Transition energy and lifetime for the ground-state hyperfine splitting of high-Z lithiumlike ions

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The ground-state hyperfine splitting values and the transition probabilities between the hyperfine structure components of high-Z lithiumlike ions are calculated in the range $Z=49$–83. The relativistic, nuclear, QED, and interelectronic interaction corrections are taken into account. It is found that the Bohr-Weisskopf effect can be eliminated in a combination of the hyperfine splitting values of the hydrogenlike and lithiumlike ions of an isotope. This gives a possibility for testing the QED effects in a combination of the strong electric and magnetic fields of the heavy nucleus. Using the experimental result for the $1s$ hyperfine splitting in $^{209}Bi^{82+}$, the $2s$ hyperfine splitting in $^{209}Bi^{80+}$ is calculated to be $\Delta E=0.7976(2)$ eV. [S1050-2947(97)05412-7]

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I. INTRODUCTION

Recently, laser spectroscopic measurements of the ground state hyperfine splitting in high-Z hydrogenlike ions became possible at the electron storage ring [1] and at the electron beam ion trap [2]. The present status of theory of the hyperfine splitting in high-Z hydrogenlike ions was discussed in Ref [3]. One of the possible directions of further experiments is an extension of the investigations to high-Z lithiumlike ions. Recently, the hyperfine structure values of lithiumlike ions were calculated in the range $Z=7$–30 [4] in connection with astrophysical search, and for $^{209}Bi^{80+}$ (without the QED correction) [5] in connection with experiments in Darmstadt [1]. In Sec. II of the present paper, we refine the calculation of Ref. [5] for $^{209}Bi^{80+}$, considering a more accurate treatment of the nuclear effects and taking into account the QED corrections, and extend it to lithiumlike ions in the range $Z=49$–83, which are likely candidates for the experiments. In addition, a method based on using the experimental values of the $1s$ hyperfine splitting for determination of the Bohr-Weisskopf effect in the lithiumlike ions is proposed. This method is used to reduce the uncertainty of the ground state hyperfine splitting in $^{209}Bi^{80+}$ and $^{165}Ho^{64+}$. It gives a possibility for testing the magnetic sector of QED. In Sec. III the transition probabilities between the hyperfine structure components are calculated.

II. HYPERFINE SPLITTING VALUES

The energy difference between the ground-state hyperfine splitting components of a lithiumlike ion is conveniently written in the form [5]

$$\Delta E_{(1s)^2 2s}=\tfrac{1}{6}\alpha(\alpha Z)^3\frac{m}{m_p}\frac{\mu}{\mu_N}\frac{2I+1}{2I}mc^2 \times\left\{[A(\alpha Z)(1-\delta)(1-\varepsilon)+x_{\rm rad}] +\frac{1}{Z}B(\alpha Z)+\frac{1}{Z^2}C(\alpha Z)+\cdots\right\}. \quad (1)$$

Here α is the fine-structure constant, I is the nuclear spin, μ is the nuclear magnetic moment, μ_N is the nuclear magneton, and m_p is the proton mass. $A(\alpha Z)$ is the one-electron relativistic factor,

$$A(\alpha Z)=\frac{2[2(1+\gamma)+\sqrt{2(1+\gamma)}]}{(1+\gamma)^2\gamma(4\gamma^2-1)} =1+\tfrac{17}{8}(\alpha Z)^2+\tfrac{449}{128}(\alpha Z)^4+\cdots, \quad (2)$$

and $\gamma=\sqrt{1-(\alpha Z)^2}$. δ and ε denote the nuclear charge and magnetization distribution corrections. $x_{\rm rad}$ is the one-electron radiative correction. The terms $B(\alpha Z)/Z$ and $C(\alpha Z)/Z^2$ correspond to interelectronic interaction contributions.

A. One-electron contribution

The one-electron contribution is enclosed in the square brackets of Eq. (1). We denote it by a_{2s}:

$$a_{2s}=A^{(2s)}(\alpha Z)(1-\delta^{(2s)})(1-\varepsilon^{(2s)})+x_{\rm rad}^{(2s)}. \quad (3)$$

To calculate the nuclear charge distribution correction δ, we used the two-parameter Fermi model with the parameters taken from Ref. [6].

