Ground-state hyperfine splitting of high-Z hydrogenlike ions

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The ground-state hyperfine splitting values of high-Z hydrogenlike ions are calculated. The relativistic, nuclear, and QED corrections are taken into account. The nuclear magnetization distribution correction (the Bohr-Weisskopf effect) is evaluated within the single-particle model with the g_S factor chosen to yield the observed nuclear moment. An additional contribution caused by the nuclear-spin-orbit interaction is included in the calculation of the Bohr-Weisskopf effect. It is found that the theoretical value of the wavelength of the transition between the hyperfine-splitting components in $^{165}Ho^{66+}$ is in good agreement with experiment. [S1050-2947(97)08306-6]

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I. INTRODUCTION

Laser spectroscopic measurement of the ground-state hyperfine splitting in hydrogenlike $^{209}Bi^{82+}$ [1] has triggered great interest in calculations of this value (see [2–7] and references therein). Recently the transition between the $F=4$ and 3 hyperfine splitting levels of the ground state in hydrogenlike $^{165}Ho^{66+}$ was observed [8], and its wavelength was determined to be 572.79(15) nm. It was found [8] that this value is in disagreement with commonly tabulated values of the nuclear dipole magnetic moment of ^{165}Ho (see, e.g., [9]), and in good agreement with the value that was measured by Nachtsheim [10] and compiled by Peker [11].

The hyperfine splitting values of $^{165}Ho^{66+}$ (for the magnetic moment from [9]) and other possible candidates for such experiments were evaluated, without QED corrections, in [4]. In the present paper we refine the calculations of [4] considering a more accurate treatment of the nuclear effects and taking into account the QED corrections.

II. BASIC FORMULAS AND CALCULATIONS

The ground-state hyperfine splitting of hydrogenlike ions is conveniently written in the form [4,12]

$$\Delta E_{\mu}=\tfrac{4}{3}\alpha(\alpha Z)^3\frac{\mu}{\mu_N}\frac{m}{m_p}\frac{2I+1}{2I}mc^2\{A(\alpha Z)(1-\delta)(1-\varepsilon)+x_{\rm rad}\}. \tag{1}$$

Here α is the fine-structure constant, Z is the nuclear charge, m is the electron mass, m_p is the proton mass, μ is the nuclear magnetic moment, μ_N is the nuclear magneton, and I is the nuclear spin. $A(\alpha Z)$ denotes the relativistic factor [13]

$$A(\alpha Z)=\frac{1}{\gamma(2\gamma-1)}=1+\tfrac{3}{2}(\alpha Z)^2+\tfrac{17}{8}(\alpha Z)^4+\cdots, \tag{2}$$

where $\gamma=\sqrt{1-(\alpha Z)^2}$. δ is the nuclear charge distribution correction, ε is the nuclear magnetization distribution correction (the Bohr-Weisskopf correction) [14], and $x_{\rm rad}$ is the QED correction.

To calculate the nuclear charge distribution correction δ we used the two-parameter Fermi model

$$\rho(r)=\frac{\rho_0}{1+\exp[(r-c)/a]}. \tag{3}$$

The parameters c, a, and $\langle r^2\rangle^{1/2}$ have been taken from [15]. We found that the error due to an uncertainty of the nuclear charge distribution parameters is much smaller than an uncertainty of the Bohr-Weisskopf effect. The Bohr-Weisskopf effect was calculated assuming that the magnetizations can be ascribed to the single-particle structure of the nucleus, with the effective g_S factor chosen to yield the observed nuclear magnetic moment. The nucleon wave functions were calculated by the Schrödinger equation with the Woods-Saxon potential [16,17]

$$U(r)=V(r)+V_{\rm SO}(r)+V_{\rm Coul}(r), \tag{4}$$

where

$$V(r)=-V_0 f(r)\ ,$$

$$V_{\rm SO}=\lambda V_0(\hbar/2m_pc)^2\boldsymbol{\sigma}\cdot\mathbf{l}\ \ r^{-1}df_{\rm SO}(r)/dr\,,$$

