Two-Loop Self-Energy Correction in High-Z Hydrogenlike Ions

V. A. Yerokhin,^{1,2} P. Indelicato,² and V. M. Shabaev¹

¹Department of Physics, St. Petersburg State University, Oulianovskaya 1, St. Petersburg 198504, Russia

²Laboratoire Kastler-Brossel, Unité Mixte de l'École Normale Supérieure, du CNRS et l'Université Pierre et Marie Curie,

Case 74, 4 Place Jussieu, F-75252, CEDEX 05, France

(Received 28 February 2003; published 15 August 2003)

A complete evaluation of the two-loop self-energy diagrams to all orders in $Z\alpha$ is presented for the ground state of H-like ions with $Z \ge 40$.

DOI: 10.1103/PhysRevLett.91.073001

The calculation of the two-loop self-energy correction to the Lamb shift is at present one of the most challenging problems in bound-state QED. Until very recently, this project has been addressed to mainly within the $Z\alpha$ -expansion approach. In it, the two-loop selfenergy contribution is represented as an expansion over $Z\alpha$ and $\ln(Z\alpha)$,

$$F(Z\alpha) = B_{40} + (Z\alpha)B_{50} + (Z\alpha)^2[L^3B_{63} + L^2B_{62} + LB_{61} + B_{60}] + \cdots,$$
(1)

where $F(Z\alpha) = \Delta E / [m(\alpha/\pi)^2 (Z\alpha)^4], \quad L = \ln(Z\alpha)^{-2}.$ Whereas the lowest-order term B_{40} has been known for a long time, calculations of higher-order contributions have not been accomplished until recently. The correction B_{50} was found to be surprisingly large [1,2], $B_{50} =$ -24.27. This result has significantly changed the theoretical prediction for the Lamb shift in hydrogen and resolved the disagreement with the experimental value existing at that time. The leading logarithmic term B_{63} was derived first in [3] and later confirmed in [4,5]. (It should be noted that the first evaluation [3], while yielding the right result, is not completely correct, as will be discussed below.) The two remaining logarithmic corrections B_{62} and B_{61} have also been elaborated lately by Pachucki [5]. Again, as in order $(Z\alpha)^5$, the result obtained turned out to be surprisingly large. The numerical value of B_{61} is 49.8, which reverses the sign of the overall logarithmic contribution for hydrogen. This indicates that the convergence of the $Z\alpha$ expansion for the twoloop self-energy correction is remarkably slow, and a conclusion has been drawn in [5] that a numerical evaluation with Dirac-Coulomb propagators is desirable even for hydrogen.

The calculation of the two-loop self-energy diagrams (Fig. 1) without an expansion in $Z\alpha$ started with the irreducible contribution of the diagram (a) [known also as the loop-after-loop (LAL) correction], which is by far the simplest part of the total set. Such an evaluation was first accomplished in [6] for high-Z ions, and later in [7] for all ions, including hydrogen. The latter investigation demonstrated a rather peculiar behavior of the LAL correction in the low-Z region. It was shown that for

PACS numbers: 31.30.Jv, 31.10.+z

hydrogen its actual value was of a different sign and magnitude than the value based on the first two terms of the $Z\alpha$ expansion. In addition, a different result was found in [7] for the leading logarithmic contribution B_{63} as compared to the analytical evaluation [3]. (We note that in the latter work the B_{63} term was evaluated for the whole set of two-loop self-energy diagrams. However, it was argued that it originated from the LAL contribution only.) As a result, a question was raised in [7] about the possibility that the $Z\alpha$ expansion for the two-loop selfenergy could be inadequate even for hydrogen. This speculation attracted attention and several investigations followed. The subsequent numerical calculation [8] claimed to be compatible with the analytical result. However, the third numerical evaluation by one of us [9] confirmed the first result [7]. At the same time, the total value of the B_{63} contribution was confirmed independently by several groups, e.g., in [4]. To throw light on this intricate situation, we performed [10] an analytic calculation of the B_{63} term separately for the LAL correction and found agreement both with our previous numerical result and with that of [7]. Our conclusion was that the LAL correction provided an additional cubed logarithmic contribution that had been omitted in the original analytical calculation [3]. However, this additional term vanishes when the whole set of two-loop self-energy diagrams is taken into account. Recently, analogous additional terms were reported for the leading logarithmic contribution for *P* states [11].

