Complete two-loop binding correction to the Lamb shift

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The binding correction of the two–loop contribution to the Lamb shift in hydrogen–like atoms is calculated by a combined analytical and numerical method. A new theoretical value for the Lamb shift is given and the proton radius puzzle is solved in favor of the value obtained by the Mainz group.

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I. INTRODUCTION

The Lamb shift is playing a fundamental role in testing bound state quantum electrodynamics. Radio–frequency measurements of the 2S-2P splitting in hydrogen have reached an accuracy of several kHz. Further progress is limited by the linewidth of $2P_{1/2}$ state, which is of the order of 100 MHz. In contrast, optical high resolution spectroscopy based on two–photon transitions between hydrogen S-states has no such restrictive barrier. In fact, the most recent measurement of Hänsch *et.al.* [1] of 1S ground state Lamb shift:

$$E_L(1S) = 8172.86(6)\,\mathrm{MHz} \tag{1}$$

has a relative accuracy greater than the best radio–frequency measurement of the 2S-2P splitting, see Eq. (31).

For the comparison with theoretical values, we have two contradicting experimental results for the proton charge radius: $r_p = 0.805(11)\,\mathrm{fm}$, $r_p = 0.862(12)\,\mathrm{fm}$, given by references two and three, respectively. As it is know [1,4], the theoretical predictions derived with the newer measurement of $r_p = 0.862(12)$ fm are not in a good agreement with the Lamb shift experiments. In order to improve the theoretical predictions we complete the evaluation of the nonrecoil corrections of order $\alpha^2\,(Z\,\alpha)^5$, where α is the fine structure constant and Z is the atomic number. We show that this correction explains this discrepancy, and agreement between theory and experiment is achieved.

The remaining corrections of comparable magnitude are known with a precision of order 1 kHz for 2S-2P Lamb shift. For example, the pure recoil correction of order $m/M(Z\,\alpha)^6$ has been calculated by Doncheski, Grotch and Erickson [4], in spite of the fact that there is still no satisfactory and effective scheme for the two body problem. The binding corrections to the one loop self–energy of order $\alpha\,(Z\,\alpha)^6$ have been calculated to high precision in [5] where a novel analytical method has been introduced. For other corrections see the very good review of Sapirstein and Yennie [6]. The two–loop correction to the hyperfine splitting in hydrogen and muonium, similar to that presented here, has been recently calculated by T. Kinoshita [7].

We concentrate now on the binding correction to the two–loop contribution. It is a general feature of bound state calculations in quantum electrodynamics that, in addition to a lower order contribution, each diagram also gives higher orders in $Z\,\alpha$ and $Z\,\alpha\,\ln(Z\,\alpha)$ terms. In the two–loop contribution, for example (we put electron mass $m=1$, speed of light $c=1$, and proton mass $M=\infty$):

$$\Delta E = \left(\frac{\alpha}{\pi}\right)^2\,\frac{(Z\,\alpha)^4}{n^3}(B_{40} + Z\alpha\,B_{50} + \cdots)\,. \tag{2}$$

The lowest order term is given by B_{40} and the binding correction by B_{50}; the first index gives the power in $Z\,\alpha$ and the second the power in the $\ln(Z\,\alpha)$. The B_{40} coefficient has been known for a long time [9], and for its calculation one can use the so called on–shell approximation. For an introduction to two–loop Lamb shift calculations see [10]. Under the on–shell approximation, B_{40} is determined by the value and derivative of the two–loop electron form factors F_2 and F_1' (for their definition see [8]) at $q^2 \equiv \mathbf{q}^2 = 0$

$$B_{40} = \left(\frac{\pi}{\alpha}\right)^2\,\left(4\,F_1'(0) + F_2(0)\right)\,. \tag{3}$$

The binding corrections to the two–loop contribution with a closed fermion loop have been calculated in the series of papers by M. Eides and coworkers [11] and by us in [12]. The present paper provides an evaluation of the most difficult and dominant two–loop corrections: those with the two photon loops. Some partial results have been already obtained [13]. The remaining three–loop contribution, although not yet calculated, is expected to give less then 1 kHz for 2S state (roughly α/π times the two–loop contribution), below the current experimental precision, Eqs. (30–32).

