Complete two-loop correction to the bound-electron g factor

Krzysztof Pachucki,[1] Andrzej Czarnecki,[2] Ulrich D. Jentschura,[3] and Vladimir A. Yerokhin[4,5]

[1] *Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, 00–681 Warsaw, Poland*

[2] *Department of Physics, University of Alberta, Edmonton, AB, Canada T6G 2J1*

[3] *Max–Planck–Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany*

[4] *Department of Physics, St. Petersburg State University, Oulianovskaya 1, Petrodvorets, St. Petersburg 198504, Russia*

[5] *Center for Advanced Studies, St. Petersburg State Polytechnical University, Polytekhnicheskaya 29, St. Petersburg 195251, Russia*

Within a systematic approach based on the dimensionally regularized nonrelativistic quantum electrodynamics, we derive the complete result for the two-loop correction to order $(\alpha/\pi)^2(Z\alpha)^4$ for the g factor of an electron bound in an nS state of a hydrogenlike ion. The results obtained significantly improve the accuracy of the theoretical predictions for the hydrogenlike carbon and oxygen ions and influence the value of the electron mass inferred from g factor measurements.

PACS numbers: 12.20.Ds, 31.30.Jv, 06.20.Jr, 31.15.-p

I. INTRODUCTION

The g factor of a bound electron is the coupling constant of the spin to an external, homogeneous magnetic field. In natural units $\hbar = c = \varepsilon_0 = 1$, it is defined by the relation

$$\delta E = -\frac{e}{2\,m}\,\left\langle \vec{\sigma}\cdot\vec{B}\right\rangle\,\frac{g}{2}\,, \tag{1}$$

where δE is the energy shift of the electron due to the interaction with the magnetic field $\vec{B}$, m is the mass of the electron, and e is the physical electron charge ($e < 0$). The matrix $\vec{\sigma}\cdot\vec{B}$ contains the Pauli spin matrices $\vec{\sigma}$ and has eigenvalues $\pm|\vec{B}|$.

Studies of the free-electron g factor play an important role in modern physics. Together with the discovery of the Lamb shift in hydrogen, the observation of the electron magnetic moment anomaly led to the development of quantum electrodynamics (QED). After decades of intensive theoretical and experimental studies, the free-electron g factor provides one of the most accurate and stringent tests of QED [1]. With the increased experimental and theoretical precision, it presently yields the most accurate determination of the fine-structure constant α [2].

It has not been until recently that investigations of the *bound*-electron g factor came into prominence. As was demonstrated in Ref. [3], the theoretical value of the bound-electron g factor can be used for the determination of the mass of the electron when combined with an experimental value for the ratio of the electronic Larmor precession frequency $\omega_{\rm L}$ and the cyclotron frequency of the ion in the trap $\omega_{\rm c}$,

$$m = m_{\rm ion}\,\frac{g}{2}\,\frac{|e|}{q}\,\frac{\omega_{\rm c}}{\omega_{\rm L}}\,, \tag{2}$$

where q is the charge of the ion and $m_{\rm ion}$ is its mass. The accuracy of the best experimental results for light hydrogenlike ions [4, 5] is already below the 1 part per billion level and is likely to be improved in the future. According to the recent adjustment of fundamental constants [2], these measurements provide the most accurate method for the determination of the electron mass.

In order to match the experimental precision achieved, various binding and QED corrections to the bound-electron g factor have to be calculated. It has been found long ago [6] that in a relativistic (Dirac) theory, the g factor of a bound electron differs from the value $g = 2$ due to the so-called binding corrections. For an nS state, they are given by

$$\begin{aligned} g^{(0)} &= \frac{2}{3}\left(1 + 2\,\frac{E}{m}\right) \\ &= 2 - \frac{2}{3}\,\frac{(Z\,\alpha)^2}{n^2} + \left(\frac{1}{2\,n} - \frac{2}{3}\right)\frac{(Z\,\alpha)^4}{n^3} + \dots\,, \end{aligned} \tag{3}$$

where E is the Dirac energy. Other corrections to the bound-electron g factor arise from the QED theory. They were the subject of extensive theoretical investigations during the last decade. Accurate calculations of the one-loop self-energy [7–11], vacuum-polarization [8, 9, 12, 13], nuclear-recoil [14–16], and nuclear-polarizability [17] corrections have been carried out. Detailed g factor investigations have been performed also for other systems that could be of experimental interest in the near future, in particular, for Li-like ions [18] and hydrogenlike ions with a non-zero nuclear spin [19].

The subject of this work is the two-loop QED correction, which is presently the main source of the uncertainty of theoretical predictions for the g factor of hydrogenlike ions. We present a complete calculation of this correction up to the order of $(\alpha/\pi)^2\,(Z\,\alpha)^4$. This two-loop correction has already been addressed to in our former work [20], where an incomplete calculation using a photon-mass regularization was presented and an estimate for the total contribution up to the order $(\alpha/\pi)^2\,(Z\,\alpha)^4$ was obtained. The present computational method is based on the dimensionally-regularized nonrelativistic quantum electrodynamics (NRQED), which is a relatively new and very powerful approach for the calculation of higher-order relativistic and radiative effects. It has already been successfully applied to several challenging problems, e.g., to the calculation of the positronium hyperfine splitting [21] and the ground-state energy of the helium atom [22].

II. DIMENSIONALLY REGULARIZED NRQED

As is customary in dimensionally regularized QED, we here assume that the dimension of the space-time is $D = 4 - 2\,\varepsilon$, and that of the space $d = 3 - 2\,\varepsilon$. The parameter ε is considered as small, but only on the level of matrix elements, where an analytic continuation to a noninteger spatial dimension is allowed.

Let us briefly discuss the extension of the basic formulas of NRQED to the case of an arbitrary number of dimensions. The momentum-space representation of the photon propagator preserves its form, namely $g_{\mu\nu}/k^2$. The Coulomb interaction is [21]

$$\begin{aligned} V(r) &= -Z\,e^2 \int \frac{d^d k}{(2\,\pi)^d}\,\frac{e^{\mathrm{i}\,\vec{k}\cdot\vec{r}}}{k^2} \\ &= -\frac{Z\,e^2}{4\,\pi\,r^{1-2\,\varepsilon}}\,\left[(4\,\pi)^\varepsilon\,\frac{\Gamma(1-2\,\varepsilon)}{\Gamma(1-\varepsilon)}\right] \equiv -\frac{Z_\varepsilon\,\alpha}{r^{1-2\,\varepsilon}}\,, \end{aligned} \tag{4}$$

where the latter representation provides an implicit definition of Z_ε, and we have used the formula for the surface area of a d-dimensional unit sphere

$$\Omega_d = \frac{2\,\pi^{d/2}}{\Gamma(d/2)}\,. \tag{5}$$

The nonrelativistic Hamiltonian of the hydrogenic system is

$$H_0 = \frac{\vec{p}^{\,2}}{2\,m} - \frac{Z_\varepsilon\,\alpha}{r^{1-2\,\varepsilon}}\,. \tag{6}$$

The operator $\vec{p}^{\,2}$ is well defined in any integer dimension. If we restrict our consideration to the spherically symmetric states, $\vec{p}^{\,2}$ can be continued to an arbitrary real dimension by

$$\vec{p}^{\,2} = -\frac{1}{r^{d-1}}\,\frac{\partial}{\partial r}\,r^{d-1}\,\frac{\partial}{\partial r}\,. \tag{7}$$

In the following, we will not need the explicit (unknown) form of the solution of the Schrödinger equation in d dimensions. It will be sufficient to use instead its scaling properties, which we obtain by introducing the dimensionless radial variable ρ

$$\rho = (m\,\alpha)^{\frac{1}{1+2\,\varepsilon}}\,r\,. \tag{8}$$

In atomic units, i.e. expressed as a function of the dimensionless ρ, the Schrödinger Hamiltonian takes the form

$$H_0 = \alpha^{\frac{2}{1+2\,\varepsilon}}\,m^{\frac{1-2\,\varepsilon}{1+2\,\varepsilon}}\left(\frac{\vec{p}_\rho^{\,2}}{2} - \frac{Z_\varepsilon}{\rho^{1-2\,\varepsilon}}\right). \tag{9}$$

We now turn to relativistic corrections to the Schrödinger Hamiltonian in an arbitrary number of dimensions. These corrections can be obtained from the Dirac Hamiltonian by the Foldy-Wouthuysen transformation. In order to incorporate a part of radiative effects right from the beginning, we use an effective Dirac Hamiltonian modified by the electromagnetic form factors F_1 and F_2 (see, e.g., Ch. 7 of [23])

$$\begin{aligned} H =& \vec{\alpha}\cdot\left[\vec{p} - e\,F_1(\vec{\nabla}^2)\,\vec{A}\right] + \beta\,m + e\,F_1(\vec{\nabla}^2)\,A_0 \\ &+ F_2(\vec{\nabla}^2)\,\frac{e}{2\,m}\,\left(\mathrm{i}\,\vec{\gamma}\cdot\vec{E} - \frac{\beta}{2}\,\Sigma^{ij}\,B^{ij}\right)\,, \end{aligned} \tag{10}$$

where

$$B^{ij} = \nabla^i\,A^j - \nabla^j\,A^i\,, \tag{11}$$

$$\Sigma^{ij} = \frac{\mathrm{i}}{2}\,[\gamma^i,\gamma^j]\,. \tag{12}$$

We use three-dimensional notations here, namely $\nabla^i \equiv \partial_i = \partial/\partial x^i$. Formulas for the electromagnetic form factors $F_{1,2}$ can be found in Appendix A.