The evaluation of the remaining contributions in Fig. 1 is by far more difficult. These contributions are the reducible part of the diagram (a), the overlapping diagram (b), and the nested diagram (c). The first attempt to evaluate them to all orders in $Z\alpha$ was made by



FIG. 1. Two-loop self-energy diagrams. Double line indicates an electron propagating in the Coulomb nuclear field. It is understood that the corresponding mass counterterms are subtracted from the diagrams.

© 2003 The American Physical Society 073001-1

Mallampalli and Sapirstein [12]. In that work, the contribution of interest was rearranged in three parts, referred to by the authors as the "*M*," "*P*," and "*F*" terms. (We will discuss this separation in more detail below.) Mallampalli and Sapirstein calculated only the M and Fterms, while the P term was left out since a new numerical technique had to be developed for its computation. In addition, since the numerical procedure turned out to be very time consuming, the actual calculation of the Mterm was carried out only for two ions, uranium and bismuth. Subsequently, in the investigation by two of us [13], we accomplished the computation of the remaining P term for Z = 83, 90, and 92, which formally completed the calculation of the two-loop self-energy. However, as we will see, the rearrangement of the whole correction into the M, P, and F terms is artificial since all three are divergent. A proper treatment should include these terms simultaneously. In addition, more than two points (in Z) are needed in order to analyze the Z dependence of the correction and to compare it with the known terms of the $Z\alpha$ expansion. All these issues are addressed in the present investigation.

Let us now turn to the evaluation of the two-loop selfenergy diagrams. The first problem to be solved is the separation of ultraviolet (UV) divergences. The standard method of renormalization in QED is developed for diagrams involving only free-electron propagators, treating them in momentum space. Therefore, our strategy is to subtract similar diagrams with electron propagators containing zero or one interaction with the nuclear Coulomb field in order to make the corresponding point-by-point difference UV finite. The subtracted diagrams can be then evaluated in momentum space or in the mixed momentum-coordinate representation. For the first-order self-energy, this approach was first implemented in [14]. The situation is much more difficult in the case of the two-loop self-energy. Here, for the first time, we encounter the overlapping UV divergences. For example, the diagram in Fig. 1(b) can be considered as consisting of two overlapping vertex subdiagrams, each of which is UV divergent. The presence of the overlapping divergences makes the structure of subtraction terms much more elaborate than that in the first order. Moreover, some of these terms contain both bound-electron propagators and UV-divergent subdiagrams. Such a situation had never been encountered before, and a new numerical technique had to be developed for the evaluation of these subtraction terms.

Following [12], we rearrange the contribution of the diagrams in Fig. 1 in four parts: the LAL part, the M, P, and F terms. The LAL correction is defined by the irreducible part of the diagram (a). Since its evaluation is relatively easy and has been performed by several groups, we do not discuss it here. The M term is diagrammatically represented by Fig. 2. It consists of three parts originating from the nested diagram, the overlapping



FIG. 2. Diagrammatic representation of the *M* term. The dashed line denotes the interaction with the Coulomb nuclear field. ΔE_{SE} is the first-order self-energy correction.

diagram, and the reducible part of the diagram (a). The subtractions in the *M* term are chosen so that each of these three parts is separately UV finite. Next, we should account for the subtracted terms. Those that contain only free-electron propagators can be treated in momentum space using the standard Feynman-parametrization technique. For those that involve bound-electron propagators, we introduce additional subtractions that remove the overlapping UV divergences. This is graphically represented by Fig. 3. The corresponding contribution is referred to as the P term. It consists of three parts, each containing only single UV-divergent subgraphs. Taking the first part as an example, we see that the difference shown in the figure is UV divergent only due to the inner self-energy loop, while the divergence due to the outer self-energy loop is canceled. Finally, we collect all terms we have subtracted and denote them as the F term depicted in Fig. 4. It consists of Feynman diagrams that contain free-electron propagators only.



FIG. 3. Diagrammatic representation of the P term. The last part should be counted twice, accounting for two equivalent terms.



FIG. 4. Diagrammatic representation of the F term. The last diagrams on the right in the first two rows should be counted twice, accounting for two equivalent diagrams.

