Speeding Up Spin-Flip: Tensor Contractions and Parameter Extractions

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We have recently introduced the RAS-nSF-IP/EA scheme, which allows unambiguous and relatively inexpensive extraction of coupling parameters for strongly correlated systems with spin and spatial degeneracies. Using a diagrammatic approach, we have derived equations for an excitation-rank version of this scheme, and we have built an implementation in Q-Chem and in an open-source Python package that interfaces with Psi4. By using the derived equations, we hope to speed up the expensive sigma vector construction step in the Davidson algorithm, allowing applications of our method to larger transition metal systems. We have also implemented a Bloch effective Hamiltonian, allowing us to extract useful coupling information for multi-site systems. We will discuss several applications of our new code to strongly-correlated systems, specifically focusing on comparison of the tensor-contraction approach to traditional string-based approaches and extraction of model Hamiltonian parameters.