NUCLEAR SIZE EFFECT AND QED CORRECTIONS TO ENERGY LEVELS OF HEAVY AND SUPERHEAVY Li-, Cu-LIKE IONS

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A consistent quantum electrodynamics (QED) perturbation theory (PT) approach is used for studying the spectra of heavy and superheavy multicharged ions. The Lamb shift polarization part is accounted for in the Uehling-Serber approximation. The 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. Calculations of spectra for Li-, Cu-like multicharged ions are carried out.

The present paper is devoted to studying spectra of heavy and superheavy Li-like and Cu-like multicharged ions within a consistent QED approach with an accurate account of the nuclear size effects and QED corrections. A full review of heavy and superheavy multicharged ions spectra calculations is given in Refs. [1–7]. Let us describe some specific features of our approach. The zeroth order QED PT one-particle wave functions are found from the solution of the relativistic Dirac equation which can be written in the central field in a two-component form:

$$\frac{\partial F}{\partial r}+(1+\chi)\frac{F}{r}-(\varepsilon+m-v)G=0$$

$$\frac{\partial G}{\partial r}+(1-\chi)\frac{G}{r}+(\varepsilon-m-v)F=0 \qquad (1)$$

Here the fine structure constant $\alpha=1$. To take into account the nuclear size effect, we fulfil the simulation of real distribution of the charge in the nucleus. We set the charge distribution in the nucleus $\rho(r)$ by the Gaussian function. With regard to normalization we have:

$$\rho(r|R)=\left(4\gamma^{3/2}/\sqrt{\pi}\right)\exp\left(-\gamma r^2\right) \quad (2)$$

$$\int_0^\infty dr r^2\rho(r|R)=1; \quad \int_0^\infty dr r^3\rho(r|R)=R \quad (3)$$

Here $\gamma=4/\pi R^2$, R is the effective nucleus radius. The Coulomb potential for the spherically symmetric density $\rho(r|R)$ is:

$$V_{nucl}(r|R)=-\left((1/r)\int_0^r dr' r'^2\rho\left(r'|R\right)+\int_r^\infty dr' r'\rho\left(r'|R\right)\right) \qquad (4)$$

It is determined by the following system of differential equations:

$$V'nucl(r,R)=\left(1/r^2\right)\int_0^r dr' r'^2\rho\left(r',R\right)\equiv\left(1/r^2\right)y(r,R)$$

$$y'(r,R)=r^2\rho(r,R)$$

$$\rho'(r,R)=-8\gamma^{5/2}r/\sqrt{\pi}\exp\left(-\gamma r^2\right)=-2\gamma r\rho(r,R)=-\frac{8r}{\pi r^2}\rho(r,R)$$

with the boundary conditions:

$$V_{nucl}(0,R) = -4/(\pi r); \quad \rho(0,R) = 4\gamma^{3/2}/\sqrt{\pi} = 32/R^3$$

The system of equations (5) includes the equations for the function of density distribution.

To take into account the polarization correction we use the Uehling potential. It is determined as a quadrature

$$U(r) = -\frac{2\alpha}{3\pi r}\int_1^\infty dt \exp(-2rt/\alpha Z)\left(1+1/2t^2\right)\frac{\sqrt{t^2-1}}{t^2} \equiv -\frac{2\alpha}{3\pi r}C(g), \qquad (5)$$

where $g = \frac{r}{\alpha Z}$. According to Refs. [3, 8], we determine the asymptotics of the function $C(g)$ in two limiting cases:

$$C(g) \underset{g\to 0}{\to} \tilde{C}_1(g) = \ln(g/2) + 1.410548 - 1.037845g$$

$$C(g) \underset{g\to \infty}{\to} \tilde{C}_2(g) = -1.8800\exp(-g)/g^{3/2}$$

The matching of the two limiting expressions for $C(g)$ was made as follows [2, 8]:

$$\tilde{C}(g) = \tilde{C}_1(g)\tilde{C}_2(g)/\left(\tilde{C}_1(g) + \tilde{C}_2(g)\right)$$

For the ground state of a hydrogen-like ion the error caused by the approximation (8) did not exceed 2–5% of the total polarization shift over the whole range of variation $Z = 10 \div 170$. The corrected matching is:

$$\tilde{\tilde{C}}(g) = \tilde{C}_1(g)\tilde{\tilde{C}}_2(g)/\left(\tilde{C}_1(g) + \tilde{\tilde{C}}_2(g)\right)$$

$$\tilde{\tilde{C}}_2(g) = \tilde{C}_2(g)f(g)$$

$$f(g) = \left((1.1022/g - 1.3362)/g + 0.8028\right).$$

The use of the new approximation of the Uehling potential permits one to decrease the calculation errors for this term down to 0.7%. For specific calculations with a finite nucleus it is necessary to turn from the point Uehling potential to the bulk one. The mathematical procedure of the polarization potential distribution over the nucleus ball is expressed as follows:

$$U(r|R) = \int U(|\vec{r}' - \vec{r}|)\rho(\vec{r}')d\vec{r}' \ .$$

In our calculation scheme we must only write out the differential equation for the function $U(r|R)$, according to Ivanov-Ivanova idea [2]:

$$U(r|R) = U(r)\int_0^r d\vec{r}'\rho(\vec{r}') + \int_r^\infty d\vec{r}'U(\vec{r}')\rho(\vec{r}').$$