Having the Foldy-Wouthuysen transformation defined by the operator S (see Ref. [24], and $\kappa \equiv F_2(0)$)

$$\begin{aligned} S = -\frac{\mathrm{i}}{2\,m}\,\Big\{&\beta\,\vec{\alpha}\cdot\vec{\pi} - \frac{1}{3\,m^2}\,\beta\,(\vec{\alpha}\cdot\vec{\pi})^3 \\ &+ \frac{e(1+\kappa)}{2\,m}\,\mathrm{i}\,\vec{\alpha}\cdot\vec{E} - \frac{e\,\kappa}{8\,m^2}\,[\vec{\alpha}\cdot\vec{\pi},\beta\,\Sigma^{ij}\,B^{ij}]\Big\}\,, \end{aligned} \tag{13}$$

the new Hamiltonian is obtained via

$$H' = e^{\mathrm{i}\,S}\,(H - i\,\partial_t)\,e^{-\mathrm{i}\,S} \tag{14a}$$

and takes the form

$$\begin{aligned} H' =& \frac{\vec{\pi}^{\,2}}{2\,m} + e\,[1 + F'_1(0)\,\vec{\nabla}^2]A^0 - \frac{e}{4\,m}\,(1+\kappa)\,\sigma^{ij}\,B^{ij} \\ &- \frac{\vec{\pi}^{\,4}}{8\,m^3} - \frac{e}{8\,m^2}\,(1+2\,\kappa)\,\left[\vec{\nabla}\cdot\vec{E} + \sigma^{ij}\,\{E^i,\pi^j\}\right] \\ &+ \frac{e}{8\,m^3}\,\left[(1+\kappa)\,p^2\,\sigma^{ij}\,B^{ij} + 2\,\kappa\,p^k\,\sigma^{ki}\,B^{ij}\,p^j\right] \\ &- \frac{e}{8\,m^2}\,[F'_1(0) + 2\,F'_2(0)]\,\sigma^{ij}\,\{\vec{\nabla}^2 E^i,\pi^j\} + \dots\,, \end{aligned} \tag{14b}$$

where by dots we denote the omitted higher-order terms, $\{X,Y\} \equiv X\,Y + Y\,X$, and $\sigma^{ij} = [\sigma^i,\,\sigma^j]/(2\,\mathrm{i})$. The Hamiltonian H' is a generalization of the Foldy-Wouthuysen Hamiltonian H_{FW} [24] to an arbitrary number of dimensions. The electromagnetic field in H' is the sum of the external Coulomb field, the external (constant) magnetic field, and a slowly varying field of the radiation. For practical calculations, it is more convenient to have a Hamiltonian expressed in terms of the gauge-independent field strengths. To achieve this, we separate out the Coulomb field and perform the Power-Zienau transformation of the Hamiltonian H' with the operator S' of the form [24]

$$S' = -e\int_0^1 du\,\vec{r}\cdot\vec{A}(u\,\vec{r},t)\,. \tag{15}$$

After neglecting irrelevant spin-independent terms, the transformed Hamiltonian becomes

$$H'' = \frac{p^2}{2\,m} + V - e\,\vec{r}\cdot\vec{E} + \frac{(1+2\,\kappa)}{8\,m^2}\,\frac{V'}{r}\,\sigma^{ij}\,L^{ij} - \frac{e}{4\,m}\,\left[L^{ij} + (1+\kappa)\,\sigma^{ij}\right]\,B^{ij}$$
$$+ \frac{e}{8\,m^3}\left[(1+\kappa)\,p^2\,\sigma^{ij}\,B^{ij} + 2\,\kappa\,p^k\,\sigma^{ki}\,B^{ij}\,p^j\right] - \frac{e\,(1+2\,\kappa)}{8\,m^2}\,\frac{V'}{r}\,\sigma^{ij}\,r^j\,B^{ik}\,r^k$$
$$+ \frac{e^2\,(1+2\,\kappa)}{8\,m^2}\,\sigma^{ij}\,E^j\,B^{ik}\,r^k - \frac{e\,(1+\kappa)}{4\,m}\,\sigma^{ij}\,r^k\,B^{ij}_{,k} - \frac{e\,(1+2\,k)}{4\,m^2}\,\sigma^{ij}\,E^i\,p^j$$
$$+ F'_1(0)\,4\,\pi\,Z\,\alpha\,\delta^d(r) - \frac{e}{8\,m^2}\,[F'_1(0) + 2\,F'_2(0)]\,\sigma^{ij}\,\nabla^j[4\,\pi\,Z\,\alpha\,\delta^d(r)]\,B^{ik}\,r^k\,. \tag{16}$$

Here, $L^{ij} = r^i\,p^j - r^j\,p^i$ and $B_{,k} \equiv \nabla^k B$. H'' is the generalization of the Power-Zienau Hamiltonian H_{PZ} [24] to an arbitrary number of dimensions.

The Hamiltonian H'' includes most of the radiative corrections that are needed for our calculation, but not all of them. First, the higher-order terms with the anomalous magnetic moment are omitted in H''. This contribution is more conveniently calculated with the exact Dirac-Coulomb wave functions, starting directly from the Hamiltonian (10). Furthermore, there is an additional correction that cannot be accounted for by the F_1 and F_2 form factors. It is represented by an effective local operator that is quadratic in the field strengths. This operator is derived separately by evaluating a low-energy limit of the electron scattering amplitude off the Coulomb and the magnetic fields. Details of this calculation are presented in Appendix B. The result is

$$\delta H = \frac{e^2}{2\,m}\,\left[2\,\sigma^{ij}\,B^{ik}\,\nabla^j E^k\,\eta + \sigma^{ij} B^{ij}\,\nabla^k E^k\,\xi\right]\,, \tag{17}$$

where $B = \text{const}$, E is an arbitrary electric field, and the functions η and ξ are given by Eqs. (B16) and (B17), respectively.

III. ONE-LOOP SELF-ENERGY CORRECTION

The dimensionally regularized NRQED approach formulated in the previous section will be first employed for a derivation of the self-energy correction to order $(\alpha/\pi)\,(Z\,\alpha)^4$ for the bound-electron g factor. This derivation will serve us as a test of the new approach (as this result has been already obtained in our previous work [20]) and also as a basis for the two-loop calculation.

As in [20], we separate the one-loop self-energy correction up to the order of $(\alpha/\pi)\,(Z\,\alpha)^4$ into three parts,

$$g^{(1)} = g_1^{(1)} + g_2^{(1)} + g_3^{(1)}\,, \tag{18}$$

where the first part is the the contribution due to the free-electron form factors F_1 and F_2, the second part is the contribution induced by the additional Hamiltonian (17), and the third part is the contribution coming from low-energy photons, i.e. a Bethe-logarithm type contribution.

We start with the form-factor part $g_1^{(1)}$. The anomalous magnetic moment $F_2(0)$ in the modified Dirac-Coulomb Hamiltonian (10) leads to the following energy shift linear in the magnetic field ($d = 3$)

$$\delta E_{1A} = \left\langle -F_2^{(1)}(0)\,\frac{e}{2\,m}\,\beta\,\vec{\Sigma}\cdot\vec{B}\right\rangle + 2\,\left\langle F_2^{(1)}(0)\,\frac{\mathrm{i}\,e}{2\,m}\,\vec{\gamma}\cdot\vec{E}\,\frac{1}{(E-H)'}\,(-e)\,\vec{\alpha}\cdot\vec{A}\right\rangle\,, \tag{19}$$

where $\vec{A} = (\vec{B}\times\vec{r})/2$, and we denote the one-loop components of the form factors by the corresponding superscript. The corresponding correction to the g factor is

$$g_{1A}^{(1)} = 2\,F_2^{(1)}(0)\left[1 + \frac{(Z\,\alpha)^2}{6\,n^2} + \left(\frac{3}{2} - \frac{5}{24\,n}\right)\frac{(Z\,\alpha)^4}{n^3}\right]. \tag{20}$$

In obtaining this result, we used the closed-form expression [25, 26] for the component of the Dirac wave function perturbed by the magnetic interaction, which has the same relativistic angular momentum, as the reference state.

