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Calculation of atomic properties using the non-linear coupled-cluster method RUPSI CHANDRA, MARIANNA SAFRONOVA, University of Delaware, W.R. JOHNSON, University of Notre Dame — One high-precision method to calculate atomic properties of one- electron systems and to study parity nonconservation (PNC) in heavy atoms is the relativistic linearized coupled-cluster method that sums infinite sets of many-body perturbation theory terms. In the present formulation of this method, single and double (SD) excitations are included completely and certain classes of triple excitations are partially added. The properties of alkali-metal atoms calculated using this method have generally been found to agree very well with experiments. However, further progress in the study of fundamental symmetries in heavy atoms calls for the improvement of the current methodology. This work is aimed at the complete restoration of the non-linear coupled-cluster terms at the SD level. Among the numerous types of non-linear coupled- cluster terms, only six will contribute to the single or double all-order equations. We have derived expressions for all six of those terms, conducted the angular reduction, and modified the single and double all-order equations accordingly. Special care has been taken to ensure proper symmetry of the double excitation coefficients. Numerical evaluation of these terms is in progress.

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