To calculate the self-energy part of the Lamb shift we suppose that in an atomic system the radiative shift and the relativistic part of the energy are, in. principle, determined by one and the same physical field. It may be supposed that there exists some universal function that connects the self-energy correction and the relativistic energy. The self-energy correction for the hydrogen-like ions states was presented by Mohr (cf. [2]). It has the following form:

$$E_{SE}(H|Z,nlj) = 0.027148\frac{Z^4}{n^3}F(H|Z,nlj) \quad (6)$$

the values of F are given at $Z = 10-110$, $nlj = 1s, 2s, 2p_{1/2}, 2p_{3/2}$. These results are modified here for the states $1s^2 nlj$ of Li-like ions. According to Ref. [2], for any ion with nlj electron over the core of closed shells the sought value may be presented in the form:

$$E_{SE}(Z,nlj) = 0.027148\frac{\xi^4}{n^3} f(\xi,nlj)\,(\mathrm{cm}^{-1}) \quad (7)$$

The parameter $\xi = (E_R)^{1/4}$, E_R is the relativistic part of the bounding energy of the outer electron; the universal function $f(\xi,nlj)$ is not dependent upon composition of the closed shells and the actual potential of the nucleus. The procedure of generalization of the Mohr's results [2] for the case of Li-like ions with the finite nucleus consists of the following steps [2]:

1) calculation of the values E_R and ξ for the states *nlj* of H-like ions with the point nucleus (in accordance with the Sommerfeld formula); 2) construction of an approximating function $f(\xi,nlj)$ and the appropriate $F(H|Z,nlj)$ [7]; 3) calculation of E_R and ξ for the states *nlj* of Li-like ions with the finite nucleus; 4) calculation of E_{SE} for the sought states by formula (47). The approximating function is determined as:

$$f(\xi,nlj) = X_0 + X_1/\xi + X_2/\xi^2 + X_3/\xi^3$$

The parameters X_0, X_1, X_2, X_3, are determined by specially chosen four reference points and more justified in comparison with the method of expansion over the parameter αZ. Construction of the QED perturbation theory is standard. The key moment of our approach is checking of the fulfilling the gauge invariance for the zeroth order QED PT basis. We use here a consistent QED procedure, developed in Ref. [3, 5].

We have applied our method in the calculation of the 1s(2)2lj,3lj,4lj energy levels for Li-like ions with nuclear charge Z=26-92. In Table 1 the results of our work for two lower transitions are compared with the available experimental data as well with the results of other calculations. In the region of $Z<36$ all results differ from each other by the means of account of the inter-electron interaction. In table 2 we present measured and calculated wavelengths (in Å) for transitions in Cu-like ions of Pb and Bi.

Table 1. Calculation results for the energies of 2s1/2-2p1/2 transitions (in cm^{-1}) in Li-like ions A- multi-configuration Hartree-Fock-Dirac method; B- the relativistic perturbation theory over the total inter-electron interaction; C – the expansion over the parameter $1/Z$; D – the semiempirical calculation; E – calculation within the relativistic perturbation theory with model zeroth approximation; F – our data.

Z	A	B	C	D	E	F	Exp. data
26	393349	391582	391699	392034	392960	392490	392003
28	428432	426635	426680	427179	427890	427453	426985
30	464248		462277	462994	463450	463085	
36	576276		573251	575137	574550	574290	574380
41	675717				672100	671890	
59	1099427				1094670	1094230	
69	1396756				1389200	138820	
79	1751903				1740100	1739875	
92	2279524				2263600	2263490	

Table 2. Measured and calculated wavelengths for transitions in Cu-like ions of Pb and Bi: A – experiment [1]; B,C, D- theory (calculations on the basis of Dirac-Fock multi-configuration method [1], QED PT [5], relativistic PT [4])

Transition	$Pb^{52+} - Pb^{53+}$ A	B	C	D	$Bi^{53+} - Bi^{54+}$ A	B	C	D
$4s^2S_{1/2} - 4p^2P_{1/2}$	104,94	103,9	104,6	104,7	102,55	101,52	102,2	102,3
$4s^2S_{1/2} - 4p^2P_{3/2}$	42,349	42,22	42,32	42,33	40,394	40,24	40,30	40,33
$4p^2P_{1/2} - 4d^2D_{3/2}$	35,181	35,20	35,19	35,19	33,775	33,76	33,77	33,77
$4p^2P_{3/2} - 4d^2D_{5/2}$	57,751	57,77	57,76	57,76	56,272	56,25	56,26	56,26
$4d^2D_{3/2} - 4f^2F_{5/2}$	-----	55,07	55,05	55,04	-----	53,70	53,67	53,66
$4d^2D_{5/2} - 4f^2F_{7/2}$	-----	62,46	62,39	62,36	-----	61,18	61,13	61,10
$4s^2S_{1/2} - 5p^2P_{3/2}$	-----	-----	9,12	9,10	-----	-----	8,72	8,69
$4s^2S_{1/2} - 5p^2P_{1/2}$	-----	-----	8,82	8,79	-----	-----	8,49	8,46

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ЕФЕКТ ЯДЕРНОГО РОЗМІРУ ТА QED ПОПРАВКИ ДО РІВНІВ ЕНЕРГІЇ ВАЖКИХ ТА НАДВАЖКИХ Li-, Cu-ПОДІБНИХ ІОНІВ

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Послідовний підхід, який базується на QED теорії збурень, використується для вивчення спектрів важких та надважких багатозарядних іонів. Власноенергетичну частину лембівського зсуву враховано ефективно за допомогою точного розрахунку H-подібних іонів з точковим ядром. Поляризаційну частину враховано у наближенні Уелінга-Сербера. Ефект скінченного розміру ядра враховано в електричному та поляризаційному потенціалах. На підставі методу виконано розрахунок спектрів важких Li- та Cu-подібних багатозарядних іонів.