Loop-After-Loop Contribution to the Second-Order Self-Energy in Hydrogen

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Abstract. We investigate the loop-after-loop contribution to the second-order Lamb shift for the ground state of hydrogenlike atoms with low nuclear charge numbers Z. The calculation is carried out in the Fried-Yennie gauge and without an expansion in $Z\alpha$. Our calculation confirms the results of Mallampalli and Sapirstein and disagrees with the calculation by Goidenko and co-workers. A fit to the numerical results provides a detailed comparison with analytical calculations based on an expansion in the parameter $Z\alpha$. We confirm the analytic results of order $\alpha^2(Z\alpha)^5$ but disagree with Karshenboim's calculation of the $\alpha^2(Z\alpha)^6\ln^3(Z\alpha)^{-2}$ contribution.

Introduction

In the present work we investigate a part of the two-loop self-energy correction to the Lamb shift in hydrogen, namely the irreducible part of diagram Fig. 1(a), referred to as the *loop-after-loop* correction. This contribution has been the subject of a recent debate in the literature. Analytic calculations of its $Z\alpha$-expansion coefficients were carried out by Eides and co-workers [1] and Pachucki [2] in order $\alpha^2(Z\alpha)^5$ and by Karshenboim [3] in order $\alpha^2(Z\alpha)^6\ln^3(Z\alpha)^{-2}$. A direct numerical calculation of this correction to all orders in $Z\alpha$ in the low-Z region was reported by Mallampalli and Sapirstein [4]. A fit to the data in Ref. [4] is consistent with the analytical result in order $\alpha^2(Z\alpha)^5$ but it is in a significant disagreement with Karshenboim's calculation of the leading logarithmic contribution. As a consequence, a question was raised in Ref. [4] about the breakdown of the $Z\alpha$ expansion for the two-loop self-energy correction even for hydrogen. The subsequent calculation by Goidenko *et al.* [5], also nonperturbative in $Z\alpha$, shows to be compatible with the analytical results. A recent evaluation by Manohar and Stewart [6] also confirms Karshenboim's value of the leading logarithmic contribution for the total two-loop self energy[1]. However, our recent nonperturbative (in $Z\alpha$) calculation [7] exhibits a good agreement with the results of Ref. [4] and yields the corresponding logarithmic contribution which is approximately 3 times larger than Karshenboim's result. In this paper, we present some additional details of our calculation and investigate possible reasons for the existing discrepancy between different studies.

[1] We note that it is not clear whether this result can be directly compared to our calculation since the authors do not specify the gauge which was used in their derivation.

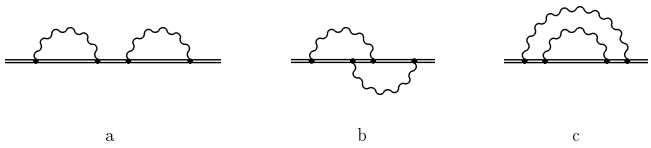

Fig. 1. One-electron self-energy Feynman diagrams of second order in α

1 Loop-after-loop contribution

The energy shift corresponding to the irreducible part of diagram Fig. 1(a) (the loop-after-loop contribution) is given by

$$\Delta E_{\rm lal} = \langle a|\Sigma_R(\varepsilon_a)G_{\rm red}\Sigma_R(\varepsilon_a)|a\rangle \tag{1}$$

where $\Sigma_R(\varepsilon)$ is the renormalized self-energy operator, $G_{\rm red}$ denotes the reducible Dirac Coulomb Green function, and a indicates the initial state. Since the present investigation is aimed to an evaluation of this correction in the low-Z region, we use the fact that the loop-after-loop contribution is invariant in any covariant gauge and perform our calculations in the Fried-Yennie gauge. It is known (see, e.g., Ref. [8]) that in this gauge the potential expansion does not lead to any spurious gauge-dependent terms of order $Z\alpha$, as is the case in all other covariant gauges. This choice of the gauge makes the numerical evaluation of the self-energy matrix elements much easier for low-Z systems. The basic numerical

Table 1. The loop-after-loop contribution to the second-order Lamb shift of the ground state of hydrogenlike atoms expressed in terms of the function $G_{\rm lal}(Z\alpha)$ defined by Eq. (2)

