Symmetry-Aware Counterdiabatic Quantum Algorithm for Ground-State Energy Estimation in Quantum Chemistry

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Quantum algorithms for molecular ground-state energy estimation are limited on near-term hardware by two main factors: (i) the large qubit overhead introduced by fermion-to-qubit mappings, and (ii) deep state-preparation circuits that accumulate noise. While the variational quantum eigensolver (VQE) and chemically motivated ansatz families such as UCCSD variants are widely used, their practical performance often degrades in strongly correlated regimes and when larger active spaces are required.

We present a resource-efficient workflow that simultaneously reduces qubit counts and circuit depth by combining three ingredients. First, we exploit molecular point-group symmetry to project the electronic Hamiltonian onto a selected irreducible representation, enabling symmetry-adapted qubit encoding. Second, we apply complete active space (CAS) selection to retain only chemically relevant orbitals and electrons. Third, we introduce a digitized counterdiabatic (CD) ansatz that accelerates convergence by suppressing non-adiabatic excitations along an interpolating evolution.

Starting from a Hartree–Fock reference, we define a CAS active space and construct the second-quantized Hamiltonian, then use point-group symmetry to compress the Hilbert space and reduce qubit requirements. We implement an interpolating Hamiltonian path whose initial Hamiltonian is designed to be compatible with the Hartree–Fock state, and we augment the digitized evolution with a variationally optimized CD correction built from a compact operator pool connected to the adiabatic gauge potential. The resulting circuits are shallow and their depth can be tuned via the number of Trotter steps and CD layers.

We validate the approach on bond-dissociation curves for three representative systems: N2, a standard strong-correlation benchmark that develops pronounced multi-reference character at stretched geometries; C2H4, a prototypical organic molecule sensitive to correlation and geometry; and C6H6, a symmetry-rich conjugated system that provides a stringent test of qubit compression.

Across simulated geometries, the combined symmetry and CAS compression enables simulations using only 7 qubits for N2, 4 qubits for C2H4, and 4 qubits for C6H6, far below conventional mappings for comparable orbital choices. For most geometries, the ground-state energy error remains within chemical accuracy, approximately 1 kilocalorie per mole (about 1.6 millihartree), including challenging stretched-bond regimes. Compared with standard adiabatic state preparation and UCCSD-style circuits at similar depths, the digitized CD ansatz typically reaches target energies in fewer layers and shows improved robustness under device-oriented noise models. In IBM-style hardware simulations, error-mitigation protocols further stabilize the energy estimates in many cases.

By unifying symmetry compression, active-space optimization, and counterdiabatic acceleration, this framework provides a scalable path toward chemically relevant quantum simulations under near-term depth and noise constraints, and it is naturally compatible with both near-term error mitigation and future fault-tolerant improvements.

References

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[3] J. M. Martin-Guerrero et al., Physical Review Research 4, 013141 (2022).

Figure

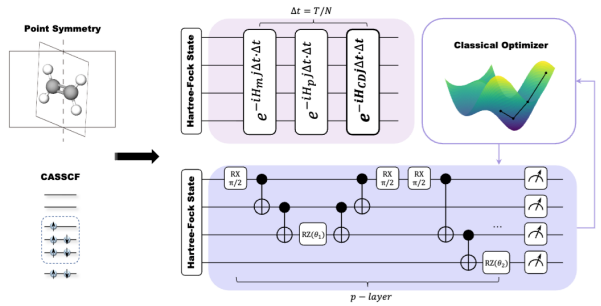

Figure 1: Schematic of synergistic approach combining symmetry encoding, active space selection, and CD ansatz.

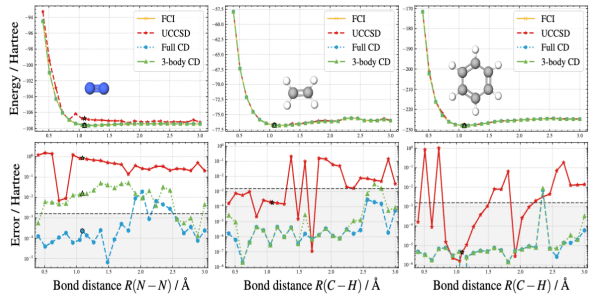

Figure 2: Potential energy curves calcaulted from our methods.