Nonrelativistic QED Approach to the Bound-Electron g Factor

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Within a systematic approach based on nonrelativistic quantum electrodynamics, we derive the one-loop self-energy correction of order $\alpha(Z\alpha)^4$ to the bound-electron g factor. In combination with numerical data, this analytic result improves theoretical predictions for the self-energy correction for carbon and oxygen by an order of magnitude. Basing on one-loop calculations, we obtain the logarithmic two-loop contribution of order $\alpha^2(Z\alpha)^4 \ln[(Z\alpha)^{-2}]$ and the dominant part of the corresponding constant term. The results obtained improve the accuracy of the theoretical predictions for the $1S$ bound-electron g factor and influence the value of the electron mass determined from g-factor measurements.

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There has been significant progress in experimental investigations of the bound-electron g factor during recent years [1,2]. The g-factor value in these measurements is obtained from the ratio of the electronic Larmor precession frequency ω_{L} and the cyclotron frequency of the ion in the trap ω_{c}, according to

$$\frac{\omega_{\mathrm{L}}}{\omega_{\mathrm{c}}} = \frac{g}{2}\frac{|e|}{q}\frac{m_{\mathrm{ion}}}{m}, \tag{1}$$

where e is the elementary charge, q is the charge of the ion, m_{ion} is the ion mass, and m is the electron mass. The present accuracy of the experimental results for carbon and oxygen is already below the 1 part per billion level and is likely to be improved in the near future. In order to match the experimental precision, accurate calculations of the one-loop self-energy [3–6], vacuum-polarization [4,7], and nuclear-recoil [8,9] corrections have been performed during the last decade. An important result of these studies is the possibility to extract the electron mass from the experimental value for ω_L/ω_c according to Eq. (1). Such a determination was presented in Refs. [2,5,10] based on the experimental result for H-like carbon and oxygen. It provided an improvement of the accuracy of the electron mass by a factor of 4, as compared to the previous value based on measurements involving protons and electrons in Penning traps [11]. As a result, the present recommended value for the electron mass [12] is derived mainly from the bound-electron g factor.

The current uncertainty of the theoretical values for the g factor in H-like carbon and oxygen originates predominately from the two-loop binding QED correction. This correction is presently known [13] only to its leading order in $Z\alpha$, namely $\alpha^2(Z\alpha)^2$, the corresponding contribution being of pure kinematical origin. The next correction enters in order $\alpha^2(Z\alpha)^4$ and results from nontrivial two-loop binding QED effects that have not been addressed theoretically up to now.

The goal of the present investigation is to formulate an approach for the systematic derivation of higher-order QED corrections to the g factor of a bound electron. Applicability of this approach is demonstrated for the one-loop self-energy correction, for which direct numerical calculations to all orders in $Z\alpha$ are available. The analytical contribution derived here is used in order to reduce the uncertainty of the numerical results for carbon and oxygen by an order of magnitude. The developed method is then applied to the evaluation of the two-loop self-energy correction. We derive the complete result for the logarithmic contribution of order $\alpha^2(Z\alpha)^4 \ln[(Z\alpha)^{-2}]$ and a large part of the corresponding constant term. The results obtained improve the accuracy of the theoretical values for the $1S$ bound-electron g factor in carbon and oxygen and influence the electron-mass determination derived from the corresponding experimental results.

The computational approach is based on the Dirac-Coulomb Hamiltonian that is modified by the presence of the free-electron form factors F_1 and F_2 [14],

$$H = \alpha \cdot [\mathbf{p} - eF_1(\Delta)\mathbf{A}] + \beta m + eF_1(\Delta)A_0 + F_2(\Delta)\frac{e}{2m}(\mathrm{i}\gamma \cdot \mathbf{E} - \beta\Sigma \cdot \mathbf{B}), \tag{2}$$

where Δ denotes the Laplacian operator. This Hamiltonian accounts only partly for the interaction of the electron with high-frequency photons. The remaining high-energy contribution can be represented as a local type of effective interaction. It is obtained by matching the low-energy limit of scattering amplitudes derived from the Hamiltonian (2) and from full QED in a way that will be discussed below.

