P H Y S I C A L   R E V I E W   L E T T E R S

Electron Self-Energy in the Presence of a Magnetic Field: Hyperfine Splitting and *g* Factor

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A high-precision numerical calculation is reported for the self-energy correction to the hyperfine splitting and to the bound-electron *g* factor in hydrogenlike ions with low nuclear charge numbers. The binding nuclear Coulomb field is treated to all orders, and the nonperturbative remainder beyond the known $Z\alpha$-expansion coefficients is determined. For the $^3\text{He}^+$ ion, the nonperturbative remainder yields a contribution of -450 Hz to the normalized difference of the 1*S* and 2*S* hyperfine-structure intervals, to be compared with the experimental uncertainty of 71 Hz and with the theoretical error of 50 Hz due to other contributions. In the case of the *g* factor, the calculation provides the most stringent test of equivalence of the perturbative and nonperturbative approaches reported so far in the bound-state QED calculations.

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The hyperfine structure (hfs) of the ground state of hydrogen is experimentally known with a relative accuracy of 1×10^{-12} [1], this measurement having for a long time been among the most precise ones in physics. One of the remarkable features of the hfs is an important role of the binding effects in its theoretical description. For the self-energy (SE) correction to the hfs, the binding effects change the sign of the correction already for a nuclear charge number $Z = 8$ and make the expansion in the binding-strength parameter $Z\alpha$ completely inadequate for high values of Z (here, α is the fine-structure constant). Large coefficients of the $Z\alpha$ expansion and the high accuracy of experimental results call for an all-order (in $Z\alpha$) approach in the theoretical description of the hfs even for systems as light as hydrogen.

The high-precision all-order calculation of radiative corrections for hydrogen is a notoriously difficult problem. This point can be illustrated by considering the SE correction to the Lamb shift. Its accurate evaluation to all orders in $Z\alpha$ was first accomplished by Mohr in 1974 [2] for $Z \geq 10$, while an analogous calculation for $Z = 1$ was not realized until two decades later [3].

All-order calculations of the SE correction to the hfs started in late 1990s [4–6]. The first attempt at a numerical evaluation for hydrogen was made at the same time in Ref. [7]. Because of insufficient numerical accuracy at $Z = 1$ in that work, the goal was reached in an indirect way: the known terms of the $Z\alpha$ expansion were subtracted from the all-order numerical results for $Z \geq 5$, and the higher-order remainder thus inferred was extrapolated towards $Z = 1$. The result obtained was used as an important theoretical input for the determination of the muon mass from the muonium hfs measurements [8].

The accuracy of the numerical evaluation of the SE correction to the hfs was improved by several orders of magnitude during the past years [9,10]. However, the precision obtained was still insufficient for a direct determination of the higher-order SE remainder at $Z = 1$, and an extrapolation procedure was again employed. The studies [9,10] provided a remainder value for the normalized difference of the 1*S* and 2*S* hfs intervals, $\Delta_2 = 8\Delta E_{2S} - \Delta E_{1S}$ [11], in $^3\text{He}^+$ and demonstrated a 2σ deviation of the theoretical prediction from the experimental result [12,13]. The accuracy of the extrapolation procedure of Refs. [9,10] has recently become a subject of some concern. In particular, there is an opinion [14] that the error of the extrapolation is 4 times larger than given in Refs. [9,10], which would bring theory and experiment back into agreement.

The main goal of the present investigation is to perform the first direct, high-precision theoretical determination of the higher-order remainder of the SE correction to the hfs of the 1*S* and 2*S* states of light hydrogenlike ions. In addition, we carry out a related study of the SE correction in the presence of an external homogeneous magnetic field, i.e., the SE correction to the *g* factor of an electron bound by a spinless nucleus.

