Two-loop self-energy for the ground state of medium-Z hydrogenlike ions

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The two-loop self-energy correction to the ground-state Lamb shift is calculated for hydrogenlike ions with the nuclear charge $Z=10-30$ without any expansion in the binding field of the nucleus. A calculational technique is reported for treatment of Feynman diagrams in the mixed coordinate-momentum representation, which yields significant improvement in numerical accuracy as compared to previous results. An extrapolation of the all-order numerical data yields a result for the higher-order remainder function for hydrogen. The previously reported disagreement between the all-order and the perturbative approaches is reduced to the marginal agreement.

Calculations of the two-loop QED corrections to all orders in the binding-strength parameter of the nucleus $Z\alpha$ (Z is the nuclear charge and α is the fine structure constant) were motivated almost two decades ago by progress in the experimental spectroscopy of heavy lithiumlike ions [1]. To date, experimental investigations of the $2p_J$-$2s$ transitions in high- and medium-Z lithiumlike ions are sensitive to the two-loop QED effects on the level of about 10% [2,3]. All-order calculations of the two-loop Lamb shift were recently accomplished in Ref. [4] for high-Z hydrogenlike ions and in Ref. [5] for high-Z lithiumlike ions.

The ratio of the QED effects to the binding energy scales as Z^2 so that the relative QED contribution gets smaller for lighter ions. However, the experimental precision is also better there and the two-loop QED effects in light systems have long being observed. The best studied case is atomic hydrogen, whose spectroscopy is nowadays carried out with an accuracy of a few parts in 10^{14} [6].

Until recently, calculations of the QED effects in hydrogen relied on the approach perturbative in the binding-strength parameter $Z\alpha$. Technical difficulties of this approach, however, grow rapidly with the increase in the order of the perturbative expansion. The state of the art of such calculations is the evaluation of the dominant part of the $\alpha^2 (Z\alpha)^6$ correction [7–9]. An alternative way is to perform a numerical calculation to all orders in $Z\alpha$ and to identify the higher-order remainder by subtracting the known low-order terms from the all-order results. The problems on this way are, first, significant internal cancellations in numerical calculations, which grow as Z decreases, and second, additional losses of accuracy occurring when the higher-order remainder is inferred from the all-order results.

The first attempt at the evaluation of the all-order two-loop remainder for the ground state of hydrogen was made in Ref. [10]. In that work, a numerical calculation of the two-loop self-energy correction was reported for $Z \geq 10$. This correction is expected to give the dominant contribution to the two-loop remainder. An extrapolation toward $Z=1$ performed in Ref. [10] yielded a result approximately twice as large as the estimate based on the analytical calculations [8]. This disagreement is presently the main source of the theoretical uncertainty of the ground-state Lamb shift in hydrogen and influences the values of the Rydberg constant and

the proton charge radius obtained from the hydrogen spectroscopic data [11].

This investigation presents an attempt to resolve the disagreement between the numerical and analytical approaches by improving the calculational accuracy of the all-order results. To this end, we develop a scheme for the evaluation of Feynman diagrams in the mixed coordinate-momentum representation (the corresponding part of the two-loop self-energy is conventionally termed as the P term). This is the most nontrivial part of the evaluation of the two-loop self-energy correction as it has no analog in the one-loop calculations.

For the first time the P term was calculated in Ref. [12] with help of a finite basis set representation of the spectrum of the Dirac equation. Later investigations [4,5,10] proceeded along the same way with adopting an improved (dual kinetically balanced) basis set [13]. The main problem of the basis-set approach is a relatively slow convergence with respect to the number of basis functions. In order to overcome this limitation, in this work we employ the analytical representation of the Dirac-Coulomb Green's function (DCGF) in terms of the Whittaker functions. As a result, the numerical accuracy of the P term is improved by more than an order of magnitude, the error now being mainly due to the termination of the partial-wave expansion.

In the present investigation, we perform a reevaluation of the two-loop self-energy correction for the ground state of hydrogenlike ions with the nuclear charge numbers in the interval $Z=10-30$. The calculation of the P term is carried out with the technique developed in this work. The other parts of the correction are evaluated by the methods described previously [14] but with the increased number of partial waves included and with denser integration grids. The nonperturbative remainder incorporating terms of order $\alpha^2 (Z\alpha)^6$ and higher is inferred from the numerical results and extrapolated toward $Z=0$ and $Z=1$.