In the calculation of electron self-energy corrections, it is often convenient to evaluate contributions due to the high- and the low-energy virtual photons separately. The separation is achieved by introducing a certain cut-off parameter, which in our calculation is chosen to be the photon mass. The low-energy part is then identified as the

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difference of the contributions with the massless and the massive photons. In order to calculate it, we perform the Foldy-Wouthuysen transformation of the Hamiltonian H followed by the Power-Zienau transformation, as described in Ref. [15],

$$H_{\rm PZ} = \frac{\mathbf{p}^2}{2m} - \frac{Z\alpha}{r} - e\mathbf{r}\cdot\mathbf{E} - \frac{e}{2m}(1+\kappa)\sigma\cdot\mathbf{B} - \frac{e}{2m}\mathbf{L}\cdot\mathbf{B} + \frac{Z\alpha}{4m^2}(1+2\kappa)\frac{\sigma\cdot\mathbf{L}}{r^3} + \frac{p^2}{4m^3}e\sigma\cdot\mathbf{B} + \frac{e\kappa}{4m^3}(\mathbf{p}\cdot\sigma)(\mathbf{p}\cdot\mathbf{B}) - \frac{e(1+\kappa)}{2m}\sigma^i r^j \partial_j B^i - \frac{e(1+2\kappa)}{4m^2}\sigma\cdot\mathbf{E}\times\mathbf{p} - \frac{e(1+2\kappa)}{8m^2}(\sigma\times\mathbf{E})\cdot(\mathbf{r}\times\mathbf{B}) - \frac{e(1+2\kappa)}{8m^2}\frac{Z\alpha}{r^3}(\mathbf{r}\times\sigma)\cdot(\mathbf{r}\times\mathbf{B}). \quad (3)$$

Here, $\mathbf{E} = \mathbf{E}|_{\mathbf{r}=\mathbf{0}}$, $\mathbf{B} = \mathbf{B}|_{\mathbf{r}=\mathbf{0}}$, and $\kappa \equiv F_2(0)$. In the Hamiltonian $H_{\rm PZ}$ we neglected the spin independent terms and the Δ dependence of the form factors. Moreover, the terms with κ will be needed only in the two-loop calculation.

We consider now the one-loop self-energy contribution to the bound-electron g factor. It is represented by the sum of three parts, $\delta g^{(1)} = g_1^{(1)} + g_2^{(1)} + g_3^{(1)}$. The first part comes from the free-electron form factors in the Hamiltonian H, the second part is due to an additional term that matches scattering amplitudes, and the third part is a low-energy-photon contribution that originates from the Hamiltonian $H_{\rm PZ}$ and is very similar to the Bethe logarithm in the hydrogen Lamb shift. All these parts are calculated in the following.

Form-factor contribution.—We evaluate this part by separating the Hamiltonian (2) into the unperturbed (Dirac) Hamiltonian and the interaction part and applying the standard Rayleigh-Schrödinger perturbation theory. Taking into account that only the first two terms in the Δ expansion of form factors contribute to the order of interest, we write the interaction Hamiltonian as

$$\delta H = \frac{e\kappa}{2m}(i\gamma\cdot\mathbf{E} - \beta\Sigma\cdot\mathbf{B}) + eF_1'(0)\Delta A_0 + \frac{ie}{2m}F_2'(0)\Delta(\gamma\cdot\mathbf{E}), \quad (4)$$

where the slope of the form factors are known to be $F_1'(0) = \frac{\alpha}{2\pi}(-1/4 - 2/3\ln\mu)$ and $F_2'(0) = \alpha/(12\pi)$, where μ is the ratio of the photon mass to the electron mass. Applying perturbation theory in first and second orders and separating contributions linear in the magnetic field, we obtain the correction to the g factor of an nS state,

$$g_1^{(1)} = \frac{\alpha}{\pi}\left[1 + \frac{(Z\alpha)^2}{6n^2} - \frac{(Z\alpha)^4}{n^3}\left(\frac{7}{6} + \frac{5}{24n} + \frac{16}{3}\ln\mu\right)\right]. \quad (5)$$

Spin-dependent scattering amplitude.—It represents a high-energy contribution which goes beyond the on-shell form-factor treatment. Here we only sketch the idea of the derivation; the details will be presented elsewhere. We first introduce the skeleton amplitude of the free-electron scattering off both the Coulomb and the magnetic external field. Then we add an electron self-energy loop inserted into the skeleton diagram in all possible ways. Infrared divergences present in loop-momentum integration are regularized by employing the photon mass. Next, we subtract the skeleton amplitude with vertices modified by the electron form factors F_1 and F_2, expand in all external momenta, and keep terms of the third power in external momenta only. The resulting amplitude can be represented by the following effective-interaction Hamiltonian ($\mathbf{B}$ = const)

$$\delta H_2 = \frac{\alpha}{\pi}\left[\frac{e^2}{4}\sigma_i B_i \partial_j E_j + \frac{e^2}{3}\ln\mu\,\sigma_i B_j \partial_i E_j\right]. \quad (6)$$