As was first noticed by M. Eides et.al. [11], all diagrams responsible for the binding correction could be generated from the fermion line with two vertices, taking all possible two–loop dressings. The diagrams without closed fermion loops are represented in Figure 1, where the fermion external legs are on the mass shell. The expression derived from this diagram can be written in the following shortened form:

$$\Delta E = \phi(0)^2 \int \frac{d^3p}{(2\pi)^3}\, \frac{(4\,\pi\,\alpha)^2}{p^4} \mathrm{Tr}\Bigg[\Bigg(\Lambda_R(0,p,0) \\ +2\,\Gamma_R(0,p)\frac{1}{\not p - m} + \Sigma_R(p)\frac{1}{(\not p - m)^2}\Bigg)\frac{(\gamma_0 + I)}{4}\Bigg]_S , \tag{4}$$

where Λ, Γ, Σ are two–loop two–, one– and zero–vertex functions with implicit indices equal to 0. S means the separation of the constant term for $p = 0$, which is responsible for the leading order contribution. $\phi(0)$ is an electron wave function at the origin.

II. THE METHOD OF CALCULATION

The expression for the two–loop correction to energy shift can be written as:

$$\Delta E = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\,\alpha)^5}{n^3}\, F\,, \\ F = \int \frac{d^3\,p}{\pi^2} \int \frac{d^4\,k_2}{\pi^2} \int \frac{d^4\,k_1}{\pi^2}\; \frac{1}{4\,p^4}\Big(f(p,k_1,k_2) - f(0,k_1,k_2)\Big)\,, \tag{5}$$

where f is a function depending on the particular diagram. The contribution of any renormalized diagram diverges with the photon mass μ in Feynman gauge like $\mu^{-3/2}$, making numerical integration difficult. There are at least two ways to avoid this problem. The first is the use of the Yennie gauge, where each diagram gives a finite contribution. The second way is to perform the integrals with respect to k_1 and k_2 analytically for small p and numerically for larger p. The first method we apply for the gauge independent set of diagrams a, b and c from Figure 1, while the rest of the (also gauge independent) set of 16 diagrams is calculated with the second method.

A. Evaluation of reducible diagrams

The Yennie gauge is particularly useful, because of its remarkable infrared properties. This gauge also provides a simple form of the renormalized one–loop self–energy [14]:

$$\Sigma_R(p) = \frac{3\,\alpha}{4\,\pi}(\not p - 1)^2\;\; \not p\, Y(p)\,, \\ Y(p) = -\left(\frac{1}{1-p^2} + \frac{p^2\,\ln(p^2)}{(1-p^2)^2}\right)\,. \tag{6}$$

We use the nonstandard notation $p^2 \equiv \mathbf{p}^2$. Calculating the traces for the first diagram a from Figure 1 we simply get

$$F_a = 0\,, \tag{7}$$

where we introduce a notation that the index in F denotes a contribution from the related diagram from Figure 1. For the remaining two diagrams b and c from Figure 1, we need also a renormalized vertex function. We decompose it in the following way:

$$\Gamma(0,p)_R = \frac{(\gamma_0 + I)}{2}\, G_1 + \frac{(\gamma_0 + I)}{2}\boldsymbol{\gamma}\cdot\mathbf{p}\, G_2 + \ldots\,, \tag{8}$$

where the dots indicate remaining terms that contain $(\gamma_0 - I)$ on the left hand side. These do not contribute after the trace is performed. The energy shift, written in terms of G_i, reads

$$\Delta E_b = 2\,\phi(0)^2 \int \frac{d^3 p}{(2\,\pi)^3} \left(\frac{4\,\pi\,\alpha}{p^2}\right)^2 (G_1 + p^2\,G_2)\frac{3\,\alpha}{4\,\pi}\,Y(p)\,, \tag{9}$$

$$\Delta E_c = -\phi(0)^2 \int \frac{d^3 p}{(2\,\pi)^3} \left(\frac{4\,\pi\,\alpha}{p^2}\right)^2 \frac{2\,G_1^2 + 2\,p^2\,G_1\,G_2}{p^2}\,. \tag{10}$$

