

Abstract Submitted
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Relativistic coupled-cluster single-double method applied to alkali-metal atoms RUPSI PAL, M.S. SAFRONOVA, University of Delaware, W.R. JOHNSON, University of Notre Dame, ANDREI DEREVIANKO, University of Nevada, Reno, SERGEY G. PORSEV, University of Nevada, Reno and Petersburg Nuclear Physics Institute, Russia — A relativistic version of the coupled-cluster single-double (CCSD) method is developed for atoms with a single valence electron. In earlier work, a linearized version of the CCSD method (with extensions to include a dominant class of triple excitations) led to accurate predictions for energies, transition amplitudes, hyperfine constants, and other properties of monovalent atoms. Further progress in high-precision atomic structure calculations for heavy atoms calls for improvement of the linearized coupled-cluster methodology. In the present work, equations for the single and double excitation coefficients of the Dirac-Fock wave function, including all non-linear coupled-cluster terms that contribute at the single-double level are worked out. Contributions of the non-linear terms to energies, electric-dipole matrix elements, and hyperfine constants of low-lying states in alkali-metal atoms from Li to Cs were systematically investigated. The effect of the core non-linear terms was found to be not negligible for heavier alkalis, reaching nearly 1% of the total values of the Cs hyperfine constants. The final results are compared with other calculations and with precise experiments.

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