Z	This work	Ref. [4]	Ref. [5]
0.5	−1.56(7)	−1.5(1)	
1	−2.75(4)	−2.87(5)	
1.5	−3.449(9)	−3.47(2)	
2	−3.919(7)	−3.965(15)	
3	−4.476(3)	−4.50(1)	−2.101
4	−4.772(3)	−4.77(1)	−2.311
5	−4.927(2)	−4.931(5)	−2.485
7	−5.015(1)	−5.016(3)	−2.694
10	−4.902(1)	−4.9016(14)	−2.601
20	−4.122(1)	−4.1217(3)	−2.568

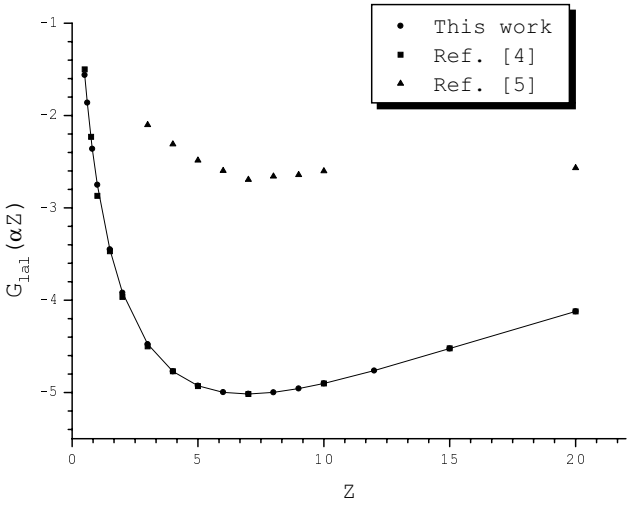

Fig. 2. The function $G_{\rm lal}(Z\alpha)$ in different studies. The solid line indicates a fit to our numerical results

procedure can be found in Ref. [7]. In Table 1 and Fig. 2 we present the results of our calculation of the loop-after-loop contribution to the second-order Lamb shift of the ground state of hydrogenlike atoms, expressed in the standard form

$$\Delta E_{\rm lal} = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^5 m}{n^3} G_{\rm lal}(Z\alpha) \; . \tag{2}$$

The results of two previous nonperturbative calculations of this correction are also presented in Table 1 and in Fig. 2. A comparison exhibits a good agreement of the present calculation with the results of Mallampalli and Sapirstein [4] and a strong deviation from the results of Goidenko *et al.* [5]. One of the possible reasons for this discrepancy may be, to our opinion, a noncovariant renormalization procedure used by Goidenko *et al.* which could provide some spurious contributions in this case. We discuss this topic in more detail in Appendix I.

In order to compare our results with calculations based on an expansion in $Z\alpha$, we approximate our data for the function $G_{\rm lal}$ by a least-squares fit with five parameters a_{50}, a_{63}, a_{62}, a_{61}, and a_{60} (the first index of the coefficients a_{ij} indicates the power of $Z\alpha$ and the second one corresponds to the power of $\ln(Z\alpha)^{-2}$). The fit yields

$$a_{50} = 2.33 \qquad a_{63} = -1.1 \; . \tag{3}$$

This is in a good agreement with the fitting coefficients from Ref. [4] ($a_{50} = 2.3$ or 2.8 for different sets of data, $a_{63} = -0.9$) but deviates significantly from Karshenboim's analytical result [3] $a_{63} = -8/27 \approx -0.296$.

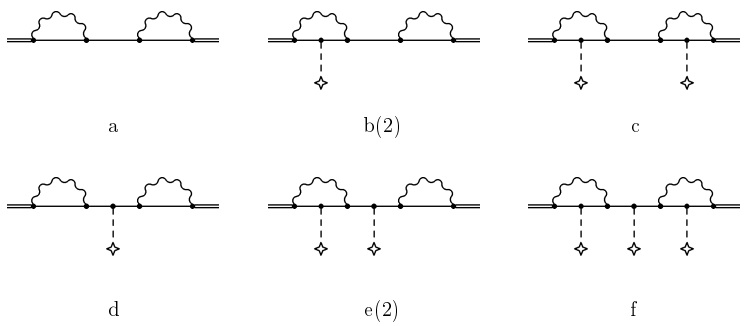

Fig. 3. Diagrams obtained from Fig. 1(a) by expansion of the inner electron propagators in terms of interactions with the nuclear binding potential. A double line denotes the electron in the field of the nucleus. A single line indicates the free electron. A dashed line denotes a Coulomb interaction with the nucleus. Some diagrams are counted twice, as is denoted by "(2)"