Both G_i can be expressed by the integral of their imaginary parts G_i^A for negative p^2, i.e.

$$G_1(p^2) = p^2 \int_0^\infty d(q^2)\,\frac{1}{q^2(p^2+q^2)}\,G_1^A(q^2)\,, \tag{11}$$

$$G_2(p^2) = -\int_0^\infty d(q^2)\frac{1}{p^2+q^2}\,G_2^A(q^2)\,, \tag{12}$$

where the index A for any function f means $f^A(q^2) = \big(f(-q^2+i\,\epsilon) - f(-q^2-i\,\epsilon)\big)\,/2\,\pi\,i$. For these imaginary parts, we derive the expressions:

$$\begin{aligned} G_1^A = \frac{3\,\alpha}{2\,\pi}\Bigg[&-\frac{2}{3} + \frac{q^2}{2\,(1+q^2)^2} + \sqrt{1-\frac{4}{q^2}}\,\frac{1}{3}\,\Theta(q-2) + \\ &\left(\frac{2}{3\,q} - \frac{q}{6}\right)\left(\arctan(q) - \Theta(q-2)\,\arccos\left(\frac{2}{q}\right)\right)\Bigg]\,, \end{aligned} \tag{13}$$

$$G_2^A = \frac{3\,\alpha}{2\,\pi}\left[\frac{1}{2\,(1+q^2)^2} + \frac{1}{6\,(1+q^2)}\right]\,, \tag{14}$$

where Θ is a step function. The remaining analytical and numerical integration gives

$$F_b = 9.28369 \tag{15}$$

$$F_c = -6.98416\,, \tag{16}$$

in agreement with the results obtained in [13].

B. The irreducible diagrams

The remaining 16 diagrams from Figure 1 we calculate using the second method. The energy shift as described by F Eq. (5) can be rewritten to the form

$$F = \frac{1}{4}\int \frac{d^3p}{\pi^2}\,\frac{1}{p^4}\,\left(f(p^2) - f(0)\right)\,, \tag{17}$$

where f is an analytical function, with a branch cut along the negative axis. From the Cauchy theorem we have

$$f(p^2) - f(0) = p^2 \int_0^\infty d(q^2)\frac{1}{q^2\,(p^2+q^2)}f^A(q^2)\,, \tag{18}$$

$$F = \int_0^\infty dq\,\frac{f^A(q^2)}{q^2}\,. \tag{19}$$

In this way we convert the integral to a form suitable for further analytical treatment. We calculate analytically the expansion of $f^A(q^2)$ up to q^{10}. This is done by writing a general procedure in symbolic language [15], which evaluates diagram by diagram. The fact that we calculate only the imaginary part of $f(-q^2)$, significantly simplified the calculation and, for example, the overall renormalization counterterms canceled automatically. The details of this calculation and what follows will be given elsewhere. The result of the expansion of f^A in q^2 is

$$\begin{aligned} f^A(q^2) = &-\frac{32\,q^2}{27} - \frac{1582\,q^4}{675} - \frac{154739\,q^6}{33075} + \frac{29253601\,q^8}{5953500} - \frac{15752340547\,q^{10}}{1440747000} + \cdots \\ &+ \left(\frac{104\,q^2}{9} - \frac{48\,q^4}{5} + \frac{41116\,q^6}{1575} - \frac{129796\,q^8}{4725} + \frac{495111\,q^{10}}{13475} + \cdots\right)\log(q^2)\,. \end{aligned} \tag{20}$$

The tests of this calculation were the cancellation of: infrared divergences (present in each separate diagram), ultraviolet divergences (counterterms were calculated independently), and the constant term in Eq. (20).