High-precision experimental investigations for the bound-electron *g* factor have a shorter history than those for the hfs but are not less important. A relative accuracy of 5×10^{-10} was reached in recent microwave measurements in hydrogenlike carbon and oxygen [15,16], thus providing a new tool for the determination of the electron mass [17]. A recent proposal [18] to employ laser spectroscopic techniques in these measurements opens perspectives for improving the experimental accuracy (particularly, for the helium ion) up to the level of 10^{-12}.

Already at the present level of experimental accuracy, the theoretical description of the bound-electron g factor has to be performed to all orders in $Z\alpha$. The numerical precision often becomes a matter of crucial importance in such calculations. So, an increase of the numerical accuracy for the SE correction to the g factor by an order of magnitude achieved in Ref. [19] as compared to the previous evaluations [6,20,21] resulted in an improvement in the electron mass value. In order to match the 10^{-12} level of accuracy anticipated in future experiments on the helium ion, the precision of numerical calculations of the SE correction should be enhanced by several orders of magnitude. This task will be accomplished in the present work.

The SE correction in the presence of an external (magnetic) potential V_{magn} is graphically represented by two topologically nonequivalent diagrams in Fig. 1. Formal expressions for them can be obtained by considering a first-order perturbation of the SE correction to the Lamb shift by V_{magn}. Perturbations of the reference-state wave function, the binding energy, and the electron propagator give rise to the irreducible, the reducible, and the vertex contributions, respectively. General formulas for these contributions are known and can be found in our previous study [10]; for a detailed analysis we direct the reader to Ref. [22]. The irreducible part reads

$$\Delta E_{\text{ir}} = \langle a|\Sigma(\varepsilon_a)|\delta a\rangle + \langle \delta a|\Sigma(\varepsilon_a)|a\rangle, \qquad (1)$$

where $\Sigma(\varepsilon_a)$ is the SE operator defined so that its diagonal matrix element $\langle a|\Sigma(\varepsilon_a)|a\rangle$ yields the one-loop SE correction to the Lamb shift [2], and $|\delta a\rangle$ is the first-order perturbation of the reference-state wave function $|a\rangle$ by V_{magn}. The reducible part is given by

$$\Delta E_{\text{red}} = \langle a|V_{\text{magn}}|a\rangle \left\langle a \left| \frac{\partial}{\partial \varepsilon} \Sigma(\varepsilon) \right| a \right\rangle \bigg|_{\varepsilon = \varepsilon_a}, \qquad (2)$$

and the vertex part is

$$\Delta E_{\text{ver}} = \frac{ie^2}{2\pi} \int_{-\infty}^{\infty} d\omega$$
$$\times \sum_{n_1 n_2} \frac{\langle n_1|V_{\text{magn}}|n_2\rangle\langle an_2|\alpha_\mu\alpha_\nu D^{\mu\nu}(\omega)|n_1 a\rangle}{(\varepsilon_a - \omega - u\varepsilon_{n_1})(\varepsilon_a - \omega - u\varepsilon_{n_2})}, \qquad (3)$$
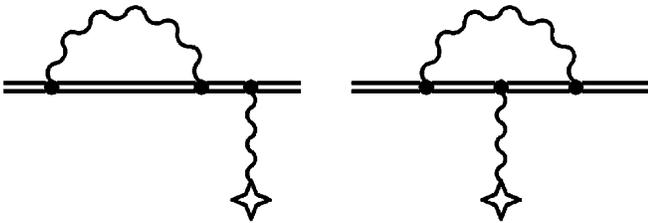
FIG. 1.　The electron self-energy in the presence of a magnetic field. The double line indicates the bound electron and the wave line with a cross is the magnetic field.

where $\alpha_\mu = (1, \boldsymbol{\alpha})$ are the Dirac matrices, $u = 1 - i0$, and $D^{\mu\nu}$ is the photon propagator.

