Improving Ground State Accuracy of Variational Quantum Eigensolvers with Soft-coded Orthogonal Subspace Representations

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We propose a new approach to improve the accuracy of ground state approximations in Variational Quantum Eigensolver (VQE) algorithms by employing subspace representations with soft-coded orthogonality constraints[1]. As in other subspace-based VQE methods, such as the Subspace-Search VQE (SSVQE)[2] and Multistate Contracted VQE (MCVQE)[3], once the parameters are optimized to maximize the subspace overlap with the low-energy sector of the Hamiltonian, one diagonalizes the Hamiltonian restricted to the subspace. Unlike these methods, where hard-coded orthogonality constraints are enforced at the circuit level among the states spanning the subspace, we consider a subspace representation where orthogonality is soft-coded via penalty terms in the cost function. We show that this representation allows for shallower quantum circuits while maintaining high fidelity when compared to single-state (standard VQE) and multi-state (SSVQE or MCVQE) representations, on two benchmark cases: a 3x3 transverse-field Ising model and random realizations of the Edwards—Anderson spin-glass model on a 4x4 lattice.

Our results demonstrate that the proposed method outperforms both standard VQE and established subspace techniques[2,3]. Specifically, compared to standard VQE, we observe a reduction in ground state infidelity by an order of magnitude for the 2D TFI model (Figure 1) and by a factor of two for the Edwards—Anderson spin-glass model.

References

[1] G. Clemente and M. Intini, arXiv:2602.05980,(2026)

[2] K. M. Nakanishi, K. Mitarai, and K. Fujii, Phys. Rev. Res. 1, 033062 (2019).

[3] R. M. Parrish, E. G. Hohenstein, P. L. McMahon, andT. J. Martinez, Phys. Rev. Lett. 122, 230401 (2019).

[4] O. Higgott, D. Wang, and S. Brierley, Quantum 3, 156 (2019).

Figures

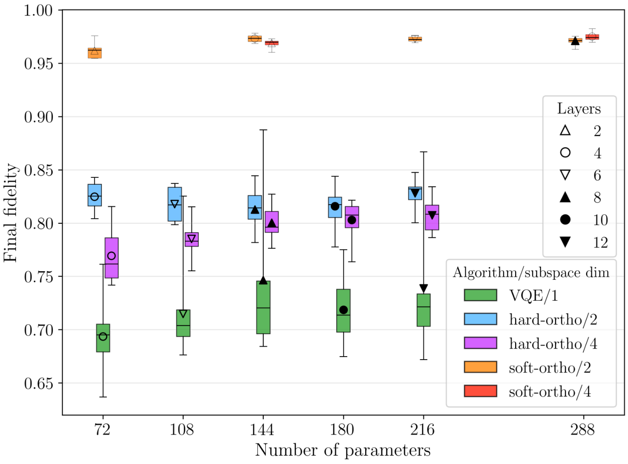

Figure 1: Box plot of the final ground state fidelities (after the optimization loops) versus the number of trainable parameters for standard VQE, hard-ortho and soft-ortho representations (subspace dimensions K=2 and K=4) on the 3x3 transverse-field Ising model varying circuit depths (Layers) of the ansatz. Each box summarizes the distribution of fidelities over 10 independent runs.