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Variational Quantum Subspace Construction via Symmetry-Preserving Cost Functions

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Determining low-lying eigenstates in correlated quantum systems is a central challenge in quantum chemistry and condensed matter physics. We propose the Variational Quantum Subspace Method (VQSM), a hybrid quantum-classical algorithm that iteratively constructs an orthonormal variational subspace from optimized trial states, in which the Hamiltonian is diagonalized classically. By employing symmetry-preserving cost functions, VQSM maintains shallow quantum circuits while ensuring rapid and robust convergence toward low-energy eigenvalues, closely resembling classical Lanczos-type methods. Benchmark calculations on hydrogen chain and ring models (H_4) demonstrate that VQSM achieves chemical accuracy with limited circuit depth and efficiently captures both ground-state energies and excited-state properties such as charge and spin gaps. These results establish VQSM as a promising and noise-resilient strategy for low-energy spectrum calculations on noisy intermediate-scale quantum (NISQ) devices.

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