

Mean-field solvable Hamiltonians: Improving quantum computing methods for quantum chemistry

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Quantum computing algorithms for solving the electronic structure problem require algebraic manipulations with the electronic Hamiltonian. Dealing with this Hamiltonian in the second quantized form poses various difficulties that we address by partitioning the Hamiltonian into a sum of mean-field solvable fragments. These fragments can be diagonalized using single-particle transformations (e.g. orbital rotations) and thus are convenient for performing algebraic manipulations. In this talk, I will illustrate how partitioning to mean-field solvable Hamiltonians can be used to improve performance of common quantum computing algorithms for quantum chemistry, Variational Quantum Eigensolver and Quantum Phase Estimation.