1. Bohr-Wesskopf effect

The Bohr-Weisskopf correction ε is given by the equations

$$\varepsilon=\frac{\langle IM_I|\Delta Q_S^z+\Delta Q_L^z+\Delta Q_{\rm SO}^z|IM_I\rangle}{\langle IM_I|Q_\mu^z|IM_I\rangle}, \tag{4}$$

$$\Delta Q_S^z=\sum_{i=1}^{A} g_{si}\left[s_{zi}K_S(r_i)+\left(\frac{\pi}{2}\right)^{1/2}[Y_{2i}\otimes\sigma_i]_z^1 \times[K_S(r_i)-K_L(r_i)]\right], \tag{5}$$

$$\Delta Q_L^z=\sum_{i=1}^{A} g_{li}l_{zi}K_L(r_i), \tag{6}$$

$$\Delta Q_{\rm SO}^z=\sum_{i=1}^{A} g_{li}\frac{2m_p}{3\hbar^2}\left[s_{zi}+\left(\frac{\pi}{2}\right)^{1/2}[Y_{2i}\otimes\sigma_i]_z^1\right]\phi(r_i)r_i^2K_L(r_i), \tag{7}$$

$$Q_\mu^z=\sum_{i=1}^{A}\left\{g_{si}s_{zi}+g_{li}l_{zi} +g_{li}\frac{2m_p}{3\hbar^2}\left[s_{zi}+\left(\frac{\pi}{2}\right)^{1/2}[Y_{2i}\otimes\sigma_i]_z^1\right]\phi(r_i)r_i^2\right\}, \tag{8}$$

where

$$K_S(r)=\frac{\int_0^r fg\,dr'}{\int_0^\infty fg\,dr'},$$

$$K_L(r)=\frac{\int_0^r\left(1-\frac{r'^3}{r^3}\right)fg\,dr'}{\int_0^\infty fg\,dr'},$$

and g and f are the radial parts of the Dirac wave function of the electron defined by

$$\psi_{n\kappa m}(\mathbf{r})=\begin{pmatrix} g_{n\kappa}(r)\Omega_{\kappa m}(\mathbf{n}) \\ if_{n\kappa}(r)\Omega_{-\kappa m}(\mathbf{n})\end{pmatrix}.$$

A is the number of nucleons. The term $\Delta Q_{\rm SO}^z$ and the related term in Eq. (8) are caused by the spin-orbit interaction

$$V_{\rm SO}(r)=\phi(r)(\mathbf{s}\cdot\mathbf{l}).$$

Neglecting these terms gives the equations derived in Ref. [7]. In the case of the single particle nuclear model Eqs. (4)–(8) were used in Ref. [3] for calculations of the Bohr-Weisskopf effect for the $1s$ state. We extended these calculations to the $2s$ state. The uncertainty due to deviation from the single-particle nuclear model was estimated in the same way as in [3]. This uncertainty gives a dominant contribution to the error bars of the hyperfine splitting values. So more accurate calculations of the Bohr-Weisskopf effect, including a consequent procedure for determination of the uncertainty, are necessary. Such calculations, based on a dynamic-correlation model [8,9], are under way, and will be published elsewhere. However, the uncertainty of the Bohr-Weisskopf effect can be considerably reduced if the $1s$ hyperfine splitting value is known from experiment with sufficient precision. To explain this point, let us consider Eqs. (4)–(8). As one can see from these equations, the Bohr-Weisskopf effect depends on the electronic structure only through the functions $K_S(r)$ and $K_L(r)$. Simple approximate expressions for these functions were derived in Ref. [10]. As follows from these expressions and is confirmed by more accurate calculations, with high precision ($\sim 0.1\%$ for $Z=83$) the functions $K_S(r)$ and $K_L(r)$ for the $2s$ state are different from those for the $1s$ state only by an overall factor denoted in Ref. [10] by b. (This fact can be easily understood if we take into account that the binding energy of the electron ($W=E-mc^2$) is small in comparison with the nuclear potential $[V(r)]$ in the nuclear region. So, the binding energy gives only a small correction to behavior of the functions $g(r)$ and $f(r)$ within the nucleus.) It follows that the Bohr-Weisskopf effect for the $2s$ state can be found by using ε for the $1s$ state and the values of the overall factors tabulated in Ref. [10] [while the relative precision of b in [10] is of order $\alpha ZR/(\hbar/mc)$, where R is the nuclear radius, the precision of the ratio $b^{(2s)}/b^{(1s)}$ is higher by orders of magnitude]. If the $1s$ hyperfine splitting is known from experiment, the Bohr-Weisskopf effect for the $1s$ state is derived from the equation

$$\varepsilon^{(1s)}=\frac{\Delta E_{\rm NS}^{(1s)}+\Delta E_{\rm QED}^{(1s)}-\Delta E_{\rm expt}^{(1s)}}{\Delta E_{\rm NS}^{(1s)}}, \tag{9}$$

where $\Delta E_{\rm NS}^{(1s)}$ is the theoretical hyperfine splitting value including the relativistic and nuclear charge distribution effects, $\Delta E_{\rm QED}^{(1s)}$ is the theoretical QED contribution, and $\Delta E_{\rm expt}^{(1s)}$ is the experimental value of the $1s$ hyperfine splitting. The Bohr-Weisskopf effect for the $2s$ state is calculated by