$$V_{\rm Coul}=\begin{pmatrix}\alpha(Z-1)(3-r^2/R_0^2)/2R_0, & r\leqslant R_0\\ \alpha(Z-1)/r\ , & r\geqslant R_0\end{pmatrix},$$

$$f(r)=\{1+\exp[(r-R_0)/a]\}^{-1},$$

$$f_{\rm SO}(r)=\{1+\exp[(r-R_{\rm SO})/a]\}^{-1}.$$

In the neutron case, the term $V_{\rm Coul}$ must be omitted. The phenomenological spin-orbit (SO) interaction, characterized by the parameter λ, is much larger than it follows from the Dirac equation. In the present paper we used the potential parameters from [17] $R_0=1.347A^{1/3}$ fm, $V_0=40.6$ MeV,

$R_{SO}=1.280A^{1/3}$ fm, and $\lambda=31.5$ for the neutron, and $R_0=1.275A^{1/3}$ fm, $V_0=58.7$ MeV, $R_{SO}=0.932A^{1/3}$ fm, and $\lambda=17.8$ for the proton. Despite the fact that these parameters were chosen to give reasonable binding energies for the lead region alone, we used them at lower Z as well. We found that the uncertainty of the Bohr-Weisskopf effect caused by possible changes of these parameters [18,19] is small in comparison with an expected error due to deviation from the single-particle model.

As is known [20], the SO interaction gives an additional contribution to the nuclear magnetic moment. Taking into account the related term in the hyperfine splitting theory gives an additional contribution to the Bohr-Weisskopf effect. If we denote the SO interaction by

$$V_{SO}(r)=\phi_{SO}(r)(\mathbf{s}\cdot\mathbf{l}), \tag{5}$$

the total expressions for the Bohr-Weisskopf correction within the single-particle approximation are given by

$$\varepsilon=\frac{g_S}{g_I}\left[\frac{1}{2I}\langle K_S\rangle+\frac{(2I-1)}{8I(I+1)}\langle K_S-K_L\rangle\right]+\frac{g_L}{g_I}\left[\frac{(2I-1)}{2I}\langle K_L\rangle+\frac{(2I+1)}{4I(I+1)}\frac{m_p}{\hbar^2}\langle\phi_{SO}r^2K_L\rangle\right] \tag{6}$$

for $I=L+\frac{1}{2}$, and

$$\varepsilon=\frac{g_S}{g_I}\left[-\frac{1}{2(I+1)}\langle K_S\rangle-\frac{(2I+3)}{8I(I+1)}\langle K_S-K_L\rangle\right]+\frac{g_L}{g_I}\left[\frac{(2I+3)}{2(I+1)}\langle K_L\rangle-\frac{(2I+1)}{4I(I+1)}\frac{m_p}{\hbar^2}\langle\phi_{SO}r^2K_L\rangle\right] \tag{7}$$

for $I=L-\frac{1}{2}$. Here

$$\langle K_S\rangle=\int_0^\infty K_S(r)|u(r)|^2r^2\,dr,$$

$$\langle K_L\rangle=\int_0^\infty K_L(r)|u(r)|^2r^2\,dr,$$

$$\langle\phi_{SO}r^2K_L\rangle=\int_0^\infty\phi_{SO}(r)r^2K_L(r)|u(r)|^2r^2\,dr,$$