We should also mention the infrared (IR) referencestate divergences that are present in the M and P terms. These singularities can occur in bound-state QED calculations when energies of the intermediate states in the spectral decomposition of electron propagators coincide with the valence-state energy. An analysis given, e.g., in [12] shows that the IR-divergent terms cancel each other in the sum of the M and the P term. To sum up our discussion of divergences, we separately write divergent contributions to the terms under consideration:

$$\Delta E_M = \Delta E_M^f - \Delta E_{\rm IR},\tag{2}$$

$$\Delta E_P = \Delta E_P^f + \Delta E_{\rm IR} + L^{(1)} \Delta E_{\rm SE}^{(2+)},\tag{3}$$

$$\Delta E_F = \Delta E_F^f + B^{(1)} \Delta E_{\rm SE}^{(2+)},\tag{4}$$

where the index f labels finite contributions, $\Delta E_{\rm IR}$ is the IR-divergent contribution, $L^{(1)}$ and $B^{(1)}$ are the one-loop renormalization constants that fulfill the Ward identity $L^{(1)} = -B^{(1)}$, and $\Delta E_{\rm SE}^{(2+)}$ is the many-potential part of the one-loop self-energy correction.

We now turn to the numerical evaluation of these terms. It was carried out in the Feynman gauge. The P term was evaluated along the lines described in detail in our previous investigation [13]. The calculation of the Fand M terms was performed in a way, in many respects similar to that of [12]. The details of the calculation will be published elsewhere. Here, we focus on major novel features of our evaluation as compared to [12]. The first point is a different treatment of the reference-state IR divergences. In [12], they were regulated by altering the valence energy ε_a to $\tilde{\varepsilon}_a = \varepsilon_a(1 - \delta)$. The actual calculations were performed keeping a finite regulator δ , and the limit $\delta \rightarrow 0$ was evaluated numerically. According to our experience, that approach, while being technically easy to handle, does not allow one to control the accuracy of the computation effectively. In our approach, we introduce some subtractions in order to make the terms under consideration finite, separating IR divergences in the form $\Delta E_{\rm IR}$. The divergent contributions cancel each other explicitly in the sum, and we can perform the whole computation without introducing any actual IR regulator. However, in order to allow the term-by-term comparison with the previous evaluation [12], we performed our calculations with the regulator δ as well.

The second new feature of our approach is a different procedure employed for the double summation over the partial waves in the *M* term. In [12], the photon angular momenta l_1 and l_2 were chosen as independent expansion parameters. We found it technically more convenient to employ for this purpose the absolute values of the relativistic angular parameter κ of two electron propagators, $|\kappa| = j + 1/2$. Thus, we turn the nested and overlapping contributions to the *M* term into tables of values $X_{|\kappa_1|,|\kappa_2|} \rightarrow Y_{ij}$, where $i = ||\kappa_1| - |\kappa_2||$, $j = (|\kappa_1| + |\kappa_2| - i)/2$. Finally, we sum up the table: First, we fix *i* and extrapolate the sum over *j* to infinity, and then sum over *i* and estimate the tail of the expansion.

Now we discuss the computer time necessary for the evaluation of the *M* term. In the previous evaluation by Mallampalli and Sapirstein, a total time of 7323 h was required for a given value of *Z*. In our numerical approach, the typical time of the evaluation of one element $X_{\kappa_1\kappa_2}$ is about 1 h for the IBM PWR3 processor with 350 MHz, both for the nested and the overlapping diagram. The typical number of elements for a given *Z* was 440 for the nested diagram and 320 for the overlapping diagram. This shows that the time consumption in our numerical procedure is smaller than that of [12], although it is still very large.

In Table I, we present the numerical results for individual contributions to the two-loop self-energy correction. The table shows that our numerical values for the LAL and F terms agree very well with the ones from [7,12] but there is a significant deviation for the M term. More specifically, our calculation for Z = 92 yields

TABLE I. Individual contributions to the two-loop selfenergy correction expressed in terms of $F(Z\alpha)$.

		•			
Ζ	LAL	F term	P term	M term	Total
40	-0.871	19.50	-30.13(15)	10.50(18)	-1.00(23)
50	-0.973	10.03	-14.42(7)	4.04(7)	-1.33(10)
		10.02 ^a			
60	-1.082	5.72	-7.48(4)	1.21(2)	-1.63(4)
70	-1.216	3.497	-4.03(3)	-0.14(1)	-1.89(3)
	-1.216^{b}				
83	-1.466	1.938	-1.831(13)	-0.990(5)	-2.349(14)
		1.937 ^a		$-1.66(1)^{a}$	
92	-1.734	1.276	-1.030(9)	-1.295(3)	-2.784(10)
	-1.733^{b}	1.274 ^a		$-1.855(7)^{a}$	
100	-2.099	0.825	-0.635(6)	-1.473(3)	-3.382(7)
		0.825 ^a			

^aRef. [12]. ^bRef. [7].