The corresponding contribution to the g factor reads:

$$g_2^{(1)} = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3}\left(4 + \frac{16}{9}\ln\mu\right). \quad (7)$$

Low-energy part.—This contribution is induced by the virtual photon of low energy. We first recall the expression for the low-energy part of the Lamb shift,

$$\delta E_L = \frac{2\alpha}{3\pi}\int dk k^3 \langle\phi|\mathbf{r}\frac{1}{E - H_S - k}\mathbf{r}|\phi\rangle = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3}\frac{4}{3}\left[\ln\frac{\mu}{(Z\alpha)^2} + \frac{5}{6} - \ln k_0\right], \quad (8)$$

where H_S is the Schrödinger Hamiltonian. In the above, we assume the implicit difference between massless and massive photons and keep only the terms that do not vanish when $\mu \to 0$. In practice, one calculates this with a cut-off $k < \epsilon$ and later performs the replacement $\ln 2\epsilon \to \ln\mu + 5/6$ [14]. We mention that this replacement is not unique and its specific form depends on the actual integrand. Equation (8) coincides with the standard definition of the Bethe logarithm $\ln k_0$, which has the explicit values $\ln k_0(1S) = 2.984\,128\,555$ and $\ln k_0(2S) = 2.811\,769\,893$.

Here, we are interested in all possible relativistic corrections to Eq. (8) induced by the Hamiltonian $H_{\rm PZ}$ which are linear in the $\mathbf{B}$ field. There are six such corrections presented in Table I. The terms involving $\mathbf{E}$ and $\partial_j B^i$ represent corrections to the vertex $(-e\mathbf{r}\cdot\mathbf{E})$, and the others yield corrections to H, E, and ϕ. The results listed in the third column of Table I involve the standard Bethe logarithm $\ln k_0$ and its modification $\ln k_3$ defined as

$$\int dk k^2 \langle\phi|\mathbf{r}\frac{1}{E - H_S - k}\frac{1}{r^3}\frac{1}{E - H_S - k}\mathbf{r}|\phi\rangle = -4\frac{(Z\alpha)^3}{n^3}\left[\ln\frac{\mu}{(Z\alpha)^2} + \frac{5}{6} - \ln k_3\right]. \quad (9)$$

We calculate $\ln k_3$ numerically, using a finite-difference representation of the Schrödinger Hamiltonian H_S, and obtain the following results for the $1S$ and $2S$ states: $\ln k_3(1S) = 3.272\,806\,545$ and $\ln k_3(2S) = 3.546\,018\,666$. Finally, we present the sum of all six contributions from Table I as

$$g_3^{(1)} = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3}\frac{32}{9}\left[\ln\frac{\mu}{(Z\alpha)^2} - \frac{5}{12} - \frac{\ln k_0}{4} - \frac{3}{4}\ln k_3\right]. \quad (10)$$

Two-loop contribution.—The complete two-loop self-energy of order $(Z\alpha)^4$ consists of contributions related to the electron form factors, to the two-photon scattering amplitude, and to the low-energy part. In the present investigation we derive an expression for the low-energy part only. This gives the complete result for the logarithmic contribution of relative order $(Z\alpha)^4$. Moreover, we observe that in the one-loop case, the low-energy part yields the dominating contribution of about 75% of the constant term. Arguably, this is a general feature of all radiative corrections, another example being the hydrogen Lamb shift. We thus assume that also in the two-loop case, the low-energy part provides the dominant contribution to the constant term. A derivation of the remaining two-loop contributions can in principle be carried out along the lines presented above.