$$\varepsilon^{(2s)}=\varepsilon^{(1s)}\frac{b^{(2s)}}{b^{(1s)}}. \tag{10}$$

High precision experimental values of the $1s$ hyperfine splitting were found for $^{209}Bi^{82+}$ [$\lambda=243.87(4)$ nm] [1] and for $^{165}Ho^{66+}$ [$\lambda=572.79(15)$ nm] [2]. Using these experimental values and the related theoretical values from Ref. [3] [with $\mu=4.1106(2)\mu_N$ for ^{209}Bi [11] and $\mu=4.132(5)\mu_N$ for ^{165}Ho [12,13,2]], Eqs. (9) and (10) give $\varepsilon^{(1s)}=0.0152(2)$ and $\varepsilon^{(2s)}=0.0164(3)$ for $^{209}Bi^{82+}$, and $\varepsilon^{(1s)}=0.0095(13)$ and $\varepsilon^{(2s)}=0.0101(14)$ for $^{165}Ho^{66+}$. For comparison, the direct calculation, based on the single particle nuclear model, gives $\varepsilon^{(1s)}=0.0118(49)$ and $\varepsilon^{(2s)}=0.0127(53)$ for $^{209}Bi^{82+}$, and $\varepsilon^{(1s)}=0.0089(27)$ and $\varepsilon^{(2s)}=0.0094(28)$ for $^{165}Ho^{66+}$.

TABLE I. The self-energy contribution to the $1s$ and $2s$ hyperfine splitting expressed in terms of the function $F(\alpha Z)$ defined by the equation (11). $\langle r^2\rangle^{1/2}$ is the root-mean-square charge radius of the nucleus [6].

Z	$\langle r^2\rangle^{1/2}$	$F^{(1s)}(\alpha Z)$	$F^{(2s)}(\alpha Z)$
49	4.598	−2.629(5)	−2.58(1)
59	4.892	−3.293(7)	−3.28(2)
67	5.190	−3.856(8)	−3.89(2)
75	5.351	−4.470(9)	−4.57(2)
83	5.533	−5.141(10)	−5.32(3)

2. QED corrections

The radiative correction is the sum of the vacuum polarization (VP) and self-energy (SE) contributions. The VP contribution is largely made up of the Uehling term. Calculation of this term was done in the same way as for the $1s$ state [3,14]. As for the Wichman-Kroll term, we calculated only the electric loop correction to the electron wave function expecting that, like the VP screening contribution for two-electron ions [15], the magnetic loop term is too small.

To calculate the SE contribution we used a covariant way based on expansion of the electron propagator in terms of the external field [16,17]. The formal expression for this contribution can easily be derived using the Green's function method (see, e.g., Ref. [5]). The contribution of the diagram with the hyperfine interaction outside the self-energy loop is divided into irreducible and reducible parts. The reducible part is the part in which the intermediate-state energy (between the self-energy loop and the hyperfine interaction) coincides with the initial-state energy. The irreducible part is the remaining one. The irreducible part is calculated in the same way as the first-order self-energy contribution. The reducible part is grouped with the vertex diagram. According to the Ward identity the counterterms for the vertex and the reducible parts cancel each other and, so, the sum of these terms regularized in the same covariant way is ultraviolet finite. To cancel the ultraviolet divergences we separate free propagators from the bound electron lines, and calculate them in the momentum representation. The remainder is ultraviolet finite but contains infrared divergences, which are explicitly separated and canceled. The results of our calculation for a finite nuclear charge distribution for the $1s$ and $2s$ states, expressed in terms of the function $F(\alpha Z)$ defined by

$$\Delta E_{\rm SE}=\frac{\alpha}{\pi}F(\alpha Z)\Delta E_{\rm NS}, \tag{11}$$

are given in Table I. A more detailed analysis of the calculation is given in Ref. [18], which also contains the results for a point nucleus. In the case of the $1s$ state the calculation of the SE contribution to the hyperfine splitting for a finite nuclear charge distribution was done first in Refs. [17,19] in a wide interval of Z. In the case of $Z=83$ and a point nucleus, such a calculation was done in Ref. [20] where it was found that $x_{\rm SE}=-3.8\alpha$. The present calculation for $Z=83$ and a point nucleus gives $x_{\rm SE}=-3.94\alpha$ (in the case of an extended nucleus, $x_{\rm SE}=-3.09\alpha$). The discrepancy of the present result with the one of Ref. [20] is caused by a spurious term which appears in the noncovariant regularization procedure used in Ref. [20]. A comparison of the present calculation for an extended nucleus with Refs. [17,19] also shows some discrepancy. So, for $Z=83$ our result is $F=-5.14(1)$, while in Refs. [17,19] it was obtained that $F=-5.098$. This discrepancy results from a small term in the vertex contribution omitted in Refs. [17,19]. For the 1s state our results are in good agreement with a recent calculation of Ref. [21], where for $Z=83$ it was found that $F=-5.1432$.

TABLE II. The one-electron contributions to the $2s$ hyperfine splitting. $A(\alpha Z)$ is the relativistic factor, δ is the nuclear charge distribution correction, ε is the Bohr-Weisskopf correction calculated within the single particle nuclear model, $x_{\rm VP}$ and $x_{\rm SE}$ are the vacuum polarization and self-energy corrections, respectively, and $x_{\rm rad}$ is the total QED correction [see Eq. (1)].

