Three-Loop Slope of the Dirac Form Factor and the 1S Lamb Shift in Hydrogen

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Abstract. The calculation of the last unknown contribution to hydrogen energy levels at order $m\alpha^7$, due to the three loop slope of the Dirac form factor, is described. The resulting shift of the nS energy level is found to be $3.16/n^3$ kHz. Adding this result to many known contributions to the $1S$ Lamb shift and comparing with experimental value, we derive the value of the proton charge radius $r_p = 0.883 \pm 0.014$ fm.

1 Introduction

Experiments with hydrogen atoms are currently very precise and, amazingly, their precision continues to increase [1,2,3,4,5,6]. Currently, the most accurate experimental value for the $1S$ Lamb shift[1] in hydrogen is [6]:

$$\Delta E(1S) = 8\ 172\ 837(22)\ \text{kHz}. \tag{1}$$

On the theoretical side, the last unknown piece at $\mathcal{O}(m\alpha^7)$, the contribution of the three loop slope of the Dirac form factor, has been computed recently [8]. In what follows that calculation is described.

The interaction of the virtual photon with the electron on its mass shell can be parameterized by the so-called Dirac and Pauli form factors:

$$\bar{u}(p_2)\Gamma_\mu u(p_1) = \bar{u}(p_2)\left(F_1(q^2)\gamma_\mu + i\sigma_{\mu\nu}\frac{q_\mu}{m}F_2(q^2)\right)u(p_1), \tag{2}$$

where the $u(p_{1,2})$ are the electron spinors in the initial and final state and q is the momentum carried away by the photon. The momenta satisfy the relation $q = p_1 - p_2$. An important consequence of QED gauge invariance and the electron charge definition is that the Dirac form factor equals unity at zero momentum transfer:

$$F_1(0) = 1, \tag{3}$$

to all orders in the coupling constant. The Pauli form factor at zero momentum transfer describes an interaction of the electron spin with the homogeneous magnetic field; it is the electron anomalous magnetic moment.

[1] We define the nS Lamb shift in a standard way, see e.g. Ref. [7].

We are interested in the value of the Dirac form factor when the momentum transfer q is small as compared to the electron mass. Then:

$$F_1(q^2) = 1 + F_1^{\rm slope}\frac{q^2}{m^2} + \mathcal{O}\left(\frac{q^4}{m^4}\right). \tag{4}$$

The slope of the Dirac form factor generates a shift in nS energy levels:

$$\Delta E(nS) = \frac{4m\alpha^4}{n^3}\left(\frac{m_r}{m}\right)^3 F_1^{\rm slope}. \tag{5}$$

To match experimental precision, the energy shift has to be computed up to $\Delta E \sim m\alpha^7$ and even higher order corrections should sometime be included. For this reason the three loop contribution to $F_1^{\rm slope}$ is required. We have previously reported on our calculation of the three loop slope of the Dirac form factor in [8], where the emphasize was on the phenomenological aspects. Here we would like to discuss some of the methods employed in that calculation in a more detailed way. Nevertheless, all important consequences of our result are presented as well.

2 Strategy of the calculation

There are approximately 40 three loop diagrams to be computed; for this reason the choice of the appropriate strategy is of significant importance. Any approach has to rely heavily on the use of symbolic manipulation computer programs. Our principal tool in this calculation is the so called *integration-by-parts* technique [9], which is common in perturbative calculations in high energy physics.

The advantage of this technique is that it allows to treat major part of the problem in a pure algebraic way; the real three loop integration has to be done for quite a few "master" integrals; the whole procedure can be easily automated and then used for various calculations.

Let us now explain the main idea behind this technique. An important point is that the applicability of the integration-by-parts requires that Feynman integrals are regularized dimensionally, so that we work in continuous space-time dimension $D = 4 - 2\epsilon$, where ϵ is the regularization parameter. Both, ultraviolet and infra-red divergences show up as poles in ϵ. If dimensional regularization is adopted, one observes that the following relation:

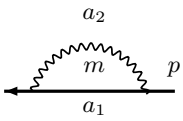
$$0 = \int \frac{\partial}{\partial k_i^\mu}\left(l_j^\mu \times \text{propagators}\right), \tag{6}$$

where k_i is one of the loop momenta and l_j is either one of the loop momenta or the external momenta, is valid. This simple equation delivers a non-trivial information, once the derivative is performed explicitly.

To illustrate how this works, we consider a simple example of the one-loop self-energy diagram on the mass shell $p^2 = m^2$, shown in Fig.1.