The value of f^A for larger q^2 was calculated numerically. We partially follow and adopt the numerical methods expanded by T. Kinoshita [16,7]. We introduce Feynman parameters to collect all the denominators, integrate with respect to k_1 and k_2 (with photon mass μ present to prevent the logarithmic infrared divergency), and perform pointwise renormalization. At this stage we perform a test by evaluating $f(p^2)$ for small p and by extrapolating to $p = 0$. This number is also known analytically because

$$\frac{f(0)}{4} = \left(\frac{\pi}{\alpha}\right)^2 (8F_1'(0) + 2\,F_2(0)) = \\ -\frac{163}{36} - \frac{85\,\pi^2}{108} + 3\,\pi^2\,\log(2) - \frac{9\,\zeta(3)}{2} = 2.81849\,, \tag{21}$$

where F_1 and F_2 are two–loop electron form factors (here without closed fermion loop).

After integration over k_1 , k_2, we obtain a sum of terms of the form: $1/(a\,p^2 + b)^n$, $n = 1, 2, 3$; $\ln(a\,p^2 + b)$, where a and b are functions of Feynman parameters. The imaginary part of the above, for negative p^2, is a delta function or its derivatives. These entities are not suitable for direct numerical integration. Thus we integrate with respect to q^2 three times by parts to convert all delta functions to theta functions. The same procedure has to be applied to the analytical part Eq. (20) in order to have the final result unchanged. Here we perform the last and most significant test and compare the numerically evaluated $f^A(q^2)$ with the analytical calculation at $q^2 = 1/2$.

Next, the integral in q^2 is done. The analytical part from 0 to 1/2 and the numerical part from 1/2 to ∞. All the diagrams are separately numerically integrated [17] using the Monte–Carlo routine VEGAS [18]. We performed up to 10^9 evaluations, for each diagram and for several values of the photon mass μ. The final result is obtained by fitting a function $f(\mu) = a + b\,\mu + c\,\mu^2$, and by extrapolating to $\mu = 0$.

The analytical part gives:

$$F_{an} = -17.03(2)\,, \tag{22}$$

where the error comes from ending the expansion Eq. (20) at q^{10}. It is estimated, based on the observation that this expansion is not far from a geometric series. The numerical part gives

$$F_{num} = -9.1(5)\,, \tag{23}$$

where the error is one standard deviation. To estimate this error we assumed that the probability distributions for different μ are correlated i.e. proportional. This is because we used the same seed for the random number generator for different value of μ^2.

The sum of all diagrams presented on Figure 1 is

$$F_I = F_{an} + F_{num} + F_a + F_b + F_c = -23.9(5) \tag{24}$$

The result for the desired coefficient B_{50} is then the sum of the results from diagrams with the closed fermion loop (calculated in the previous paper = 2.71 [12]) and of F_I:

$$B_{50} = -21.2(5)\,. \tag{25}$$

III. RESULTS AND CONCLUSION

A few words should be said about the reliability of this result. During the calculation we performed several tests: the cancellation of ultraviolet and infrared divergences, the cancellation of a constant term in Eq. (20), a comparison of the numerically calculated $f(0)$ with the analytical result from the two–loop electron vertex function, and a comparison of the numerical and analytical parts of f^A at $q^2 = 1/2$. All these tests were passed successfully, but in our opinion the confirmation of the above result by an independent group is nevertheless of great importance.

The obtained results give corrections:

$$\Delta E_L(1S) = -291(7)\,\text{kHz} \tag{26}$$
$$\Delta E_L(2S) = -36.5(9)\,\text{kHz}\,. \tag{27}$$

The new theoretical values for the Lamb shift, using for the proton radius the experimental value of Mainz group $r_p = 0.862(12)$ fm [3] are

$$E_L(2S-2P) = 1\,057\,838(6)\,\mathrm{kHz} \tag{28}$$

$$E_L(4S) - E_L(2S) - \frac{1}{4}\left(E_L(2S) - E_L(1S)\right) = 868\,623(5)\,\mathrm{kHz} \tag{29}$$

