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# Reparameterization invariance of NRQED self-energy corrections and improved theory for excited $D$ states in hydrogenlike systems

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## Abstract

Canonically, the quantum electrodynamic radiative corrections in bound systems have been evaluated in photon energy regularization, i.e., using a noncovariant overlapping parameter that separates the high-energy relativistic scales of the virtual quanta from the nonrelativistic domain. Here, we calculate the higher-order corrections to the one-photon self-energy calculation with three different overlapping parameters (photon energy, photon mass and dimensional regularization) and demonstrate the reparameterization invariance of nonrelativistic quantum electrodynamics (NRQED) using this particular example. We also present new techniques for the calculation of the low-energy part of this correction, which lead to results for the Lamb shift of highly excited states that are important for high-precision spectroscopy.

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## 1. Introduction

In 1986, Caswell and Lepage introduced the idea of nonrelativistic quantum electrodynamics (NRQED) to describe bound states [1]. The underlying notion is to reformulate the predictions of full relativistic quantum electrodynamics in terms of operators acting on nonrelativistic spinors, so that the higher-order corrections can be expressed in terms of a series of iterated operators of lower order, and additional operators which come in at every given order in the so-called  $Z\alpha$  expansion, where  $Z$  is the nuclear charge number, and  $\alpha$  is the fine-structure constant.

The development of NRQED seems to have been motivated by the well-known fact that a “usual” quantum field theory based on  $S$ -matrix elements evaluated on free states and free

propagators is not enough to describe bound states. Two energy scales are present in the problem, and these have to be separated by a so-called overlapping parameter (see §123 of Ref. [2]). The two energy domains are the high-energy relativistic scale of the virtual quanta and the nonrelativistic domain of bound-state momenta and energies.

Note that the regularization and renormalization of amplitudes in the ultraviolet (UV) at some mass scale  $\Lambda_{UV}$  has got nothing to do with the scale-separation, or overlapping, parameter. For the overlapping parameter, one can use either a photon energy  $\epsilon$ , or a photon mass  $\mu$ , or one can work in  $4 - 2\epsilon_D$  space-time dimensions (we emphasize that  $\epsilon \neq \epsilon_D$ , the index  $D$  is supplied in this work in order to facilitate the distinction of the two regularizations). Feynman [3], as well as French and Weisskopf [4] did their calculations in photon energy regularization. It turned out to be nontrivial to convert the high-energy part from a photon mass  $\mu$  to a photon energy  $\epsilon$  (see the rather well-known footnote 13 on p. 777 of Ref. [3]), while the photon energy regularization is the most natural cut-off for the low-energy part.

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All three regularizations have been used in the literature for the treatment of different bound-state QED problems. E.g., Nio and Kinoshita [5] used photon mass regularization for their calculation of the higher-order binding corrections to the muonium hyperfine structure, while Pachucki [6] used photon energy regularization for the same problem. Dimensional regularization has been described for the lowest-order Lamb shift by Pineda and Soto in 1998 [7]. Higher-order binding corrections to the Lamb shift have been evaluated in dimensional regularization in [8].

This Letter has a twofold purpose. (i) Here, for the first time to the best of our knowledge, a calculation of a non-trivial QED correction is presented in all three common (re-)parameterizations of NRQED (photon energy, photon mass and dimensional regularization). Namely, we consider the higher-order binding corrections to the one-loop self-energy in hydrogenlike systems. We thereby verify the reparameterization invariance to the full extent, for all three common regularization methods, while working on the same problem employing three different methods. (ii) As a byproduct, we develop methods to do the calculation of relativistic Bethe logarithms for arbitrary Rydberg states of hydrogenlike systems, and we evaluate these corrections for states with principal quantum numbers as high as  $n = 12$ , where the excessive number of terms has been prohibiting both numerical as well as analytic approaches in the past.