For the remaining part of the form-factor contribution, we employ the transformed Hamiltonian (16). The last term of this Hamiltonian

$$-\frac{e}{8\,m^2}\,[F'_1(0) + 2\,F'_2(0)]\,\sigma^{ij}\,\nabla^j[4\,\pi\,Z\,\alpha\,\delta^d(r)]\,B^{ik}\,r^k \tag{21}$$

gives rise to a contribution

$$g_{1B}^{(1)} = -[F'^{(1)}_1(0) + 2\,F'^{(1)}_2(0)]\,\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle\,. \tag{22}$$

The second-order correction to the energy

$$2\,\left\langle F'^{(1)}_1(0)\,4\,\pi\,Z\,\alpha\,\delta^d(r)\,\frac{1}{(E_0-H_0)'}\,\frac{e}{8\,m^3}\,p^2\,\sigma^{ij}\,B^{ij}\right\rangle \tag{23}$$

yields

$$g_{1C}^{(1)} = 2\,(3 - 8\,\varepsilon)\,F'^{(1)}_1(0)\,\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle\,. \tag{24}$$

The other second-order correction to the energy

$$2\,\left\langle F'^{(1)}_1(0)\,\vec{\nabla}^2 V\,\frac{1}{(E_0-H_0)'}\,(-1)\frac{e}{8\,m^2}\,\frac{V'}{r}\,\sigma^{ij}\,r^j\,B^{ik}\,r^k\right\rangle, \tag{25}$$

gives

$$g_{1D}^{(1)} = -(1 - 4\,\varepsilon)\,F'^{(1)}_1(0)\,\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle\,. \tag{26}$$

The total form-factor contribution is

$$g_1^{(1)} \;=\; g_{1A}^{(1)} + g_{1B}^{(1)} + g_{1C}^{(1)} + g_{1D}^{(1)}\,. \tag{27}$$

The second part of Eq. (18), denoted by $g_2^{(1)}$, is a high-energy correction that is not accounted for by the form factors. It is given by the effective Hamiltonian (17), with E being the electric Coulomb field. The corresponding correction to the g factor is

$$\begin{aligned} g_2^{(1)} &= 4\left(\frac{2}{d}\,\eta^{(1)} + \xi^{(1)}\right)\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle \\ &= \frac{\alpha}{\pi}\left(\frac{2}{9\,\varepsilon} + \frac{19}{27}\right)\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle\,, \end{aligned} \tag{28}$$

where $\eta^{(1)}$ and $\xi^{(1)}$ are the one-loop components of the coefficient functions given below in Eqs. (B16) and (B17).

The third part of Eq. (18) is a low-energy contribution that can be considered as a correction to the Bethe logarithm due to the interaction with an external magnetic field. Let us first derive the Bethe-logarithm correction to the hydrogen Lamb shift within the dimensional regularization. The correction to the energy is

$$\begin{aligned} \delta E_L =& e^2\int\frac{d^dk}{(2\,\pi)^d\,2\,k}\,\delta_T^{ij}\left\langle\frac{p^i}{m}\,\frac{1}{E_0-k-H_0}\,\frac{p^j}{m}\right\rangle \\ =& e^2\int\frac{d^dk}{(2\,\pi)^d\,2\,k}\,\delta_T^{ij}\,k^2\left\langle r^i\,\frac{1}{E_0-k-H_0}\,r^j\right\rangle\,. \end{aligned} \tag{29}$$

Here, $\delta_T^{ij} = \delta^{ij} - k^i\,k^j/k^2$ is the transverse delta function, and $k = |\vec{k}|$. After performing the integration over k and dropping a common overall factor of $(4\,\pi)^\varepsilon\,\Gamma(1+\varepsilon)$, δE_L becomes

$$\begin{aligned} \delta E_L =& \frac{\alpha}{\pi}\,\frac{1}{6\,\varepsilon}\,\frac{\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle}{m^2} \\ &+ m\,\frac{\alpha}{\pi}\,\frac{(Z\,\alpha)^4}{n^3}\left[\frac{10}{9} - \frac{4}{3}\,\ln(Z\,\alpha)^2] - \frac{4}{3}\,\ln k_0\right]\,, \end{aligned} \tag{30}$$

where the Bethe logarithm $\ln k_0$ is given by

$$\ln k_0 = \frac{\left\langle\vec{p}\,(H_0-E_0)\ln\left[\frac{2\,(H_0-E_0)}{m\,(Z\,\alpha)^2}\right]\,\vec{p}\right\rangle}{\langle\vec{p}\,(H_0-E_0)\,\vec{p}\rangle}\,. \tag{31}$$

We now consider all corrections to δE_L due to the presence of the external magnetic field. The first one is induced by the correction to the Hamiltonian [the fifth term on the right-hand side of Eq. (16)]

$$\delta_A H = \frac{p^2}{8\,m^3}\,e\,\sigma^{ij}\,B^{ij}\,. \tag{32}$$

The corresponding energy shift is given by

$$\delta_A E = e^2\int\frac{d^dk}{(2\,\pi)^d\,2\,k}\,\delta_T^{ij}\,k^2\,\delta_A\left\langle r^i\,\frac{1}{E_0-k-H_0}\,r^j\right\rangle\,, \tag{33}$$

where by $\delta_A\langle\ldots\rangle$ we denote the first-order correction to the matrix element induced by the perturbing Hamiltonian $\delta_A H$. This matrix element is calculated using the scaling properties of the Schrödinger Hamiltonian given by Eq. (9), and the corresponding correction to the g factor is found to be

$$\begin{aligned} g_{3A}^{(1)} =& \frac{\alpha}{\pi}\,\frac{1}{3\,\varepsilon}\,\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle \\ &- \frac{\alpha}{\pi}\,\frac{(Z\,\alpha)^4}{n^3}\left[\frac{8}{3}\,\ln(Z\,\alpha)^2 + \frac{8}{3}\,\ln k_0 + \frac{100}{9}\right]\,. \end{aligned} \tag{34}$$

The second correction to the interaction with the magnetic field is [sixth term in Eq. (16)]

$$\begin{aligned} \delta_B H =& -\frac{e}{8\,m^2}\,\frac{V'}{r}\,\sigma^{ij}\,r^j\,B^{ik}\,r^k \\ =& -\frac{d-2}{d}\,\frac{e}{8\,m^2}\,V\,\sigma^{ij}\,B^{ij}\,, \end{aligned} \tag{35}$$

where the last part of the equation holds only for S-states. The corresponding contribution to the g factor is

$$\begin{aligned} g_{3B}^{(1)} =& -\frac{\alpha}{\pi}\,\frac{2}{9\,\varepsilon}\,\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle \\ &+ \frac{\alpha}{\pi}\,\frac{(Z\,\alpha)^4}{n^3}\left[\frac{16}{9}\,\ln(Z\,\alpha)^2 + \frac{16}{9}\,\ln k_0 + \frac{64}{27}\right]\,. \end{aligned} \tag{36}$$

The third correction is due to the coupling with the radiation field, [seventh term in Eq. (16)],

$$\delta_C H = \frac{e^2}{8\,m^2}\,\sigma^{ij}\,E^j\,B^{ik}\,r^k = [-e\,\vec{r}\cdot\vec{E}]\left[\frac{-e\,\sigma^{ij}\,B^{ij}}{8\,m^2\,d}\right]\,. \tag{37}$$

Here, the last expression is obtained by d-dimensional angular averaging. The corresponding energy shift is written as

$$\begin{aligned} \delta_C E =& 2\left[\frac{-e\,\sigma^{ij}\,B^{ij}}{8\,m^2\,d}\right] \\ &\times e^2\int\frac{d^dk}{(2\,\pi)^d\,2\,k}\,\delta_T^{ij}\,k^2\left\langle r^i\,\frac{1}{E_0-k-H_0}\,r^j\right\rangle\,. \end{aligned} \tag{38}$$

The contribution to the g factor is

$$\begin{aligned} g_{3C}^{(1)} =& \frac{\alpha}{\pi}\,\frac{1}{9\,\varepsilon}\,\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle \\ &- \frac{\alpha}{\pi}\,\frac{(Z\,\alpha)^4}{n^3}\left[\frac{8}{9}\,\ln(Z\,\alpha)^2 + \frac{8}{9}\,\ln k_0 - \frac{28}{27}\right]\,. \end{aligned} \tag{39}$$

The fourth contribution involves both the correction to the coupling with the radiation field and the interaction with the magnetic field, [the fourth and the ninth term of Eq. (16)],

$$\delta_D H = -\frac{e}{4\,m^2}\,\sigma^{ij}\,E^i\,p^j - \frac{e}{4\,m}\,L^{ij}\,B^{ij} \tag{40}$$

and is of the form

$$\begin{aligned} \delta_D E =& 2\,e^2\int\frac{d^dk}{(2\,\pi)^d\,2\,k}\,\delta_T^{ij}\,k^2 \\ &\times\left\langle r^i\frac{1}{E_0-k-H_0}\left[\frac{-e}{4\,m}L^{ab}B^{ab}\right]\frac{1}{E_0-k-H_0}\,\frac{\sigma^{jk}\,p^k}{4\,m^2}\right\rangle\,. \end{aligned} \tag{41}$$

The corresponding correction to the g factor is

$$g_{3D}^{(1)} = \frac{\alpha}{\pi}\,\frac{1}{3\,\varepsilon}\,\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle - \frac{\alpha}{\pi}\,\frac{(Z\,\alpha)^4}{n^3}\,\left[\frac{8}{3}\,\ln(Z\,\alpha)^2 + \frac{8}{3}\,\ln k_0 - \frac{20}{9}\right]. \quad (42)$$

