Sub-system self-consistency in coupled cluster theory

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In this talk, we discuss details of the sub-system embedding sub-algebra coupled cluster (CC) formalism. In particular, we provide numerical evidence indicating that the single-reference coupled-cluster energies can be calculated alternatively to its copybook definition. We demonstrate that the CC energy can be reconstructed by diagonalizing the effective Hamiltonians describing correlated sub-systems of the many- body system in special classes of active spaces. In the extreme case, we provide numerical evidence that the CC energy can be reproduced through the diagonalization of the effective Hamiltonian describing sub-system composed of a single electron. These properties of CC formalism can be exploited to design protocols to define effective interactions in sub-systems used as probes to calculate the energy of the entire system and introduce a new type of self-consistency for approximate CC approaches. We also discuss how these formulations can capture the sparsity of the interacting quantum systems.