## 2. Reparameterization invariance (general remarks)

Our final goal is to express the self-energy shift  $\Delta E(nL_j)$  of a general hydrogenic state with orbital angular momentum quantum number  $L \geq 2$ , total angular momentum  $j$  and principal quantum number  $n$ ,

$$\Delta E(nL_j) = \frac{\alpha (Z\alpha)^4}{\pi n^3} F(nL_j), \quad (1)$$

in terms of the reference state quantum numbers (we use natural units with  $\hbar = c = \epsilon_0 = 1$ , and we choose the energy scale so that the electron mass  $m = 1$ ). The scaled self-energy function  $F(nL_j)$  has the following semi-analytic expansion (it is not analytic because of the presence of logarithms),

$$F(nL_j) = A_{40} + (Z\alpha)^2 \{ A_{61} \ln[(Z\alpha)^{-2}] + A_{60} \}, \quad (2)$$

where the first index of the  $A$  coefficients counts the number of factors  $Z\alpha$ , whereas the second counts the power of the logarithm  $\ln[(Z\alpha)^{-2}]$ .

The reparameterization invariance of NRQED implies that the  $F$  function should be expressible as the sum of a regularized high-energy part  $F_H$  and a regularized low-energy part  $F_L$ , where  $F_H$  and  $F_L$  can be formulated in photon energy, photon mass or in dimensional regularization, as follows,

$$\begin{aligned} F &= F_H(\epsilon) + F_L(\epsilon) = F_H(\mu) + F_L(\mu) \\ &= F_H(\epsilon_D) + F_L(\epsilon_D). \end{aligned} \quad (3)$$

## 3. High-energy part

In the treatment of the one-loop self-energy, we start with the high-energy part, which corresponds to photon energies of the order of the electron mass, and electron momenta of the order of the atomic momentum scale  $Z\alpha$ , where  $Z$  is the nuclear charge, and  $\alpha$  is the fine-structure constant. We identify all operators that contribute at the order  $\alpha(Z\alpha)^6$ , and evaluate these for a general state in a hydrogenlike system with orbital angular momentum quantum number  $L \geq 2$ , in photon energy, photon mass, and also in dimensional regularization. We find that the final expressions simplify considerably for these states, and indeed very compact final results can be indicated.

The different contributions to the high-energy part, for states with nonvanishing orbital angular momentum, can be described as follows, in terms of the electron Dirac form factor  $F_1$  and the electron magnetic form factor  $F_2$ . Here, we give only an indication of these corrections, detailed formulas corresponding to the terms mentioned below can be found in Ref. [8]. First, we have an  $F'_1(0)$  correction evaluated on the relativistic wave function, where the latter has to be expanded up to the relative order of  $(Z\alpha)^2$ . This correction can be rewritten as the sum of several effective operators acting on the nonrelativistic wave function. Then, we have an  $F''_1(0)$  correction evaluated on the nonrelativistic wave function. From the magnetic form factor, we have an  $F_2(0)$  correction evaluated on the relativistic wave function, and an  $F'_2(0)$  correction on its nonrelativistic counterpart. The form factors are known in photon mass [9,10] as well as dimensional [11,12] regularization. For dimensional regularization, all the relevant formulas are explicitly given in [8], and the terms corresponding to the above mentioned form factors are indicated. In order to go over to photon energy regularization, one has to convert the photon mass to a noncovariant cutoff. For the lowest-order form factor slope contributing to the leading  $\alpha(Z\alpha)^4$  correction to the Lamb shift (in units of the electron mass), this is described in the textbook of Itzykson and Zuber [13]. For a general hydrogenic state, we use a different ansatz, namely a generalization of the approach described previously for  $P$  and  $D$  states in Refs. [14,15], in order to express the high-energy part as a function of  $\epsilon$  for a general state of the hydrogen atom.