Ion	A	δ	ε	$x_{\rm VP}$	$x_{\rm SE}$	$x_{\rm rad}$
^{113}In	1.3425	0.0174	0.0048	0.0034	−0.0079	−0.0045
^{121}Sb	1.3791	0.0195	0.0053	0.0037	−0.0085	−0.0048
^{123}Sb	1.3791	0.0195	0.0014	0.0037	−0.0085	−0.0048
^{127}I	1.4188	0.0218	0.0054	0.0040	−0.0092	−0.0052
^{133}Cs	1.4620	0.0243	0.0018	0.0044	−0.0099	−0.0055
^{139}La	1.5089	0.0271	0.0026	0.0048	−0.0107	−0.0059
^{141}Pr	1.5601	0.0302	0.0078	0.0052	−0.0115	−0.0063
^{151}Eu	1.6770	0.0379	0.0084	0.0063	−0.0134	−0.0071
^{159}Tb	1.7440	0.0424	0.0073	0.0069	−0.0145	−0.0076
^{165}Ho	1.8175	0.0477	0.0094	0.0075	−0.0156	−0.0081
^{175}Lu	1.9879	0.0603	0.0006	0.0091	−0.0183	−0.0092
^{181}Ta	2.0871	0.0679	0.0018	0.0100	−0.0199	−0.0098
^{185}Re	2.1973	0.0745	0.0130	0.0111	−0.0216	−0.0104
^{203}Tl	2.6141	0.1048	0.0193	0.0152	−0.0278	−0.0126
^{205}Tl	2.6141	0.1049	0.0193	0.0152	−0.0278	−0.0126
^{207}Pb	2.6994	0.1114	0.0451	0.0161	−0.0291	−0.0130
^{209}Bi	2.7904	0.1181	0.0127	0.0169	−0.0304	−0.0134

In addition to the nuclear charge distribution correction, there is also a nuclear magnetization distribution correction to the QED effect (a combined QED–Bohr-Weisskopf effect). This correction is expected to be negligible compared with the uncertainty of the first-order Bohr-Weisskopf effect.

Comparing the VP and SE contributions for $1s$ and $2s$ states we found that, within a few percent, they are related by

$$\frac{x^{(2s)}_{\rm VP,SE}}{A^{(2s)}}\approx\frac{x^{(1s)}_{\rm VP,SE}}{A^{(1s)}}. \tag{12}$$

This means that, like the nuclear corrections (δ and ε) [10], a dominant contribution to the QED corrections to the hyperfine splitting arises from distances where the binding energy of the electron is small compared with the nuclear potential.

The values of the one-electron corrections to the $2s$ hyperfine splitting, with the Bohr-Weisskopf effect calculated within the single-particle nuclear model, are listed in Table II.

B. Interelectronic interaction corrections

To find the function $B(\alpha Z)$, we have to calculate the Feynman diagrams containing, in addition to the hyperfine

TABLE III. The function $B(\alpha Z)$ defined by Eq. (1). $B_0(\alpha Z)$ is the point nucleus value, δ_B is the nuclear charge distribution correction, $B_{\rm NS}(\alpha Z)=B_0(\alpha Z)(1-\delta_B)$, and $B_{\rm NS,BW}(\alpha Z)=B_0(\alpha Z)(1-\delta_B)(1-\varepsilon)$.

Ion	$B_0(\alpha Z)$	δ_B	$B_{\rm NS}(\alpha Z)$	$B_{\rm NS,BW}(\alpha Z)$
$^{113}In^{46+}$	−3.677	0.019	−3.607	−3.590
$^{121}Sb^{48+}$	−3.788	0.021	−3.708	−3.688
$^{123}Sb^{48+}$	−3.788	0.021	−3.708	−3.703
$^{127}I^{50+}$	−3.909	0.024	−3.817	−3.796
$^{133}Cs^{52+}$	−4.042	0.026	−3.935	−3.928
$^{139}La^{54+}$	−4.186	0.029	−4.063	−4.052
$^{141}Pr^{56+}$	−4.344	0.033	−4.201	−4.168
$^{151}Eu^{60+}$	−4.707	0.041	−4.513	−4.475
$^{159}Tb^{62+}$	−4.916	0.046	−4.690	−4.655
$^{165}Ho^{64+}$	−5.147	0.052	−4.881	−4.835
$^{175}Lu^{68+}$	−5.687	0.066	−5.314	−5.310
$^{181}Ta^{70+}$	−6.003	0.074	−5.560	−5.550
$^{185}Re^{72+}$	−6.357	0.081	−5.841	−5.765
$^{203}Tl^{78+}$	−7.711	0.114	−6.829	−6.697
$^{205}Tl^{78+}$	−7.711	0.114	−6.829	−6.697
$^{207}Pb^{79+}$	−7.992	0.122	−7.020	−6.703
$^{209}Bi^{80+}$	−8.292	0.129	−7.223	−7.131

