurity Anderson model and the 12-qubit hydrogen fluoride molecular system from the corresponding noise-free and noisy MMCC quantum computations. We also outline the extension of the MMCC formalism to the case of a unitary CC wave-function Ansatz



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Reference

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