Symmetry Dilemmas in Quantum Computing: A Comprehensive Analysis

Muhan Zhang, **Ilias Magoulas, Francesco A. Evangelista**

Department of Chemistry and Cherry Emerson Center for Scientific Computation, Emory University, Atlanta, Georgia 30322, USA

Exploiting symmetries (spatial, spin, etc.) can significantly decrease the dimension of the many-electron Hilbert space, resulting in reduced computational resources. In the realm of quantum computing, implementing circuits for spin-adapted many-body operators remains an open problem. For example, simple Trotterization of spin-preserving operators leads to spin symmetry breaking. To circumvent this challenge, state-of-the-art quantum algorithms typically enforce total spin symmetry either by employing a compact operator pool consisting of spin-adapted generalized single and perfect-pairing double (saGSpD) excitations or by relying on the complete generalized singles and doubles (GSD) pool and incorporating a spin-penalty term in the Hamiltonian. However, as this presentation will demonstrate, these solutions, while useful, are not without limitations. As shown in our numerical analysis, tightly converged wavefunctions built upon saGSpD pool with spatial symmetry enforced remain orthogonal to configuration state functions that have a substantial weight in the exact eigenvectors. These observations reveal the compromise of universality of the saGSpD pool once spatial symmetry is imposed. Additionally, our numerical simulations demonstrate that, despite the drastic suppression of spin-symmetry contaminants, spin-penalty terms result in slower convergence to the exact solution and a considerable increase in the number of Pauli measurements. In an effort to combine the advantages of both approaches, we consider the following split operator pool approach: Initially, a symmetry-adapted wavefunction is constructed iteratively using operators from the saGSpD pool, with point group symmetry enforced. Subsequently, a spin-penalty term is introduced to the Hamiltonian, and the wavefunction is further developed using operators from the GSD pool, maintaining point group symmetry.