Second-Order Electron Self-Energy in Hydrogenlike Ions

Igor Goidenko,* Leonti Labzowsky,* and Andrei Nefiodov†
Max-Plank-Institut für Physik komplexer Systeme, Nöthnitzer Strasse 38, D-01187 Dresden, Germany

Günter Plunien and Gerhard Soff
Institut für Theoretische Physik, Technische Universität Dresden, Mommsenstrasse 13, D-01062 Dresden, Germany
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A calculation of the loop after loop irreducible contribution of the second-order electron self-energy for hydrogenlike ions with nuclear charge numbers $3 \leq Z \leq 92$ is presented. The interaction with the nuclear Coulomb potential is treated nonperturbatively in the coupling constant $Z\alpha$. Our results are in strong disagreement with recent calculations of Mallampalli and Sapirstein for low-Z values but are compatible with the two known terms of the analytical $Z\alpha$ expansion.

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The numerical evaluation of the complete set of radiative corrections of order α^2 but to all orders in $Z\alpha$ for hydrogenlike ions with arbitrary nuclear charge numbers Z is a challenging theoretical problem. It is important to provide theoretical results for the Lamb shift for the comparison with available experimental data for highly charged ions. But also in the low-Z region exact numerical data are highly appreciated since they allow one to test the reliability of results obtained by means of analytical $Z\alpha$ expansions. For a general review of the current theoretical and experimental situation in hydrogenlike heavy systems, we refer to Ref. [1]. With respect to the various two-loop corrections only the subset of the second-order electron self-energy (SESE) remains uncalculated until now. These contributions to the Lamb shift are represented by the Feynman diagrams in Fig. 1. The first diagram depicted in Fig. 1(a), i.e., the loop after loop irreducible contribution, has been calculated previously for selected values of $Z = 70$, 80, 90, and 92 [2] and more recently for the entire range of nuclear charge numbers between $1 \leq Z \leq 92$ [3]. Employing the Feynman gauge commonly used in calculations of QED corrections, the diagram [Fig. 1(a)] can be renormalized and thus the corresponding energy shift can be evaluated separately. In Ref. [3] it was denoted as a "perturbed orbital" contribution. A fair agreement between the results obtained in Refs. [2,3] has been achieved.

The calculation of the remaining graphs depicted in Figs. 1(b)–1(d) is a much more difficult task. This is predominantly due to the fact that only the sum of all these diagrams allows for a renormalization leading to gauge-invariant expressions. Accordingly, their contributions to the total energy shift have to be evaluated simultaneously. A specific part of it has been calculated recently for $Z = 92$ within the framework of a generalized potential-expansion approach [4]. However, it is not obvious whether this part is the dominant one or not.

Our final goal is to calculate the remaining SESE corrections depicted in Figs. 1(b)–1(d). We decided to employ the renormalization scheme developed in Ref. [5] (see also Ref. [6]) in combination with the partial-wave renormalization method [7,8]. In view of the complexity of the evaluations, it is highly desirable to compare the results obtained within different numerical approaches. Since the corresponding numerical calculations are extremely time consuming (the same holds true for the calculations performed in Ref. [4]), one has to develop appropriate numerical methods. One approach which simplifies the calculations considerably has been applied recently for the evaluation of the first-order electron self-energy (SE) [9,10]. We plan to apply similar techniques for calculating the complete two-photon self-energy as well. This approach is based on the multiple commutator expansion method [11].

One motivation for the present studies has been to test this approach in the case of the irreducible SESE (a) correction. In addition, we had to elaborate the most time-saving procedure compatible with the required level of accuracy. Therefore we employed a minimal number of grid points and partial waves that could guarantee an accuracy of 10%.