There are two recurrence relations. Let us look at the one that corresponds to $(\partial/\partial k)\ k$. Explicit calculation gives:

$$\left(D - 2a_2 - a_1 - a_1\mathbf{2}^-\mathbf{1}^+\right) I(a_1, a_2) = 0, \tag{7}$$



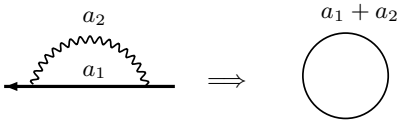
$$I(a_1,a_2) = \int \frac{\mathrm{d}k^D}{(2\pi)^D} \frac{1}{(k^2+2pk)^{a_1}(k^2)^{a_2}}$$

Fig. 1. The one-loop on shell mass shell diagram

where $\mathbf{1}^{\pm} I(a_1,a_2) = I(a_1 \pm 1, a_2)$ and similar for $\mathbf{2}^{\pm}$. Let us assume that a_2 is positive. Then, we rewrite Eq.(7) as:

$$I(a_1,a_2) = \frac{a_1}{D-2a_2-a_1} I(a_1+1,a_2-1). \tag{8}$$

By repeated application of this identity index a_2 can be reduced to zero (see Fig.2) which implies that the calculation of $I(a_1,a_2)$ is reduced to the calculation of vacuum bubble integrals that do not dependent on the external momentum p. That is a significant simplification.



$$I(a_1,a_2) \Longrightarrow I(a_1+a_2,0),$$

Fig. 2. A reduction of the on-shell one-loop integrals to vacuum integrals

Amazingly, this simple logic generalizes on to much more difficult cases and is now the main tool in perturbative calculations in high energy physics. We use it for the required calculation of the three loop slope of the Dirac form factor.

The first thing to realize is that all Feynman integrals that have to be computed can be expressed through four basic topologies shown in Fig.3 (obviously, only if arbitrary powers of all propagators are allowed).

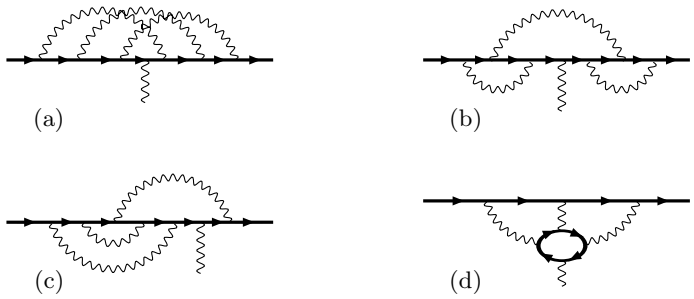


Fig. 3. Examples of electron-photon vertex diagrams that correspond to the four different integration topologies

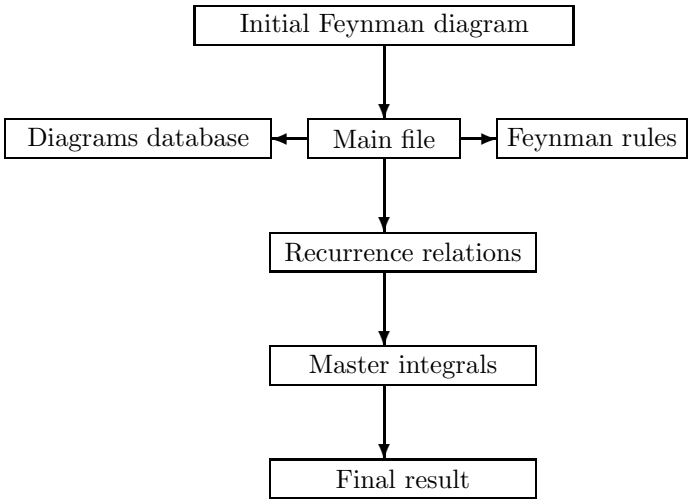
We then solve the recurrence relations for all of these topologies and, as the result, we have the mapping:

$$\text{Any three loop on} - \text{shell QED Feynman integral}$$
$$\Longrightarrow 17 \text{ master three loop integrals.}$$

These seventeen integrals have been computed in the course of the calculation of the anomalous magnetic moment of the electron [10] and we can borrow them from that reference. In the next section we present the structure of the computer program in which this strategy is realized.

