Techniques in Analytic Lamb Shift Calculations

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Abstract
Quantum electrodynamics has been the first theory to emerge from the ideas of regularization and renormalization, and the coupling of the fermions to the virtual excitations of the electromagnetic field. Today, bound-state quantum electrodynamics provides us with accurate theoretical predictions for the transition energies relevant to simple atomic systems, and steady theoretical progress relies on advances in calculational techniques, as well as numerical algorithms. In this brief review, we discuss one particular aspect connected with the recent progress: the evaluation of relativistic corrections to the one-loop bound-state self-energy in a hydrogenlike ion of low nuclear charge number, for excited non–S states, up to the order of $\alpha (Z\alpha)^6$ in units of the electron mass. A few details of calculations formerly reported in the literature are discussed, and results for 6F, 7F, 6G and 7G states are given.

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1 Introduction

The bound-state self-energy of an electron in a hydrogenlike atom has been one of the key theoretical and experimental cornerstones in the development of modern field theory. During the last decade, the techniques available for calculations have dramatically advanced, and the accuracy of today’s predictions is several orders of magnitude better than in the early days of quantum electrodynamics (QED). The advances would be impossible without the combined theoretical efforts toward the description of the hydrogen spectrum, which have involved generations of physicists. The aim of the current brief review is threefold: first, to give an overview of some recent advances in Lamb shift calculations and self-energy calculations in particular, second, to describe a few details of recent calculations, for higher excited non–S states, which may be useful in an independent recalculation of the higher-order binding corrections, and third, to supplement previously available data for higher-order corrections by results for 6F, 7F, 6G and 7G states.

In “usual” calculations of virtual loops, we are used to the association: “the number of loops equals the power of the coupling constant.” For hydrogenic bound states, the situation is different, and the expansion of a bound-state energy, including QED effects, is actually a double expansion in terms of the QED $\alpha \approx 1/137.036$ and the electron-nucleus coupling parameter $Z\alpha$, where $Z$ is the nuclear charge number.
Specifically, the leading one-loop energy shifts (due to self-energy and vacuum polarization) in hydrogenlike systems are of order $\alpha (Z \alpha)^4 mc^2$, where $m$ is the electron mass and $c$ is the speed of light. The complete correction in this order was obtained first in the years 1948 and 1949 [1, 2, 3, 4]. The leading two-loop energy shifts are of order $\alpha^2 (Z \alpha)^4 mc^2$; the paradigm is that $\alpha$ counts the number of loops, whereas $Z\alpha$ is a measure of the relativistic corrections that enter the loop corrections and are typical of the bound-state problem.

When scanning the literature, one should be aware that sometimes, the QED energy shifts are expressed in terms of atomic units, for which the fundamental energy scale is that of the Hartree, which equals $\alpha^2 mc^2$, and therefore the leading QED shift is of order $Z^4 \alpha^3$ in atomic units.

The current paper will be concerned mainly with the calculation of the correction of order $\alpha (Z \alpha)^6$, which is effectively a relativistic correction to the one-loop correction (sic!) due to the binding of the electron to the nucleus (hence the name “binding corrections”). We thus have to consider the relativistic atomic physics aspect of the problem in addition to the usual loop calculation.

The separation of the problem into high- and low-energy virtual photon contributions has been discussed (e.g.) in §123 of Ref. [5]. In the context of NRQED [6, 7, 8, 9], the general paradigm is to map the high-energy effects onto effective operators. By contrast, the low-energy effects are mapped onto the transverse degrees of freedom of the electromagnetic field and are integrated up to some cutoff scale. The systematic expansion of the Wilson coefficients multiplying the effective operators is rather nontrivial. In the current context, we start from the fully relativistic expression of the self-energy, and do appropriate expansions for both domains. For the problem at hand, this conceptually simpler approach has certain pragmatic advantages.

One might well ask why we would need information on the Lamb shift of higher excited states in the first place, especially because the most accurately measured hydrogenic transition involves the 1S and the metastable 2S level [10]. The answer is that one transition is not enough to determine fundamental constants like the Rydberg to sufficient accuracy: one needs at least two transitions. We would like to cite from Ref. [11], a system of equations that illustrates this fact in a particularly clear way. One combines two of the most accurately measured frequencies ($f_{1S-2S}$ [10] and a $f_{2S-8D}$ [12] transition), where we can either use $8D_{3/2}$ and $8D_{5/2}$ for the 8D level, for a determination of the Rydberg. Defining $\epsilon_D$ as a dimensionless relativistic Dirac energy, we can schematically establish the following equations,

$$f_{1S-2S} = R_{\infty} c \{ \epsilon_D(2S) - \epsilon_D(1S) \} + \mathcal{L}_{2S} - \mathcal{L}_{1S},$$