interaction line, a photon line corresponding to the interelectronic interaction. Such a calculation for a point nucleus with an approximate evaluation of the finite nuclear size effect was done in Ref. [5]. In the present paper we calculate this function with an accurate treatment of the nuclear charge distribution effect. For that, formulas from Ref. [5] and the finite basis set method for the Dirac equation [22–24] are used. Like the one-electron contribution, it is convenient to represent the function $B(\alpha Z)$ in the form

$$B(\alpha Z)=B_0(\alpha Z)(1-\delta_B)(1-\varepsilon_B), \tag{13}$$

where $B_0(\alpha Z)$ is the point nucleus approximation of $B(\alpha Z)$, δ_B is the nuclear charge distribution correction to this function, and ε_B is the nuclear magnetization distribution correction. The values B_0 and δ_B are given in the second and third columns of Table III. As one can see from Tables II and III, in agreement with an approximate evaluation of the nuclear size effect for $B(\alpha Z)$ given in Ref. [5], the values δ_B are very close to the related one-electron values δ. It is natural to assume that the nuclear magnetization correction ε_B is also close to the related one-electron value ε (this assumption can be argued in the same way as the corresponding assumption for δ in Ref. [5]). So, in the last column of Table III we give the values $B(\alpha Z)$ corrected by the factor $(1-\varepsilon)$.

The term $C(\alpha Z)/Z^2$ in Eq. (1) is small enough, and was estimated in the nonrelativistic approximation

$$\frac{C(\alpha Z)}{Z^2}\approx\frac{C(0)}{Z^2}. \tag{14}$$

The coefficient $C(0)$ was found from the configuration interaction Hartree-Fock (CI-HF) calculation of Ref. [4] to be $C(0)=0.87\pm0.05$.

C. Complete theoretical values

In Table IV we give theoretical values of the energies and wavelengths of the transition between the ground-state hyperfine splitting components of high-Z lithiumlike ions,

TABLE IV. The energies (ΔE) and the wavelengths (λ) of the transition between the hyperfine structure components of the ground state of lithiumlike ions, with the Bohr-Weisskopf effect calculated within the single-particle nuclear model. a_{2s} is the total one-electron contribution defined by Eq. (3). $B(\alpha Z)/Z$ and $C(0)/Z^2$ are the interelectronic interaction contributions defined by Eq. (1). $\eta=8\Delta E_{(1s)^2 2s}/\Delta E_{1s}$. The nuclear magnetic moments are taken from Refs. [11–13].

Ion	$\frac{\mu}{\mu_N}$	a_{2s}	$\frac{B(\alpha Z)}{Z}$	$\frac{C(0)}{Z^2}$	ΔE (eV)	$\lambda(\mu$m)	η
$^{113}In^{46+}$	5.5289(2)	1.3083	−0.0733	0.0004	0.11744(18)	10.56(2)	1.0270(2)
$^{121}Sb^{48+}$	3.3634(3)	1.3402	−0.0723	0.0003	0.08931(15)	13.88(2)	1.0368(2)
$^{123}Sb^{48+}$	2.5498(2)	1.3455	−0.0726	0.0003	0.06473(9)	19.15(3)	1.0369(2)
$^{127}I^{50+}$	2.81327(8)	1.3752	−0.0716	0.0003	0.08620(15)	14.38(2)	1.0468(2)
$^{133}Cs^{52+}$	2.58202	1.4183	−0.0714	0.0003	0.08700(14)	14.25(2)	1.0573(2)
$^{139}La^{54+}$	2.78305	1.4583	−0.0711	0.0003	0.10749(20)	11.53(2)	1.0681(2)
$^{141}Pr^{56+}$	4.2754(5)	1.4949	−0.0707	0.0002	0.1974(5)	6.280(16)	1.0789(2)
$^{151}Eu^{60+}$	3.4717(6)	1.5928	−0.0710	0.0002	0.2085(6)	5.946(16)	1.1026(2)
$^{159}Tb^{62+}$	2.014(4)	1.6502	−0.0716	0.0002	0.1531(5)	8.10(3)	1.1150(2)
$^{165}Ho^{64+}$	4.132(5)	1.7064	−0.0722	0.0002	0.3053(10)	4.061(13)	1.1278(3)
$^{175}Lu^{68+}$	2.2327(11)	1.8577	−0.0748	0.0002	0.2142(7)	5.79(2)	1.1562(3)
$^{181}Ta^{70+}$	2.3705(7)	1.9320	−0.0760	0.0002	0.2573(9)	4.82(2)	1.1709(3)
$^{185}Re^{72+}$	3.1871(3)	1.9968	−0.0769	0.0002	0.407(2)	3.043(13)	1.1857(4)
$^{203}Tl^{78+}$	1.62226	2.2823	−0.0829	0.0001	0.499(3)	2.485(15)	1.2360(6)
$^{205}Tl^{78+}$	1.63821	2.2821	−0.0829	0.0001	0.504(3)	2.461(15)	1.2359(6)
$^{207}Pb^{79+}$	0.592583(9)	2.2775	−0.0817	0.0001	0.1887(9)	6.57(3)	1.2427(5)
$^{209}Bi^{80+}$	4.1106(2)	2.4162	−0.0859	0.0001	0.800(4)	1.549(9)	1.2553(5)

