# Improving the Efficiency and Robustness of Quantum Algorithms for Computational Chemistry

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One of the promising areas where quantum computers are anticipated to have an advantage over their classical counterparts is the simulation of quantum many-body systems. However, standard quantum circuits implementing anti-Hermitian excitations contain a number of CNOT gates that scales exponentially with the many-body rank of the excitation operators. Given that two-qubit gates, such as CNOTs, dominate gate errors in current noisy intermediate-scale quantum devices, minimizing their number is crucial for experimental realization of hybrid quantum–classical algorithms. Inspired by the work of Yordanov *et al.* [1], who constructed CNOT-efficient quantum circuits performing single and double excitations, we introduce CNOT-efficient representations of operators with arbitrary excitation rank [2]. Our classical numerical simulations demonstrate that the replacement of traditional quantum circuits by their CNOT-efficient counterparts leads to a decrease in the CNOT count by factors as large as 15 in molecular simulations using adaptive hybrid quantum–classical algorithms. To achieve a linear scaling of the CNOT count with the many-body rank, we consider approximate implementations of our compact circuits [3]. Our numerical results show that the approximants faithfully reproduce the energies obtained with the full quantum circuits, while the ensuing symmetry breaking is essentially negligible. To further reduce the quantum resources for ansatz-dependent quantum algorithms, we explore the usefulness of non-iterative energy corrections [4]. We demonstrate that chemically accurate energies can be obtained with substantially more compact circuits, implying enhanced resilience to gate and decoherence noise.

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