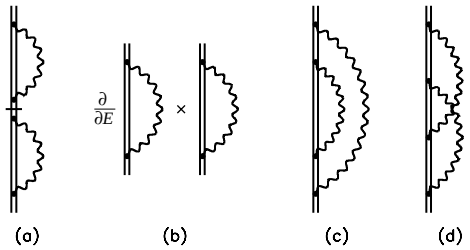

FIG. 1. The second-order electron self-energy Feynman diagrams. The double solid line denotes the electron in the field of the nucleus, the wavy line denotes the photon. The double line with the bar denotes the electron propagator with the reference state being excluded from the summation over the complete Dirac spectrum. The symbol $\frac{\partial}{\partial E}$ in (b) denotes the derivative of the self-energy graph with respect to the energy parameter E in the bound-electron propagator. The graphs (a) and (b) correspond to the irreducible and reducible parts of the loop after loop contribution, the graph (c) corresponds to the loop inside loop contribution, and the graph (d) corresponds to the crossed loops contribution.

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Using the exact expressions for SESE (a) we are in the position to compare with recent results reported by Mallampalli and Sapirstein [3]. Agreement is found for large values of Z; however, serious discrepancies (more than 50% deviation) between our results for the energy shifts and those presented in Ref. [3] are obtained in the low-Z region. The significant disagreement with previous calculations performed by Mallampalli and Sapirstein is indeed a crucial point. In Ref. [3] numerical results for the energy shift have been obtained up to $Z = 1$ and compared with the analytically known terms of the $Z\alpha$ expansion. From the observed discrepancies a strong indication for a nonperturbative nature of the SESE correction was deduced even in the case for hydrogen. However, perturbation theory has been employed intensively in many calculations of radiative corrections to test QED for weakly bound atomic electrons. Considerable success was achieved in this direction during the past several years [12–14]. In contrast to the results and the conclusions drawn in Ref. [3], our numerical results are consistent with the perturbation theory expansion for small Z. Based on exact calculations we can establish the validity of the $Z\alpha$ expansion in the low-Z region which represents the most important outcome of the present investigation.

The renormalized SE expression for the atomic state $|a\rangle$ is given by [9,10]

$$\Delta E_a = \langle a|\hat{\Sigma}_b(E_a)|a\rangle_{\rm ren} = \langle a|\hat{\Sigma}_b(E_a)|a\rangle - \langle a|\hat{\Sigma}_f|a\rangle = \sum_{l=0}^{\infty}\langle a|\hat{\Sigma}_b^{(l)}(E_a)|a\rangle_{\rm ren} = \sum_{l=0}^{\infty}[\langle a|\hat{\Sigma}_b^{(l)}(E_a)|a\rangle - \langle a|\hat{\Sigma}_f^{(l)}|a\rangle], \quad (1)$$

where $\hat{\Sigma}_b$ and $\hat{\Sigma}_f$ are the bound- and free-electron self-energy operators, and $\hat{\Sigma}_b^{(l)}$ and $\hat{\Sigma}_f^{(l)}$ are terms of the corresponding partial-wave expansions. The matrix element of $\hat{\Sigma}_b^{(l)}$ can be written as the sum of a logarithmic and a sign terms:

$$\langle a|\hat{\Sigma}_b^{(l)}(E_a)|a\rangle = \frac{\alpha}{\pi}(2l+1)\sum_n \Delta_{na}\ln|\Delta_{na}|\,\langle a|\alpha_{1\mu}j_l(\Delta_{na}r_1)\boldsymbol{C}_1^l|n\rangle\cdot\langle n|\alpha_2^\mu j_l(\Delta_{na}r_2)\boldsymbol{C}_2^l|a\rangle$$
$$-\frac{\alpha}{2}(2l+1)\sum_n \mathrm{sgn}(E_n)\Delta_{na}\langle an|\alpha_{1\mu}\alpha_2^\mu j_l(\Delta_{na}r_<)n_l(\Delta_{na}r_>)\boldsymbol{C}_1^l\cdot\boldsymbol{C}_2^l|na\rangle. \quad (2)$$

Here $\Delta_{na} = E_n - E_a$, $\alpha_{1\mu}\alpha_2^\mu = 1 - \boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2$, $j_l(z)$ and $n_l(z)$ are spherical Bessel and Neumann functions, respectively, and $\boldsymbol{C}_i^l$ $(i = 1, 2)$ are the standard spherical tensors. Relativistic units $\hbar = c = 1$ are used together with the fine-structure constant α. The index n runs over the entire spectrum of the Dirac equation in the external nuclear field.