TABLE V. The individual contributions to the ground-state hyperfine splitting in $^{209}Bi^{80+}$ for $\Delta E^{(1s)}_{\rm expt}=5.0840(8)$ eV [1] and $\mu=4.1106(2)\mu_N$ [11], and in $^{165}Ho^{64+}$ for $\Delta E^{(1s)}_{\rm expt}=2.1645(6)$ eV [2] and $\mu=4.132(5)\mu_N$ [12,13,2]. The Bohr-Weisskopf effect is found by using the experimental values of the $1s$ hyperfine splitting (see the text).

Contribution	$^{209}Bi^{80+}$	$^{165}Ho^{64+}$
Nonrelativistic one-electron value	0.34349(2) eV	0.1868(2) eV
Relativistic one-electron value	0.958 50(5) eV	0.3395(4) eV
Nuclear size	−0.1132(2) eV	−0.0162(1) eV
Bohr-Weisskopf	−0.0139(2) eV	−0.0032(5) eV
One-electron QED	−0.0046 eV	−0.0015 eV
Interelectronic interaction	−0.02936(4) eV	−0.0134 eV
Interelectronic interaction QED	0.000 16(8) eV	0.00006(3) eV
Total value	0.7976(2) eV	0.3052(1) eV

based on using the single-particle nuclear model in the calculation of the Bohr-Wesskopf effect. The error bars given in the table are mainly defined by the uncertainty of the Bohr-Weisskopf effect discussed in Ref. [3]. As is known (see Tables I and II in Ref. [10]), the nuclear corrections ε and δ are weakly dependent functions of the the principal quantum number n for the s states and, so, cancel considerably in the the ratio of the $2s$ and $1s$ hyperfine splitting values. This means that, if the value ε is calculated in the same nuclear model for the $1s$ and $2s$ states, the ratio has a higher precision than the individual hyperfine splitting values. In this connection, in the last column of Table IV we give the values η defined by

$$\eta=\frac{8\Delta E_{(1s)^2 2s}}{\Delta E_{1s}} =\frac{A^{(2s)}(1-\delta^{(2s)})(1-\varepsilon^{(2s)})+x^{(2s)}_{\rm rad}+\dfrac{B(\alpha Z)}{Z}+\dfrac{C(0)}{Z^2}}{A^{(1s)}(1-\delta^{(1s)})(1-\varepsilon^{(1s)})+x^{(1s)}_{\rm rad}}. \tag{15}$$

These values can be useful for comparing experimental values of the hyperfine splitting in the hydrogenlike and lithiumlike ions of an isotope. According to Eq. (12), the one-electron QED corrections are also considerably canceled in ratio (15) and, so, the value η is mainly defined by the functions $A(\alpha Z)$ and $B(\alpha Z)$.

More accurate calculations can be done for $^{209}Bi^{80+}$ and $^{165}Ho^{64+}$ by using the values of the Bohr-Weisskopf effect found above from the $1s$ hyperfine splitting experiments. In addition, a combined interelectronic interaction QED correction can roughly be estimated, assuming

$$\Delta E^{(2s)}_{\rm int,QED}\sim\frac{B(\alpha Z)}{Z}\,\frac{\Delta E^{(2s)}_{\rm QED}}{A(\alpha Z)}. \tag{16}$$

This formula can be understood if we take into account that the interelectronic interaction correction is mainly defined by the direct Coulomb interaction of a $2s$ electron with a closed $1s$ shell [5]. Since a dominant contribution to the QED correction arises from distances where the Coulomb potential of the nucleus is to be alone [see the text after Eq. (12)], the interaction of the $2s$ electron with the spherically symmetric potential of the closed $1s$ shell almost does not change the relative value of the QED correction (it mainly changes the normalization factor of the wave function for small distances). The precision of estimate (16) is taken to be 50%. Combining these corrections with the other contributions from Tables II–IV gives $\Delta E=$ 0.7976(2) eV [$\lambda=$ 1.5544(3) μm] for $^{209}Bi^{80+}$, and $\Delta E=$ 0.3052(1) eV [$\lambda=$ 4.062(1) μm] for $^{165}Ho^{64+}$. The values of the individual contributions are given in Table V. It should be stressed here that the uncertainty of the total hyperfine splitting values is not equal to the sum of the uncertainties of the individual contributions given in Table V. This is caused by the fact that the total hyperfine splitting value found in this way is stable enough in respect to possible changes of the nuclear charge radius and the magnetic moment. For explanation, let us represent the $2s$ hyperfine splitting value in the form

