Title of Research: Electronic Structure Calculations using Quantum Computing

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Abstract

The computation of electronic structure properties at the quantum level is a crucial aspect of modern physics research. However, conventional methods can be computationally demanding for larger, more complex systems. To address this issue, we present a hybrid Classical-Quantum computational procedure that uses the Variational Quantum Eigensolver (VQE) algorithm. By mapping the quantum system to a set of qubits and utilising a quantum circuit to prepare the ground state wavefunction, our algorithm offers a streamlined process requiring fewer computational resources than classical methods. Our algorithm demonstrated similar accuracy in rigorous comparisons with conventional electronic structure methods, such as Density Functional Theory and Hartree-Fock Theory, on a range of molecules while utilising significantly fewer resources. These results indicate the potential of the algorithm to expedite the development of new materials and technologies. This work paves the way for overcoming the computational challenges of electronic structure calculations. It demonstrates the transformative impact of quantum computing on advancing our understanding of complex quantum systems.