The matrix elements $\langle a|\hat{\Sigma}_f^{(l)}|a\rangle$ represent the mass counterterms in the framework of the partial-wave renormalization method [7,8]. Accordingly, the relevant counterterms for Eq. (2) read

$$\langle a|\hat{\Sigma}_f^{(l)}|a\rangle = \frac{\alpha}{\pi}(2l+1)\int d\boldsymbol{p}|\langle\boldsymbol{p}\,|\,a\rangle|^2\int d\boldsymbol{q}\,\Delta_{qp}\ln|\Delta_{qp}|\,\langle\boldsymbol{p}|\alpha_{1\mu}j_l(\Delta_{qp}r_1)\boldsymbol{C}_1^l|\boldsymbol{q}\rangle\cdot\langle\boldsymbol{q}|\alpha_2^\mu j_l(\Delta_{qp}r_2)\boldsymbol{C}_2^l|\boldsymbol{p}\rangle$$
$$-\frac{\alpha}{2}(2l+1)\int d\boldsymbol{p}|\langle\boldsymbol{p}\,|\,a\rangle|^2\int d\boldsymbol{q}\,\mathrm{sgn}(E_q)\Delta_{qp}\langle\boldsymbol{pq}\,|\,\alpha_{1\mu}\alpha_2^\mu j_l(\Delta_{qp}r_<)n_l(\Delta_{qp}r_>)\boldsymbol{C}_1^l\cdot\boldsymbol{C}_2^l|\boldsymbol{qp}\rangle, \quad (3)$$

where $\Delta_{qp} = E_q - E_p$. The states $|\boldsymbol{p}\rangle$ and $|\boldsymbol{q}\rangle$ denote the spherical-wave solutions of the free-electron Dirac equation. Integration over $\boldsymbol{p}$ is interpreted as integration over the energies $E_p = \pm\sqrt{m_e^2 + p^2}$, where m_e is the electron mass, and p is the absolute value of the electron momentum. The summation over angular quantum numbers is also implicitly assumed. The free-electron wave functions are normalized to δ functions in the energy variable. Equations (1)–(3) are also valid for arbitrary electron states $|a\rangle$ as well as for nondiagonal matrix elements of the type $\langle a|\hat{\Sigma}(E_a)|n\rangle$ provided that $|a\rangle$ refers to the ground state.

In Refs. [9,10] the B-spline approach [15] has been employed to approximate numerically the sums involved in Eq. (2) and the integrals over $\boldsymbol{q}$ and $\boldsymbol{p}$ in Eq. (3). The following set of parameters was chosen: The number of grid points was $N = 140$, the order of splines $k = 9$, and the number of partial waves $s = 16$ [9]. The accuracy achieved in Ref. [9] compared to the exact results of Mohr [16] for the pointlike nuclei was found to be 0.1% for $Z = 10$ and 0.001% for $Z = 92$.

The renormalized expression for the energy shift due to the SESE (a) correction can be expressed as [2,3]

$$\Delta E_a^{\rm irr} = \sum_{l_1,l_2=0}^{\infty}{\sum_n}' \frac{\langle a|\hat{\Sigma}_b^{(l_1)}(E_a)|n\rangle_{\rm ren}\langle n|\hat{\Sigma}_b^{(l_2)}(E_a)|a\rangle_{\rm ren}}{E_a - E_n}. \quad (4)$$

It involves two independent summations over partial waves (l_1, l_2) and a summation over the complete Dirac spectrum for electrons (n) in the external field of the nucleus, where the prime indicates that the term with $E_n = E_a$ is excluded. For the evaluation of the matrix elements involved, formulas (2) and (3) can be applied. In total we have to perform threefold (or even fourfold, for counterterms) summations over the spline Dirac spectrum.

