Efficient Preparation of Ansatz States on Near-Term Quantum Computers for Quantum Chemistry

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Abstract
Quantum computing has promised quantum advantage in quantum chemistry applications to solve molecular many-body problems. For example, quantum phase estimation has shown to have exponential speedup over its classical counterparts with the success probability that is determined by the overlap of a trial ansatz state with the eigenstate of interest [1]. However, quantum ansatz state preparation was quickly identified as a major bottleneck step that prohibits quantum algorithms from fulfilling their potential [1]. Widely-used quantum ansatzes including the Slater determinants [3] and Unitary Coupled Cluster [4] employ parameterized fermionic excitation gates, with the latter resulting in deep quantum circuits that scale at least polynomially in two-qubit gate depth with the system size N, which exacerbate errors due to quantum noise and decoherence. As quantum computers are yet to become fault-tolerant, it is thus important to have depth-efficient preparation of quantum ansatz for near-term quantum computing applications in chemistry. Here we propose an alternate paradigm for fermionic ansatz state preparation [5] inspired by data-loading circuit methods developed for quantum machine learning [6]. We show how a shallow, yet scalable sequence of parameterised fermionic excitation operators $\hat{C}_i$ can be used to prepare Slater determinants and correlated ansatzes yielding subexponential reduction in the two-qubit gate depth compared to previous approaches, as shown in Fig. 1. Moreover, our approach is designed to be compatible on existing quantum devices with planar qubit architectures without requiring any expensive qubit swapping overheads, thereby enabling the use of more qubits needed for high-precision quantum chemistry studies on near-term quantum devices.

References

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Figures

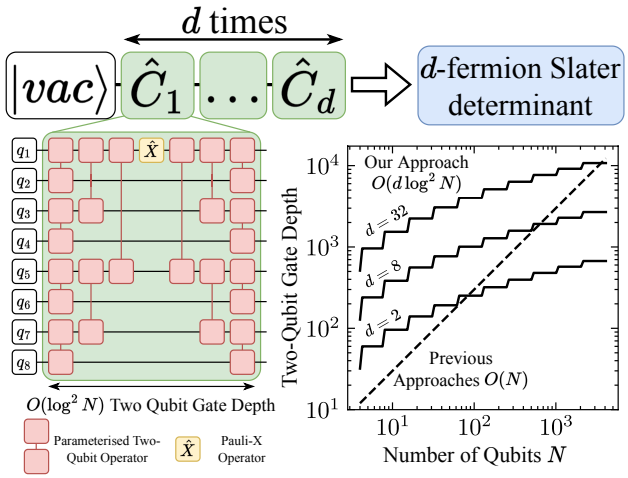

Figure 1: Proposed efficient approach and the estimated two-qubit gate depth for preparing d-fermion Slater determinant on a quantum computer with N qubits.