(1a)

$$f_{2S-8D} = R_{\infty} c \{ \epsilon_D(8D) - \epsilon_D(2S) \} + \mathcal{L}_{8D} - \mathcal{L}_{2S}.$$  

(1b)

By $L$, we refer to the Lamb shift [see Eq. (67) of Ref. [13] for an often-used definition of this effect]. We can eliminate $L_{2S}$ using the combination

$$L_{2S} = \frac{L_{1S} + W_{21}}{8}$$

(2)

where

$$W_{21} = 8L_{2S} - L_{1S}$$

(3)

is independent of the nuclear-size correction (proton radius) and can therefore be determined theoretically to high accuracy. We can now solve the system of equations (1) for two unknowns:
provided we have theoretical values for the weighted combination $W_{21}$ and $L_{SD}$. The evaluation of an important contribution to the latter will be one of the issues discussed in the current brief review.

A generalization of this rather elementary exercise involves a least-squares analysis \[14\]. Roughly speaking, one tries to find the “best fit,” in the sense of least squares, to a set of experimental results representing the most accurately measured transitions in hydrogen and deuterium. For the 2002 adjustment \[15\], a total of 23 transitions in hydrogen and deuterium have been used as input data. The least-squares analysis includes covariances among the theoretical uncertainties. One thus obtains theoretical values, including standard uncertainties, for the proton radius and the Rydberg, and one can make optimal predictions for other transition frequencies not used in the adjustment of the constants. Some of the predicted frequencies are currently more accurate \[14\] than the predictions for the anomalous magnetic moment of the electron.

There is another aspect which is relevant to calculations for higher excited states: the extrapolation of the data to higher quantum numbers, for given manifolds of states. For example, we can extrapolate to higher principal quantum numbers $n$ for given angular momenta (orbital and spin). In an apparently not widely known paper (Ref. \[16\]), the one-loop Bethe logarithm has been evaluated, in terms of a (slowly convergent) integral representation, in the limit of $n \to \infty$. From this point onwards, the extrapolation to higher principal quantum numbers of the one-loop nonrelativistic Bethe logarithm, based on a few known low-$n$ results, becomes an interpolation. However, this calculation uses a few particular properties of the nonrelativistic Bethe logarithm [order $\alpha(Z\alpha)^4$], which are not applicable to the much more involved correction of order $\alpha(Z\alpha)^6$ (relativistic Bethe logarithm). Nevertheless, it has recently been observed that a large number of relativistic effects and loop corrections can actually be expressed as an inverse power series in the principal quantum number \[17, 18\]. This is not irrelevant because it gives confidence that such fits, applied to other corrections like the relativistic Bethe logarithm provide us with an accurate representation of the corrections for large $n$, where the complex structure of the wave function leads to a prohibitively large number of terms in intermediate steps of the calculation, which makes an evaluation impossible even if today’s computer algebra systems \[19\] are used.

This brief review follows two investigations \[18, 20\] in which previous treatments of the one-loop problem were extended to higher quantum numbers, and some general expressions relevant to selected manifolds of bound states were presented. Here, we supplement the results obtained previously by explicit numerical calculations for 6F, 7F, 6G and 7G states. Furthermore, in Sec. 2, we discuss some general ideas relevant to the calculation, before dwelling on the low-energy part in Sec. 3. This part, mediated by ultrasoft virtual photons, is one of the key elements in the treatment of higher excited non-S states. Throughout the paper, we restrict the discussion to states with nonvanishing orbital angular momentum. Numerical results are presented in Sec. 4 and conclusions are drawn in Sec. 5.

2 General Ideas

We first take the opportunity to refer the reader to the two most comprehensive treatments of the one-loop self-energy problem for a bound state, which have appeared in the literature up to
now and which we are aware of. These are Refs. [21] and [22]. Here, we briefly mention a few particular aspects of interest which may be useful in finding a general access to the calculations, also with regard to a possible independent verification. We fix the units so that $\hbar = c = \epsilon_0 = 1$, which implies that $e^2 = 4\pi \alpha$. The electron charge is $e$, not $-e$.

In Feynman gauge, the one-loop bound-state self-energy reads

$$E = i e^2 \int_{C_F} \frac{d^4k}{(2\pi)^4} D_{\mu\nu}(k) \left\langle \bar{\psi} \gamma^\mu \gamma_5 \frac{1}{p - k - m - \gamma^0 V} \gamma_\nu \psi \right\rangle - \left\langle \bar{\psi} | \delta m | \psi \right\rangle ,$$

where $D_{\mu\nu}(k)$ is the photon propagator, and $C_F$ is the Feynman contour. Lorentz covariance is explicitly broken by the Coulomb potential $V = -Z\alpha/r$. The quantity $\delta m$ is the mass counter term, and $m$ is the electron mass.