FIG. 5. The results of our numerical evaluation to all orders to $Z\alpha$ (dots) together with the first two terms of the $Z\alpha$ expansion (solid line) and all known terms of the $Z\alpha$ expansion (dashed line).

-2.137, 4.679(2), and -3.837(2) for the reducible, nested, and overlapping contributions to the *M* term, respectively. These results should be compared correspondingly with -2.137, 4.669(5), and -4.387(5) from [12]. We see that the leading source of discrepancy is the overlapping diagram. Taking into account the complexity of the computation, it is difficult to suppose what the reason for this disagreement could be.

As in the case of the one-loop self-energy, the evaluation becomes problematic very fast as Z decreases. It is due in part to the fact that some individual contributions exhibit a nearly Z-independent behavior, while the total correction scales as $(Z\alpha)^4$. Numerical problems restricted our calculation to the region $Z \ge 40$. In Fig. 5, we compare our nonperturbative results with the known terms of the $Z\alpha$ expansion. Although we cannot as yet say anything conclusive about the higher-order terms, the figure suggests that the results obtained by two different methods could be compatible.

In summary, we have evaluated all contributions to the two-loop self-energy correction for H-like ions with $Z \ge 40$. As this correction has been the major source of the uncertainty of theoretical values for the ground-state Lamb shift in these systems, our evaluation improves their accuracy by an order of magnitude [13]. While the experimental precision for H-like uranium is not presently sufficient to probe the new contribution, this should become possible when the experiment currently planned at Gesellschaft für Schwerionenforschung (Germany) [15] is completed. The question of utmost importance is to extend the present evaluation to low-Z ions, where higher-order terms could enter at the level of experimental interest even at Z = 1 [5], as well as to excited states. For the $2p_{1/2}$ -2s transition in Li-like high-Z ions, the two-loop self-energy presently defines the uncertainty of the theoretical prediction [13] and can be probed by comparing with available experimental data.

This study was supported in part by RFBR (Grant No. 01-02-17248), by Ministry of Education (Grant No. E02-3.1-49), and by the program "Russian Universities" (Grant No. UR.01.01.072). V.Y. acknowledges the support from the Ministère de l'Education Nationale et de la Recherche, the foundation "Dynasty," and International Center for Fundamental Physics. The computation was performed on the CINES and IDRIS national computer centers.

- [1] K. Pachucki, Phys. Rev. Lett. 72, 3154 (1994).
- [2] M. Eides and V. Shelyuto, Phys. Rev. A 52, 954 (1995).
- [3] S. G. Karshenboim, Zh. Eksp. Teor. Fiz. 103, 1105 (1993)
 [Sov. Phys. JETP 76, 541 (1993)].
- [4] A.V. Manohar and I.V. Stewart, Phys. Rev. Lett. 85, 2248 (2000).
- [5] K. Pachucki, Phys. Rev. A 63, 042503 (2001).
- [6] A. Mitrushenkov, L. Labzowsky, I. Lindgren, H. Persson, and S. Salomonson, Phys. Lett. A 200, 51 (1995).
- [7] S. Mallampalli and J. Sapirstein, Phys. Rev. Lett. 80, 5297 (1998).
- [8] I. Goidenko, L. Labzowsky, A. Nefiodov, G. Plunien, and G. Soff, Phys. Rev. Lett. 83, 2312 (1999).
- [9] V. A. Yerokhin, Phys. Rev. A 62, 012508 (2000).
- [10] V. A. Yerokhin, Phys. Rev. Lett. 86, 1990 (2001).
- [11] U. D. Jentschura and I. Nándori, Phys. Rev. A 66, 022114 (2002).
- [12] S. Mallampalli and J. Sapirstein, Phys. Rev. A 57, 1548 (1998).
- [13] V. A. Yerokhin and V. M. Shabaev, Phys. Rev. A 64, 062507 (2001).
- [14] N. J. Snyderman, Ann. Phys. (N.Y.) 211, 43 (1991); S. A. Blundell and N. J. Snyderman, Phys. Rev. A 44, R1427 (1991).
- [15] T. Stöhlker et al., Phys. Rev. Lett. 85, 3109 (2000).