3 Basics of the program

All the above steps have been automated (in simple terms this means, that getting either the three loop $g-2$ or the slope of the Dirac form factor is just a matter of changing a single line in the computer code). The program is written in Form, a symbolic manipulation language created by J.A.M. Vermaseren. Organization of the program is as follows:



When the calculation of specific diagram is requested, the program pulls it out of the database, uses Feynman rules to substitute vertices and propagators, applies recurrence relations to map the diagram into the master integrals, substitutes these master integrals from a separate database and prints out the result. A typical run of the program looks like (diagram Fig.1b as an example):

```
> form2.3 runChargeRad
...
Time=10 sec          Generated terms = 5531
EXPR                  Terms in output = 5531
```

expand line 4 Bytes used = 799972
....
Time = 1919.10 sec Generated terms = 32
EXPR Terms in output = 32
Bytes used = 608

$$\begin{aligned}\mathrm{EXPR} = & -\frac{13}{288\epsilon^3} - \frac{683}{3456\epsilon^2} + \frac{1}{\epsilon}\left(-\frac{8675}{20736} + \frac{1}{32}\zeta_3 - \frac{\pi^2}{48}\log 2 - \frac{53}{1152}\pi^2\right) \\ & + \left(\frac{672619}{497664} + \frac{17}{72}\zeta_3\pi^2 - \frac{2503}{576}\zeta_3 - \frac{5}{6}\zeta_5 + \frac{459}{320}\pi^2\log 2\right. \\ & \left. - \frac{101}{72}\pi^2\log^2 2 - \frac{12809}{7200}\pi^2 + \frac{793}{4320}\pi^4 - \frac{23}{144}\log^4 2 - \frac{23}{6}a_4\right) .\end{aligned}$$

The program has been tested on several QED and QCD motivated examples such as: electron $g-2$ in QED, gauge independence of the electron wave function renormalization in QED, a relation between the pole and the $\overline{\mathrm{MS}}$ mass in QCD, exponentiation of the infra-red asymptotic of the heavy fermion propagator. Many details concerning these checks and other technical aspects of our calculations can be found in Ref. [11] which the interested reader should consult.

4 Results

We now summarize the results of the calculation. For the slope of the Dirac form factor we obtain:

$$F_1^{\mathrm{slope}} = \sum_{n=1}^{\infty}\left(\frac{\alpha}{\pi}\right)^n A_{\mathrm{slope}}^{(n)}, \tag{9}$$

and

$$A_{\mathrm{slope}}^{(1)} = -\frac{1}{8} - \frac{1}{6\epsilon}, \tag{10}$$

$$A_{\mathrm{slope}}^{(2)} = -\frac{4819}{5184} - \frac{3}{4}\zeta_3 + \frac{1}{2}\pi^2\log 2 - \frac{49}{432}\pi^2, \tag{11}$$

$$\begin{aligned}A_{\mathrm{slope}}^{(3)} = & -\frac{77513}{186624} - \frac{17}{24}\zeta_3\pi^2 - \frac{2929}{288}\zeta_3 + \frac{25}{8}\zeta_5 + \frac{41671}{2160}\pi^2\log 2 - \frac{217}{216}\log^4 2 \\ & - \frac{103}{1080}\pi^2\log^2 2 - \frac{454979}{38880}\pi^2 + \frac{3899}{25920}\pi^4 - \frac{217}{9}a_4,\end{aligned} \tag{12}$$

where $a_4 = \sum\limits_{n=1}^{\infty} 1/(2^n n^4)$ and $\zeta_k = \sum\limits_{n=1}^{\infty} 1/(n^k)$ denotes the Riemann zeta function. Note, that the one-loop slope $A_{\mathrm{slope}}^{(1)}$ is divergent as $\epsilon \to 0$. This infrared divergence is transformed to $\log\alpha$, if other contributions to the Lamb shift at order $m\alpha^5$ are taken into account. The results for $A_{\mathrm{slope}}^{(2,3)}$ show explicitly that in higher orders of perturbation theory this problem is absent.

The correction to the S-wave energy levels induced by the three-loop slope of the Dirac form factor is then:

$$\Delta E^{\rm slope}_{\alpha^3(Z\alpha)^4}(n) = \frac{4m\alpha^7}{\pi^3 n^3}\left(\frac{m_r}{m}\right)^3 A^{(3)}_{\rm slope} \to \frac{8cR_\infty\alpha^5}{\pi^3 n^3}\left(\frac{m_r}{m}\right)^3 A^{(3)}_{\rm slope},$$

where cR_∞ is the Rydberg constant in MHz.