The fifth contribution is due to another correction to the coupling with the radiation field and the same interaction with the magnetic field,

$$\delta_E H = -\frac{e}{4\,m}\,\sigma^{ij}\,r^k\,B^{ij}_{,k} - \frac{e}{4\,m}\,L^{ij}\,B^{ij}\,, \quad (43)$$

and is of the form

$$\delta_E E = \frac{4\,e^2}{d}\int\frac{d^dk}{(2\,\pi)^d\,2\,k}\,k^2\,\left\langle r^i\,\frac{1}{E_0-k-H_0}\left[-\frac{e}{4\,m}L^{ab}\,B^{ab}\right]\frac{1}{E_0-k-H_0}\,\frac{\mathrm{i}\,k\,\sigma^{ij}r^j}{4\,m^2}\right\rangle. \quad (44)$$

The corresponding correction to the g factor is

$$g_{3E}^{(1)} = -\frac{\alpha}{\pi}\,\frac{4}{9\,\varepsilon}\,\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle + \frac{\alpha}{\pi}\,\frac{(Z\,\alpha)^4}{n^3}\,\left[\frac{32}{9}\,\ln(Z\,\alpha)^2 + \frac{32}{9}\,\ln k_0 - \frac{136}{27}\right]. \quad (45)$$

The sixth and the last contribution is due to the spin-orbit interaction and the interaction to the magnetic field,

$$\delta_F H = \frac{1}{8\,m^2}\,\frac{V'}{r}\,\sigma^{ij}\,L^{ij} - \frac{e}{4\,m}\,L^{ij}\,B^{ij}\,. \quad (46)$$

This correction involves a more complicated matrix element with three propagators,

$$\delta_F E = 2\,e^2\int\frac{d^dk}{(2\,\pi)^d\,2\,k}\,\delta_T^{ij}\,k^2\,\left\langle r^i\,\frac{1}{E_0-k-H_0}\left[\frac{1}{8\,m^2}\,\frac{V'}{r}\,\sigma^{ij}\,L^{ij}\right]\frac{1}{E_0-k-H_0}\left[-\frac{e}{4\,m}\,L^{ij}\,B^{ij}\right]\frac{1}{E_0-k-H_0}\,r^j\right\rangle. \quad (47)$$

The corresponding correction to the g factor is

$$g_{3F}^{(1)} = \frac{\alpha}{\pi}\,\frac{1}{3\,\varepsilon}\,\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle - \frac{\alpha}{\pi}\,\frac{(Z\,\alpha)^4}{n^3}\,\left[\frac{8}{3}\,\ln(Z\,\alpha)^2 + \frac{8}{3}\,\ln k_3 - \frac{20}{9}\right], \quad (48)$$

where $\ln k_3$ is implicitly defined by the relation

$$\int_0^\epsilon dk\,k^2\,\left\langle \vec{r}\,\frac{1}{E_0-H_0-k}\,\frac{1}{r^3}\,\frac{1}{E_0-H_0-k}\,\vec{r}\right\rangle = \epsilon\,\left\langle\frac{1}{r}\right\rangle - 4\,\frac{(Z\,\alpha)^3}{n^3}\left[\ln\frac{2\,\epsilon}{(Z\,\alpha)^2} - \ln k_3\right], \quad (49)$$

which holds in the limit of large ϵ.

Finally, the total Bethe-logarithm type contribution to the g factor is a sum of calculated terms

$$g_3^{(1)} = g_{3A}^{(1)} + g_{3B}^{(1)} + g_{3C}^{(1)} + g_{3D}^{(1)} + g_{3E}^{(1)} + g_{3F}^{(1)}\,. \quad (50)$$

The complete one-loop self-energy correction to the bound-electron g factor is then

$$g^{(1)} = \frac{\alpha}{\pi}\left\{1 + \frac{(Z\alpha)^2}{6n^2} + \frac{(Z\alpha)^4}{n^3}\left[\frac{32}{9}\ln[(Z\alpha)^{-2}] + \frac{73}{54} - \frac{5}{24n} - \frac{8}{9}\ln k_0 - \frac{8}{3}\ln k_3\right]\right\}, \quad (51)$$

in full agreement with the former result in Eq. (12) of Ref. [20].

IV. TWO-LOOP CONTRIBUTION

The derivation of the two-loop corrections to the bound-electron g factor is performed in full analogy to the one-loop calculations. The total two-loop correction of the order $(\alpha/\pi)^2\,(Z\,\alpha)^4$ can be separated into four parts,

$$g^{(2)} = g_1^{(2)} + g_2^{(2)} + g_3^{(2)} + g_4^{(2)}\,. \quad (52)$$

The first part $g_1^{(2)}$ is a form-factor contribution. The second part $g_2^{(2)}$ is an additional high-energy contribution not accounted for by the form factors. The third part arises from a contribution in which one of the two virtual photons is of low energy. The second photon effectively modifies the vertex, which can be accounted for by the anomalous magnetic moment. The fourth contribution $g_4^{(2)}$ involves the closed fermion loops and is called the vacuum polarization part.

We start with the form-factor contribution. The two-loop anomalous magnetic moment correction is obtained from the corresponding one-loop contribution, Eq. (20)

$$g^{(2)}_{1A} = 2\,F^{(2)}_2(0)\,\left[1+\frac{(Z\,\alpha)^2}{6\,n^2}+\left(\frac{3}{2}-\frac{5}{24\,n}\right)\frac{(Z\,\alpha)^4}{n^3}\right]. \tag{53}$$

The one-loop anomalous magnetic moment in the modified Dirac-Coulomb Hamiltonian (10) leads to the following energy shift,

$$\begin{aligned}\delta E_{1B} = [F^{(1)}_2(0)]^2 \Bigg\{ &\left\langle \frac{-e}{2\,m}\,\beta\,\vec\Sigma\cdot\,\vec B\,\frac{1}{(E-H)'}\,\frac{\mathrm{i}\,e}{2\,m}\,\vec\gamma\cdot\vec E\right\rangle \\ &+2\left\langle \frac{\mathrm{i}\,e}{2\,m}\vec\gamma\cdot\vec E\frac{1}{(E-H)'}\frac{\mathrm{i}\,e}{2\,m}\vec\gamma\cdot\vec E\frac{1}{(E-H)'}(-e)\,\vec\alpha\cdot\vec A\right\rangle \\ &+\left\langle \frac{\mathrm{i}\,e}{2\,m}\,\vec\gamma\cdot\vec E\,\frac{1}{(E-H)'}\,(-e)\,\vec\alpha\cdot\vec A\,\frac{1}{(E-H)'}\,\frac{\mathrm{i}\,e}{2\,m}\,\vec\gamma\cdot\vec E\right\rangle \\ &-\left\langle -e\,\vec\alpha\cdot\vec A\right\rangle\left\langle \frac{\mathrm{i}\,e}{2\,m}\,\vec\gamma\cdot\vec E\,\frac{1}{(E-H)'^{\,2}}\,\frac{\mathrm{i}\,e}{2\,m}\,\vec\gamma\cdot\vec E\right\rangle \\ &-2\left\langle \frac{\mathrm{i}\,e}{2\,m}\,\vec\gamma\cdot\vec E\right\rangle\left\langle (-e)\,\vec\alpha\cdot\vec A\,\frac{1}{(E-H)'^{\,2}}\,\frac{\mathrm{i}\,e}{2\,m}\,\vec\gamma\cdot\vec E\right\rangle\Bigg\}. \end{aligned} \tag{54}$$

The corresponding correction to the g factor is

$$g^{(2)}_{1B} = -\frac{2}{3}\,[F^{(1)}_2(0)]^2\,\frac{(Z\,\alpha)^4}{n^3}. \tag{55}$$

The other contributions due to the two-loop form factors are immediately obtained from the corresponding one-loop expressions in Eqs. (22), (24) and (26)

$$g^{(2)}_{1C} = -\,[F'^{(2)}_1(0)+2\,F'^{(2)}_2(0)]\,\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle\,, \tag{56}$$

$$g^{(2)}_{1D} = 2\,(3-8\,\varepsilon)\,F'^{(2)}_1(0)\,\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle\,, \tag{57}$$

$$g^{(2)}_{1E} = -\,(1-4\,\varepsilon)\,F'^{(2)}_1(0)\,\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle\,. \tag{58}$$

The second-order corrections involving the slope of the one-loop form factors and the one-loop anomalous magnetic moment vanish. It becomes clear if we notice that the coupling of the anomalous magnetic moment to the magnetic field, as obtained from the Hamiltonian (16), is

$$\begin{aligned}\delta V =&\frac{e\,\kappa}{8\,m^3}\,\Big[p^2\,\sigma^{ij}\,B^{ij}+2\,p^k\,\sigma^{ki}\,B^{ij}\,p^j \\ &-2\,m\,\frac{V'}{r}\,\sigma^{ij}\,r^j\,B^{ik}\,r^k\Big]\end{aligned} \tag{59}$$

and for S-states

$$\delta V = \frac{d-2}{d}\,\frac{e\,\kappa}{4\,m^2}\,\sigma^{ij}\,B^{ij}\,\left[\frac{\vec p^{\,2}}{2\,m}-\frac{Z_\epsilon\,\alpha}{r^{1-2\,\epsilon}}\right]. \tag{60}$$