Let us now identify the two-loop low-energy correction. When *both* photons are of low energy, the **B**-dependent part is of a higher order and thus negligible. The contribution of interest comes when only *one* photon is of low energy. The second photon effectively modifies the vertex, and only the part with the anomalous magnetic moment is relevant, as the slope of the form factors contributes to higher orders. There are two equivalent contributions obtained by interchanging the photons, which results in an additional factor of 2. The effective Hamiltonian that accounts for the anomalous magnetic moment is given by Eq. (3). The calculation of the Bethe-logarithmic contributions is the same as for the one-loop case, but involves different overall factors for each term, which are listed in the fourth column of Table I. Using the one-loop results, we obtain for the sum of all low-energy contributions,

$$g_3^{(2)} = \left(\frac{\alpha}{\pi}\right)^2\frac{(Z\alpha)^4}{n^3}\left[\frac{56}{9}\ln\frac{\mu}{(Z\alpha)^2} + \frac{44}{27} - \frac{8}{9}\ln k_0 - \frac{16}{3}\ln k_3\right], \quad (11)$$

where the numerical value of the constant term is $a_{40}^{(2)}(1S) = -18.477\,948\,664(1)$ and $a_{40}^{(2)}(2S) = -19.781\,820\,939(1)$. The term with $\ln\mu$ is canceled by corresponding contributions coming from the slope of the form factors and the two-loop scattering amplitude.

Results and discussion.—We first summarize our calculation for the *one-loop* self-energy correction. The total analytic result for an nS state is

$$\delta g^{(1)} = \frac{\alpha}{\pi}\left\{1 + \frac{(Z\alpha)^2}{6n^2} + \frac{(Z\alpha)^4}{n^3}\left[\frac{32}{9}\ln((Z\alpha)^{-2}) + \frac{73}{54} - \frac{5}{24n} - \frac{8}{9}\ln k_0 - \frac{8}{3}\ln k_3\right] + (Z\alpha)^5 G_n(Z)\right\}, \quad (12)$$

where the remainder function $G_n(Z)$ incorporates all contributions of higher orders in $Z\alpha$, and the numerical value of the constant term in order $(Z\alpha)^4$ is $a_{40}^{(1)} = -10.236\,524\,318(1)$ for the $1S$ state and $a_{40}^{(1)} = -10.707\,715\,607(1)$ for the $2S$ state. The first two terms in Eq. (12) are well known; the first one is the famous Schwinger correction and the second was derived previously for the $1S$ state in Ref. [13].

By subtracting all known terms of the $Z\alpha$ expansion in Eq. (12) from numerical data [5,6], one can isolate the one-loop self-energy remainder $G_n(Z)$ and improve its numerical accuracy for carbon and oxygen by extrapolating results for higher values of Z. The higher-order contribution extracted directly from numerical results of Ref. [5] reads $G_1(6) = 22.19(24)$ and $G_1(8) = 21.86(6)$. An extrapolation of numerical data [5] for $Z > 8$ yields the results for the self-energy remainder $G_1(6) = 22.160(10)$ and $G_1(8) = 21.859(4)$, which are significantly more accurate. In addition, we obtain the following result for the total contribution of order $(Z\alpha)^5$: $G_1(0) = 23.0$.

The result for the *two-loop* self-energy contribution is given by Eq. (11). We estimate the uncertainty due to uncalculated parts $g_1^{(2)}$ and $g_2^{(2)}$ as 30% of the constant term. Explicitly, the two-loop self-energy correction for

TABLE I. Breakdown of the low-energy contribution to the bound-electron g factor.

#	δH	δg	two-loop prefactor
1	$\frac{p^2}{2m}\frac{e\sigma\cdot\mathbf{B}}{2m^2}$	$\frac{8}{3}[-\frac{1}{6} - \ln k_0 - \ln(Z\alpha)^2 + \ln\mu]$	$\kappa/3$
2	$-\frac{e}{8m^2}(\mathbf{r}\times\sigma)\cdot(\mathbf{r}\times\mathbf{B})$	$-\frac{16}{9}[\frac{1}{3} - \ln k_0 - \ln(Z\alpha)^2 + \ln\mu]$	2κ
3	$-\frac{e}{8m^2}(\sigma\times\mathbf{E})\cdot(\mathbf{r}\times\mathbf{B})$	$\frac{8}{9}[\frac{5}{6} - \ln k_0 - \ln(Z\alpha)^2 + \ln\mu]$	2κ
4	$-\frac{e}{4m^2}\sigma\cdot\mathbf{E}\times p - \frac{e}{2m}\mathbf{L}\cdot\mathbf{B}$	$\frac{8}{3}[\frac{1}{2} - \ln k_0 - \ln(Z\alpha)^2 + \ln\mu]$	2κ
5	$-\frac{e}{2m}\sigma^i r^j\partial_j B^i - \frac{e}{2m}\mathbf{L}\cdot\mathbf{B}$	$-\frac{32}{9}[\frac{13}{12} - \ln k_0 - \ln(Z\alpha)^2 + \ln\mu]$	κ
6	$\frac{Z\alpha}{4m^2}\frac{\sigma\cdot\mathbf{L}}{r^3} - \frac{e}{2m}\mathbf{L}\cdot\mathbf{B}$	$\frac{8}{3}[\frac{1}{2} - \ln k_3 - \ln(Z\alpha)^2 + \ln\mu]$	2κ

