HIGH-PRECISION CALCULATIONS OF ATOMIC PROPERTIES AND PARITY NONCONSERVATION IN SYSTEMS WITH ONE VALENCE ELECTRON

Abstract

by

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High-precision calculations of atomic properties of systems with one valence electron outside of a closed core are carried out using a relativistic all-order method. The method used here is a linearized version of coupled-cluster method which sums infinite sets of many-body perturbation theory terms.

Energy levels are calculated for the ground state and five excited states of sodium and sodium-like ions with nuclear charges $Z$ in the range 12 – 16 and are found to be in precise agreement with experimental values (to 0.002% – 0.01%). The resulting fine structures are also in excellent agreement with experiment.

A systematic study of atomic properties of alkali-metal atoms from sodium to francium, which includes the calculations of energy levels, fine structures, electric-dipole matrix elements, hyperfine constants, static polarizabilities of the ground states and first excites $s$ states, scalar transition polarizabilities, and vector transition polarizabilities, is conducted. This study provides benchmark values for a large number of yet unmeasured properties. We find that the single-double (SD) all-order method, with an added dominant class of the triple excitations, gives accurate results for energy levels and fine structures. Our results for electric-dipole matrix elements agree with precise experiments to 0.1% – 0.3% for all primary transitions
for alkali-metal atoms from Na to Fr with the exception of the $7p_{3/2} - 7s$ transition in francium, where the difference is 0.8%. To obtain accurate values for the $ns$ and $np_{1/2}$ magnetic-dipole hyperfine constants, we partially include triple excitations in the SD wave functions. The resulting values for $ns$ and $np_{1/2}$ hyperfine constants of Na, K, Rb, and Cs agree with experiment to 0.1% – 1%. Our values for static polarizabilities are in excellent agreement with alternative theoretical calculations and experiment. We recommend values of scalar and vector transition polarizabilities for the $6s - 7s$ transition in Cs and the $7s - 8s$ transition in Fr.

We carry out calculations of the PNC amplitude in Cs and Fr at the 1% level of accuracy. The dependence of PNC amplitudes on the parameters of the nuclear distribution is investigated. We also carry out calculations of the spin-dependent part of the PNC amplitudes for four Fr isotopes with $A = 207, 209, 211, 213$ and for $^{133}$Cs. Our results for the francium PNC amplitude can be used in conjunction with future measurements for atomic-physics tests of the Standard Model.