Shortcuts for Adiabatic and Variational Algorithms in Molecular Simulation

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Quantum algorithms are prominent in the pursuit of achieving quantum advantage in various computational tasks. However, addressing challenges such as limited qubit coherence and high error rate in near-term devices requires extensive efforts. In this paper, we present a significant advancement in quantum chemistry [1] by integrating shortcuts to adiabaticity techniques into adiabatic and variational algorithms for calculating molecular ground state properties. Our approach includes a counterdiabatic [2] term that accelerates adiabatic evolution, reducing Trotter errors and enabling faster computations. Additionally, we introduce the counterdiabatic term as the adiabatic gauge ansatz for variational quantum eigensolver, the *Adiabatic Gauge Ansatz* (AGA) and the Reduced-AGA, which exhibits favourable convergence properties with a fewer number of parameters, thereby reducing the number of qubits and circuit depth. Our approach achieves comparable accuracy to the established ansatz, while advancing practical applications in material science, drug discovery, and molecular simulations.

References

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[2] D. Guéry-Odelin, A. Ruschhaupt, A. Kiely, E. Torrontegui, S. Martínez-Garaot, and J. G. Muga, Rev. Mod. Phys. 91, 045001 (2019).

Figures

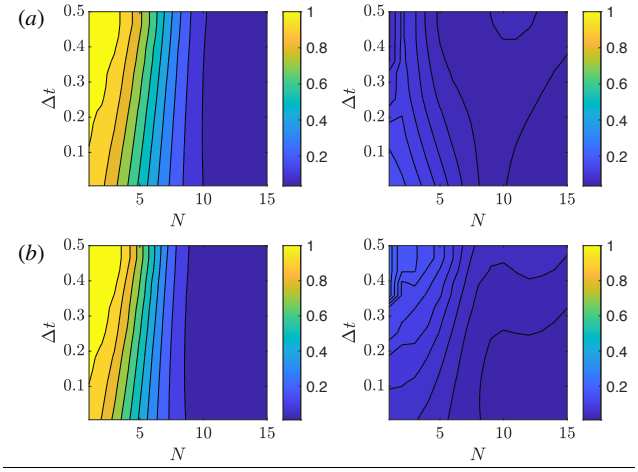

Figure 1: Adiabatic ground state energy deviation in *LiH*-(a) and *BeH_2*-(b) molecules with (right) and without (left) counterdiabatic assistance w.r.t the time steps Δt and the number of steps N.

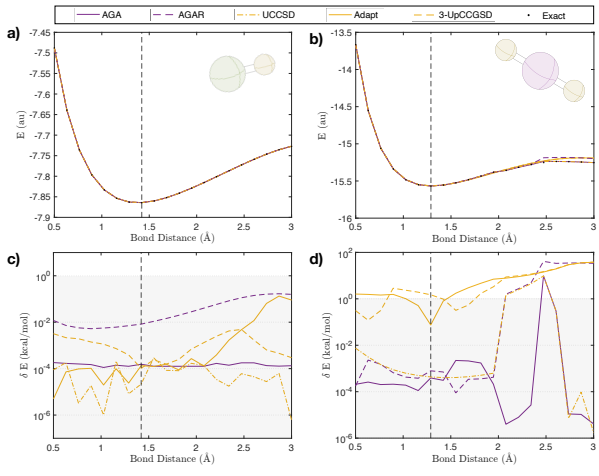

Figure 2: VQE ansatzes comparation for *LiH* (left) and *BeH_2* (right) energy ground state simulation. (c)-(d) figures represents the discrepancy among the simulated energy and the exact for the different ansatzes.