The calculation of the irreducible part is similar to the evaluation of the diagonal matrix element of the SE operator. It is performed here by a generalization of the approach of Ref. [3], with the use of the closed form analytical representation for the perturbed wave function $|\delta a\rangle$ [23]. The evaluation of the reducible and vertex parts is more difficult. It is carried out after splitting them into several parts,

$$\Delta E_{\text{red}} = \Delta E_{\text{red}}^{(a)} + \Delta E_{\text{red}}^{(0)} + \Delta E_{\text{red}}^{(1+)}, \qquad (4)$$

$$\Delta E_{\text{ver}} = \Delta E_{\text{ver}}^{(a)} + \Delta E_{\text{ver}}^{(0)} + \Delta E_{\text{ver}}^{(1)} + \Delta E_{\text{ver}}^{(2+)}, \qquad (5)$$

where the upper index (a) labels the contributions induced by the reference-state part of the electron propagators and the other indices specify the total number of interactions with the binding field in the electron propagators [the index $(i+)$ labels the terms generated by $\geq i$ such interactions]. The reference-state contributions $\Delta E_{\text{red}}^{(a)}$ and $\Delta E_{\text{ver}}^{(a)}$ are separately infrared divergent. The divergences disappear when the contributions are regularized in the same way and evaluated together. The zero-potential parts $\Delta E_{\text{red}}^{(0)}$ and $\Delta E_{\text{ver}}^{(0)}$ are separately ultraviolet divergent. They are covariantly regularized by working in an extended number of dimensions and calculated in momentum space. The remainder of the reducible part $\Delta E_{\text{red}}^{(1+)}$ contains at least one interaction with the binding field in the electron propagators and is finite. In its evaluation, advantage was taken of a generalization of the numerical procedures originally developed in Ref. [3].

The remaining vertex contributions $\Delta E_{\text{ver}}^{(1)}$ and $\Delta E_{\text{ver}}^{(2+)}$ contain three electron propagators and represent the most difficult part of the calculation. The key to the success was to isolate the one-potential vertex contribution $\Delta E_{\text{ver}}^{(1)}$ and to calculate it without any partial-wave expansion in momentum space. For the SE correction to the g factor, such a calculation has been carried out in Ref. [19], employing the fortunate fact that in momentum space, the interaction with the homogeneous magnetic field is expressed in terms of the (gradient of the) δ-function. This is not the case for the hfs, and the calculation of this contribution is much more difficult. The general expression for $\Delta E_{\text{ver}}^{(1)}$ reads

$$\Delta E_{\text{ver}}^{(1)} = -8\pi i\alpha \int \frac{d\boldsymbol{p}\,d\boldsymbol{p}'\,d\boldsymbol{p}''}{(2\pi)^9} \int \frac{d^4k}{(2\pi)^4} \frac{V_C(\boldsymbol{p}'')}{k^2}$$
$$\times \bar{\psi}_a(\boldsymbol{p})\gamma_\sigma S(p - k)\gamma_0 S(p - p'' - k)\gamma_0$$
$$\times V_{\text{magn}}(\boldsymbol{p}''')S(p' - k)\gamma^\sigma \psi_a(\boldsymbol{p}'), \qquad (6)$$

where $p''' = p - p' - p''$, $p_0 = p_0' = \varepsilon_a$, $p_0'' = p_0''' = 0$, $S(p) = 1/(\not{p} - m)$ is the free electron propagator, and V_C

is the Coulomb potential. Effectively, $\Delta E_{\text{ver}}^{(1)}$ is a two-loop contribution because two momentum integrations (over d^4k and $d\boldsymbol{p}''$) need to be performed analytically. They are carried out after joining denominators by introducing 4 auxiliary Feynman parameters. Next, we integrate over all angular variables except $\boldsymbol{p} \cdot \boldsymbol{p}'$, which leaves 7 integrations (3 over the kinematic variables and 4 over the auxiliary parameters) to be carried out numerically. The numerical evaluation is rather time-consuming (about a month of processor time for each value of Z) but the crucial point is that it does not involve any partial-wave summations.

