

## Recoil Correction to the Bound-Electron $g$ Factor in H-Like Atoms to All Orders in $\alpha Z$

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(Received 18 October 2001; published 11 February 2002)

The nuclear-recoil correction to the bound-electron  $g$  factor in H-like atoms is calculated to first order in  $m/M$  and to all orders in  $\alpha Z$ . The calculation is performed in the range  $Z = 1-100$ . A large contribution of terms of order  $(\alpha Z)^5$  and higher is found. Even for hydrogen, the higher-order correction exceeds the  $(\alpha Z)^4$  term, while for uranium it is above the leading  $(\alpha Z)^2$  correction. As a result, one of the main sources of the theoretical uncertainty for the bound-electron  $g$  factor is eliminated.

DOI: 10.1103/PhysRevLett.88.091801

PACS numbers: 12.20.Ds, 31.30.Gs, 31.30.Jv

Recent progress in high-precision measurements of the bound-electron  $g$  factor for H-like carbon [1,2] and the related theoretical investigations [3–11] provide a new independent determination of the electron mass. The accuracy of this determination presented in [11] is 3 times better than that of the accepted value for the electron mass [12]. This result can be improved if the theoretical and experimental uncertainties for the  $g$  factor are reduced. From the experimental side, an improvement of the accuracy by an order of magnitude is anticipated in the near future, as well as an extension of the measurements to higher- $Z$  systems [13]. Investigations of the bound-electron  $g$  factor in high- $Z$  systems are of particular importance since they can provide a new determination of the fine structure constant [8,13], nuclear magnetic moments [13], and nuclear charge radii. They would also create a good possibility for testing the magnetic sector of QED in a strong Coulomb field. At present, the theoretical uncertainty of the bound-electron  $g$  factor in H-like ions is mainly determined by four factors: a numerical error in evaluation of the QED correction of first order in  $\alpha$ , an error caused by employing the  $\alpha Z$  expansion for the QED correction of second order in  $\alpha$ , an error resulting from the  $\alpha Z$  expansion of the nuclear recoil correction, and, for very heavy ions, an error due to the finite nuclear size correction. The main goal of this Letter is to evaluate the nuclear-recoil correction to the  $1s$   $g$  factor to all orders in  $\alpha Z$  and, therefore, to eliminate one of the main sources of the uncertainty for the corresponding theoretical predictions.

As is known [14], in the nonrelativistic limit the recoil correction to the  $1s$   $g$  factor vanishes. The leading relativistic recoil correction is of order  $(\alpha Z)^2 m/M$  and was evaluated in [15,16] (see also [17], and references therein). General formulas for the nuclear-recoil effect valid to all orders in  $\alpha Z$  were derived recently in [9]. These results

were confirmed by Yelkhovsky [10] by employing a different method. In addition, Yelkhovsky presented some arguments for the assertion that the recoil correction up to order  $(\alpha Z)^4 m/M$  is completely defined by the so-called lower-order term (which was evaluated analytically in [9] and re-derived in [10]). As a result, in [10] the total theoretical uncertainty for the  $g$  factor in  $C^{5+}$  was reduced to the level of  $1.2 \times 10^{-9}$ . This leads to improving the precision of the electron-mass determination by a factor of 2. In this Letter, we numerically evaluate the higher-order contribution to the recoil correction to all orders in  $\alpha Z$ . Our results confirm the statement of [10] that the expansion of this term starts with  $(\alpha Z)^5$ . However, we find that the  $(\alpha Z)^5$  behavior of the higher-order term is a result of a cancellation of terms of order  $(\alpha Z)^3$  and  $(\alpha Z)^4$  (see a discussion below), while the argumentation of [10] does not contain any indication of the appearance of such terms. We also observe that for all H-like atoms in the range  $Z = 1-100$  the higher-order term exceeds the  $(\alpha Z)^4 m/M$  contribution. In particular, for the case of carbon this term is about 5 times larger than the  $(\alpha Z)^4 m/M$  term and by a factor of 10 exceeds its estimation given in [10]. It is caused by the fact that the  $(\alpha Z)^4 m/M$  term has a numerically small coefficient while the higher-order term exhibits the  $(\alpha Z)^5 \log(\alpha Z) m/M$  behavior with a numerically large coefficient.