There is a further two-vertex operator which is given by the diagrams in Fig. 5 of Ref. [8]. It corresponds to the following Hamiltonians in the three regularizations,

$$H(\epsilon) = \frac{\alpha}{\pi} \left[ \frac{2}{3} \ln\left(\frac{1}{2\epsilon}\right) - \frac{2}{3\epsilon} + \frac{34}{45} \right] (\vec{\nabla}V)^2, \quad (4a)$$

$$H(\mu) = \frac{\alpha}{\pi} \left[ \frac{2}{3} \ln\left(\frac{1}{\mu}\right) - \frac{3\pi}{16\mu} - \frac{1}{6} \right] (\vec{\nabla}V)^2, \quad (4b)$$

$$H(\epsilon_D) = \frac{\alpha}{\pi} \left( \frac{1}{6} - \frac{1}{3\epsilon_D} \right) (\vec{\nabla}V)^2. \quad (4c)$$

The above formulas, however, are of little use for a comparison to experiments unless complemented by their evaluation on a general hydrogenic state in terms of actual quantum numbers. A general result for the high-energy part in dimensional regularization, valid for all states with nonvanishing angular

momentum and for the weighted difference of  $nS$  states (where  $n$  is the principal quantum number), has been given in Ref. [8]. We here refer to Eq. (3.35) of Ref. [8], with partial results given in Eqs. (3.32) and (3.34) of Ref. [8], and the latter term corresponds to our  $H(\varepsilon_D)$ . This result is expressed in terms of matrix elements to be evaluated on the reference state, which is manifestly taken as a nonrelativistic Schrödinger eigenstate. These matrix elements, as given in [8], constitute rather complicated expressions and are not evaluated in terms of quantum numbers. In photon energy regularization, the general form of the result for the high-energy part has been indicated in Eq. (8) of Ref. [15], but the quantities  $\mathcal{K}$  and  $\mathcal{C}$  in that equation were given in general form only for selected submanifolds of states.

In this Letter, we are in the position to note that the final results for the high-energy part, in all three regularizations, can be expressed in a very compact form for all states with orbital angular momentum  $L \geq 2$ ,

$$F_H(\epsilon) = \mathcal{E} + (Z\alpha)^2 A_{61} \left[ \ln\left(\frac{1}{2\epsilon}\right) - \frac{1}{\epsilon} + \frac{17}{15} \right], \quad (5a)$$

$$F_H(\mu) = \mathcal{E} + (Z\alpha)^2 A_{61} \left[ \ln\left(\frac{1}{\mu}\right) - \frac{9}{32\mu} - \frac{1}{4} \right], \quad (5b)$$

$$F_H(\varepsilon_D) = \mathcal{E} + (Z\alpha)^2 A_{61} \left( \frac{1}{4} - \frac{1}{2\varepsilon_D} \right). \quad (5c)$$

The  $A_{61}$  coefficient is defined in Eq. (2) and can be given as ( $L \geq 2$ )

$$A_{61} = \frac{2}{3} \frac{n^3}{(Z\alpha)^4} \langle \phi | \frac{1}{r^4} | \phi \rangle = \frac{3n^2 - L(L+1)}{3n^2(L + \frac{3}{2})(L+1)(L + \frac{1}{2})L(L - \frac{1}{2})}, \quad (6)$$

where  $|\phi\rangle$  is the Schrödinger eigenstate. Note that  $A_{61}$  is independent of  $j$  for  $L \geq 2$ . The matrix element  $\mathcal{E}$  is derived from the magnetic form factor correction to the Lamb shift and can be expressed either as a sum of various effective operators acting on the nonrelativistic hydrogenic wave function, or as a single operator acting on the full relativistic Dirac wave function, appropriately expanded in powers of  $Z\alpha$ . The latter approach leads to the most compact expression, and the resulting matrix element can be related to the integral denoted as  $C_{nk,n\kappa}^{-2}$  on p. 4483 of [16] and evaluated using generalized virial relations for the Dirac equation. Indeed, the result reads, expanded in subleading order in the  $Z\alpha$ -expansion ( $\vec{E} = -\vec{\nabla}V$  is the electric field generated by the atomic nucleus with  $V = -Z\alpha/r$ ),