The remaining vertex contribution $\Delta E_{\text{ver}}^{(2+)}$ contains bound-electron propagators, and so the partial-wave expansion in its evaluation is unavoidable. However, the convergence of this expansion turns out to be very good, provided that the integrations over all radial variables are first carried out. For instance, at $Z = 1$, the sum of only the first two partial waves for the hfs yields a result with a relative accuracy of 10^{-5}. The good convergence is due to the separation of the one-potential contribution $\Delta E_{\text{ver}}^{(1)}$ introduced in this work. About 120 partial waves included in the actual calculation and the extended-precision arithmetics employed allowed us to control the calculation to a level of 10^{-9}.

The results for the SE correction to the hfs can be conveniently represented as

$$\Delta E_n = E_F(n) \frac{\alpha}{\pi} [a_{00} + (Z\alpha)a_{10} + (Z\alpha)^2(L^2 a_{22} + L a_{21}$$
$$+ a_{20}) + (Z\alpha)^3 L a_{31} + (Z\alpha)^3 F_n(Z\alpha)], \qquad (7)$$

where $E_F(n)$ is the nonrelativistic hfs value, $L = \ln[(Z\alpha)^{-2}]$, and a_{ij} are coefficients of the $Z\alpha$-expansion known today: $a_{00}(nS) = 1/2$, $a_{10}(nS) = -8.03259003$, $a_{22}(nS) = -2/3$, $a_{21}(1S) = -1.334504$, $a_{21}(2S) = 0.317104$, $a_{20}(1S) = 17.122339$, $a_{20}(2S) = 11.901105$, $a_{31}(nS) = -13.307416$; see recent works [11,24], and references therein for earlier studies. F_n is the higher-order remainder, which should addressed in a numerical all-order approach.

The results of our numerical calculation of the SE correction to the hfs of the $1S$ and $2S$ states of light hydrogenlike ions with $Z \leq 5$ are presented in Table I. The fine-structure constant of $\alpha^{-1} = 137.03599911$ [8] was employed in the calculation. Since the current uncertainty of α (3 ppb) does not influence the numerical accuracy of the higher-order remainders, α is assumed to attain exactly the value indicated. Good agreement is observed with the extrapolated values of the higher-order remainder obtained previously [7,9,10] and with the $Z\alpha$-expansion result of Ref. [25], but their accuracy is increased by several orders of magnitude.

Our calculation removes a significant source of uncertainty in the theoretical predictions for the normalized difference of the $1S$ and $2S$ hfs intervals in hydrogen and

TABLE I. SE correction to the hfs of nS states of hydrogenlike ions. $\delta E_n = \Delta E_n/[(\alpha/\pi)E_F(n)]$ and F_n is defined in Eq. (7).

n	Z	δE_n	F_n	Ref.
1	1	0.438 101 842 (2)	-13.8308 (42)	
			-13.8 (3)	[10]
			-15.9 (1.6)	[25]
			-12 (2)	[7]
	2	0.373 467 603 (3)	-14.1159 (10)	
	3	0.307 583 837 (4)	-14.4120 (4)	
	4	0.241 005 729 (6)	-14.6962 (2)	
	5	0.174 026 210 (7)	-14.9673 (2)	
2	1	0.438 692 275 (3)	-6.1205 (84)	
			-6.2 (9)	[10]
			-7.8 (1.4)	[9]
	2	0.375 352 040 (4)	-6.9129 (11)	
			-6.9 (4)	[10]
			-8.2 (9)	[9]
	3	0.311 203 192 (5)	-7.5833 (5)	
	4	0.246 665 422 (7)	-8.1698 (3)	
	5	0.181 938 683 (10)	-8.7069 (2)	