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

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

g and f are the radial parts of the Dirac wave function of the electron, and $u(r)$ is the radial part of the wave function of the odd nucleon. The functions $K_S(r)$ and $K_L(r)$ are calculated by using simple approximate formulas from [4] (the relative precision of such a calculation is of order $\alpha ZR_0/(\hbar/mc)$). Taking $g_L=0$ for the neutron and $g_L=1$ for the proton, we choose g_S to give the experimental value of the magnetic moment within the single-particle approximation

$$\frac{\mu}{\mu_N}=\frac{1}{2}g_S+\left[I-\frac{1}{2}+\frac{2I+1}{4(I+1)}\frac{m_p}{\hbar^2}\langle\phi_{SO}r^2\rangle\right]g_L \tag{8}$$

for $I=L+\frac{1}{2}$ and

$$\frac{\mu}{\mu_N}=-\frac{I}{2(I+1)}g_S+\left[\frac{I(2I+3)}{2(I+1)}-\frac{2I+1}{4(I+1)}\frac{m_p}{\hbar^2}\langle\phi_{SO}r^2\rangle\right]g_L \tag{9}$$

TABLE I. The Bohr-Weisskopf effect within the single-particle model of the nucleus: with taking into account the SO term in Eqs. (6)–(9), without the SO term in Eqs. (6)–(9), and taken from [4].

Ion	Nucleon state	g_S	ε (with SO)	ε (without SO)	ε (from [4])
$^{113}In^{48+}$	$1g_{9/2}$	3.67	0.0047	0.0045	0.0039
$^{121}Sb^{50+}$	$2d_{5/2}$	3.04	0.0052	0.0051	0.0046
$^{123}Sb^{50+}$	$1g_{7/2}$	4.21	0.0014	0.0019	0.0016
$^{127}I^{52+}$	$2d_{5/2}$	1.95	0.0052	0.0051	0.0047
$^{133}Cs^{54+}$	$1g_{7/2}$	4.14	0.0017	0.0024	0.0020
$^{139}La^{56+}$	$1g_{7/2}$	3.64	0.0025	0.0032	0.0027
$^{141}Pr^{58+}$	$2d_{5/2}$	4.88	0.0075	0.0073	0.0072
$^{151}Eu^{62+}$	$2d_{5/2}$	3.27	0.0080	0.0079	0.0079
$^{159}Tb^{64+}$	$2d_{3/2}$	−0.203	0.0069	0.0074	0.0073
$^{165}Ho^{66+}$	$1f_{7/2}$	2.90	0.0089	0.0085	0.0086
$^{175}Lu^{70+}$	$1g_{7/2}$	5.10	0.0006	0.0020	0.0018
$^{181}Ta^{72+}$	$1g_{7/2}$	4.76	0.0017	0.0032	0.0030
$^{185}Re^{74+}$	$2d_{5/2}$	2.71	0.0122	0.0120	0.013
$^{203}Tl^{80+}$	$3s_{1/2}$	3.47	0.0179	0.0177	0.020
$^{205}Tl^{80+}$	$3s_{1/2}$	3.50	0.0179	0.0177	0.020
$^{207}Pb^{81+}$	$3p_{1/2}$	−3.56		0.0419	0.036
$^{209}Bi^{82+}$	$1h_{9/2}$	2.80	0.0118	0.0133	0.011

TABLE II. The radiative corrections to the ground-state hyperfine splitting in terms of x defined by Eq. (1). x_{VP}^{UE} is the Uehling electric loop contribution, x_{VP}^{UM} is the Uehling magnetic loop contribution, x_{VP}^{WKE} is the WK electric loop contribution, x_{VP} is the total VP contribution without the WK magnetic loop part, x_{SE} is the SE contribution found by interpolation of the related values from [26], and x_{rad} is the total radiative correction.

Z	x_{VP}^{UE}	x_{VP}^{UM}	x_{VP}^{WKE}	x_{VP}	x_{SE}	x_{rad}
49	0.0020	0.0011	−0.0000	0.0031	−0.0074	−0.0043
53	0.0024	0.0013	−0.0000	0.0036	−0.0084	−0.0048
57	0.0029	0.0014	−0.0000	0.0043	−0.0096	−0.0053
63	0.0037	0.0017	−0.0001	0.0054	−0.0116	−0.0062
67	0.0044	0.0020	−0.0001	0.0063	−0.0132	−0.0069
71	0.0053	0.0022	−0.0001	0.0074	−0.0150	−0.0076
75	0.0064	0.0026	−0.0002	0.0088	−0.0171	−0.0083
82	0.0089	0.0033	−0.0003	0.0119	−0.0218	−0.0099
83	0.0094	0.0034	−0.0003	0.0125	−0.0226	−0.0101