The two-loop self-energy correction is shown in Fig. 1. In this work, we concentrate on the part of the correction that is treated in the mixed coordinate-momentum representation and is referred to as the P term. The corresponding Feynman diagrams are shown in Fig. 2. They arise from the diagrams in Fig. 1 when the bound-electron propagators are expanded in terms of the interaction with the binding field. The distinct feature of the diagrams contributing to the P term is that

FIG. 1. The two-loop self-energy correction. The double line represents the electron propagator in the Coulomb binding field of the nucleus.

ultraviolet divergences in them originate from the one-loop subgraphs only. These subgraphs are covariantly regularized and calculated in the momentum space, whereas the remaining part of the diagrams does not need any regularization and is treated in the coordinate space.

In order to illustrate the calculational technique used for the evaluation of the P term, we consider one of the simplest diagrams in Fig. 2, graph (b). Its contribution can be written as

$$
\begin{aligned}
\Delta E_{N1b,P} = 4i\alpha \int_{C_F} d\omega \int \frac{d\boldsymbol{p}}{(2\pi)^3} \int dx_1 dx_4 D(\omega, x_{14}) \\
\times \psi_a^\dagger(\boldsymbol{x}_1) \alpha_\mu [G_V(E, \boldsymbol{x}_1, \boldsymbol{p}) - G_V^{(0)}(E, \boldsymbol{x}_1, \boldsymbol{p})] \\
\times \frac{1}{\gamma^0 E - \boldsymbol{\gamma} \cdot \boldsymbol{p} - m} \Sigma_R^{(0)}(E, \boldsymbol{p}) G^{(0)}(E, \boldsymbol{p}, \boldsymbol{x}_4) \\
\times \alpha^\mu \psi_a(\boldsymbol{x}_4),
\end{aligned}
\tag{1}
$$

where $E = \varepsilon_a - \omega$, ε_a is the reference-state energy, $D(\omega, x_{14})$ is the scalar part of the photon propagator in the Feynman gauge defined by $D^{\mu\nu}(\omega, x_{14}) \equiv g^{\mu\nu} D(\omega, x_{14})$, $\Sigma_R^{(0)}$ is the renormalized free self-energy operator (see, e.g., Ref. [14] for its definition and evaluation), $G_V(\varepsilon, \boldsymbol{x}_1, \boldsymbol{p})$ is the Fourier transform of the product of the DCGF $G(\varepsilon, \boldsymbol{x}_1, \boldsymbol{x}_2)$ and the Coulomb potential V_C,

$$
G_V(\varepsilon, \boldsymbol{x}_1, \boldsymbol{p}) = \int d\boldsymbol{x}_2 e^{i\boldsymbol{p}\cdot\boldsymbol{x}_2} G(\varepsilon, \boldsymbol{x}_1, \boldsymbol{x}_2) V_C(\boldsymbol{x}_2),
\tag{2}
$$

the function $G_V^{(0)}$ is given by an analogous expression with the DCGF substituted by the free Dirac Green's function $G^{(0)}$, and $G^{(0)}(E, \boldsymbol{p}, \boldsymbol{x}_4)$ is the Fourier transform of the free Dirac Green's function.

The main problem of the evaluation of Eq. (1) is the absence of a convenient representation for the function $G_V(\varepsilon, \boldsymbol{x}_1, \boldsymbol{p})$. Because of this, we have to start with the coordinate-space representation of the Green's function and perform the Fourier transformation numerically. The DCGF
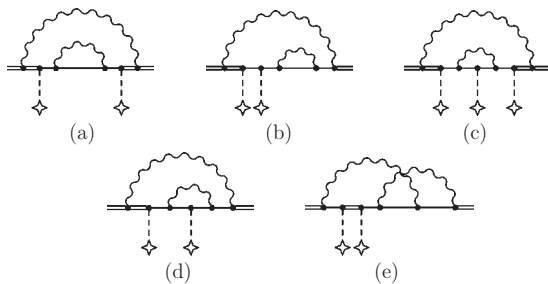

FIG. 2. The P term. The single line represents the free electron propagator. The dashed line with a cross indicates the interaction with the Coulomb field of the nucleus.

