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Application of the dual-kinetic-balance sets in the relativistic many-body problem of atomic structure[1] KYLE BELOY, ANDREI DEREVIANKO, University of Nevada, Reno — The dual-kinetic-balance (DKB) finite basis set method for solving the Dirac equation for hydrogen-like ions [V. M. Shabaev *et al.*, Phys. Rev. Lett. 93, 130405 (2004)] is extended to problems with a non-local spherically-symmetric Dirac-Hartree-Fock potential. We implement the DKB method using B-spline basis sets and compare its performance with the widely-employed approach of Notre Dame (ND) group [W.R. Johnson, S.A. Blundell, J. Sapirstein, Phys. Rev. A 37, 307-15 (1988)]. We compare the performance of the ND and DKB methods by computing various properties of Cs atom: energies, hyperfine integrals, the parity-non-conserving amplitude of the $6s_{1/2} - 7s_{1/2}$ transition, and the second-order many-body correction to the removal energy of the valence electrons. We find that for a comparable size of the basis set the accuracy of both methods is similar for matrix elements accumulated far from the nuclear region. However, for atomic properties determined by small distances, the DKB method outperforms the ND approach.

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