TABLE III. The energies (ΔE) and the wavelengths (λ) of the transition between the hyperfine structure components of the ground state of the hydrogenlike ions. A is the relativistic factor, δ is the nuclear charge distribution correction, ε is the nuclear magnetization distribution correction (the Bohr-Weisskopf correction), and $x_{\rm rad}$ is the radiative correction [see Eq. (1)].

Ion	$\frac{\mu}{\mu_N}$	A	δ	ε	$x_{\rm rad}$	ΔE (eV)	λ (nm)
$^{113}In^{48+}$	5.5289(2)	1.2340	0.0170	0.0047	−0.0043	0.9148(13)	1355.3(1.9)
$^{121}Sb^{50+}$	3.3634(3)	1.2582	0.0191	0.0052	−0.0045	0.6891(11)	1799.3(2.8)
$^{123}Sb^{50+}$	2.5498(2)	1.2582	0.0191	0.0014	−0.0045	0.4994(7)	2482.5(3.5)
$^{127}I^{52+}$	2.813 27(8)	1.2843	0.0213	0.0052	−0.0048	0.6587(10)	1882.2(3.0)
$^{133}Cs^{54+}$	2.582 02	1.3125	0.0237	0.0017	−0.0051	0.6582(11)	1883.6(3.0)
$^{139}La^{56+}$	2.783 05	1.3430	0.0263	0.0025	−0.0053	0.8052(14)	1539.9(2.6)
$^{141}Pr^{58+}$	4.2754(5)	1.3761	0.0292	0.0075	−0.0056	1.464(3)	847.0(1.9)
$^{151}Eu^{62+}$	3.4717(6)	1.4509	0.0365	0.0080	−0.0062	1.513(4)	819.4(2.0)
$^{159}Tb^{64+}$	2.014(4)	1.4933	0.0407	0.0069	−0.0065	1.099(3)	1128(3)
$^{165}Ho^{66+}$	4.132(5)	1.5395	0.0456	0.0089	−0.0069	2.166(7)	572.5(1.7)
$^{175}Lu^{70+}$	2.2327(11)	1.6453	0.0575	0.0006	−0.0076	1.482(4)	836.6(2.4)
$^{181}Ta^{72+}$	2.3705(7)	1.7061	0.0645	0.0017	−0.0080	1.758(5)	705.3(2.2)
$^{185}Re^{74+}$	3.1871(3)	1.7731	0.0706	0.0122	−0.0083	2.749(10)	451.0(1.7)
$^{203}Tl^{80+}$	1.622 26	2.0217	0.0988	0.0179	−0.0096	3.229(18)	384.0(2.1)
$^{205}Tl^{80+}$	1.638 21	2.0217	0.0989	0.0179	−0.0096	3.261(18)	380.2(2.1)
$^{207}Pb^{81+}$	0.592 583(9)	2.0718	0.1049	0.0419	−0.0099	1.215(5)	1020.5(4.5)
$^{209}Bi^{82+}$	4.1106(2)	2.1250	0.1111	0.0118	−0.0101	5.101(27)	243.0(1.3)

for $I=L-\frac{1}{2}$.