The minimal set of parameters for the numerical spline calculations was chosen to be $N = 28$, $k = 9$, and $s = 7$,

TABLE I. Convergence of the partial contributions $\sum_l \Delta E_{1s}^{(l)}$ in the first-order self-energy correction ΔE_{1s} for $Z = 10$. The number of the grid points was chosen to be $N = 28$.

Even		Odd		ΔE_{1s} (eV)	
l	$\sum_{l'=0}^{l} \Delta E_{1s}^{(l')}$ (eV)	l	$\sum_{l'=0}^{l} \Delta E_{1s}^{(l')}$ (eV)	This work	Ref. [16]
0	0.1269	1	0.1769	0.1688	0.1566
2	0.1615	3	0.1715		
4	0.1659	5	0.1702		
6	0.1672				

while in Ref. [3] $N = 50$ and $12 \leq s \leq 40$. However, in our approach even this minimal set allowed us to keep the controlled accuracy better than 10%. The convergence of our method for the SE correction (1) is exemplified in Table I for the ground state of the ion with $Z = 10$. The accumulated sums of partial-wave contributions $\sum_{l'=0}^{l} \Delta E_{1s}^{(l')}$ for odd and even l values have been assumed to converge to a common limit. The accuracy of the calculation amounts to 7.8% for the minimal basis set.

We should stress that within our approach, unlike the potential expansion method [3], no cancellations and no loss of accuracy occur for small values of Z. However, the numerical stability becomes poorer in the low-Z region, which is a distinct but less dangerous numerical problem. The loss of stability for small Z values arises because we generate the spline spectrum in a large spatial box with the same minimal number of the grid points ($N = 28$). For $Z = 1$ and 2, the inaccuracy turned out to be above the prescribed limit of 10%.

The results of our calculations of the SESE (a) correction (4) for the $1s$-ground state are given in Table II. For $Z = 70$, 80, and 92, our results coincide rather well with those presented in Refs. [2,3]. The mean deviation is about 1.5%, while the corrresponding energy shifts listed in [2] and [3] coincide with each other within three digits. However, for $Z = 20$ the deviation from Ref. [3] amounts to about 50%, and for $Z = 10$ it is as large as 70%.

To control the stability of our numerical procedure, we compared the results calculated with a different order of splines k but keeping the number of grid points N and the number of partial waves s fixed. For $k = 4$, the deviation from the results obtained in basis set with $k = 9$ is increased from 1.5% for $Z = 92$ up to 9.5% for $Z = 3$. In view of the adopted 10% inaccuracy limit, the results for $Z = 1, 2$ have to be considered as unstable. In consequence, we retained only the values for $Z \geq 3$.

Let us now examine the question concerning the perturbative nature of QED effects in the low-Z region. For small values of Z we can compare the numerical results for the SESE (a) correction with the known leading terms of the $Z\alpha$ expansion [12–14]. We present the energy correction in the standard form:

$$\Delta E_a^{\mathrm{irr}} = m_e \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^5}{n^3} G_a^{\mathrm{irr}}(Z\alpha), \qquad (5)$$

where n is the principal quantum number of the state $|a\rangle$. According to the $Z\alpha$ expansion the following terms are known for small Z values:

$$G_a^{\mathrm{irr}}(Z\alpha) = 2.29953 - \frac{8}{27}(Z\alpha)\ln^3(Z\alpha)^{-2}. \qquad (6)$$

The constant term in Eq. (6) has been derived in Refs. [12,13] and the cubic logarithmic term has been

TABLE II. Comparison of the SESE (a) correction for the $1s$ ground state with previous calculations.