We consider a H-like atom with a spinless nucleus that is put into the classical homogeneous magnetic field,  $\mathbf{A}_{cl}(\mathbf{r}) = [\mathcal{H} \times \mathbf{r}]/2$ . For simplicity, we assume that  $\mathcal{H}$  is directed along the  $z$  axis. The energy shift of a state  $a$  to first order in  $\mathcal{H}$  and to first order in  $m/M$  is conveniently written as the sum of the lower-order and the higher-order term [9,10],  $\Delta E = \Delta E_L + \Delta E_H$ , where ( $\hbar = c = 1, e < 0$ )

$$\begin{aligned} \Delta E_L = & \frac{1}{M} \langle \delta a | \left\{ \mathbf{p}^2 - \frac{\alpha Z}{r} [\boldsymbol{\alpha} \cdot \mathbf{p} + (\boldsymbol{\alpha} \cdot \mathbf{n})(\mathbf{n} \cdot \mathbf{p})] \right\} | a \rangle \\ & + \frac{e}{2} \frac{\mathcal{H}}{M} \langle a | \left( [\mathbf{r} \times \mathbf{p}]_z - \frac{\alpha Z}{2r} [\mathbf{r} \times \boldsymbol{\alpha}]_z \right) | a \rangle, \end{aligned} \quad (1)$$

$$\begin{aligned} \Delta E_H = & \frac{i}{2\pi M} \int_{-\infty}^{\infty} d\omega \left\{ \langle \delta a | \left( D^k(\omega) - \frac{[p^k, V]}{\omega + i0} \right) G(\omega + \varepsilon_a) \left( D^k(\omega) + \frac{[p^k, V]}{\omega + i0} \right) | a \rangle \right. \\ & + \langle a | \left( D^k(\omega) - \frac{[p^k, V]}{\omega + i0} \right) G(\omega + \varepsilon_a) \left( D^k(\omega) + \frac{[p^k, V]}{\omega + i0} \right) | \delta a \rangle \\ & \left. + \langle a | \left( D^k(\omega) - \frac{[p^k, V]}{\omega + i0} \right) G(\omega + \varepsilon_a) (\delta V - \delta \varepsilon_a) G(\omega + \varepsilon_a) \left( D^k(\omega) + \frac{[p^k, V]}{\omega + i0} \right) | a \rangle \right\}. \end{aligned} \quad (2)$$

Here,  $p^k = -i\nabla^k$ ,  $\mathbf{n} = \mathbf{r}/r$ ,  $V(r) = -\alpha Z/r$  is the Coulomb potential of the nucleus,  $\delta V(\mathbf{x}) = -e\boldsymbol{\alpha} \cdot \mathbf{A}_{cl}(\mathbf{x})$ ,  $D^k(\omega) = -4\pi\alpha Z\alpha^l D^{lk}(\omega)$ ,

$$\begin{aligned} D^{il}(\omega, \mathbf{r}) = & -\frac{1}{4\pi} \left\{ \frac{\exp(i|\omega|r)}{r} \delta_{il} \right. \\ & \left. + \nabla^i \nabla^l \frac{[\exp(i|\omega|r) - 1]}{\omega^2 r} \right\} \end{aligned} \quad (3)$$

is the transverse part of the photon propagator in the Coulomb gauge,  $G(\omega) = \sum_n |n\rangle \langle n| [\omega - \varepsilon_n(1 - i0)]^{-1}$  is the Dirac-Coulomb Green function,  $\delta \varepsilon_a = \langle a | \delta V | a \rangle$ ,  $|\delta a\rangle = \sum_{n \neq \varepsilon_a} |n\rangle \langle n | \delta V | a \rangle (\varepsilon_a - \varepsilon_n)^{-1}$ , and  $\boldsymbol{\alpha}$  is a vector incorporating the Dirac matrices. In Eq. (2), the summation over the repeated indices ( $k = 1, 2, 3$ ), which enumerate components of three-dimensional vectors, is implicit. The recoil correction to the bound-electron  $g$  factor is defined as  $\Delta g = \Delta E/(\mu_0 \mathcal{H} m_j)$ , where  $\mu_0 = |e|/(2m)$  is the Bohr magneton and  $m_j$  is the angular momentum projection of the state under consideration.

For the  $1s$  state, the analytical evaluation of the lower-order term yields [9,10]

$$\Delta g_L = \frac{m}{M} (\alpha Z)^2 - \frac{m}{M} \frac{(\alpha Z)^4}{3[1 + \sqrt{1 - (\alpha Z)^2}]^2}. \quad (4)$$

The first term in the right-hand side of this equation reproduces the result of [15,16], while the second term contributes to order  $(\alpha Z)^4$  and higher.