In order to investigate the discrepancy between different methods in more detail, we note that the analytical calculations of the loop-after-loop correction in Refs. [1,2,3] have been performed in the Fried-Yennie gauge similar to the present work. Therefore, it is possible to compare all calculations on intermediate stages. Aiming this, we expand the inner electron propagators in diagram Fig. 1(a) in terms of interactions with the nuclear binding potential. While the potential expansion of electron propagators inside the loops is straightforward, some care should be taken for the middle propagator from which the contribution of the initial state a is subtracted. We discuss the potential expansion of the reducible Green function in Appendix II.

Table 2. Fitting results for the first coefficients of the $Z\alpha$-expansion of the diagrams Fig. 3 in comparison with the analytical calculations [1–3]

Z	Fig. 3(a)	Fig. 3(b)	Fig. 3(c)	Fig. 3(d)	Fig. 3(e)	Fig. 3(f)	Fig. 3(a-f)
Analytical results:							
a_{50}	0	9.284	−6.984	0	0	0	2.300
a_{63}	0	0	0	0	0	−0.296	−0.296
Fitting results:							
a_{50}	0.000	9.284	−6.985	0.000	0.000	0.001	2.300
a_{63}	0.000	0.001	−0.658	0.002	-0.003	−0.304	−0.963

The Feynman diagrams corresponding to the first six terms of the potential expansion of the loop-after-loop diagram are shown in Fig. 3. Each of these diagrams as well as the nonperturbative remainder are calculated separately. The sum of all contributions is in good agreement with the results of the direct calculation of the diagram Fig. 1(a). For the evaluation of the middle electron propagator in the diagrams of Fig. 3 we use the analytical momentum-space representation of the Dirac Green function with zero and one Coulomb interaction. This is essentially different from the method employed in the calculation of the diagram Fig. 1(a), where the Green function was first constructed with B-splines in coordinate space and then numerically transformed into momentum space. The resulting agreement shows that the B-splines basis set method is very reliable in this case. To provide an accurate fitting of the numerical results which behave nearly singularly in the vicinity of $Z = 0$, we extend our calculation up to very low fractional Z, namely $Z = 0.1$. This appeared to be technically possible since the diagrams under consideration contain only free electron propagators which are known in a closed analytical form.

The results of the least-squares fit of our numerical results are presented in Table 2. The fitting was carried out with eight parameters a_{50}, a_{6i} $(i = 3, \dots, 0)$, a_{7i} $(i = 3, 2, 1)$. In order to reduce the statistical uncertainty of the fitting procedure, a large number of points (twenty or more) was used. We note that the fitting results are remarkable stable with respect to the number of fitting parameters, number of nodes and to the choice of the minimal and maximal nuclear charge numbers. The same fitting procedure was applied to all diagrams Fig. 3. As one can see from the Table 2, the fitting results for the coefficients a_{50} and a_{63} are in a very good agreement with analytical calculations for all diagrams except one. We can deduce that the existing discrepancy between different methods originates only from diagram Fig. 3(c). While this diagram should not contribute to order $\alpha^2(Z\alpha)^6 \ln^3(Z\alpha)^{-2}$ according to Karshenboim, our calculation shows the presence of the cubed logarithm with a coefficient $a_{63} = -0.652(30)$. The reason for this disagreement is not known at present.

Although our analysis does not explain the existing discrepancy, we localized its origin. A conclusion can be drawn already that this disagreement can not be ascribed to any nonperturbative effects, as was originally surmised by Mallampalli and Sapirstein [4]. Still, the existing discrepancy looks to be quite surprising since the diagram under consideration is relatively simple both for the direct numerical calculation and for the analytical evaluation of the leading logarithm. Moreover, the derivation method for the leading-logarithmic contributions used by Karshenboim [3] is considered as a standard tool for this type of calculations at present. In the next section, we perform a similar calculation for the combined self-energy vacuum-polarization diagram and demonstrate an agreement achieved in that case for the leading-logarithmic contribution.