In the third and fourth columns of Table I, we present the values g_S and ε calculated by Eqs. (6)–(9). As one can see from the table, except for ^{159}Tb and ^{127}I, the values g_S lie between the free Dirac and free real g factors. For comparison, in the fifth column we give the values ε found in disregarding the spin-orbit terms in Eqs. (6)–(9) (it corresponds to the calculation using the original Bohr-Weisskopf formulas [14]). In the last column we give the values ε found in [4] by using a simple, homogeneous over the nucleus, distribution of $|u(r)|^2$. (We note here that in the case of $^{209}Bi^{82+}$ in [4] a more accurate evaluation of ε was also presented which gave $\varepsilon=0.013$ and $\lambda=242.0$ nm, without the QED correction. The same value was found in [21].) Taking into account that the single-particle model with the effective g_S factor gives reasonable agreement with experiment for neutral atoms [22,23], we assume the following errors bars for ε. For the ions where the spin and orbital parts in Eqs. (6) and (7) are of the same sign (it results in relatively large values of ε) the uncertainty is about 30% of ε. For the ions where the spin and orbital parts in Eqs. (6) and (7) are of opposite sign (it results in relatively small values of ε) the uncertainty is about 20% of $\langle K_S\rangle$ ($0.2\langle K_S\rangle\sim 0.03\alpha Zb$, where b is a factor tabulated in [4]). In the case of Pb the uncertainty is assumed to be about 10% of ε. It should be stressed, however, that the uncertainty found in this way is to be considered only as the order of the expected error. More accurate calculations of the Bohr-Weisskopf effect must be based on many-particle nuclear models, and must include a more consequent procedure for a determination of the error bars.

The radiative correction is the sum of the vacuum polarization (VP) and self-energy (SE) contributions. The VP contribution can easily be calculated within the Uehling approximation. We calculated this effect for a finite nucleus charge distribution, and found that for $Z=82$ and 83 our results are in good agreement with the results of [3,6]. The values of the electric loop and magnetic loop contributions in the Uehling approximation are given in the second and third columns of Table II. The Wichman-Kroll (WK) contribution is also the sum of two terms. The first term is given by the WK electric

TABLE IV. The individual contributions to the ground-state hyperfine splitting in $^{165}Ho^{66+}$ for $\mu=4.132(5)\mu_N$ [10,11,8].

Nonrelativistic value	1.4945(18) eV
Relativistic value (point nucleus)	2.3007(28) eV
Nuclear size effect	−0.1050(7) eV
Bohr-Weisskopf effect	−0.0195(59) eV
Vacuum polarization	0.0094 eV
Self-energy	−0.0197 eV
Total theoretical value	2.1659(66) eV [λ = 572.5(1.7) nm]
Experiment [8]	2.1645(6) eV [λ = 572.79(15) nm]

loop correction to the electron wave function. The calculation of this term can be done in the same way as the calculation of the first-order WK contribution. The results of such a calculation, based on using the approximate formulas for the WK potential for a point nucleus [24], are given in the fourth column of the table. The second term is the WK magnetic loop contribution. Calculation of this term is a more complex problem. However, calculations of the corresponding term in the VP screening diagrams for two-electron ions [25] allow us to expect that this term is small enough. In the fifth column of Table II the total VP contribution, without the WK magnetic loop term, is given. The SE contribution was evaluated in [6,26] in a wide interval of Z for a finite nuclear size distribution. The values of this contribution given in the sixth column of Table II are found by interpolation of the related values from [26]. In the last column of the table the total radiative correction is listed.

In Table III we give the theoretical values of the energies and the wavelengths of the transition between the ground-state hyperfine splitting components of high-Z hydrogenlike ions. The error bars given in the table are mainly defined by the uncetainty of the Bohr-Weisskopf effect discussed above. The magnetic moment values, except Ho [10,11,8], are taken from [9]. In the case of Ho, the theoretical value constitutes $\lambda = 572.5(1.7)$ nm, and is in good agreement with experiment $\lambda = 572.79(15)$ nm [8]. The values of the individual contributions are listed in Table IV. In the case of Bi the difference between the experimental value [$\lambda = 243.87(2)$ nm [1]], and the theoretical value given in Table III is within the expected error of the Bohr-Weisskopf effect. We expect that these theoretical results will be refined by including the random-phase approximation in a more elaborate treatment of the Bohr-Weisskopf effect [5], based on the dynamic-correlation model [27]. Such calculations are underway and will be published elsewhere.

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