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Complete treatment of the non-linear terms in the single-double all-order method RUPSI CHANDRA, M.S. SAFRONOVA, University of Delaware, W.R. JOHNSON, University of Notre Dame — The implementation of the single-double (SD) relativistic all-order method yielded accurate results for a number of atomic properties in alkali-metal atoms and other systems with one valence electron. This method is a linearized coupled-cluster method, where single and double excitations of Dirac-Fock wavefunctions are included to all orders of perturbation theory. Partial triples excitations are also included in the SDpT extension of the SD method. However, further progress in the study of fundamental symmetries in heavy atoms calls for the improvement of the current methodology. This work represents a complete restoration of all six non-linear coupled-cluster terms that contribute at the SD level. The contributions of the non-linear terms to various atomic properties is investigated.

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