helium-3 ion, $\Delta_2 = 8\Delta E_2 - \Delta E_1$. For $^3\text{He}^+$, the SE remainder determined in this work amounts to -0.450 kHz. Combining this result with other theoretical contributions to Δ_2 described in detail in Refs. [11,26,27], we obtain the total theoretical value $\Delta_2(^3\text{He}^+)_{\text{theo}} = -1190.135(50)$ kHz, to be compared with the experimental result $\Delta_2(^3\text{He}^+)_{\text{exp}} = -1189.979(71)$ kHz [12,13]. Our calculation of the SE remainder improves the accuracy of the theoretical prediction by a factor of 3, as compared with Ref. [26]. For hydrogen, the theoretical and experimental results read $\Delta_2(\text{H})_{\text{theo}} = 48.9541(23)$ kHz and $\Delta_2(\text{H})_{\text{exp}} = 49.13(13)$ kHz [1,28], correspondingly.

For the g factor, the results of our numerical evaluation can be parameterized as

$$\Delta g_n = \frac{\alpha}{\pi} [1 + (Z\alpha)^2 b_{20} + (Z\alpha)^4 (L b_{41} + b_{40})$$
$$+ (Z\alpha)^5 H_n(Z\alpha)], \qquad (8)$$

where b_{ij} are known coefficients of the $Z\alpha$ expansion: $b_{20}(nS) = \frac{1}{6}n^{-2}$, $b_{41}(nS) = \frac{32}{9}n^{-3}$, $b_{40}(1S) = -10.236524$, $b_{40}(2S) = -1.338464$; see Ref. [29] and references therein. H_n is the remainder incorporating all higher-order contributions. It is remarkable that for the g factor, the higher-order remainder enters in the relative order $(Z\alpha)^5$ rather than in the relative order $(Z\alpha)^3$, as in the case of the hfs. This means that cancellations in extracting the remainder from numerical results for $Z = 1$ are by 4 orders of magnitude larger for the g factor than for the hfs.

The results of our numerical calculation of the SE correction for the $1S$ bound-electron g factor are presented in Table II. For hydrogen, they are consistent with values reported previously [19,21] but are by 2 orders of magni-

TABLE II. SE correction to the 1S bound-electron g factor, in units of 10^{-6} (ppm). H_1 is the higher-order remainder defined by Eq. (8) and obtained by a direct evaluation; H_1(extr.) denotes the extrapolated results. The results of Refs. [19,21] are scaled for the present value of α [8].

Z	Δg_1	H_1	H_1 (extr.)	Ref.
1	2 322.840 245 (1)	12 (31)	23.39 (80)	
	2 322.840 3 (1)			[19]
	2 322.840 2 (9)			[21]
2	2 322.904 052 (4)	23.1 (2.8)	23.03 (44)	
3	2 323.014 310 (8)	22.88 (70)		
4	2 323.175 54 (2)	22.57 (30)		
5	2 323.392 99 (2)	22.35 (16)		

tude more accurate. At the same time, all ten digits of our numerical all-order result for $Z = 1$ coincide with the value obtained within the $Z\alpha$-expansion. The fact of this coincidence can be considered as one of the most stringent tests of consistency of the two main theoretical approaches presently developed in bound-state QED. Similar agreement between the $Z\alpha$-expansion and the all-order approach was observed for the 2S state; the corresponding results will be presented elsewhere.

The accuracy of the direct numerical determination of the g-factor remainder H_1 for $Z = 1$ and 2 can be increased by extrapolating our results obtained for the higher-Z region. We employ the extrapolation procedure described in Refs. [9,10] and the numerical data for the remainder H_1 for Z as high as 20 in order to obtain the improved results listed in Table II under the label H_1(extr.).

To conclude, we have performed high-precision all-order calculations for the SE correction to the hfs and to the bound-electron g factor in light hydrogenlike systems, improving the numerical accuracy by several orders of magnitude as compared to the previous evaluations. Accurate nonperturbative results have been obtained for the higher-order SE remainder for the hfs. We remove an important source of uncertainty in theoretical predictions for the normalized difference of the 1S and 2S hfs intervals in hydrogen and the helium-3 ion and increase the theoretical accuracy by a factor of 3.

