Downfolding of many-body Hamiltonians using active-space models

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Despite the grand effort in quantum chemistry and materials science communities to develop methods for describing complicated electron correlation effects, the applicability of these methods is still defined by a trade-off between accuracy and computational costs. Mathematically rigorous models where correlation effects are downfolded into a low-dimensional space offer a unique change to eliminate the inherent bias/biases of current many-body methods. In this presentation, I will discuss the extension of recently introduced the sub-system embedding sub-algebras coupled cluster (SES-CC) formulation[1] to unitary CC formalisms,[2,3] which allows one to include the dynamical (outside the active space) correlation effects in an SES induced complete active space (CAS) effective Hamiltonian. In contrast to the standard single-reference SES-CC theory, the unitary CC approach results in a Hermitian form of the effective Hamiltonian. I will discuss a particular form of the unitary ansatz needed in order to accomplish this called the double unitary CC formalism (DUCC) where the corresponding CAS eigenvalue problem provides a rigorous separation of external cluster amplitudes that describe dynamical correlation effects – used to define the effective Hamiltonian – from those corresponding to the internal (inside the active space) excitations that define the components of eigenvectors associated with the energy of the entire system. The proposed formalism can be viewed as an efficient way of downfolding many-electron Hamiltonian to the low-energy model represented by a particular choice of CAS. In principle, this technique can be extended to any type of complete active space representing an arbitrary energy window of a quantum system. The Hermitian character of low-dimensional effective Hamiltonians makes them an ideal target for several types of full configuration interaction (FCI) type eigensolvers, such as those used in quantum algorithms and DMRG methods. I will demonstrate the power and effectiveness of this downfolding technique through examples of energies obtained with quantum algorithms for several atomic and molecular systems. In addition, I will illustrate the utility of these Hamiltonians with correlated approaches such as Green's function CC methods.[4]

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[1] K. Kowalski, *J. Chem. Phys.* **148**, 094104 (2018).

[2] N. P. Bauman, E. J. Bylaska, S. Krishnamoorthy, G. H. Low, N. Weibe, C. E. Grenade, M. Roetteler, M. Troyer, and K. Kowalski, *J. Chem. Phys.* **151**, 014107 (2019).

[3] N. P. Bauman, G. H. Low, and K. Kowalski, *J. Chem. Phys.* [recently accepted], preprint *arXiv:1909.06404* (2019).

[4] N. P. Bauman, B. Peng, K. Kowalski, *Mol. Phys.* [submitted], preprint *arXiv:1910:00394* (2019).