Symmetry breaking slows convergence of the ADAPT Variational Quantum Eigensolver

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Variational quantum eigensolvers (VQEs) are a class of hybrid classical-quantum computing methods which prepare and measure a parameterized state on quantum hardware and optimize the wavefunction parameters on classical hardware. While many VQEs begin with a predetermined wavefunction ansatz, ADAPT-VQE builds a problem-tailored ansatz by iteratively adding operators from a predefined pool in a way determined by the problem Hamiltonian. This leads to shorter circuits, making ADAPT-VQE advantageous in the current regime of noisy intermediate-scale quantum simulation. Because quantum simulation of molecular systems is expected to provide the strongest advantage over classical computing methods for systems exhibiting strong electron correlation, it is critical that the performance of VQEs be assessed for strongly correlated systems. For classical simulation, strong correlation often results in symmetry-breaking of the Hartree-Fock reference, leading to Löwdin's well known “symmetry dilemma” whereby accuracy in the energy can be increased by breaking spin or spatial symmetries. Here, we explore the impact of symmetry breaking on the performance of ADAPT-VQE using two strongly correlated systems: (i) the “fermionized” anisotropic Heisenberg model, where the anisotropy parameter controls the correlation in the system, and (ii) symmetrically stretched linear H_4, where correlation increases with increasing H-H separation. In both of these cases, increasing the level of correlation of the system leads to spontaneous symmetry breaking (parity and S^2 respectively) of the mean-field solutions. We analyze the role that symmetry breaking in the reference states and orbital mappings of the fermionic Hamiltonians has on the compactness and performance of ADAPT-VQE. We observe that improving the energy of the reference states by breaking symmetry has a deleterious effect on ADAPT-VQE by increasing the length of the ansatz necessary for energy convergence and exacerbating the problem of “gradient troughs”.