Downfolding of Many-Body Hamiltonians: Recent Advancements and Applications

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The double unitary coupled cluster (DUCC) ansatz [J. Chem. Phys. 151; 014107 (2019)], an extension of the sub-system embedding sub-algebras coupled cluster (SES-CC) formalism [J. Chem. Phys. 148; 094104 (2018)], allows one to include dynamical (outside the active space) correlation effects in a complete active space 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, which has been promising for quantum computing applications, among others. I will review the DUCC theory in this presentation and discuss its time-dependent extension [J. Chem. Phys. 152; 244127 (2020)] and the recent high-performance implementation. I will discuss the effect of the commutator expansion in approximations [J. Chem. Phys. 156; 094106 (2022)) and demonstrate the applicability of the DUCC approach through several ground- and excited-state applications.