Considering the loop-after-loop diagram Fig. 1(a), one should keep in mind that the corresponding contribution is not completely gauge invariant. It is invariant in any covariant gauge but not, e.g., in the Coulomb gauge. This means that, strictly speaking, the loop-after-loop contribution has no well-defined phys-

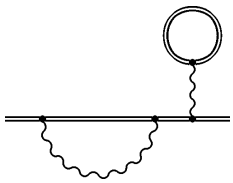

Fig. 4. Combined self-energy vacuum-polarization diagram

ical meaning when considered separately. Therefore, if any "physical" assumptions are made in analytic evaluation of the leading-logarithmic contribution, one could expect the correct result only for the whole gauge invariant set of diagrams but not for the loop-after-loop contribution alone.

2 Combined self-energy vacuum-polarization diagram

In this section we report a numerical evaluation of the combined self-energy vacuum-polarization diagram Fig. 4 in the low-Z region without an expansion in $Z\alpha$. Analytical evaluation of its leading logarithmic contribution of order $\alpha^2(Z\alpha)^6 \ln^2(Z\alpha)^{-2}$ was carried out by Karshenboim [9]. This diagram can be considered as a good "test case" for an investigation of the leading logarithm. While it is significantly easier for the analytical analysis than the loop-after-loop diagram, at the same time the derivation of the leading logarithm for these two diagrams is very similar.

Numerical results for the diagram Fig. 4 are presented in Table 3 for several values of Z. The calculation was carried out in the Fried-Yennie gauge similarly to that for the loop-after-loop diagram. A least-squares fit to our numerical results yields

$$a_{50} = 0.611(4) \qquad a_{62} = 0.15(4)\ . \tag{4}$$

This is in a reasonable agreement with the Karshenboim's result for the leading logarithmic contribution $a_{62} = 8/45 \approx 0.178$. A detailed analysis similar to that for the loop-after-loop contribution shows that the diagram corresponding to diagram Fig 3(c) does not contribute to order $\alpha^2(Z\alpha)^6 \ln^2(Z\alpha)^{-2}$ in this case.

Table 3. The contribution of the combined self-energy vacuum-polarization diagram for the ground state of hydrogenlike atoms expressed in terms of the function $G(Z\alpha)$ defined by Eq. (2)

Z	1	2	3	4	5	7	10
$G(Z\alpha)$	0.67	0.691	0.704	0.712	0.718	0.723	0.722

Conclusion

In the present investigation, we reported the numerical evaluation of the loop-after-loop contribution to the Lamb shift of the ground state for hydrogenlike low-Z ions. The calculation was carried out in the Fried-Yennie gauge and without an expansion in parameter $Z\alpha$. Our study confirms the results of Mallampalli and Sapirstein [4] and disagrees with the calculation by Goidenko and co-workers [5]. A fit to our numerical results confirms the analytical result of Refs. [1,2] for the coefficient a_{50} but deviates significantly from the Karshenboim's value of the leading logarithmic contribution a_{63} [3]. A detailed analysis shows that the existing discrepancy originates from one diagram in the potential expansion of the loop-after-loop contribution. While the reason for this discrepancy remains unknown, we concluded that it can not be ascribed to any nonperturbative effects.

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Appendix I: Partial Wave Renormalization

