Quasi-Hermitian Hamiltonian Simulation: Transcorrelated Electronic Hamiltonians

Cheng-Lin Hong[1,2], Werner Dobrautz[1,2,3,4]
[1] *Center for Advanced Systems Understanding, 02826 Görlitz, Germany*

[2] *Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany*

[3] *Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig, 01069 Dresden, Germany*
[4] *Technical University Dresden, 01069 Dresden, Germany*

One challenge in quantum chemistry on quantum computers is the large number of qubits required to achieve accurate results near the complete basis set (CBS) limit. The transcorrelated (TC) method [1,2] addresses this issue by using a non-unitary similarity transformation to incorporate electron-correlation effects, such as the cusp condition, directly into the Hamiltonian. This approach accelerates convergence toward the CBS limit even when using small basis sets, significantly reducing the qubit overhead. However, the non-unitary nature of the transformation leads to a non-Hermitian Hamiltonian in the standard Hilbert space [3,4], whose structure and corresponding physical quantities depend sensitively on the chosen Jastrow factor.

We investigate such non-Hermitian transcorrelated Hamiltonians in both quantum-computing and tensor network contexts. We analyze how different single-parameter Jastrow factors [5] affect the structure of the final Hamiltonian and evaluate the quantum resources [6] required to solve them. Finally, we employ perturbation theory to derive an approximate solution for these non-Hermitian transcorrelated systems.

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