is known in terms of the partial-wave expansion over the relativistic angular parameter κ, with the radial part given by [15]

$$
G_\kappa(\varepsilon, x_1, x_2) = \begin{cases} -\phi_\kappa^0(\varepsilon, x_1) \phi_\kappa^{\infty T}(\varepsilon, x_2), & \text{for } x_1 < x_2 \\ -\phi_\kappa^\infty(\varepsilon, x_1) \phi_\kappa^{0T}(\varepsilon, x_2), & \text{for } x_2 < x_1, \end{cases}
\tag{3}
$$

where ϕ_κ^0 and ϕ_κ^∞ are the two-component solutions of the radial Dirac equation regular at the origin and at the infinity, respectively, and normalized in such a way that their Wronskian is unity. The radial part of the Fourier transform of the DCGF over the second radial variable can be represented as

$$
G_\kappa(\varepsilon, x_1, p) = -\phi_\kappa^\infty(\varepsilon, x_1) \psi_\kappa^{0T}(\varepsilon, p; x_1) - \phi_\kappa^0(\varepsilon, x_1) \psi_\kappa^{\infty T}(\varepsilon, p; x_1),
\tag{4}
$$

with

$$
\psi_\kappa^0(\varepsilon, p; x_1) = 4\pi \int_0^{x_1} dx_2 x_2^2 \begin{pmatrix} j_l(px_2) \phi_{\kappa,+}^0(\varepsilon, x_2) \\ -\frac{\kappa}{|\kappa|} j_{\bar{l}}(px_2) \phi_{\kappa,-}^0(\varepsilon, x_2) \end{pmatrix}
\tag{5}
$$

and

$$
\psi_\kappa^\infty(\varepsilon, p; x_1) = 4\pi \int_{x_1}^\infty dx_2 x_2^2 \begin{pmatrix} j_l(px_2) \phi_{\kappa,+}^\infty(\varepsilon, x_2) \\ -\frac{\kappa}{|\kappa|} j_{\bar{l}}(px_2) \phi_{\kappa,-}^\infty(\varepsilon, x_2) \end{pmatrix},
\tag{6}
$$

where $\phi_{\kappa,\pm}^0$ and $\phi_{\kappa,\pm}^\infty$ denote the upper and lower components of ϕ_κ^0 and ϕ_κ^∞, respectively, $l = |\kappa + 1/2| - 1/2$ and $\bar{l} = |\kappa - 1/2| - 1/2$.

The integration over x_2 in the functions $\psi_\kappa(\varepsilon, p; x_1)$ has to be performed numerically. The problems here are that (i) the integration interval depends on x_1 and (ii) the integrand contains the spherical Bessel function which oscillates rapidly in the high-momenta region. Clearly, a straightforward use of Eqs. (5) and (6) would lead to a re-evaluation of the integral for each new value of x_1, making the calculation prohibitively expensive. One can observe, however, that if the function $\psi_\kappa(\varepsilon, p; x)$ is known for a particular set of ε, p, and x, then the evaluation of $\psi_\kappa(\varepsilon, p; x')$ can be done by computing the Bessel transform integral over the interval (x, x') only. So, introducing an ordered radial grid $\{x_i\}$, one can store the set of values $\{\psi_\kappa(\varepsilon, p; x_i)\}$ by performing just one Bessel transform over the interval $(0, \infty)$. This shows that for a fixed values of ε and p, the integration over x_1 can be performed without a recalculation of the Bessel transform integral. Still, the evaluation of the functions ψ_k was one of the most problematic parts of the computation since a controllable accuracy was required for momenta as high as $p = 10^6$.

The next problem to be solved in the numerical evaluation of Eq. (1) is that the free Dirac Green's function $G^{(0)}(E, \boldsymbol{p}, \boldsymbol{x}_4)$ contains a spherical Bessel function $j_L(px_4)$ and thus is highly oscillating too in the high-momenta region. It can be observed that the radial integration over x_4 resembles the Bessel transform integral over x_2 and so can be

TABLE I. The two-loop self-energy correction for the ground state of hydrogenlike ions, in units of $\Delta E/[m\alpha^2(Z\alpha)^4/\pi^2]$. "LAL" denotes the loop-after-loop correction. Definitions and detailed description of individual contributions can be found in Ref. [14].