The higher-order term, defined by equation Eq. (2), is represented by the sum of the Coulomb, one-transverse-photon, and two-transverse-photon contributions,  $\Delta E_H = \Delta E_H^{\text{Coul}} + \Delta E_H^{\text{tr1}} + \Delta E_H^{\text{tr2}}$ . The wave-function correction  $|\delta a\rangle$  can be found analytically by the method of generalized virial relations for the Dirac equation [18]. The explicit form for the component of  $|\delta a\rangle$ , which has the same angular quantum numbers as the reference state  $|a\rangle$ , is presented in [9] (only this component contributes to the effect under consideration). The numerical evaluation of the expression (2) was carried out similar to our previous calculations of the nuclear-recoil correction to the Lamb shift [19–21]. After integration over angles, the finite basis set method was used to evaluate infinite summations over the electron spectrum. Basis functions were constructed from  $B$  splines by employing the procedure proposed in [22]. The integration over  $\omega$  was carried out analytically for the Coulomb and one-transverse-photon contributions and numerically for the two-transverse-photon contribution. The number of  $B$  splines used in actual calculations was varied from 70 to 110. The estimated uncertainty corresponds to the dependence of the results on grid parameters and the number of splines and integration points.

The correction to the  $1s$   $g$  factor induced by the higher-order term  $\Delta E_H$  is expressed in terms of the function  $P(\alpha Z)$ ,

TABLE I. The higher-order recoil correction to the  $1s$   $g$  factor, expressed in terms of the function  $P(\alpha Z)$  defined by Eq. (5).

$Z$	$P_{\text{Coul}}$	$P_{\text{tr1}}$	$P_{\text{tr2}}$	$P$
1	-1.11414	100.701(2)	-80.8200(3)	18.769(2)
2	-1.09754	53.5278(6)	-36.98689	15.4434(6)
3	-1.08183	37.44949(6)	-22.80837	13.55928(6)
4	-1.06693	29.24592(4)	-15.91960	12.25940(4)
5	-1.05277	24.23027(3)	-11.90049	11.27702(3)
6	-1.03931	20.82713(1)	-9.29387	10.49395(1)
8	-1.01429	16.47349	-6.15902	9.30018(1)
10	-0.99161	13.78331	-4.37646	8.41524(1)
20	-0.90647	8.09979	-1.22907	5.96425(1)
30	-0.85834	6.08456	-0.41612	4.81010(1)
40	-0.84048(1)	5.09672(1)	-0.08937	4.16687(1)
50	-0.85209(1)	4.58136(3)	0.07843	3.80770(3)
60	-0.89803(3)	4.36161(3)	0.18668(1)	3.65025(4)
70	-0.99173(9)	4.39148(9)	0.27839(1)	3.6781(1)
80	-1.1647(1)	4.7153(3)	0.38378(3)	3.9344(3)
90	-1.4962(9)	5.525(3)	0.5459(2)	4.575(3)
100	-2.228(9)	7.48(3)	0.883(2)	6.14(3)

$$\Delta g_H = \frac{m}{M} (\alpha Z)^5 P(\alpha Z). \quad (5)$$

The corresponding numerical results are presented in Table I. It is noteworthy that the one-transverse-photon contribution and the two-transverse-photon contribution separately are of the order  $(\alpha Z)^4$  for small  $Z$ , while their sum exhibits the  $(\alpha Z)^5$  behavior. This fact is clearly demonstrated in Fig. 1, where the numerical results for the ratio  $\Delta g_H/[(m/M)(\alpha Z)^4]$  are plotted. We also note that the one-transverse-photon contribution contains terms of order  $(\alpha Z)^3$  which are cancelled when added together. Namely, the part corresponding to the perturbation of the reference state  $a$  and the part corresponding to the perturbation of the electron propagator exhibit the  $(\alpha Z)^3$  behavior, when taken separately. We note that, in contrast to our results, the argumentation of [10], where the same gauge is considered, does not indicate the appearance of terms of order lower than  $(\alpha Z)^5$ . For this reason, we can not consider the argumentation of Yelkhovsky, in the form it is given in [10], as complete. Fitting our numerical results for small  $Z$  to the form  $P(\alpha Z) = C_{51} \log(\alpha Z) + C_{50} + \alpha Z(\dots)$  yields  $C_{51} = -5.3 \pm 0.5$  and  $C_{50} = -6.5 \pm 1.0$ . The uncertainties of the coefficients were estimated by analyzing the dependence of the results on the number of parameters in the fit and the number of fitting points.