All other possible two-loop corrections, which involve one-loop form-factors, are of higher order in the $Z\,\alpha$ expansion. Therefore, the total form-factor contribution is given by the sum

$$g^{(2)}_1 \;=\; g^{(2)}_{1A}+g^{(2)}_{1B}+g^{(2)}_{1C}+g^{(2)}_{1D}+g^{(2)}_{1E}\,. \tag{61}$$

The second part of Eq. (52) is a high-energy correction that is not accounted for by the form factors. This contribution is induced by the effective Hamiltonian δH in Eq. (17), with E being the electric Coulomb field. The corresponding correction to the g factor is

$$\begin{aligned}g^{(2)}_2 =&4\left(\frac{2}{d}\,\eta^{(2)}+\xi^{(2)}\right)\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle \\ =&\left(-\frac{5}{9\,\varepsilon}+\frac{5455}{972}+\frac{833}{1296}\,\pi^2-\frac{31}{9}\,\pi^2\,\ln 2+\frac{31}{6}\,\zeta(3)\right) \\ &\times\langle 4\,\pi\,Z\,\alpha\,\delta^d(r)\rangle\,.\end{aligned} \tag{62}$$

The third part of Eq. (52) $g^{(2)}_3$ is obtained from the formulas for the one-loop Bethe-logarithm corrections. The overall coefficients in these formulas are modified by the presence of the anomalous magnetic moment κ, in accordance with the corresponding terms in the effective Hamiltonian (16). The resulting corrections to the Hamiltonian describing the interaction with the magnetic field are given by (for S-states)

$$\begin{aligned}\delta^{(2)}_A H =&\frac{e\,\kappa}{8\,m^3}\,[p^2\,\sigma^{ij}\,B^{ij}+2\,p^k\,\sigma^{ki}\,B^{ij}\,p^j] \\ =&\left[\kappa\,\frac{(d-2)}{d}\right]\,\frac{p^2}{8\,m^3}\,e\,\sigma^{ij}\,B^{ij}\,,\end{aligned} \tag{63a}$$

$$\delta^{(2)}_B H =[2\,\kappa]\,\left(-\frac{d-2}{d}\,\frac{e}{8\,m^2}\,V\,\sigma^{ij}\,B^{ij}\right), \tag{63b}$$

$$\delta^{(2)}_C H =[2\,\kappa]\,\frac{e^2}{8\,m^2}\,\sigma^{ij}\,E^j\,B^{ik}\,r^k\,, \tag{63c}$$

$$\delta^{(2)}_D H =[2\,\kappa]\,\left(-\frac{e}{4\,m^2}\,\sigma^{ij}\,E^i\,p^j\right)-\frac{e}{4\,m}\,L^{ij}\,B^{ij}\,, \tag{63d}$$

$$\delta^{(2)}_E H =[\kappa]\,\left(-\frac{e}{4\,m}\,\sigma^{ij}\,r^k\,B^{ij}_{,k}\right)-\frac{e}{4\,m}\,L^{ij}\,B^{ij}\,, \tag{63e}$$

$$\delta^{(2)}_F H =[2\,\kappa]\,\frac{1}{8\,m^2}\,\frac{V'}{r}\,\sigma^{ij}\,L^{ij}-\frac{e}{4\,m}\,L^{ij}\,B^{ij}\,. \tag{63f}$$

The resulting two-loop corrections to the g factor are

$$g^{(2)}_{3A} \;=\; \left[\kappa\,\frac{(d-2)}{d}\right]\,g^{(1)}_{3A}\,, \tag{64a}$$

$$g^{(2)}_{3B} \;=\; 2\,\kappa\,g^{(1)}_{3B}\,, \tag{64b}$$

$$g^{(2)}_{3C} \;=\; 2\,\kappa\,g^{(1)}_{3C}\,, \tag{64c}$$

$$g^{(2)}_{3D} \;=\; 2\,\kappa\,g^{(1)}_{3D}\,, \tag{64d}$$

$$g^{(2)}_{3E} \;=\; \kappa\,g^{(1)}_{3E}\,, \tag{64e}$$

$$g^{(2)}_{3F} \;=\; 2\,\kappa\,g^{(1)}_{3F}\,. \tag{64f}$$

The total two-loop Bethe-logarithm contribution is

$$g^{(2)}_3 = g^{(2)}_{3A}+g^{(2)}_{3B}+g^{(2)}_{3C}+g^{(2)}_{3D}+g^{(2)}_{3E}+g^{(2)}_{3F}\,. \tag{65}$$

The last part of Eq. (52) $g^{(2)}_4$ involves the vacuum-polarization correction. The contribution of the diagrams with the closed fermion loop on the self-energy photon is accounted for by the corresponding parts of the electromagnetic form factors F_1, F_2 and η, ξ. The two-loop vacuum polarization correction can be obtained from the correction due to

$F_1'^{(2)}(0)$ by the replacement

$$F_1'^{(2)}(0) \to v^{(2)} = \left(\frac{\alpha}{\pi}\right)^2 \left(-\frac{82}{81} \times \frac{1}{4}\right). \tag{66}$$

The corresponding contribution to the g factor is

$$g_{4A}^{(2)} = -\left(\frac{\alpha}{\pi}\right)^2 \frac{82}{81} \left\langle 4\,\pi\, Z\,\alpha\,\delta^d(r)\right\rangle . \tag{67}$$

The mixed self-energy and vacuum-polarization correction can be obtained in a similar way by the replacement

$$F_2'^{(2)}(0) \to F_2^{(2)}(0)\, v^{(1)} = F_2^{(2)}(0)\, \frac{\alpha}{\pi} \left(-\frac{1}{15}\right). \tag{68}$$

The corresponding contribution to the g factor is

$$g_{4B}^{(2)} = \left(\frac{\alpha}{\pi}\right)^2 \frac{1}{15} \left\langle 4\,\pi\, Z\,\alpha\,\delta^d(r)\right\rangle . \tag{69}$$

The total vacuum-polarization contribution beyond the one accounted for by the form factors and η, ξ is

$$g_4^{(2)} = g_{4A}^{(2)} + g_{4B}^{(2)} . \tag{70}$$

Finally, the complete two-loop correction to the bound-electron g factor is given by the sum of four parts in Eq. (52), which yields

$$\begin{aligned} g^{(2)} \;=\; & \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\,\alpha)^4}{n^3} \left\{ \frac{28}{9}\,\ln[(Z\,\alpha)^{-2}] + \frac{258917}{19440} - \frac{4}{9}\,\ln k_0 - \frac{8}{3}\,\ln k_3 + \frac{113}{810}\,\pi^2 \right. \\ & \left. - \frac{379}{90}\,\pi^2\,\ln 2 + \frac{379}{60}\,\zeta(3) + \frac{1}{n}\left[-\frac{985}{1728} - \frac{5}{144}\,\pi^2 + \frac{5}{24}\,\pi^2\,\ln 2 - \frac{5}{16}\,\zeta(3)\right]\right\}. \end{aligned} \tag{71}$$

The numerical values for $\ln k_0$ and $\ln k_3$ for the first 7 S states are

$$\ln k_0(1S) = 2.984\,128\,556\,, \quad \ln k_3(1S) = 3.272\,806\,545\,, \tag{72a}$$

$$\ln k_0(2S) = 2.811\,769\,893\,, \quad \ln k_3(2S) = 3.546\,018\,666\,, \tag{72b}$$

$$\ln k_0(3S) = 2.767\,663\,612\,, \quad \ln k_3(3S) = 3.881\,960\,979\,, \tag{72c}$$

$$\ln k_0(4S) = 2.749\,811\,840\,, \quad \ln k_3(4S) = 4.178\,190\,961\,, \tag{72d}$$

$$\ln k_0(5S) = 2.740\,823\,727\,, \quad \ln k_3(5S) = 4.433\,243\,558\,, \tag{72e}$$

$$\ln k_0(6S) = 2.735\,664\,206\,, \quad \ln k_3(6S) = 4.654\,608\,237\,, \tag{72f}$$

$$\ln k_0(7S) = 2.732\,429\,129\,, \quad \ln k_3(7S) = 4.849\,173\,615\,, \tag{72g}$$

The total numerical value of the nonlogarithmic term in Eq. (71) for the $1S$ state is $-16.436\,842$. All terms involving the closed fermion loop contribute $-3.278\,177$ to this result, with the dominant contribution originating from the two-loop vacuum-polarization correction $g_{4A}^{(2)}$.

V. RESULTS AND DISCUSSION

In Table I, we collect all contributions available for the $1S$ bound-electron g factor in three specific hydrogenlike ions which are important from an experimental point of view. For two of them, carbon and oxygen, accurate experimental results are presently available [4, 5], whereas the experiment on calcium is planned for the future [27].

The errors of the point-nucleus Dirac value and of the free part of the one-loop QED correction indicated in the table originate from the uncertainty of the fine-structure constant, $\alpha^{-1} = 137.035\,999\,11(46)$ [2]. The finite-nuclear-size correction was re-evaluated in this work using the most recent values for the root-mean-square (rms) nuclear radii [28]. The error ascribed to this correction originates both from the uncertainty of the rms radius and from the estimated model dependence for the nuclear-charge distribution.