Z	LAL	F term	P term	M term	Total	2005 results [10]
10	−0.358	822.138(5)	−721.311(6)	−100.297(35)	0.172(36)	0.25(16)
12	−0.417	519.603(2)	−439.065(6)	−80.117(38)	0.004(38)	
15	−0.495	292.901(2)	−235.211(4)	−57.406(11)	−0.212(12)	−0.164(85)
17	−0.541	211.052(1)	−164.280(3)	−46.567(9)	−0.336(10)	
20	−0.602	136.909(1)	−102.029(2)	−34.780(4)	−0.501(5)	−0.481(58)
25	−0.686	74.501(1)	−51.982(2)	−22.560(6)	−0.728(6)	
30	−0.756	44.728(1)	−29.414(3)	−15.468(3)	−0.910(5)	−0.903(26)

efficiently calculated by introducing analogs of the functions ψ_k. Details of the numerical procedure will be published elsewhere.

The results of our numerical evaluation of the two-loop self-energy correction to the ground-state Lamb shift of middle-Z hydrogenlike ions are presented in Table I. They are consistent with but improve upon the data obtained previously [10,16].

In the present investigation we are concerned with the higher-order remainder function that incorporates contributions of all orders starting with $\alpha^2(Z\alpha)^6$ and is denoted as $G_{\text{SESE}}^{\text{h.o.}}$. It is obtained from the two-loop self-energy correction ΔE_{SESE} by separating out the first terms of its $Z\alpha$ expansion,

$$\Delta E_{\text{SESE}} = m\left(\frac{\alpha}{\pi}\right)^2 (Z\alpha)^4 \{B_{40} + (Z\alpha)B_{50} + (Z\alpha)^2$$
$$\times [L^3 B_{63} + L^2 B_{62} + LB_{61} + G_{\text{SESE}}^{\text{h.o.}}(Z)]\}, \quad (7)$$

where $L \equiv \ln[(Z\alpha)^{-2}]$ and the expansion of the remainder starts with a constant, $G_{\text{SESE}}^{\text{h.o.}}(Z) = B_{60} + Z\alpha(\dots)$. The results for the expansion coefficients (see Refs. [7–9,11] and references therein) are: $B_{40} = 1.409244$, $B_{50} = -24.2668(31)$, $B_{63} = -8/27$, $B_{62} = 16/27 - (16/9)\ln 2$, $B_{61} = 48.388913$, and $B_{60} = -61.6(9.2)$. The remainder function inferred from our numerical results is plotted in Fig. 3.

In order to obtain a value of the remainder function for hydrogen, we have to extrapolate the numerical data obtained for $Z \geq 10$. For this we use a variant of the procedure first employed in Ref. [17]. The extrapolation toward the required value of $Z = Z_0$ (=0 and 1 in our case) is performed in two steps. First, we apply an (exact) linear fit to each pair of two consecutive points from our data set and store the resulting values at $Z = Z_0$. Second, we perform a global parabolic least-squares fit to the set of data obtained on the first step and take the fitted value at $Z = Z_0$ as a final result. Similar procedure applied to the determination of the B_{50} coefficient reproduces the known analytical result with the accuracy of about 1%. For comparison, a global polynomial fit yields a result for the B_{50} coefficient accurate within 5% only.

When applied to the remainder function $G_{\text{SESE}}^{\text{h.o.}}(Z)$, the extrapolation procedure described above gives

$$G_{\text{SESE}}^{\text{h.o.}}(Z=0) \equiv B_{60} = -84(15), \quad (8)$$

$$G_{\text{SESE}}^{\text{h.o.}}(Z=1) = -86(15). \quad (9)$$

The extrapolated value for $Z=1$ [Eq. (9)] is higher than but marginally consistent with the 2005 result of $-127(42)$ [10]. The shift of the central value is due to two reasons. First, the analytical result for the B_{61} coefficient was recently changed by $\delta B_{61} = -1.4494\dots$ [9], thus pushing the higher-remainder higher up. Second, the improved numerical accuracy of the present calculation and the increased number of data points allowed us to identify the upward trend in the numerical data, which influenced the extrapolated values considerably. A result of this improvement is that the difference between the previous numerical result of $-127(42)$ and the analytical value of $B_{60} = -62(9)$ [8] is now significantly reduced. The present result for $Z=0$ [Eq. (8)] is consistent (but still not in perfect agreement) with the analytical value.