TABLE II. Individual contributions to the $1s$ bound-electron g factor, $1/\alpha$ from [12] is 137.035 999 11(46).

	$12C^{5+}$	$16O^{7+}$
Dirac value (point)	1.998 721 354 39(1)	1.997 726 003 06(2)
Finite nuclear size	0.000 000 000 41	0.000 000 001 55
Free QED, $\sim(\alpha/\pi)$	0.002 322 819 47(1)	0.002 322 819 47(1)
Binding SE, $\sim(\alpha/\pi)$	0.000 000 852 97	0.000 001 622 67(1)
Binding VP, $\sim(\alpha/\pi)$	−0.000 000 008 51	−0.000 000 026 37(1)
Free QED, $\sim(\alpha/\pi)^2 \cdots (\alpha/\pi)^4$	−0.000 003 515 10	−0.000 003 515 10
Binding QED, $\sim(\alpha/\pi)^2(Z\alpha)^2$	−0.000 000 001 13	−0.000 000 002 01
Binding QED, $\sim(\alpha/\pi)^2(Z\alpha)^4$	0.000 000 000 41(11)	0.000 000 001 06(35)
Recoil	0.000 000 087 63	0.000 000 116 97
Total	2.001 041 590 52(11)	2.000 047 021 28(35)

the $1S$ state is

$$\delta g^{(2)} = \left(\frac{\alpha}{\pi}\right)^2 (Z\alpha)^4 \left\{\frac{56}{9} \ln[(Z\alpha)^{-2}] - 18.5(5.5)\right\}. \quad (13)$$

We now turn to the experimental consequences of our calculation. A previous compilation of theoretical contributions to the $1S$ bound-electron g factor was given in Ref. [5]. In the present work we modify it in several ways, with the corresponding contributions listed in Table II: (i) we employ the new, more accurate results for the one-loop self-energy remainder; (ii) we use the analytic result of Ref. [7] for the leading term of the $Z\alpha$ expansion of the first-order magnetic-loop vacuum-polarization correction; (iii) we include the leading part of the two-loop self-energy correction of order $\alpha^2(Z\alpha)^4$ obtained in this work [Eq. (13)]. We assume that the uncertainty due to other uncalculated two-loop corrections is absorbed into the error bars of the constant term in Eq. (13).

As compared to the previous compilation [5], the accuracy of the theoretical value for carbon is improved by a factor of 3. In case of oxygen, only a small improvement of accuracy is achieved, but the theoretical value is shifted slightly outside of the error bars given in Ref. [5]. The described modification of the theoretical predictions for the bound-electron g factor influences the electron-mass values derived from the experiments on carbon [1] and oxygen [2]. Following Refs. [2,10] and using the g-factor values from Table II, we obtain the following results for the electron mass,

$$m(^{12}C^{5+}) = 0.000\,548\,579\,909\,41(29)(3)\ \text{u}, \quad (14)$$

$$m(^{16}O^{7+}) = 0.000\,548\,579\,909\,87(41)(10)\ \text{u}, \quad (15)$$

where the first uncertainty originates from the experimental value for the ratio ω_L/ω_c and the second uncertainty comes from the theoretical result for the bound-electron g factor.

In summary, we have presented an approach for a systematic derivation of higher-order QED corrections to the g factor of a bound electron. We obtained the complete result for the one-loop self-energy correction of order $\alpha(Z\alpha)^4$. The derived contribution is in excellent agreement with the previous numerical calculation. The developed approach was then applied to the most problematic two-loop self-energy correction. We obtained the logarithmic contribution to order $\alpha^2(Z\alpha)^4 \ln(Z\alpha)^{-2}$ and the dominant part of the corresponding constant term. As a result, we improved the accuracy of the theoretical predictions for the $1S$ bound-electron g factor for carbon and oxygen and presented new values for the electron mass derived from the corresponding measurements.

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