	$\Delta E_{1s}^{\mathrm{irr}}$ (eV)			G_{1s}^{irr}	
Z	Ref. [2]	Ref. [3]	This work	Ref. [3]	This work
3		-0.6237×10^{-7}	-0.2913×10^{-7}	−4.50	−2.101
4		-0.2786×10^{-6}	-0.1351×10^{-6}	−4.77	−2.311
5		-0.8792×10^{-6}	-0.4431×10^{-6}	−4.931	−2.485
6			-0.1153×10^{-5}		−2.599
7		-0.4808×10^{-5}	-0.2584×10^{-5}	−5.016	−2.694
8			-0.4972×10^{-5}		−2.659
9			-0.8903×10^{-5}		−2.642
10		-0.2796×10^{-4}	-0.1483×10^{-4}	−4.9016	−2.601
20		-0.7525×10^{-3}	-0.4688×10^{-3}	−4.1217	−2.568
30			-0.3454×10^{-2}		−2.491
50			-0.4407×10^{-1}		−2.472
70	−0.2283	−0.2282	−0.2314	−2.3804	−2.413
80	−0.4474	−0.4472	−0.4512	−2.3923	−2.413
92	−0.9712	−0.9706	−0.9599	−2.581	−2.553

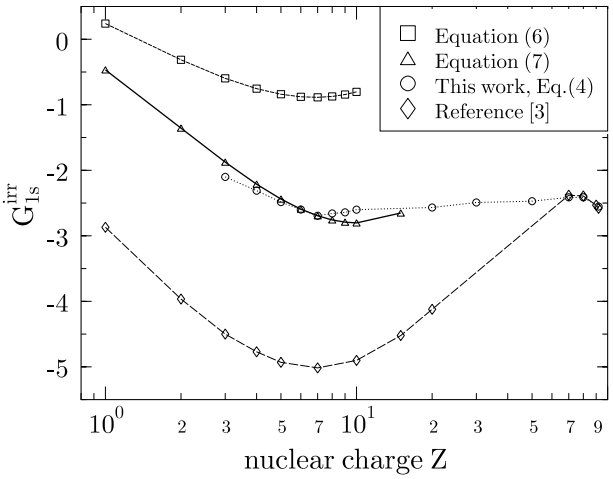

FIG. 2. Different calculations for $G_{1s}^{\rm irr}$ as a function of the nuclear charge number Z.

deduced in Ref. [14]. The results of our numerical calculation for the $G_{1s}^{\rm irr}$ function are indicated in Table II and Fig. 2. The function $G_{1s}^{\rm irr}$ obtained in Ref. [3] is depicted in the same figure. In addition, we also plot the results of the nonrelativistic limit (6). To determine whether our results are compatible with the nonrelativistic limit (6), we tried to use an expression incorporating a quadratic logarithmic term:

$$\tilde{G}_{1s}^{\rm irr} = 2.299\,53 - \frac{8}{27}(Z\alpha)\ln^3(Z\alpha)^{-2} + C(Z\alpha)\ln^2(Z\alpha)^{-2}. \quad (7)$$

In order to determine the coefficient C, we require the condition $\tilde{G}_{1s}^{\rm irr} = G_{1s}^{\rm irr}$ for different values of Z, where $G_{1s}^{\rm irr}$ signifies the exact numerical function. For the range $3 \le Z \le 20$ we obtained nearly the same value for the coefficient C. Averaging over Z yields $C = -1.0 \pm 0.1$. We also display in Fig. 2 the curve corresponding to Eq. (7) with the coefficient $C = -1$ deduced from the matching prescription described above. The magnitude of the coefficient reveals that our results are consistent with the $Z\alpha$-expansion perturbation theory [12–14]. A more detailed comparison with the outcome obtained in Ref. [3] indicates that the total difference results from the sum over negative-energy states in Eq. (4) [17]. The reason for this discrepancy could be not only the difference in the spline spectrum but also the difference in the evaluation of the off-diagonal self-energy for the negative-energy states. The latter part is very difficult to compare explicitly since the methods employed here for the evaluation and those used in Ref. [3] are quite different. In summary, we can state that our numerical results presented for low-Z systems are consistent with existing results obtained from $Z\alpha$ expansions and that there is no indication for a nonperturbative nature of the electron self-energy in the low-Z limit.

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*Permanent address: St. Petersburg State University, 198904 St. Petersburg, Russia.
†Permanent address: Petersburg Nuclear Physics Institute, 188350 Gatchina, St. Petersburg, Russia.

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