Physically motivated enhancements of variational quantum eigensolvers for quantum chemistry

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The Adaptive Derivative-Assembled Pseudo-Trotter Variational Quantum Eigensolver (ADAPT-VQE) [1] has emerged as a promising approach in quantum chemistry. Nevertheless, the application of ADAPT-VQE with noisy quantum devices requires to enhance its efficacy. Leveraging insights from electronic structure theory, we concentrate on optimizing state preparation without added computational burden and guiding ansatz expansion (Figure 1) to yield more concise wavefunctions with expedited convergence toward exact solutions. These advancements culminate in shallower circuits and reduced number of measurements. The performance of the new ADAPT-VQE variants will be assessed across mono, di, and tridimensional arrangements of H4 models, as well as in the ground state calculation of the water molecule. Ultimately, this work attests to the viability of physically-motivated strategies in fortifying ADAPT-VQE's efficiency, marking a significant stride in quantum chemistry simulations.

References

[1] Grimsley, H. R.; Economou, S. E.; Barnes, E.; Mayhall, N. J., Nat. Commun., 10 (2019) 3007.

Figures

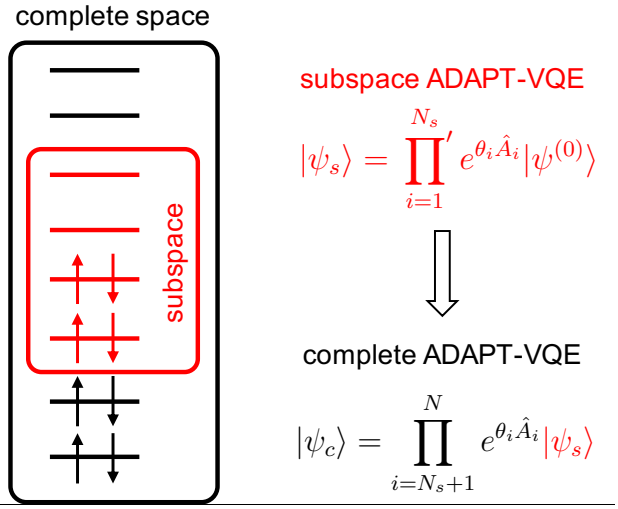

Figure 1: Representation of the orbital subspace strategy to guide ansatz growth in ADAPT-VQE.