The one-loop QED correction up to the order of $(Z\,\alpha)^4$ is given by the sum of the self-energy part [Eq. (51)] and the vacuum-polarization part [29],

$$g_{\rm VP}^{(1)} = \frac{\alpha}{\pi}\,(Z\,\alpha)^4 \left(-\frac{16}{15}\right). \tag{73}$$

The higher-order one-loop self-energy correction was inferred from the results of the all-order numerical calculation [10, 11]. For carbon and oxygen, the results presented in the table were obtained in Ref. [20] by an extrapolation of the numerical results [10] for $Z > 8$, after subtracting the known terms of the $Z\alpha$ expansion. The one-loop vacuum-polarization correction consists of two parts, the electric-loop contribution that is due to the vacuum-polarization insertion into the electron line and the magnetic-loop contribution, which corresponds to the insertion of the vacuum-polarization loop into the interaction with the external magnetic field. The values for the higher-order electric-loop contribution presented in the table were inferred from the all-order numerical results of Ref. [30],

TABLE I: Individual contributions to the $1s$ bound-electron g factor. The abbreviations used are as follows: "h.o." stands for a higher-order contribution, "SE" – for the self-energy correction, "VP-EL" – for the electric-loop vacuum-polarization correction, "VP-ML" – for the magnetic-loop vacuum-polarization correction, "TW" indicates the results obtained in this work. $\langle r^2\rangle^{1/2}$ is the root-mean-square nuclear charge radius.

		$^{12}C^{5+}$	$^{16}O^{7+}$	$^{40}Ca^{19+}$	Ref.
$\langle r^2\rangle^{1/2}$[fm]		2.4703 (22)	2.7013 (55)	3.4764 (10)	[28]
Dirac value (point nucleus)		1.998 721 354 39 (1)	1.997 726 003 06 (2)	1.985 723 203 7 (1)	
Finite nuclear size		0.000 000 000 41	0.000 000 001 55 (1)	0.000 000 113 0 (1)	
1-loop QED	$(Z\alpha)^0$	0.002 322 819 47 (1)	0.002 322 819 47 (1)	0.002 322 819 5	
	$(Z\alpha)^2$	0.000 000 742 16	0.000 001 319 40	0.000 008 246 2	[31]
	$(Z\alpha)^4$	0.000 000 093 42	0.000 000 240 07	0.000 002 510 6	[20]
	h.o., SE	0.000 000 008 28	0.000 000 034 43 (1)	0.000 003 107 7 (2)	[10]+[20]
	h.o., VP-EL	0.000 000 000 56	0.000 000 002 24	0.000 000 172 7	[30]
	h.o., VP-ML	0.000 000 000 04	0.000 000 000 16	0.000 000 014 6	[13]
≥2-loop QED	$(Z\alpha)^0$	−0.000 003 515 10	−0.000 003 515 10	−0.000 003 515 1	[2]
	$(Z\alpha)^2$	−0.000 000 001 12	−0.000 000 002 00	−0.000 000 012 5	[31]
	$(Z\alpha)^4$	0.000 000 000 06	0.000 000 000 08	−0.000 000 010 9	TW
	h.o.	0.000 000 000 00 (3)	0.000 000 000 00 (11)	0.000 000 000 0 (100)	
Recoil	m/M	0.000 000 087 70	0.000 000 117 07	0.000 000 297 3	[16]
	h.o.	−0.000 000 000 08	−0.000 000 000 10	−0.000 000 000 3	[15]
Total		2.001 041 590 18 (3)	2.000 047 020 32 (11)	1.988 056 946 6 (100)	

whereas the magnetic-loop contribution was taken from the recent evaluation [13].

The $(Z\alpha)^0$ and $(Z\alpha)^2$ parts of the two- and more-loop QED correction comprise the two-, three-, and four-loop contributions to the free-electron g factor, multiplied by a kinematic factor of the electron [31]. The $(Z\alpha)^4$ part of the two-loop QED contribution was derived in the present work. The uncertainty due to higher-order two-loop contributions was estimated as

$$g^{(2)}_{\rm h.o.} = 2\, g^{(1)}_{\rm h.o.}\, \frac{g^{(2)}[(Z\alpha)^2]}{g^{(1)}[(Z\alpha)^2]}\,, \tag{74}$$

where $g^{(n)}_{\rm h.o.}$ is the n-loop higher-order QED contribution and $g^{(n)}[(Z\alpha)^2]$ is the n-loop $(Z\alpha)^2$ QED contribution.

The nuclear recoil correction to first order in the mass ratio m/M but to all order in $Z\alpha$ was calculated in Refs. [14, 16]. The leading recoil corrections to order $(m/M)^2$ and $\alpha\, m/M$ were derived in Refs. [32, 33] for a nuclear spin $I = 1/2$ and recently generalized for an arbitrary nuclear spin in Ref. [15].

Based on the data presented in Table I, we conclude that our evaluation of the one- and two-loop QED corrections to order $(Z\alpha)^4$ improves the accuracy of the theoretical prediction for carbon by an order of magnitude, as compared to the previous compilation [10]. The resulting QED contribution to order $(Z\alpha)^4$ turns out to be rather small for carbon and oxygen, as a result of a cancellation between the logarithmic and the nonlogarithmic parts of this correction [see Eq. (71)]. For calcium, to the contrary, the numerical contribution of the two-loop $(Z\alpha)^4$ correction is large and of the same order as the $(Z\alpha)^2$ correction. This indicates that the perturbative $Z\alpha$-expansion approach is no longer effective in this region of Z, and a direct all-order numerical evaluation would be highly desirable.

It is remarkable that among different sources of the theoretical uncertainty for calcium, the error due to the higher-order two-loop QED correction is by far the dominant one. This means that, if the prospective experimental investigation of the bound-electron g factor in calcium is performed on the same level of accuracy as for carbon, namely 10^{-9}, a comparison of the theoretical and experimental results would allow one to identify the contribution of the non-perturbative (in $Z\alpha$) two-loop QED effects with a 10% accuracy.

The comparison of the theoretical and experimental results for the $1S$ bound-electron g factor in carbon and oxygen yields the presently most accurate method for determination of the electron mass [2]. Based on the theoretical g factor values presented in Table I, we obtain the following values for the electron mass derived from the experiments on carbon [4] and oxygen [5] (in atomic mass units):

$$m(^{12}C^{5+}) = 0.000\,548\,579\,909\,32\,(29)\,, \tag{75}$$

$$m(^{16}O^{7+}) = 0.000\,548\,579\,909\,60\,(41)\,. \tag{76}$$

The uncertainty of these results originates from the experimental value for the ratio of the electronic Larmor precession frequency and the cyclotron frequency of the ion in the trap; the uncertainty due to the theoretical prediction is more than by an order of magnitude smaller and thus negligible.

Acknowledgments

Valuable discussions with W. Quint are gratefully acknowledged. This work was supported by EU grant No. HPRI-CT-2001-50034 and by RFBR grant No. 04-02-17574. A.C. acknowledges the support by Science and Engineering Research Canada. V.A.Y. acknowledges support by the foundation "Dynasty". U.D.J. acknowledges support from the Deutsche Forschungsgemeinschaft via the Heisenberg program.

APPENDIX A: ELECTROMAGNETIC FORM FACTORS

We consider the form factors defined by

$$\gamma_\mu \to \Gamma_\mu = F_1(q^2)\gamma_\mu + \frac{i}{2m} F_2(q^2) \left(\frac{i}{2}\right) [\not{q}, \gamma_\mu] \,, \quad \text{(A1)}$$

where q is the outgoing photon momentum. The form factors are expanded in α up to second order,

$$\begin{aligned} F_1(q^2) &= 1 + F_1^{(1)}(q^2) + F_1^{(2)}(q^2) \,, \\ F_2(q^2) &= F_2^{(1)}(q^2) + F_2^{(2)}(q^2), \end{aligned} \quad \text{(A2)}$$

where the superscript corresponds to the loop order, i.e. to the power of α. They have recently been calculated analytically by Bonciani, Mastrolia and Remiddi in [34]. The results for the form factors expanded into powers of q^2 up to q^4 read (in $D = 4 - 2\varepsilon$):

$$F_1^{(1)}(q^2) = \frac{\alpha}{\pi} \left[q^2 \left(-\frac{1}{8} - \frac{1}{6\varepsilon} - \frac{1}{2}\varepsilon \right) + q^4 \left(-\frac{11}{240} - \frac{1}{40\varepsilon} - \frac{5}{48}\varepsilon \right) \right] , \quad \text{(A3a)}$$

$$F_2^{(1)}(q^2) = \frac{\alpha}{\pi} \left[\frac{1}{2} + 2\varepsilon + q^2 \left(\frac{1}{12} + \frac{5}{12}\varepsilon \right) + q^4 \left(\frac{1}{60} + \frac{11}{120}\varepsilon \right) \right] , \quad \text{(A3b)}$$