$$\Delta E^{(2s)}=\Delta E^{(2s)}_{\rm NS}+\Delta E^{(2s)}_{\rm int,NS}+\nu(\Delta E^{(1s)}_{\rm expt}-\Delta E^{(1s)}_{\rm NS})+\Delta E^{(2s)}_{\rm QED} +\Delta E^{(2s)}_{\rm int,QED}-\nu\Delta E^{(1s)}_{\rm QED}, \tag{17}$$

where

$$\nu=\frac{b^{(2s)}}{b^{(1s)}}\,\frac{\Delta E^{(2s)}_{\rm NS}+\Delta E^{(2s)}_{\rm int,NS}}{\Delta E^{(1s)}_{\rm NS}}, \tag{18}$$

$\Delta E^{(2s)}_{\rm int,NS}$ is the interelectronic interaction contribution for a finite nuclear charge distribution. [We note here that the theoretical value of the Bohr-Weisskopf effect is eliminated completely in Eq. (17).] Taking, for example, a small variation of the magnetic moment $\delta\mu$, we obtain

$$\delta(\Delta E^{(2s)})=\frac{\delta\mu}{\mu}\left[(\Delta E^{(2s)}_{\rm NS}+\Delta E^{(2s)}_{\rm int})\left(1-\frac{b^{(2s)}}{b^{(1s)}}\right)+\Delta E^{(2s)}_{\rm QED} +\Delta E^{(2s)}_{\rm int,QED}-\nu\Delta E^{(1s)}_{\rm QED}\right]. \tag{19}$$

Because the factor $[1-(b^{(2s)}/b^{(1s)})]$ is small (it constitutes -0.078 for $Z=83$), the ratio $\delta(\Delta E^{(2s)})/\Delta E^{(2s)}$ is smaller, at least, by orders of magnitude than $\delta\mu/\mu$. Considering in the same way a small variation of the nuclear charge radius, and taking into account that $\delta^{(1s)}$, $\delta^{(2s)}$, and δ_B are considerably

canceled in Eq. (18) [e.g., in the case $Z=83$, $(\delta^{(2s)}-\delta^{(1s)})/(\delta^{(1s)})=0.063$ and $(\delta_B-\delta^{(1s)})/(\delta^{(1s)})=0.16$], we obtain a similar result. As to the small variation of the $1s$ experimental hyperfine splitting value, we find $\delta(\Delta E^{(2s)})/\Delta E^{(2s)}=\delta(\Delta E^{(1s)}_{\rm expt})/\Delta E^{(1s)}_{\rm expt}$. So the uncertainty of the total hyperfine splitting value is mainly defined by $\delta(\Delta E^{1s}_{\rm expt})$, and the combined interelectronic interaction QED term estimated by Eq. (16).

D. Testing QED effects

One of the main objects of the investigations of the hyperfine splitting of highly charged ions consists in testing QED effects in the strong electric and magnetic fields of heavy nuclei. As one can see from Table V, the QED contributions for the $2s$ state are larger than the uncertainties of the hyperfine splitting values with the Bohr-Weisskopf effect found from the $1s$ hyperfine splitting. However, since the calculation of the Bohr-Weisskopf effect includes the QED correction of the $1s$ state, it is natural to consider, as a value derived from QED, the sum of the last three terms in Eq. (17). (Strictly speaking, division of the contributions into QED and non-QED parts is not uniquely defined. So, a part of the interelectronic interaction contribution [the function $B(\alpha Z)$] can be considered as a two-electron QED effect [5].) We find that the value derived from QED is 0.0002(1) eV for $^{209}Bi^{80+}$ and 0.0001 eV for $^{165}Ho^{64+}$. Comparing these values with the uncertainty of the complete theoretical values discussed in the preceding subsection (see also Table V) we conclude that high-precision measurements of the ground-state hyperfine splitting in hydrogenlike and lithiumlike ions of an isotope would give a possibility for testing QED effects in a combination of the strong electric and magnetic fields.

III. TRANSITION PROBABILITIES

As is well known [25–27], the transition between the hyperfine splitting components of an atomic level is a $M1$ transition. In the hydrogenlike approximation, which corresponds to the zeroth order in $1/Z$, in the case of one electron over a closed shell the transition probability is given by the formula

$$w_{F\to F'}=\alpha\frac{\omega^3}{c^2}\frac{(2F'+1)(2j+1)^3}{3j(j+1)}\times\begin{Bmatrix} j & F' & I\\ F & j & 1\end{Bmatrix}^2\left[\int_0^\infty g(r)f(r)r^3dr\right]^2, \quad (20)$$

where ω is the transition frequency, j is the electron moment, F and F' are the total atomic moments in the initial and final states, respectively, and $g(r)$ and $f(r)$ are the upper and lower radial components of the hydrogenlike Dirac wave function. For a point nucleus, using formulas from Ref. [28], one simply finds

$$\int_0^\infty g(r)f(r)r^3dr=\frac{2\kappa\epsilon-mc^2}{4mc^2}\frac{\hbar}{mc}. \quad (21)$$

