Towards Efficient Simulation of Strongly Correlated Materials Using Hybrid Quantum–Classical Algorithms

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Abstract

Understanding and predicting the properties of strongly correlated materials remains one of the central challenges in modern condensed matter and materials science. Traditional density functional theory (DFT) methods often struggle with these systems because they fail to accurately describe strong electron–electron correlations.[1,2] While quantum computing offers promising new opportunities, its practical applications are still constrained by current hardware capabilities.[3]

In this ongoing work, we explore a hybrid quantum–classical approach that combines classical electronic structure methods with quantum algorithms to address these limitations.[4] Using BigDFT's support-function formalism,[5] we generate compact, localized representations of electronic wavefunctions, which naturally lead to sparse Hamiltonians suitable for quantum processing.[6] As part of our initial studies, we analyze model systems to investigate the relationship between locality, orthonormality of the orbital basis set, and the sparsity and graph representation of the single-body and many-body Hamiltonians. These insights are essential for constructing Hamiltonians that can be efficiently tackled using quantum algorithms such as the Variational Quantum Eigensolver (VQE), Quantum Krylov methods, or Quantum Phase Estimation (QPE).[7]

This contribution focuses on the construction of many-body Hamiltonian derived from BigDFT's wavelet-based support-function formalism and the quantitative characterization of their sparsity and locality properties. By extending the atom-centered support-function representation beyond the one-body level through explicit inclusion of Coulomb interaction tensors, we investigate how the inherent spatial localization of the basis impacts the structure, conditioning, and effective sparsity of the resulting Hamiltonian. Metrics such as norm-based sparsity measures, orbital variance, and overlap conditioning are used to characterize the Hamiltonian in view of its suitability for quantum simulation workflows. The presentation will highlight the practical methodology, numerical behavior, and implications for reducing quantum resource overhead in near-term algorithms.

The long-term goal is to develop a scalable and hardware-efficient simulation pipeline capable of addressing materials of industrial and technological relevance. By bridging classical and quantum techniques, this work aims to contribute to the broader effort of making quantum simulations practical for real-world materials science problems.

References

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