There is an excellent agreement with the very recent experiment of Hagley and Pipkin [19], where the Lamb shift has been extracted from the measured $2S_{1/2} - 2P_{3/2}$ fine structure interval

$$E_L(2S-2P) = 1\,057\,839(12)\,\mathrm{kHz}\,. \tag{30}$$

While we have a good agreement with a direct measurement of Lundeen and Pipkin [20]

$$E_L(2S-2P) = 1\,057\,845(9)\,\mathrm{kHz}\,, \tag{31}$$

and with the recent high precision Doppler–free two–photon measurement of Weitz *et. al.* [1]

$$E_L(4S) - E_L(2S) - \frac{1}{4}\left(E_L(2S) - E_L(1S)\right) = 868\,630(12)\,\mathrm{kHz}\,. \tag{32}$$

In contrast to our previous paper [5] we do not include in the above theoretical results the values of $A_{71}\,, A_{70}$ coefficients. This is because, in our opinion, the current numerical results P. Mohr [21] have unsufficient accuracy, to estimate these higher order terms from the extrapolation. We also do not include the uncertainty from these terms to the above errors. There is an additional uncertainty from three–loop correction which is also not included in the above errors. This correction is determined by the value and derivative of three–loop form factors at $q^2 = 0$ (Eq. (3)) and can be calculated in a similar way to the electron anomalous magnetic moment.

Our calculation indicates that the older experimental value for the proton radius $r_p = 0.805(11)$ [2], which decreases the 2S Lamb shift by about 18 kHz, is incorrect.

The main uncertainty for the hydrogen Lamb shift is now given by the error in the proton radius (3.5 kHz); a reduction of this uncertainty is of crucial importance for future tests of QED in the hydrogen atom. The reliable measurement of nuclear radii is important also, because for the hydrogen–deuterium isotope shift [22] the difference between the theoretical and experimental value is 108 kHz, what is 5 times more than the experimental error.

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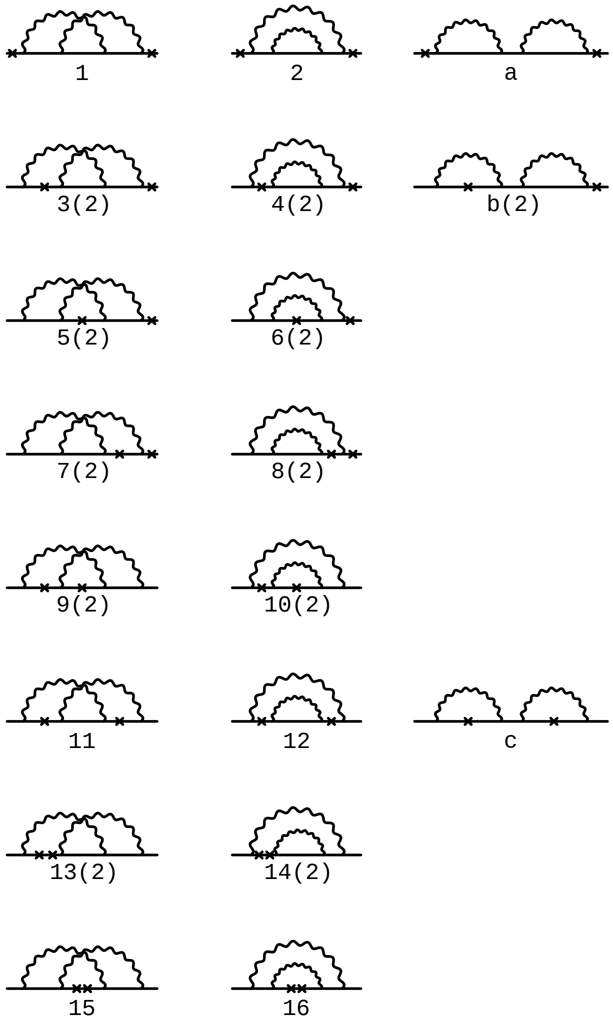

FIG. 1. Diagrams representing two–loop binding corrections to the Lamb shift. The closed fermion loops are excluded here. Crosses mean insertion of Coulomb vertex. Some diagrams are counted twice, as is denoted by '(2)'. All diagrams are implicitly renormalized, thus there is no loop on external legs.