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Reducing the complexity of quantum algorithms: the effect of single-particle basis transformation on the 1-norm of the electronic structure Hamiltonian.

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Reducing the complexity of quantum algorithms to treat quantum chemistry problems is essential to demonstrate an eventual quantum advantage of Noisy-Intermediate Scale Quantum (NISQ) devices over their classical counterpart. Significant improvements have been made recently to simulate the time-evolution operator $U(t) = e^{iHt}$ where H is the electronic structure Hamiltonian, or to simulate H directly (when written as a linear combination of unitaries) by using block encoding or "qubitization" techniques [1,2]. A fundamental measure quantifying the practical implementation complexity of these quantum algorithms is the so-called "1-norm" of the qubit-representation of the Hamiltonian, which can be reduced by writing the Hamiltonian in factorized or tensor-hypercontracted forms for instance [2,3]. The 1-norm also dictates the number of shots of preparation and measurements in the so-called Variational Quantum Eigensolver (VQE) algorithm [4-6]. In this contribution, we describe a simple strategy to reduce the 1-norm which consists in a classical pre-optimization of the electronic structure Hamiltonian representation via single-particle basis transformation [7]. We derived a new formula for the 1-norm as a function of the electronic integrals, and used this quantity as a cost function for an orbital-optimization scheme that improves over standard localization schemes. To summarize, this contribution gives more insights about the importance of the 1-norm in quantum computing for quantum chemistry, and provides simple ways of decreasing its value to reduce the complexity of quantum algorithms.

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