[1] L. Essen *et al.*, Nature (London) **229**, 110 (1971); Metrologia **9**, 128 (1973).
[2] P. J. Mohr, Ann. Phys. (N.Y.) **88**, 26 (1974); **88**, 52 (1974).
[3] U. D. Jentschura, P. J. Mohr, and G. Soff, Phys. Rev. Lett. **82**, 53 (1999); Phys. Rev. A **63**, 042512 (2001).
[4] H. Persson *et al.*, Phys. Rev. Lett. **76**, 1433 (1996).
[5] V. M. Shabaev and V. A. Yerokhin, Pis'ma Zh. Eksp. Teor. Fiz. **63**, 309 (1996) [JETP Lett. **63**, 316 (1996)].
[6] S. A. Blundell, K. T. Cheng, and J. Sapirstein, Phys. Rev. A **55**, 1857 (1997).
[7] S. A. Blundell, K. T. Cheng, and J. Sapirstein, Phys. Rev. Lett. **78**, 4914 (1997).
[8] P. J. Mohr and B. N. Taylor, Rev. Mod. Phys. **77**, 1 (2005).
[9] V. A. Yerokhin and V. M. Shabaev, Phys. Rev. A **64**, 012506 (2001).
[10] V. A. Yerokhin, A. N. Artemyev, V. M. Shabaev, and G. Plunien, Phys. Rev. A **72**, 052510 (2005).
[11] S. G. Karshenboim and V. G. Ivanov, Eur. Phys. J. D **19**, 13 (2002); Phys. Lett. B **524**, 259 (2002).
[12] H. A. Schuessler, E. N. Fortson, and H. G. Dehmelt, Phys. Rev. **187**, 5 (1969); Phys. Rev. A **2**, 1612(E) (1970).
[13] M. H. Prior and E. C. Wang, Phys. Rev. A **16**, 6 (1977).
[14] S. G. Karshenboim and V. G. Ivanov, Can. J. Phys. **83**, 1063 (2005).
[15] H. Häffner *et al.*, Phys. Rev. Lett. **85**, 5308 (2000).
[16] J. Verdu *et al.*, Phys. Rev. Lett. **92**, 093002 (2004).
[17] As a result, the latest values of the mass of the electron and of the ratio of the electron to proton mass are derived mainly from these experiments (see Ref. [8]).
[18] W. Quint, B. Nikoobakht, and U. D. Jentschura, Pis'ma Zh. Eksp. Teor. Fiz. **87**, 36 (2008) [JETP Lett. **87**, 30 (2008)].
[19] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Phys. Rev. Lett. **89**, 143001 (2002); Phys. Rev. A **69**, 052503 (2004).
[20] H. Persson *et al.*, Phys. Rev. A **56**, R2499 (1997).
[21] T. Beier *et al.*, Phys. Rev. A **62**, 032510 (2000).
[22] P. Sunnergren *et al.*, Phys. Rev. A **58**, 1055 (1998).
[23] V. M. Shabaev, J. Phys. B **24**, 4479 (1991).
[24] K. Pachucki, Phys. Rev. A **54**, 1994 (1996); M. Nio and T. Kinoshita, Phys. Rev. D **55**, 7267 (1997).
[25] M. Nio, in *Quantum Electrodynamics and Physics of the Vacuum*, AIP Conf. Poc. No. 564 (AIP, Melville, NY, 2001), p. 178.
[26] S. G. Karshenboim, Phys. Rep. **422**, 1 (2005).
[27] U. D. Jentschura and V. A. Yerokhin, Phys. Rev. A **73**, 062503 (2006).
[28] N. Kolachevsky *et al.*, Phys. Rev. Lett. **92**, 033003 (2004).
[29] K. Pachucki, U. D. Jentschura, and V. A. Yerokhin, Phys. Rev. Lett. **93**, 150401 (2004); **94**, 229902(E) (2005); K. Pachucki *et al.*, Phys. Rev. A **72**, 022108 (2005).