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Triple excitations in the relativistic coupled-cluster formalism and calculation of Na properties[1] SERGEY PORSEV, UNR & PNPI, ANDREI DEREVIANKO, UNR — The coupled-cluster (CC) formalism is a highly-accurate method of atomic, molecular and nuclear structure. We have implemented a CC-inspired relativistic method for univalent atoms that includes a nonperturbative treatment of single and double excitations from the core and single, double, and triple excitations involving valence electron. Triple excitations of core electrons are included in the fourth order of many-body perturbation theory. In addition, we incorporate all-order dressing of lines and vertices of the matrix-element diagrams. The resulting formalism for matrix elements is complete through the fourth order and subsumes certain chains of diagrams in all orders. With the developed method we computed removal energies, magnetic-dipole hyperfine-structure constants, and electric- dipole amplitudes for atomic Na. We find that the removal energies are reproduced within 0.01-0.03% and the hyperfine constants of the $3s_{1/2}$ and $3p_{1/2}$ states with a better than 0.1% accuracy. The computed dipole amplitudes for the principal $3s_{1/2} - 3p_{1/2;3/2}$ transitions are in an agreement with 0.05%-accurate experimental data. Details can be found in the paper: S.G.Porsev and A.Derevianko, Phys. Rev. A 73, 012501 (2006)

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