Finally, we account for the contribution from the diagrams with closed fermion loops calculated recently in Ref. [18]. The total value of the remainder function for hydrogen is

$$G^{\text{h.o.}}(Z=1) = -86(15) - 15(2) = -101(15). \quad (10)$$

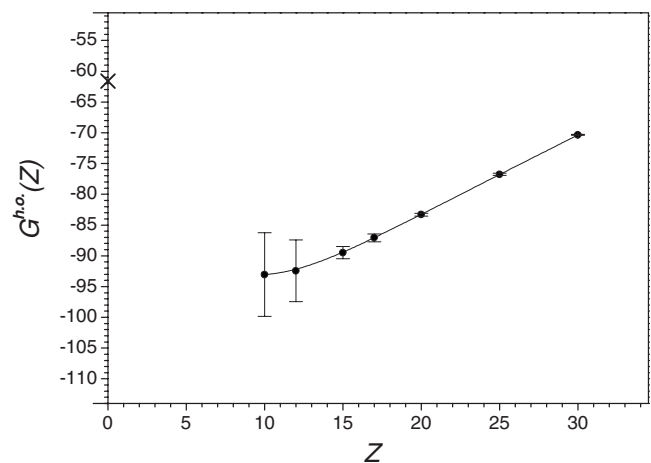To conclude, the present investigation reports a technique

FIG. 3. The higher-order remainder function of the two-loop self-energy correction. The cross on the y axis indicates the analytical result.

for the evaluation of Feynman diagrams in the mixed coordinate-momentum representation, which allows one to significantly improve the numerical accuracy. A complete re-calculation of the diagrams of the two-loop self-energy is presented for the ground state of hydrogenlike ions with the nuclear charge number $Z=10-30$. The higher-order (in $Z\alpha$) remainder function is inferred from numerical all-order re-sults and extrapolated toward $Z=0$ and 1. The extrapolated value of the higher-order remainder function is in marginal agreement with the analytical result obtained within the per-turbative approach.

[1] J. Schweppe, A. Belkacem, L. Blumenfeld, N. Claytor, B. Feinberg, H. Gould, V. E. Kostroun, L. Levy, S. Misawa, J. R. Mowat, and M. H. Prior, Phys. Rev. Lett. **66**, 1434 (1991).

[2] P. Beiersdorfer, H. Chen, D. B. Thorn, and E. Träbert, Phys. Rev. Lett. **95**, 233003 (2005).

[3] S. W. Epp, J. R. Crespo López-Urrutia, G. Brenner, V. Mäckel, P. H. Mokler, R. Treusch, M. Kuhlmann, M. V. Yurkov, J. Feldhaus, J. R. Schneider, M. Wellhöfer, M. Martins, W. Wurth, and J. Ullrich, Phys. Rev. Lett. **98**, 183001 (2007).

[4] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Phys. Rev. Lett. **91**, 073001 (2003).

[5] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Phys. Rev. Lett. **97**, 253004 (2006).

[6] M. Niering, R. Holzwarth, J. Reichert, P. Pokasov, T. Udem, M. Weitz, T. W. Hänsch, P. Lemonde, G. Santarelli, M. Ab-grall, P. Laurent, C. Salomon, and A. Clairon, Phys. Rev. Lett. **84**, 5496 (2000).

[7] K. Pachucki, Phys. Rev. A **63**, 042503 (2001).

[8] K. Pachucki and U. D. Jentschura, Phys. Rev. Lett. **91**, 113005 (2003).

[9] U. D. Jentschura, A. Czarnecki, and K. Pachucki, Phys. Rev. A **72**, 062102 (2005).

[10] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Phys. Rev. A **71**, 040101(R) (2005).

[11] P. J. Mohr, B. N. Taylor, and D. B. Newell, Rev. Mod. Phys. **80**, 633 (2008).

[12] V. A. Yerokhin and V. M. Shabaev, Phys. Rev. A **64**, 062507 (2001).

[13] V. M. Shabaev, I. I. Tupitsyn, V. A. Yerokhin, G. Plunien, and G. Soff, Phys. Rev. Lett. **93**, 130405 (2004).

[14] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Eur. Phys. J. D **25**, 203 (2003).

[15] P. J. Mohr, G. Plunien, and G. Soff, Phys. Rep. **293**, 227 (1998).

[16] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Zh. Eksp. Teor. Fiz. **128**, 322 (2005) [JETP **101**, 280 (2005)].

[17] P. J. Mohr, Phys. Rev. Lett. **34**, 1050 (1975).

[18] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Phys. Rev. A **77**, 062510 (2008).