Relativistic calculations of the isotope shifts in highly charged Li-like ions

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In the past years a great progress was achieved in experimental study of the isotope shifts in highly charged ions. This was done in the dielectronic recombination (DR) experiments at ESR (GSI) [1] as well as applying a high-resolution grating spectrometer at EBIT [2]. The joint analysis of the results obtained in the high-precision theoretical and experimental investigations of isotope shifts in highly charged ions provides determination of nuclear charge radii differences and enables tests of quantum electrodynamics (QED) at strong fields. With the FAIR facilities the isotope shift measurements in heavy ions will be further improved in accuracy and extended to radioactive isotopes with a lifetime longer than about 10 s.

From the theoretical side, to obtain the total value of the isotope shift one needs to evaluate the nuclear size (field shift) and nuclear recoil (mass shift) contributions, including the relativistic and QED effects. Since there exists some discrepancy in the results obtained in Refs. [3] and [4] for heavy ions, we develop an alternative method which merges the perturbative and CI-DFS (configuration-interaction Dirac-Fock-Sturm) calculations [5]. Namely, we calculate the nuclear recoil contributions within the Breit approximation to zeroth and first orders in $1/Z$ and add the related contributions of second and higher orders in $1/Z$, obtained using the CI-DFS method. To derive the nuclear recoil contributions to the binding energies of Li-like ions by perturbation theory, we use the two-time Green’s function method [6] with the $(1s)^2$ shell regarded as belonging to a redefined vacuum. The obtained non-QED results are combined with the corresponding QED contributions of the zeroth order in $1/Z$ to get the most accurate theoretical data for the mass shifts in highly charged Li-like ions. In addition, the field shifts are calculated in the framework of the Dirac-Coulomb-Breit Hamiltonian. These calculations, being performed by the CI-DFS method, are compared with the corresponding MCDF (multiconfiguration Dirac-Fock) calculations of Ref. [3]. The QED corrections to the field shifts are also evaluated. In addition, we consider the nuclear deformation and nuclear polarization corrections. As the result, the most precise theoretical values of the isotope shifts for the $2p_{1/2} - 2s$ and $2p_{3/2} - 2s$ transitions in Li-like ions are presented in our paper [5]. The theoretical contributions to the isotope shifts in Li-like thorium and uranium are given in Table 1.

Table 1: Individual contributions to the isotope shifts for the $2p_{1/2} - 2s$ and $2p_{3/2} - 2s$ transitions in Li-like $^{232,230}\mathrm{Th}^{88+}$ and $^{238,234}\mathrm{U}^{89+}$(in meV) with given values of $\delta\langle r^2\rangle$.

	$^{232,230}\mathrm{Th}^{87+}$	
	$^{232,230}\delta\langle r^2\rangle$=0.2050 fm^2	
	$2\mathrm{p}_{1/2} - 2\mathrm{s}$	$2\mathrm{p}_{3/2} - 2\mathrm{s}$
Main contributions		
Field shift	-116.1	-128.7
Mass shift	0.1	0.3
FS plus MS	-116.0	-128.4
QED		
Field shift	0.6	0.9
Mass shift	0.4	0.4
Others		
Nuclear polarization	1.6	1.7
Nuclear deformation	1.5	1.5
Total IS theory	-111.9(22)	-123.9(22)
	$^{238,234}\mathrm{U}^{89+}$	
	$^{238,234}\delta\langle r^2\rangle$=0.334 fm^2	
	$2\mathrm{p}_{1/2} - 2\mathrm{s}$	$2\mathrm{p}_{3/2} - 2\mathrm{s}$
Main contributions		
Field shift	-227.8	-254.5
Mass shift	0.2	0.6
FS plus MS	-227.6	-253.9
QED		
Field shift	1.2	1.8
Mass shift	0.9	0.8
Others		
Nuclear polarization	2.3	2.6
Nuclear deformation	-2.4	-2.7
Total IS theory	-225.6(32)	-251.4(33)

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