$$\begin{aligned} F_1^{(2)}(q^2) = {} & \left(\frac{\alpha}{\pi}\right)^2 \left\{ q^2 \left[\left(-\frac{1099}{1296} + \frac{77}{144}\zeta(2) \right)_{\rm VP} - \frac{47}{576} + 3\,\zeta(2)\,\ln 2 - \frac{175}{144}\zeta(2) - \frac{3}{4}\zeta(3) \right] \right. \quad \text{(A3c)} \\ & \left. + q^4 \left[\left(-\frac{491}{1440} + \frac{5}{24}\zeta(2) \right)_{\rm VP} + \frac{1721}{12960} + \frac{1}{72\,\varepsilon^2} + \frac{1}{48\,\varepsilon} + \frac{11}{10}\zeta(2)\,\ln 2 - \frac{14731}{28800}\zeta(2) - \frac{11}{40}\zeta(3) \right] \right\} , \end{aligned}$$

$$\begin{aligned} F_2^{(2)}(q^2) = {} & \left(\frac{\alpha}{\pi}\right)^2 \left\{ \left(\frac{119}{36} - 2\zeta(2) \right)_{\rm VP} - \frac{31}{16} - 3\,\zeta(2)\,\ln 2 + \frac{5}{2}\zeta(2) + \frac{3}{4}\zeta(3) \right. \\ & + q^2 \left[\left(\frac{311}{216} - \frac{7}{8}\zeta(2) \right)_{\rm VP} - \frac{77}{80} - \frac{1}{12\,\varepsilon} - \frac{23}{10}\zeta(2)\,\ln 2 + \frac{61}{40}\zeta(2) + \frac{23}{40}\zeta(3) \right] \\ & \left. + q^4 \left[\left(\frac{533}{1080} - \frac{3}{10}\zeta(2) \right)_{\rm VP} - \frac{1637}{5040} - \frac{19}{720\,\varepsilon} - \frac{15}{14}\zeta(2)\,\ln 2 + \frac{689}{1050}\zeta(2) + \frac{15}{56}\zeta(3) \right] \right\} . \end{aligned} \quad \text{(A3d)}$$

The subscript VP denotes the contribution to the two-loop form factors which involves a closed fermion loop.

APPENDIX B: THE LOW-ENERGY LIMIT OF THE SCATTERING AMPLITUDE

In this section we describe the evaluation of the low-energy limit of the spin-dependent part of the scattering amplitude that gives rise to the effective Hamiltonian (17). The scattering amplitude under consideration is schematically depicted in Fig. 1, where the leftmost graph is the "tree" diagram and the remaining graphs represent the tree diagram "dressed" by a self-energy photon. The two-loop diagrams are not shown explicitly; they can be obtained from the one-photon ones in a standard way. Each graph contains two interactions with the external field, one of which is the interaction with the homogeneous magnetic field (a γ^i vertex) and the other is the interaction with the Coulomb field of the nucleus (a γ^0 vertex). From the one- and two-loop scattering amplitudes we additionally subtract a tree amplitude with the vertices modified by the electromagnetic form factors F_1 and F_2. This procedure removes the part that is already accounted for by the Hamiltonian (16) and leads to a simple polynomial expression for the resulting amplitude.

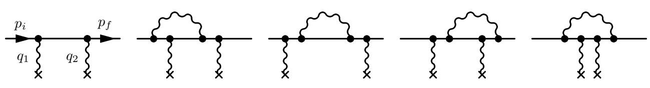

FIG. 1: Feynman diagrams representing the scattering amplitude of a free electron on both the Coulomb and the magnetic field, at the tree and the one-loop level.

In order to extract the spin dependent part of the scattering amplitude, we construct the projection operator. Let us first consider a general non-relativistic operator Q,

$$Q = Q^0 + Q^i\,\sigma^i \,. \quad \text{(B1)}$$

The spin-dependent part of Q can be retrieved by the following projection operator:

$$Q^i = \frac{1}{2}\,{\rm Tr}[Q\,\sigma^i] \,. \quad \text{(B2)}$$

In d dimensions, the nonrelativistic expansion of the Hamiltonian involves $\sigma^{ij} = [\sigma^i, \sigma^j]/(2\,\mathrm{i})$. The extension of the spin-projection operator to an arbitrary number of dimensions is

$$Q^{ij} = \frac{1}{4}\,\mathrm{Tr}[Q\,\sigma^{ij}]\,, \tag{B3}$$

with $Q = Q^{ij}\,\sigma^{ij}$. We assume here the following properties of the trace to hold:

$$\begin{aligned}\mathrm{Tr}[\sigma^{ij}] &= 0\,,\\ \mathrm{Tr}[\mathrm{I}] &= 2\,,\\ \mathrm{Tr}[\sigma^{ij}\,\sigma^{kl}] &= 2\,(\delta^{ik}\,\delta^{jl} - \delta^{jk}\,\delta^{il})\,.\end{aligned} \tag{B4}$$

We now consider the operator Q sandwiched between the positive-energy solutions of the free Dirac equation normalized by $\bar{u}\,u = 1$. The following identity holds,

$$\bar{u}(p_\mathrm{f}, s_\mathrm{f})\,Q\,u(p_\mathrm{i}, s_\mathrm{i}) = \mathrm{Tr}[Q\,u(p_\mathrm{i}, s_\mathrm{i})\,\bar{u}(p_\mathrm{f}, s_\mathrm{f})]\,. \tag{B5}$$

Since our aim is to calculate the low-energy limit of the amplitude only, we can use an approximate form for $u(p,s)$,

$$u(p,s) \approx \begin{pmatrix} \phi(s) \\ \frac{1}{2}\,\vec{\sigma}\cdot\vec{p}\,\phi(s)\end{pmatrix}\,, \tag{B6}$$

where ϕ is a nonrelativistic spinor. Using a replacement that extracts the spin dependence

$$\phi(s_\mathrm{i})\,\phi^{+}(s_\mathrm{f}) \to \frac{\sigma^{ij}}{4}\,, \tag{B7}$$

the projection operator becomes (in units $m = 1$)

$$\begin{aligned}u(p_\mathrm{i}, s_\mathrm{i})\,\bar{u}(p_\mathrm{f}, s_\mathrm{f}) &\to \frac{1}{4}\begin{pmatrix}\sigma^{ij}, & -\frac{1}{2}\,\sigma^{ij}\,\vec{\sigma}\cdot\vec{p}_\mathrm{f}\\ \frac{1}{2}\,\vec{\sigma}\cdot\vec{p}_\mathrm{i}\,\sigma^{ij}, & -\frac{1}{4}\,\vec{\sigma}\cdot\vec{p}_\mathrm{i}\,\sigma^{ij}\,\vec{\sigma}\cdot\vec{p}_\mathrm{f}\end{pmatrix}\\ &\approx \frac{1}{16}\,(\not{p}_\mathrm{i}+1)\,\Sigma^{ij}\,(\not{p}_\mathrm{f}+1)\,.\end{aligned} \tag{B8}$$

Therefore,

$$Q^{ij} = \frac{1}{16}\,\mathrm{Tr}\left[(\not{p}_\mathrm{f}+1)\,Q\,(\not{p}_\mathrm{i}+1)\,\Sigma^{ij}\right]\,. \tag{B9}$$

We now turn to the scattering amplitude of the free electron on the Coulomb and magnetic fields. The spin-dependent part of this amplitude is written as

$$Q = Q^{\mu\nu\rho}\,e\,A_0(q_1)\,e\,A_\mu(q_2)\,\sigma_{\nu\rho}\,, \tag{B10}$$

where q_1 and q_2 denote the exchange momenta. The amplitude corresponding to the tree diagram in Fig. 1 is given by

$$\begin{aligned}Q_0^{\mu\nu\rho} = \frac{1}{16}\,\mathrm{Tr}\Bigg[&(\not{p}_\mathrm{f}+1)\,\gamma^0\,\frac{1}{\not{p}_\mathrm{i}+\not{q}_2-1}\,\gamma^\mu\,(\not{p}_\mathrm{i}+1)\,\Sigma^{\nu\rho}\\ &+(\not{p}_\mathrm{f}+1)\,\gamma^\mu\,\frac{1}{\not{p}_\mathrm{i}+\not{q}_1-1}\,\gamma^0\,(\not{p}_\mathrm{i}+1)\,\Sigma^{\nu\rho}\Bigg]\,,\end{aligned} \tag{B11}$$

where the momenta p_i, p_f are on the mass shell, and the exchange momenta are spatial, $q_1^0 = q_2^0 = 0$.

