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Break down the high-order tensors of quantum chemistry, for O(N)-depth circuit algorithm

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Abstract

Quantum chemistry is gaining more attention as a promising field of application of quantum computers because of its high affinity to the qubit representations and universal gate operations. Even so, the status is far from real-world applications. One of the reasons is that high-order tensors that describe electron interaction or correlation, e.g., the two-electron molecular integrals or double-excitation cluster amplitudes, need to be processed in quantum chemical calculations, which will be interpreted by at least O(N^4) quantum gates in the circuits, thereby making it infeasible on current and near-term quantum computers. Here, we present an efficient tensor decomposition for the above high-order tensors, and a new ansatz for the variational quantum eigensolver. The method is able to be implemented with O(N)-depth quantum circuit and at the same time considerably reduce the required number of measurements.