$$\begin{aligned} \mathcal{E} &= \frac{n^3}{(Z\alpha)^4} \langle \psi^+ | \frac{i}{4} \vec{\gamma} \cdot \vec{E} | \psi \rangle \\ &= -\frac{1}{2\kappa(2L+1)} \\ &\quad + (Z\alpha)^2 \left( -\frac{12\kappa^2 - 1}{2(2j+1)\kappa^2(2\kappa-1)(2\kappa+1)^2} \right. \\ &\quad \left. - \frac{1}{n} \frac{3}{4\kappa^2(2\kappa+1)} + \frac{1}{n^2} \frac{8\kappa-3}{2(2j+1)(2\kappa-1)(2\kappa+1)} \right) \\ &= -\frac{1}{2\kappa(2L+1)} + (Z\alpha)^2 \mathcal{E}_2, \end{aligned} \quad (7)$$

where  $\psi$  is the relativistic Dirac wave function, and  $\psi^+$ , for clarity, is its adjoint (row vector in spinor space, complex conjugated), which is different from the Dirac adjoint  $\bar{\psi} = \psi^+ \gamma^0$ . The Dirac quantum number is  $\kappa = 2(L-j)(j + \frac{1}{2})$ . We here define  $\mathcal{E}_2$  to be the coefficient of the  $(Z\alpha)^2$  term (this convention will be useful later). This completes our treatment of high-energy photons.

#### 4. Low-energy part

In a certain sense, the photon energy regularization constitutes the most natural procedure for low-energy photons. One simply expands the transition current via a Foldy–Wouthuysen transformation [14], and then one applies time-independent perturbation theory from the low-energy terms in the resulting NRQED Hamiltonian. One then integrates the photon energy to some upper cutoff  $\epsilon$  (in [17], it is explained why the expansion first in  $\alpha$ , then in  $\epsilon$  is actually an expansion for large  $\epsilon$ ).

We now describe briefly how to convert the result obtained in photon energy regularization to photon mass regularization. For the leading-order term of order  $\alpha(Z\alpha)^4$ , the by now famous substitution [3,4,13] reads  $\ln(\mu) \rightarrow \ln(2\epsilon) + \frac{5}{6}$  while for the higher-order terms, one has to be very careful in distinguishing  $k = |\vec{k}|$  from  $\omega = \sqrt{\vec{k}^2 + \mu^2}$ . The so-called quadrupole term obtained by expanding the exponential  $\exp(i\vec{k} \cdot \vec{r})$  in the nonrelativistic transition current  $p^i \exp(i\vec{k} \cdot \vec{r})$  is very sensitive to the changes in the matching of  $\mu$  and  $\epsilon$  because the power of the photon momentum  $k$  is different from the nonrelativistic dipole term. The additional terms can, however, be written in closed analytic form.

Finally, the full evaluation of the low-energy part in dimensional regularization is described in detail in Ref. [8], and we are now in the position to indicate the results as follows. We denote the (nonrelativistic) Bethe logarithm by  $\ln k_0$  and the relativistic Bethe logarithm by  $\mathcal{L}$ , following the conventions of Refs. [8,15]. Both of these quantities are of course state dependent, and they can both be evaluated only numerically. In the three different regularizations, the results read (for states with angular momenta  $L \geq 2$ )

$$F_L(\epsilon) = -\frac{4}{3} \ln k_0 + (Z\alpha)^2 \left\{ A_{61} \left[ \ln\left(\frac{\epsilon}{(Z\alpha)^2}\right) + \frac{1}{\epsilon} \right] + \mathcal{L} \right\}, \quad (8a)$$

$$F_L(\mu) = -\frac{4}{3} \ln k_0 + (Z\alpha)^2 \left\{ A_{61} \left[ \frac{83}{60} + \frac{9}{32\mu} + \ln\left(\frac{1}{2} \frac{\mu}{(Z\alpha)^2}\right) \right] + \mathcal{L} \right\}, \quad (8b)$$

$$F_L(\varepsilon_D) = -\frac{4}{3} \ln k_0 + (Z\alpha)^2 \left\{ A_{61} \left[ \frac{53}{60} + \frac{1}{2\varepsilon_D} + \ln\left(\frac{1}{2} (Z\alpha)^{-2}\right) \right] + \mathcal{L} \right\}. \quad (8c)$$