In Table II we present the ratios  $\Delta g_H/\Delta g_0$  and  $(\Delta g_L - \Delta g_0)/\Delta g_0$ , where  $\Delta g_0 = (\alpha Z)^2 m/M$  is the lowest-order correction derived in [15,16]. As can be seen from the table, the  $\Delta g_H$  term exceeds  $(\Delta g_L - \Delta g_0)$  for all  $Z$  in the range  $Z = 1-100$ . In the case of carbon,  $\Delta g_H$  amounts to

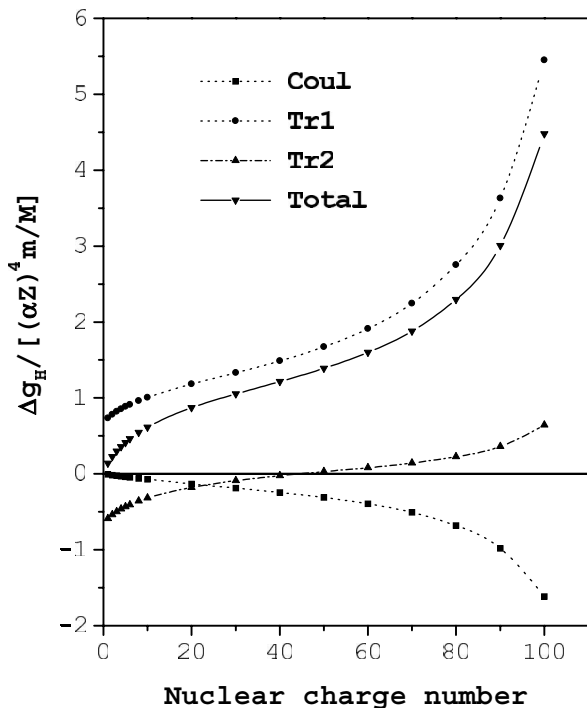


FIG. 1. The Coulomb, one-transverse-photon, and two-transverse-photon contributions to the ratio  $\Delta g_H/[(\alpha Z)^4 m/M]$ .

$7.7 \times 10^{-11}$ , which is 10 times larger than the uncertainty ascribed to this term in [10]. However, since this correction is about 10 times smaller than the current theoretical uncertainty due to the binding QED correction, it does not affect the electron-mass prediction of [11]. The higher-order recoil correction is more important for higher- $Z$  systems, since it grows very rapidly when  $Z$  increases. In particular, for uranium the higher-order recoil correction is even above the  $(\alpha Z)^2 m/M$  term.

In Table III we present the individual contributions to the  $1s$   $g$  factor for some H-like ions in the range  $Z = 6-92$ . An error ascribed to the Dirac point-nucleus value results from the current uncertainty of the fine structure constant,  $1/\alpha = 137.03599976(50)$  [12]. The uncertainty of the finite nuclear size correction was estimated as the difference between the result obtained with the Fermi model of the nuclear charge distribution and with the homogeneously charged sphere model. The nuclear charge radii were taken from [23,24]. The one-loop QED correction was taken from [4,5], where it was evaluated numerically to all orders in  $\alpha Z$ . The  $\alpha^2$  QED correction includes the existing  $\alpha Z$  expansion terms for the QED correction of second order in  $\alpha$  [7,8] and the known free QED terms of higher orders in  $\alpha$  (see, e.g., [6]). Its relative uncertainty was estimated as the ratio of the part of the one-loop QED correction, that is beyond the  $(\alpha Z)^2$  approximation, to the part that is within the  $(\alpha Z)^2$  approximation. The recoil correction incorporates the total recoil correction of first order in  $m/M$ , calculated in this paper, and the known corrections of orders  $(m/M)^2$  and  $\alpha(m/M)$  [17]. From the table, we conclude that for low  $Z$  the theoretical uncertainty is mainly determined by the numerical error of the one-loop QED correction [5,6], while for high  $Z$  it results from the  $\alpha Z$  expansion of the  $\alpha^2$  QED correction and from the finite nuclear size correction. Calculations of the QED corrections up to the desirable accuracy seem to be feasible in the near future if we consider recent progress in calculations of the corresponding corrections to the Lamb shift in H-like ions [25,26]. As to the uncertainty due to the finite nuclear size

TABLE II. The recoil corrections to the  $1s$   $g$  factor, expressed in terms of the leading correction,  $\Delta g_0 = (\alpha Z)^2 m/M$ . The difference  $\Delta g_L - \Delta g_0$  is defined by the second term in Eq. (4) and corresponds to the deviation of the lower-order term from  $(\alpha Z)^2 m/M$ .  $\Delta g_H$  is the higher-order term.