We divide the problem of calculation into two contributions, which correspond to two different photon energy regions, and two different parts of the photon energy integration contour $C_F$. The photon energy separation parameter $\epsilon$ takes the role of an infrared cutoff for the high-energy part, and it acts as an ultraviolet cutoff for the low-energy part. The low-energy part may be expressed as

$$E_L = \alpha \sum_{n \geq 4} (Z\alpha)^n f_n \left( \frac{\epsilon}{(Z\alpha)^2 m} \right) ,$$

and the high-energy part $E_H$ reads

$$E_H = \alpha \sum_{n \geq 4} (Z\alpha)^n g_n \left( \frac{\epsilon}{m} \right) .$$

The key is to first expand both contributions in $Z\alpha$ for small $Z\alpha$, then in $\epsilon$, for small $\epsilon$. By performing the expansions in that sequence, we automatically assume that $(Z\alpha)^2 m \ll \epsilon$. Counter-intuitively, this is equivalent to performing an expansion for large $\epsilon$, after scaling the powers of $Z\alpha$ out of the calculation, as will be demonstrated below in Sec. 3.3. It is also important to realize that the actual numerical value of $\epsilon$ is arbitrary. All that matters is the expansion in systematic expansion in $\epsilon$, including the logarithmic terms. In Refs. [21] and [22], it has been stressed that different gauges may be used for the evaluation of the low- and the high-energy parts. This gauge “arbitrariness” (rather than “invariance”) holds only if linear terms in $\epsilon$ are neglected. This remarkable fact is a cornerstone in the construction of nonrelativistic QED Lagrangians (NRQED), where most high-energy effective operators are taken from calculations carried out in Feynman gauge, but the ultrasoft-scale effects (where the virtual photon energy is of the order of the atomic binding energy) are calculated in Coulomb gauge.

The general structure of the one-loop energy shift $E$, for non-S states, is

$$E = E_L + E_H = \frac{\alpha}{\pi} \frac{(Z\alpha)^4 m_e e^2}{n^3} F(Z\alpha) .$$

The dimensionless function $F(Z\alpha)$ depends on the bound-state quantum numbers and has the expansion (again, for non-S states)

$$F(Z\alpha) = A_{40} + (Z\alpha)^2 \left\{ A_{61} \ln \left[ (Z\alpha)^{-2} \right] + A_{60} \right\} .$$
Here, we ignore higher-order terms irrelevant for the current \( \alpha (Z\alpha)^6 \)-calculation. The indices of the constant coefficients \( A_{XY} \) correspond to the power \( X \) of \( Z\alpha \) and the power \( Y \) of the logarithm \( \ln[(Z\alpha)^{-2}] \). The function \( F(Z\alpha) \) is obtained as the sum

\[
F(Z\alpha) = F_H(Z\alpha, \epsilon) + F_L(Z\alpha, \epsilon),
\]

where \( F_H \) corresponds to \( E_H \) and \( F_L \) corresponds to \( E_L \). The sum \( F(Z\alpha) \) is independent of the cutoff parameter \( \epsilon \).

Let us consider the concrete case of the \( 8D_{3/2} \) state. The high-energy part reads

\[
F_H(8D_{3/2}) = -\frac{1}{20} + (Z\alpha)^2 \left[ -\frac{20893}{2419200} - \frac{31}{2520} \frac{m}{\epsilon} - \frac{31}{2520} \ln \left( \frac{2\epsilon}{m} \right) \right].
\]

The calculation entails techniques familiar from high-energy physics and is described in detail in Ref. [22]. The term \( -1/20 \) is a consequence of the anomalous magnetic moment of the electron as described in detail in Chap. 7 of Ref. [23]. The low-energy part is obtained largely by atomic-physics calculational techniques and reads

\[
F_L(8D_{3/2}, Z\alpha, \epsilon) = -\frac{4}{3} \ln k_0(8D) + (Z\alpha)^2 \left[ 0.024886 + \frac{31}{2520} \frac{m}{\epsilon} + \frac{31}{2520} \ln \left( \frac{\epsilon}{(Z\alpha)^2 m} \right) \right],
\]

where \( \ln k_0 \) is the familiar nonrelativistic Bethe logarithm. The sum is

\[
F(8D_{3/2}, Z\alpha, \epsilon) = F_H(8D_{3/2}, Z\alpha) + F_L(8D_{3/2}, Z\alpha)
= -\frac{1}{20} - \frac{4}{3} \ln k_0(8D) + (Z\alpha)^2 \left[ \frac{31}{2520} \ln [(Z\alpha)^{-2}] + 0.007723 \right]
\]

and thus free of \( \epsilon \), as it should be. A comparison of Eqs. (9) and (12) reveals that

\[
A_{60}(8D_{3/2}) = +0.007723.
\]

The generalization of the term \( -1/20 - (4/3) \ln k_0(8D) \) to an arbitrary hydrogenic state is discussed in Ref. [24]. Model examples illustrating the cancellation of the cutoff parameter \( \epsilon \) can be found in Appendix A of Ref. [24] and in Section 2 of Ref. [25].