#### 5. Adding the high- and low-energy parts

It is easy to see that when adding the high- and low-energy parts from Eqs. (5) and (8), not only the regularization para-

Table 1

Explicit high- and low-energy parts for the  $8D_{3/2}$  state. The  $F_H$  is the contribution to the self-energy correction from the high-energy part, the  $F_L$  is the low-energy part, and the three regularizations are:  $\epsilon$  denotes the photon energy,  $\mu$  denotes the photon mass, and in dimensional regularization, we work in  $4 - 2\epsilon_D$  space-time dimensions

$$\begin{aligned}
 F_H(8D_{3/2}, \epsilon) &= -\frac{1}{20} + (Z\alpha)^2 \left[ -\frac{20893}{2419200} - \frac{31}{2520\epsilon} - \frac{31}{2520} \ln(2\epsilon) \right] \\
 F_L(8D_{3/2}, \epsilon) &= -\frac{4}{3} \ln k_0(8D) + (Z\alpha)^2 \left[ 0.024886 + \frac{31}{2520\epsilon} + \frac{31}{2520} \ln\left(\frac{\epsilon}{(Z\alpha)^2}\right) \right] \\
 F_H(8D_{3/2}, \mu) &= -\frac{1}{20} + (Z\alpha)^2 \left[ -\frac{20687}{806400} - \frac{31\pi}{8960\mu} - \frac{31}{2520} \ln\left(\frac{1}{\mu}\right) \right] \\
 F_L(8D_{3/2}, \mu) &= -\frac{4}{3} \ln k_0(8D) \\
 &\quad + (Z\alpha)^2 \left[ 0.033376 + \frac{31\pi}{8960\mu} + \frac{31}{2520} \ln\left[\frac{\mu}{(Z\alpha)^2}\right] \right] \\
 F_H(8D_{3/2}, \epsilon_D) &= -\frac{1}{20} + (Z\alpha)^2 \left[ -\frac{15727}{806400} - \frac{31}{5040\epsilon_D} \right] \\
 F_L(8D_{3/2}, \epsilon_D) &= -\frac{4}{3} \ln k_0(8D) \\
 &\quad + (Z\alpha)^2 \left[ 0.027226 + \frac{31}{5040\epsilon_D} + \frac{31}{2520} \ln[(Z\alpha)^{-2}] \right] \\
 (\text{Sum } F = F_H + F_L) \\
 F(8D_{3/2}) &= -\frac{1}{20} - \frac{4}{3} \ln k_0(8D) + (Z\alpha)^2 \left[ \frac{31}{2520} \ln[(Z\alpha)^{-2}] + 0.007723 \right]
 \end{aligned}$$

meters cancel, but also, a reparameterization-invariant result is obtained,

$$\begin{aligned}
 F &= -\frac{1}{2\kappa(2L+1)} - \frac{4}{3} \ln k_0 \\
 &\quad + (Z\alpha)^2 \left\{ A_{61} \left[ \ln\left(\frac{1}{2}(Z\alpha)^{-2}\right) + \frac{17}{15} \right] + \mathcal{E}_2 + \mathcal{L} \right\}. \quad (9)
 \end{aligned}$$

The reparameterization invariance of NRQED is thus verified in a nontrivial calculation beyond leading order, in all three common regularization methods. A concrete numerical example is given in Table 1, where the explicit numerical coefficients are written out for the  $8D_{3/2}$  state (this hydrogenic level is spectroscopically important [18]).