$Z$	$(\Delta g_L - \Delta g_0)/\Delta g_0$	$\Delta g_H/\Delta g_0$
1	$-4.437732 \times 10^{-6}$	$7.2935(8) \times 10^{-6}$
2	$-1.775234 \times 10^{-5}$	$4.8010(2) \times 10^{-5}$
6	$-1.599074 \times 10^{-4}$	$8.80823(1) \times 10^{-4}$
10	$-4.449468 \times 10^{-4}$	$3.27011(1) \times 10^{-3}$
20	$-1.794206 \times 10^{-3}$	$1.85414(1) \times 10^{-2}$
30	$-4.092524 \times 10^{-3}$	$5.04677(1) \times 10^{-2}$
50	$-1.190031 \times 10^{-2}$	$0.184956(2)$
70	$-2.514919 \times 10^{-2}$	$0.49025(2)$
90	$-4.672903 \times 10^{-2}$	$1.296(1)$
100	$-6.261303 \times 10^{-2}$	$2.39(1)$

TABLE III. The individual contributions to the  $1s$  bound-electron  $g$  factor in H-like ions.

	$^{12}\text{C}^{5+}$	$^{16}\text{O}^{7+}$	$^{32}\text{S}^{15+}$	$^{40}\text{Ar}^{17+}$	$^{40}\text{Ca}^{19+}$
Dirac value (point)	1.998 721 354 4	1.997 726 003 1	1.990 880 058 3(1)	1.988 447 661 3(1)	1.985 723 203 8(1)
Fin. nucl. size	0.000 000 000 4	0.000 000 001 5	0.000 000 038 9	0.000 000 070 3	0.000 000 113 1(1)
QED, order $(\alpha/\pi)$	0.002 323 663 7(9)	0.002 324 416(1)	0.002 330 920(3)	0.002 333 636(4)	0.002 336 92(1)
QED, order $(\alpha/\pi)^2$	-0.000 003 516 2(2)	-0.000 003 517 1(4)	-0.000 003 523(4)	-0.000 003 525(6)	-0.000 003 528(9)
Recoil	0.000 000 087 6	0.000 000 117 0	0.000 000 236 0	0.000 000 239 8	0.000 000 297 1
Total	2.001 041 589 9(9)	2.000 047 021(1)	1.993 208 254(5)	1.990 778 082(8)	1.988 057 01(2)
	$^{52}\text{Cr}^{23+}$	$^{74}\text{Ge}^{31+}$	$^{132}\text{Xe}^{53+}$	$^{208}\text{Pb}^{81+}$	$^{238}\text{U}^{91+}$
Dirac value (point)	1.979 392 224 9(2)	1.963 137 509 5(3)	1.892 114 650(1)	1.734 947 026(2)	1.654 846 173(3)
Fin. nucl. size	0.000 000 272 6(2)	0.000 001 231 2(10)	0.000 023 49(3)	0.000 453 3(9)	0.001 275 0(25)
QED, order $(\alpha/\pi)$	0.002 345 02(1)	0.002 369 20(1)	0.002 505 26(1)	0.002 884 38(3)	0.003 088 93(3)
QED, order $(\alpha/\pi)^2$	-0.000 003 533(16)	-0.000 003 55(4)	-0.000 003 61(19)	-0.000 003 7(6)	-0.000 003 8(9)
Recoil	0.000 000 332 4	0.000 000 426 5	0.000 000 783 5	0.000 001 723	0.000 002 491
Total	1.981 734 32(2)	1.965 504 82(4)	1.894 640 57(19)	1.738 282 7(11)	1.659 208 9(27)

effect, one may expect that, as in the case of the hyperfine splitting [27], it can be significantly reduced in a specific difference of the bound-electron  $g$  factor in H- and Li-like ions.

We thank T. Beier, S. Karshenboim, J. Kluge, W. Quint, and A. Yelkhovsky for valuable discussions, and N. Lentsman for improving the language. This work was supported in part by RFBR (Grant No. 01-02-17248), by the program ‘‘Russian Universities–Basic Research’’ (Project No. 3930), and by GSI.

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