Using the values for the Rydberg and the fine structure constant [12]

$$cR_\infty = 3\ 289\ 841\ 960.367(25)\ \text{MHz}, \quad \alpha = 1/137.035\ 999\ 76(50),$$

we arrive at:

$$\Delta E^{\rm slope}_{\alpha^3(Z\alpha)^4}(n) = \frac{3.016}{n^3}\ \text{kHz}.$$

The contribution due to the three-loop slope of the Dirac form factor was the last unknown contribution to the hydrogen energy levels at order $\alpha^3(Z\alpha)^4$. The two other contributions come from the three-loop electron anomalous magnetic moment and the three-loop vacuum polarization correction to the Coulomb propagator. These contributions can be extracted from the literature [10,13].

The effects of $\alpha^3(Z\alpha)^4$ are conveniently parameterized by the coefficient C_{40} defined by:

$$\Delta E_{\alpha^3(Z\alpha)^4} = \frac{8cR_\infty\alpha^5}{\pi^3 n^3}\left(\frac{m_r}{m}\right)^3 C_{40}.$$

Taking all the three contributions into account, we obtain the following expression for the coefficient C_{40} for the S-levels:

$$\begin{aligned} C_{40} &= \frac{679441}{93312} - \frac{252251}{9720}\pi^2 + \frac{4787}{108}\pi^2\log 2 - \frac{121}{72}\zeta_3\pi^2 - \frac{239}{135}\pi^2\log^2 2 \\ &\quad - \frac{84071}{2304}\zeta_3 + \frac{85}{24}\zeta_5 - \frac{568}{9}a_4 + \frac{1591}{3240}\pi^4 - \frac{71}{27}\log^4 2 \approx 0.417508, \end{aligned} \tag{13}$$

which results in a three-loop correction to the nS-level Lamb shift:

$$\begin{aligned} \Delta E_{\alpha^3(Z\alpha)^4}(n) &= \frac{m\alpha^7}{n^3\pi^3}\left(\frac{m_r}{m}\right)^3 C_{40} \\ &= (3.016 + 5.187 - 6.370)\ \frac{\text{kHz}}{n^3} = \frac{1.83}{n^3}\ \text{kHz}. \end{aligned}$$

We have displayed the contributions due to the three-loop slope of the Dirac form factor, the three-loop anomalous magnetic moment of the electron and the three-loop photon vacuum polarization separately. Thanks to the cancellation between these contributions, the correction turns out to be quite small numerically.

We now present our result for the $1S$ Lamb shift in hydrogen. A detailed description of all the corrections that we include to obtain the final result as well as references to the original papers are given in [8]. The final value for the $1S$-shift strongly depends on the value of the proton charge radius:

$$\Delta E(1S)_{\rm theory} = 8\ 172\ 778(16)(32)\ \ \text{kHz}, \tag{14}$$

$$\Delta E(1S)_{\rm theory} = 8\ 172\ 819(16)(66)\ \ \text{kHz}, \tag{15}$$

where the two values of $\Delta E(1S)$ are given for $r_p = 0.862(12)$ fm [14] and $r_p = 0.877(24)$ fm [15], respectively. The first error in Eqs.(14,15) is the theoretical uncertainty due to still uncalculated higher order corrections to energy levels. The second error is due to the uncertainty in the experimental values of the proton charge radius. The uncertainties in Rydberg and the fine structure constants are not relevant at the present level of precision.

Comparing the theoretical result Eqs.(14,15) with the most recent measurement of the $1S$-level Lamb shift [6]

$$\Delta E(1S)_{\rm exp} = 8\ 172\ 837(22)\ \text{kHz}, \tag{16}$$

we conclude that the larger values of the proton charge radius seem to give an agreement between the theory and experiment.

Turning the problem around, we note that the small uncertainty in the theoretical result for the $1S$ Lamb shift permits an extraction of the proton charge radius by comparing experimental and theoretical results. We then arrive at the precise value of the proton radius $r_p = 0.883 \pm 0.014$ fm. It is interesting to note that this result seems to be in good agreement with the value of the proton charge radius derived in a recent re-analysis of the electron-proton scattering data [16].

In conclusion, we have computed the three-loop slope of the Dirac form factor. Thanks to this calculation the theoretical uncertainty in the predictions for the $1S$ Lamb shift is reduced. Comparison of the theoretical and experimental results for the $1S$ level shift permits an accurate determination of the proton charge radius. Further improvements in theoretical predictions for the $1S$ level shift would be possible if subleading $\alpha^2(Z\alpha)^6 \log^2 \alpha$ corrections are calculated. Only then can the theoretical uncertainty be brought down to several kHz and can the potential of the recent measurement of the $1S - 2S$ transition frequency [6] be fully exploited.

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