Having obtained compact expressions, the question can be asked whether it is possible to evaluate, beyond leading order, the relativistic Bethe logarithms  $\mathcal{L}$  for highly excited states of hydrogenlike atoms, in approximately the same way as for the nonrelativistic counterparts (the “usual” Bethe logarithms), for which a systematic investigation has been started in Ref. [19] in relation to excited states. In order to appreciate the difficulties associated with the problem, one should recall that the relativistic Bethe logarithms represent a comparatively much more demanding calculation as compared to their nonrelativistic counterparts, and the first such evaluation was not done until 1993 (see Ref. [20]), i.e., 46 years after the evaluation of the nonrelativistic counterpart [21].

Analytic and semi-analytic calculations, where all expressions are kept in full analytic form before the final photon energy integration, are prohibitively difficult for states with higher principal quantum numbers, as already described in a number of previous works on the subject of interest. It is doubtful if the analytic approach to the evaluation of matrix elements with the hydrogenic propagator, which is commonly based on a Sturmian decomposition [22–24], can ever be generalized beyond principal quantum number  $n = 8$ , where on the order of  $10^5$  terms are encountered in intermediate steps [15]. Calculations for the relativistic corrections to higher excited states seem to be possible only via completely numerical (lattice) methods.

Table 2

Relativistic Bethe logarithms  $\mathcal{L}$  and  $A_{60}$  coefficients for highly excited  $D$  states

$n$	$\mathcal{L}(nD_{3/2})$	$\mathcal{L}(nD_{5/2})$
9	0.02504391(5)	0.02256466(5)
10	0.02518592(5)	0.02266965(5)
11	0.02528093(5)	0.02273386(5)
12	0.02535359(5)	0.02278080(5)
$n$	$A_{60}(nD_{3/2})$	$A_{60}(nD_{5/2})$
9	0.00808301(5)	0.03473588(5)
10	0.00841379(5)	0.03483271(5)
11	0.00868109(5)	0.03487638(5)
12	0.00890960(5)	0.03489667(5)

Here, a numerical approach inspired by a discretized space as used by Salomonson and Oester [25] is used, and up to eleven-point discretized representations are used in order to represent differential operators on the lattice whose coordinates are chosen to represent very accurately the origin in coordinate space. Values for the relativistic Bethe logarithms  $\mathcal{L}$  and for the  $A_{60}$  coefficients of highly excited  $D$  states are given in Table 2, where we note that the  $12D_{3/2}$  and  $12D_{5/2}$  states are of particular experimental interest [26].

## 6. Conclusions

In summary, we have completed two goals in this Letter. (i) The reparameterization invariance of NRQED has been verified through relative order  $(Z\alpha)^2$  for a rather fundamentally important QED correction to the spectrum of hydrogenlike atoms: namely, the one-photon self-energy for excited states in a hydrogenlike system with orbital angular momentum quantum number  $L \geq 2$ . It has been verified that the photon energy, the photon mass and the dimensional regularizations give the same results for the energy shift [see Eqs. (5), (8) and (9)]. Because the higher-order binding corrections to the Lamb shift involve a multitude of terms, this fact is rather nontrivial and is displayed in a particularly clear manner in the compact expressions for the self-energy effects obtained here. (ii) Numerical techniques for the calculation of the relativistic Bethe logarithm  $\mathcal{L}$  have been developed which circumvent problems associated to the growth of the number of terms in intermediate steps with the principal quantum number; these problems otherwise prohibit analytic and semi-analytic evaluations for highly excited states. With the methods described here, calculations become possible for Rydberg states of the hydrogen atom, and these are important for ultra-high-precision spectroscopy [18,26].

The two above mentioned aspects are important for two rather diverse topics:

- (i) for a fundamental reassurance regarding the internal consistency of NRQED and the consistency of overlapping parameters used in field theories in general;
- (ii) for obtaining improved theoretical predictions for transition frequencies in hydrogenlike atoms.

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