As an example of one-photon contributions, we give an expression for the rightmost diagram in Fig. 1,

$$\begin{aligned}Q_1^{\mu\nu\rho} = -i\,e^2\int\frac{d^Dk}{(2\,\pi)^D}\,\frac{1}{k^2}\,\frac{1}{16}\,\mathrm{Tr}\Bigg[&(\not{p}_\mathrm{f}+1)\,\gamma^\sigma\\ &\times\frac{1}{\not{p}_\mathrm{f}-\not{k}-1}\,\gamma^0\,\frac{1}{\not{p}_\mathrm{i}+\not{q}_2-\not{k}-1}\,\gamma^\mu\,\frac{1}{\not{p}_\mathrm{i}-\not{k}-1}\\ &\times\gamma_\sigma(\not{p}_\mathrm{i}+1)\,\Sigma^{\nu\rho}\Bigg] + \text{symmetrization}\,.\end{aligned} \tag{B12}$$

The other one- and two-loop contributions are obtained in the analogous way. From the resulting amplitude we subtract the tree amplitude $Q_F^{\mu\nu\rho}$ with vertices γ^α replaced by Γ^α,

$$\begin{aligned}Q_F^{\mu\nu\rho} &=\\ \frac{1}{16}\,\mathrm{Tr}\Bigg[&(\not{p}_\mathrm{f}+1)\,\Gamma^0(q_1)\,\frac{1}{\not{p}_\mathrm{i}+\not{q}_2-1}\,\Gamma^\mu(q_2)\,(\not{p}_\mathrm{i}+1)\,\Sigma^{\nu\rho}\\ &+(\not{p}_\mathrm{f}+1)\,\Gamma^\mu(q_2)\,\frac{1}{\not{p}_\mathrm{i}+\not{q}_1-1}\,\Gamma^0(q_1)\,(\not{p}_\mathrm{i}+1)\,\Sigma^{\nu\rho}\Bigg]\,,\end{aligned} \tag{B13}$$

where Γ^α is defined in Eq. (A1). The final expression for the total amplitude $Q^{\mu\nu\rho}$ is obtained by the expansion in small momenta $\vec{p}_\mathrm{i}\,, \vec{p}_\mathrm{f}$ and the subsequent integration over the loop momenta. The result for $Q^{\mu\nu\rho}$ can be written in the form

$$Q^{\mu\nu\rho} = \frac{1}{2}\,[\eta\,\mathcal{F}^{\mu\nu\rho} + \xi\,\mathcal{G}^{\mu\nu\rho}]\,, \tag{B14}$$

where the functions $\mathcal{F}^{\mu\nu\rho}$ and $\mathcal{G}^{\mu\nu\rho}$ are orthogonal to q_2^μ (due to the gauge invariance) and antisymmetric in ν, ρ. Their explicit expressions are

$$\begin{aligned}\mathcal{F}^{\mu\nu\rho} &= q_1^\mu\,(q_1^\rho q_2^\nu - q_1^\nu q_2^\rho) + q_1\cdot q_2\,(g^{\mu\rho}q_1^\nu - g^{\mu\nu}q_1^\rho)\,,\\ \mathcal{G}^{\mu\nu\rho} &= q_1^2\,(g^{\mu\rho}q_2^\nu - g^{\mu\nu}q_2^\rho)\,.\end{aligned} \tag{B15}$$

The results for the coefficient functions η and ξ have been obtained with the help of the symbolic program *FORM* [35] and read

$$\begin{aligned}\eta = &-\frac{\alpha}{4\pi}\,\frac{2}{3\varepsilon} + \left(\frac{\alpha}{4\pi}\right)^2\Bigg[\left(\frac{2528}{81} - \frac{169}{54}\pi^2\right)_{\mathrm{VP}}\\ &-\frac{283}{10} + \frac{169}{120}\,\pi^2 - \frac{4}{15}\,\pi^2\ln 2 + \frac{2}{5}\,\zeta(3) - \frac{16}{3\varepsilon}\Bigg]\,,\end{aligned} \tag{B16}$$

$$\begin{aligned}\xi = &\frac{\alpha}{4\pi}\left(1 + \frac{2}{3\varepsilon}\right) + \left(\frac{\alpha}{4\pi}\right)^2\Bigg[\left(\frac{2674}{81} - \frac{91}{27}\pi^2\right)_{\mathrm{VP}}\\ &-\frac{152}{15} + \frac{319}{45}\,\pi^2 - \frac{68}{5}\,\pi^2\ln 2 + \frac{102}{5}\,\zeta(3) + \frac{4}{3\varepsilon}\Bigg]\,,\end{aligned} \tag{B17}$$

where the subscript VP denotes the contribution involving a closed fermion loop. The effective local operator Q in Eq. (B10) becomes

$$\begin{aligned}Q = \;&\frac{1}{2}\,[\eta\,\mathcal{F}^{\mu\nu\rho} + \xi\,\mathcal{G}^{\mu\nu\rho}]\;e\,A_0(q_1)\,e\,A_\mu(q_2)\,\sigma_{\nu\rho}\\ \to\;&\frac{e^2}{2\,m}\,\left[2\,\sigma^{ij}\,B^{ik}\,\nabla^j E^k\,\eta + \sigma^{ij}B^{ij}\,\nabla^k E^k\,\xi\right]\,,\end{aligned} \tag{B18}$$

which corresponds to the effective Hamiltonian in Eq. (17).

[1] V. W. Hughes and T. Kinoshita, Rev. Mod. Phys. **71**, 133 (1999).
[2] P. J. Mohr and B. N. Taylor, Rev. Mod. Phys. **77**, 1 (2005).
[3] T. Beier, H. Häffner, N. Hermanspahn, S. G. Karshenboim, H.-J. Kluge, W. Quint, S. Stahl, J. Verdú, and G. Werth, Phys. Rev. Lett. **88**, 011603 (2002).
[4] H. Häffner, T. Beier, N. Hermanspahn, H.-J. Kluge, W. Quint, S. Stahl, J. Verdú, and G. Werth, Phys. Rev. Lett. **85**, 5308 (2000).
[5] J. Verdú, S. Djekic, S. Stahl, T. Valenzuela, M. Vogel, G. Werth, T. Beier, H.-J. Kluge, and W. Quint, Phys. Rev. Lett. **92**, 093002 (2004).
[6] G. Breit, Nature (London) **122**, 649 (1928).
[7] S. A. Blundell, K. T. Cheng, and J. Sapirstein, Phys. Rev. A **55**, 1857 (1997).
[8] H. Persson, S. Salomonson, P. Sunnergren, and I. Lindgren, Phys. Rev. A **56**, R2499 (1997).
[9] T. Beier, I. Lindgren, H. Persson, S. Salomonson, P. Sunnergren, H. Häffner, and N. Hermanspahn, Phys. Rev. A **62**, 032510 (2000).
[10] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Phys. Rev. Lett. **89**, 143001 (2002).
[11] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Phys. Rev. A **69**, 052503 (2004).
[12] S. G. Karshenboim and A. I. Milstein, Phys. Lett. B **549**, 321 (2002).
[13] R. N. Lee, A. I. Milstein, I. S. Terekhov, and S. G. Karshenboim, Phys. Rev. A **71**, 052501 (2005).
[14] V. M. Shabaev, Phys. Rev. A **64**, 052104 (2001).
[15] A. P. Martynenko and R. N. Faustov, Zh. Eksp. Teor. Fiz. **120**, 539 (2001) [JETP **93**, 471 (2001)].
[16] V. M. Shabaev and V. A. Yerokhin, Phys. Rev. Lett. **88**, 091801 (2002).
[17] A. V. Nefiodov, G. Plunien, and G. Soff, Phys. Rev. Lett. **89**, 081802 (2002).
[18] D. A. Glazov, V. M. Shabaev, I. I. Tupitsyn, A. V. Volotka, V. A. Yerokhin, G. Plunien, and G. Soff, Phys. Rev. A **70**, 062104 (2004).
[19] D. L. Moskovkin, N. S. Oreshkina, V. M. Shabaev, T. Beier, G. Plunien, W. Quint, and G. Soff, Phys. Rev. A **70**, 032105 (2004).
[20] K. Pachucki, U. D. Jentschura, and V. A. Yerokhin, Phys. Rev. Lett. **93**, 150401 (2004); erratum Phys. Rev. Lett. **94**, 229902(E) (2005).
[21] A. Czarnecki, K. Melnikov, and A. Yelkhovsky, Phys. Rev. Lett. **82**, 311 (1999).
[22] V. Korobov and A. Yelkhovsky, Phys. Rev. Lett. **87**, 193003 (2001).
[23] C. Itzykson and J. B. Zuber, *Quantum Field Theory*, McGraw-Hill, New York, 1980.
[24] K. Pachucki, Phys. Rev. A **69**, 052502 (2004).
[25] V. M. Shabaev, J. Phys. B **24**, 4479 (1991).
[26] V. M. Shabaev, in *Precision Physics of Simple Atomic Systems*, ed. by S. G. Karshenboim and V. B. Smirnov, Springer, Berlin, 2003, p. 97.
[27] W. Quint, private communication (2004).
[28] I. Angeli, At. Data Nucl. Data Tables **87**, 185 (2004).
[29] S. G. Karshenboim, Phys. Lett. A **266**, 380 (2000).
[30] T. Beier, Physics Reports **339**, 79 (2000).
[31] H. Grotch, Phys. Rev. Lett. **24**, 39 (1970).
[32] H. Grotch, Phys. Rev. A **2**, 1605 (1970).
[33] R. Faustov, Phys. Lett. B **33**, 422 (1970).
[34] R. Bonciani, P. Mastrolia and E.Remiddi, Nucl.Phys. **B661**, 289 (2003); Erratum-ibid. **B702** 359 (2004).
[35] J.A.M. Vermaseren, math-ph/0010025.