Here ϵ is the one-electron Dirac-Coulomb energy, $\kappa=(-1)^{j+l+1/2}(j+1/2)$, and l is the orbital electron moment. For the s states we obtain

$$w_{F\to F'}=\alpha\omega^3\frac{\hbar^2}{m^2c^4}\frac{4}{27}\frac{I}{2I+1}\left[\frac{2\epsilon}{mc^2}+1\right]^2. \quad (22)$$

Because the integrand in Eq. (20) is a strongly decreasing function of r at $r\to 0$, the finite nuclear size corrections to Eqs. (21) and (22) can be neglected. To calculate the $1/Z$ interelectronic interaction correction to the transition probability, we used the technique developed in [29,5]. We found that this correction is small enough. It increases w by 0.23% for $^{209}Bi^{80+}$, and by 0.17% for $^{165}Ho^{64+}$. We also note that a calculation of the transition probability for a many-electron atom, including an approximate treatment of the $1/Z$ term, can be done by the formula

$$w_{F\to F'}=\alpha\frac{\omega^3}{3c^2}(2F'+1)J(J+1)(2J+1)\begin{Bmatrix} JF'I\\ FJ1\end{Bmatrix}^2\gamma^2(J), \quad (23)$$

where

$$\gamma(J)=\frac{\langle JM_J|\Sigma_i[\mathbf{r}_i\times\boldsymbol{\alpha}_i]_z|JM_J\rangle}{M_J}.$$

J and M_J are the total electronic moment and its projection, respectively. Such a calculation, based on the CI-HF method [4], confirms the exact (in $1/Z$) results.

The results of the calculation of the transition probabilities and the lifetimes ($\tau=1/w$), based on using the transition energies from Table IV, are presented in Table VI. According to Eqs. (20)–(22), the uncertainty of the transition probability is three times larger than the uncertainty of the transition energy.

More accurate calculation of the transition probability for $^{209}Bi^{80+}$ and $^{165}Ho^{64+}$, based on the transition energies from Table V, gives $w=12.07(2)\ s^{-1}$ ($\tau=0.0829(1)$ s) for $^{209}Bi^{80+}$, and $w=0.675(1)\ s^{-1}$ [$\tau=1.481(2)$ s] for $^{165}Ho^{64+}$. The errors bars are chosen to include the uncalculated terms.

IV. CONCLUSION

In the present paper we calculated the ground-state hyperfine splitting values and the transition probabilities between the hyperfine structure components of high-Z lithiumlike ions. We proposed a method which allows one to eliminate completely the Bohr-Weisskopf effect in a combination of the hyperfine splitting values of the $1s$ and $2s$ states and, so, gives a possibility for testing the QED effects.

Recently [30,31], the first experimental result for the ground state hyperfine splitting in lithiumlike bismuth was reported to be $\Delta E_{\rm expt}=0.820(26)$ eV. This agrees with the theoretical value found within the single particle nuclear model [$\Delta E=0.800(4)$ eV], as well as with the value obtained by using the experimental result for the $1s$ hyperfine splitting [$\Delta E=0.7976(2)$ eV], although it is close to the limit of the error bar.

TABLE VI. The transition probabilities (w) and the lifetimes ($\tau = 1/w$) for the ground-state hyperfine splitting of high-Z lithiumlike ions calculated with the transition energies from the Table IV.

Ion	w (s^{-1})	τ (s)
$^{113}In^{46+}$	0.0404(2)	24.75(11)
$^{121}Sb^{48+}$	0.016 42(8)	60.9(3)
$^{123}Sb^{48+}$	0.006 57(3)	152.3(6)
$^{127}I^{50+}$	0.014 73(8)	67.9(4)
$^{133}Cs^{52+}$	0.015 87(8)	63.0(3)
$^{139}La^{54+}$	0.029 87(16)	33.5(2)
$^{141}Pr^{56+}$	0.1758(13)	5.69(4)
$^{151}Eu^{60+}$	0.206(2)	4.85(4)
$^{159}Tb^{62+}$	0.0733(7)	13.64(13)
$^{165}Ho^{64+}$	0.676(7)	1.479(14)
$^{175}Lu^{68+}$	0.232(2)	4.31(4)
$^{181}Ta^{70+}$	0.401(4)	2.49(3)
$^{185}Re^{72+}$	1.51(2)	0.662(8)
$^{203}Tl^{78+}$	1.65(3)	0.607(11)
$^{205}Tl^{78+}$	1.70(3)	0.590(11)
$^{207}Pb^{79+}$	0.0890(13)	11.24(17)
$^{209}Bi^{80+}$	12.2(2)	0.0820(14)

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