

Accurate QED perturbation theory calculation of the heavy and super heavy elements atoms, ions, atomic parity nonconservation

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A consistent theoretical approach, based on the quantum electrodynamics (QED) perturbation theory is developed for investigation of the spectroscopic characteristics for heavy and super heavy atomic systems, multi charged and negative ions. Zeroth approximation is generated by the effective ab initio model functional, constructed on the basis of the gauge invariance principle. The wave functions zeroth basis is found from the Dirac equation with potential which includes the core ab initio potential, the electric and polarization potentials of a spherically symmetric nucleus (the gaussian form of charge distribution in the nucleus and the uniformly charged sphere are considered). The correlation corrections of the high orders are taken into account within the Green functions method (with the use of the Feynman diagram's technique. There have taken into account all correlation corrections of the second order and dominated classes of the higher orders diagrams (electrons screening, particle-hole interaction, mass operator iterations). The magnetic inter-electron interaction is accounted in the lowest (on α^2 parameter), the Lamb shift polarization part - in the Ulling-Serber approximation, self-energy part of the Lamb shift is accounted effectively with the use of the "exact" calculation for H-like ions with point nucleus. The nuclear size effect is accounted in the electric and polarization potentials. Method is applied in calculations of the: 1) $1s(2)2l_j, 3l_j, 4l_j$ energy levels for Li-like ions in interval (nuclear charge) $Z=20-100$; 2) energy levels, hyperfine structure intervals, E1-, M1-transitions amplitudes in heavy atoms of Cs, Sn, Pb; parity nonconserving 6s-7p dipole amplitude in Cs; calculation lead to the value: $\langle 6s | D_z | 7s \rangle = -0.908 \times i 10^{-11} |e| a_0 (-Qw/N)$; 3) energy spectra of the super heavy elements atoms with $Z=110, 112, 114$; 4) bond energies in heavy elements (Sn, Pb). Method developed is testing in comparison with methods [1-4].

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