The partial wave renormalization (PWR) approach has been introduced by Persson and co-workers [10] and by Quiney and Grant [11] as a convenient method for the numerical evaluation of diagonal matrix elements of the first-order self-energy operator. In this approach, the truncation of the partial-wave expansion fulfills the role of the regularization parameter. Obviously, this regularization is noncovariant and, therefore, some *correction terms* are likely to appear due to a noncovariant nature of the procedure. While it is not the case for the diagonal matrix elements of the first-order self-energy operator, such spurious terms have been observed in numerical calculations of the screened self energy if the screening potential contains a magnetic photon (see Ref. [12] and a concluding remark in Ref. [13]). An analytic evaluation of the correction terms for the self-energy correction in the presence of an additional Coulomb-like screening potential $V_c(r)$ was reported by Persson et al. [13]. The corresponding Feynman diagrams are presented in Fig. 5. It was shown that the PWR scheme being applied to the irreducible part of diagram Fig. 5(a) provides a spurious term which can be evaluated to be

$$\mathcal{E}_1^a = -\frac{\alpha}{2\pi}\langle a|\big[V_c(r) - \overline{V}_c\big]\ln(r)|a\rangle \ , \tag{5}$$

where $\overline{V}_c = \langle a|V_c(r)|a\rangle$. For Coulomb-like potential $V_c(r)$ this correction term is exactly cancelled when considered together with the remaining contribution of Fig. 5.

A direct numerical calculation of the diagrams presented in Fig. 5 was carried out in our recent work [7] using both the PWR scheme as well as the covariant

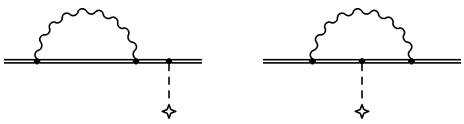

Fig. 5. Feynman diagrams representing the self-energy correction in the presence of an additional screening potential $V_c(r)$ (dashed line)

Table 4. Comparison of the correction terms obtained by a direct numerical calculation of the diagrams Fig. 5 with $V_c(r) = -\alpha/r$ and using the analytical expression (5), in atomic units

Z	Ref. [7]	Eq. (5)
20	-0.01190	-0.01187
30	-0.01832	-0.01830
50	-0.03350	-0.03349
70	-0.05501	-0.05500
92	-0.09726	-0.09726

approach. The spurious term for the irreducible contribution calculated in that work is listed in the second column of Table 4. In the third column we present the correction term evaluated according to Eq. (5). An excellent agreement[2] is found. While the cancellation of the spurious contributions does not hold anymore if the potential $V_c(r)$ contains a magnetic photon, it is possible to derive a corresponding expression for the correction term for that case [14] as well.

However, another opinion exists in the literature about the correction terms in the PWR method. In the recent work by Goidenko and co-workers [15], the authors argue that the derivation of Ref. [13] is erroneous and the corresponding correction terms should be identically zero.

[2] This fact was first pointed out to the author by G. Plunien and I. Goidenko.

Appendix II: Potential expansion of the reducible Green function

Here we examine the potential expansion of the reducible Green function $G_{\rm red}$. It is defined by

$$G_{\rm red}(\mathbf{x}_1,\mathbf{x}_2) = \lim_{\varepsilon\to\varepsilon_a}\left[G(\varepsilon,\mathbf{x}_1,\mathbf{x}_2) - \sum_{\varepsilon_n=\varepsilon_a}\frac{\psi_n(\mathbf{x}_1)\psi_n^\dagger(\mathbf{x}_2)}{\varepsilon-\varepsilon_a}\right] , \tag{6}$$

where G denotes the full Dirac Coulomb Green function. The analytical properties of $G(\varepsilon)$ in the complex ε-plane are well known. In a vicinity of a single pole $\varepsilon=\varepsilon_a$ we can write the Laurent expansion of $G(\varepsilon)$

$$G(\varepsilon) = \frac{c_{-1}}{\varepsilon-\varepsilon_a} + c_0 + (\varepsilon-\varepsilon_a)\,c_1 + \cdots . \tag{7}$$

The reducible Green function is then given by the coefficient c_0 in the Laurent expansion of the full Green function

$$G_{\rm red} = c_0 = \frac{1}{2\pi i}\oint_\Gamma d\varepsilon \frac{G(\varepsilon)}{\varepsilon-\varepsilon_a} , \tag{8}$$

where the contour Γ surrounds only the pole $\varepsilon=\varepsilon_a$ and is oriented counterclockwise. Now we can use the standard potential expansion of $G(\varepsilon)$ into zero-, one-, and many-potential terms (see, e.g., Ref. [16])

$$G(\varepsilon) = G^{(0)}(\varepsilon) + G^{(1)}(\varepsilon) + G^{(2+)}(\varepsilon) \tag{9}$$

