

Sub-system self-consistency in coupled-cluster theory

Karol Kowalski¹, Nicholas P. Bauman¹

¹ Physical Sciences Division, Pacific Northwest National Laboratory, Richland, WA 99352, USA

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The double unitary coupled cluster (DUCC) ansatz [1], an extension of the sub-system embedding sub-algebras coupled cluster (SES-CC) formalism [2], 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. We will review the DUCC theory in this presentation and discuss its time-dependent extension [3] and the recent high-performance implementation. We will discuss the effect of the commutator expansion in approximations [4] and demonstrate the applicability of the DUCC approach through several ground- and excited-state applications.

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- [2] K. Kowalski, *J. Chem. Phys.*, **148** (2018), 094104.
- [3] K. Kowalski, N. P. Bauman, *J. Chem. Phys.*, **152** (2020), 244127.
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