Multireference Fock space coupled cluster method in application to the double electron attached states

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The intermediate Hamiltonian (IH) multireference coupled cluster (CC) method with singles (S) and doubles (D) within the double electron attached (2,0) sector of the Fock space (FS) is formulated and implemented. The intermediate Hamiltonian realization of the (2,0) FS problem allows to replace the iterative scheme of the FS-CC equations based on the effective Hamiltonian with the diagonalization of the properly constructed matrix. The proposed method, IH-FS-CCSD (2,0), is rigorously size-extensive, easy to code, and numerically very efficient with the results comparable or slightly better than equation-of-motion ones at the CCSDT (T - triples) level. The performance of the method is discussed on the basis of the test calculations for potential energy curves of the systems for which double positive ions dissociate into closed-shell fragments (e.g., Na_2 dimer). Double electron attachment (DEA) scheme can be also useful in determination of the excitation spectra for difficult cases. The example is a carbon atom which has two electrons out of the closed shell structure.