to build the corresponding expansion for $G^{\rm red}$. Since both $G^{(0)}(\varepsilon)$ and $G^{(1)}(\varepsilon)$ are regular at $\varepsilon=\varepsilon_a$, we have $G^{(0)}_{\rm red} = G^{(0)}(\varepsilon_a)$ and $G^{(1)}_{\rm red} = G^{(1)}(\varepsilon_a)$. To derive the expression for $G^{(2+)}_{\rm red}$, we use the spectral representation for the function $G^{(2+)}$,

$$G^{(2+)}(\varepsilon) = \sum_{\alpha\beta n}\frac{|\alpha\rangle\langle\alpha|V|n\rangle\langle n|V|\beta\rangle\langle\beta|}{(\varepsilon-\varepsilon_\alpha)(\varepsilon-\varepsilon_n)(\varepsilon-\varepsilon_\beta)} , \tag{10}$$

where we use α, β for the summation over the free Dirac states, n for Dirac states in an external field, and V is the nuclear binding potential. Let us evaluate the contribution of the initial state $n=a$ in Eq. (10) to the reducible Green function:

$$\begin{aligned}
&\frac{1}{2\pi i}\oint_\Gamma \frac{d\varepsilon}{\varepsilon-\varepsilon_a}\sum_{\alpha\beta}\frac{|\alpha\rangle\langle\alpha|V|a\rangle\langle a|V|\beta\rangle\langle\beta|}{(\varepsilon-\varepsilon_\alpha)(\varepsilon-\varepsilon_a)(\varepsilon-\varepsilon_\beta)}\\
&= -\sum_{\alpha\beta}\left\{\frac{|\alpha\rangle\langle\alpha|V|a\rangle\langle a|V|\beta\rangle\langle\beta|}{(\varepsilon_a-\varepsilon_\alpha)^2(\varepsilon_a-\varepsilon_\beta)} + \frac{|\alpha\rangle\langle\alpha|V|a\rangle\langle a|V|\beta\rangle\langle\beta|}{(\varepsilon_a-\varepsilon_\alpha)(\varepsilon_a-\varepsilon_\beta)^2}\right\}\\
&= -\sum_{\alpha\beta}\left\{\frac{|\alpha\rangle\langle\alpha|a\rangle\langle a|\beta\rangle\langle\beta|}{\varepsilon_a-\varepsilon_\alpha} + \frac{|\alpha\rangle\langle\alpha|a\rangle\langle a|\beta\rangle\langle\beta|}{\varepsilon_a-\varepsilon_\beta}\right\} .
\end{aligned} \tag{11}$$

In the last step we employed the following identity

$$\langle\alpha|V|a\rangle = \langle\alpha|(-\mathcal{H}_0+\mathcal{H})|a\rangle = (\varepsilon_a-\varepsilon_\alpha)\langle\alpha|a\rangle \ , \tag{12}$$

where $\mathcal{H}_0$ and $\mathcal{H}$ are the free and the full Dirac Hamiltonian, respectively. Finally, we obtain

$$G_{\rm red} = G^{(0)}(\varepsilon_a) + G^{(1)}(\varepsilon_a) + G^{(2+)}_{\rm red} \ , \tag{13}$$

where

$$\begin{aligned} G^{(2+)}_{\rm red} = & \sum_{\substack{\alpha\beta \\ \varepsilon_n\neq\varepsilon_a}} \frac{|\alpha\rangle\langle\alpha|V|n\rangle\langle n|V|\beta\rangle\langle\beta|}{(\varepsilon_a-\varepsilon_\alpha)(\varepsilon_a-\varepsilon_n)(\varepsilon_a-\varepsilon_\beta)} \\ & - \sum_{\substack{\alpha \\ \varepsilon_n=\varepsilon_a}} \left\{ \frac{|n\rangle\langle n|\alpha\rangle\langle\alpha|}{\varepsilon_a-\varepsilon_\alpha} + \frac{|\alpha\rangle\langle\alpha|n\rangle\langle n|}{\varepsilon_a-\varepsilon_\alpha} \right\} \ . \end{aligned} \tag{14}$$

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