### 3 Low–Energy Part

#### 3.1 Orientation

In this brief review, we will focus on the low-energy part ("ultrasoft" scale, \( \omega \sim (Z\alpha)^2 m \)). According to Eq. (3.109) of Ref. [22], this term may be written as

\[
E_L = -\frac{e^2}{2} \int_0^\epsilon dk \frac{k^i}{(2\pi)^3} \int d\Omega_k \left( \delta^{ij} - \frac{k^i k^j}{k^2} \right) \left\langle \psi^+ \left| \alpha^i e^{ik\cdot\vec{r}} \right| \frac{1}{H_D - E_D + k} \alpha^i e^{-ik\cdot\vec{r}} \left| \psi \right\rangle,
\]

\[
(14)
\]
where the fully relativistic Dirac wave functions $\psi$ is used, and the $\alpha^i = \gamma^0\gamma^i$ matrices are a noncovariant form of the Dirac $\gamma$ matrices. The quantity $k = |\vec{k}|$ is virtual photon energy. Note that one should actually supplement a principal value prescription in this formula, because the lower-lying states generate poles in the integration region $k \in (0, \epsilon)$ with $\epsilon \gg (Z\alpha)^2m$. The ensuing problem of the accurate definition of a resonance eigenvalue has been discussed in Ref. [26], in the context of two-loop corrections.

It is well known that the Dirac Hamiltonian $H_D$ in Eq. (14) can be transformed to the Schrödinger Hamiltonian plus various relativistic corrections, using the Foldy–Wouthuysen transformation $U$, which leads to a transformed Hamiltonian $UH_DU^{-1}$. It is this transformation which is the key to the successful identification of all terms which contribute to the low-energy contribution in a given order of the $Z\alpha$ expansion. Specifically, one may apply that same transformation $U$ to the current operator [13],

$$j^j = \alpha^j \exp(i \vec{k} \cdot \vec{r}).$$

The result is

$$Uj^jU^{-1} = \frac{p^j}{m} + \delta j^j,$$

where

$$\delta j^j \sim \frac{p^j}{m} \left(1 + i \left(\vec{k} \cdot \vec{r}\right) - \frac{1}{2} \left(\vec{k} \cdot \vec{r}\right)^2 \right) - \frac{1}{2m^3}p^j \bar{p}^2 - \frac{1}{2m^2} \frac{Z\alpha}{r^3} (\vec{r} \times \vec{\sigma})^j + \frac{1}{2m} \left(\vec{k} \cdot \vec{r}\right) \left(\vec{k} \times \vec{\sigma}\right)^j - \frac{i}{2m} \left(\vec{k} \times \vec{\sigma}\right)^j.$$

Here, we have dropped terms which couple lower and upper components of the Foldy-Wouthuysen transformation and lead to vanishing energy shifts within the context of the $\epsilon$-expansion. The term proportional to $\vec{k} \times \vec{\sigma}$ entails a spin flip, but the leading-order current $p^j/m$ necessitates a change in the angular momentum of the electron. Because of angular momentum selection rules, we may thus neglect this term in the calculation.

Alternatively, one might have obtained the current (17) by considering a Foldy–Wouthuysen transformation of a Dirac Hamiltonian with a vector potential $\vec{A}$ included, i.e. a transformation of $\vec{\alpha} \cdot (\vec{p} - e\vec{A}) + \beta m + V$ instead of $\vec{\alpha} \cdot \vec{p} + \beta m + V$. The effective current operator then is the term that multiplies $\vec{A}$ in the transformed Hamiltonian. That latter approach is used, e.g., in Ref. [27]. The term

$$\frac{p^j}{m} \left(1 + i \left(\vec{k} \cdot \vec{r}\right) - \frac{1}{2} \left(\vec{k} \cdot \vec{r}\right)^2 \right)$$

leads to the so-called quadrupole correction. The other current corrections in Eq. (17) are considered separately and identifies as “relativistic corrections to the current” (see Refs. [13, 28]). Of course, these corrections have to be supplemented by relativistic corrections to the Hamiltonian and to the bound-state energy, as well as corrections to the wave function. These corrections are well defined and identify all terms relevant in the order $\alpha (Z\alpha)^6 m$. 

6
3.2 Dimensionless energy parameter

One of the advantages of the Foldy–Wouthuysen transformation is that we may carry out all further calculations using the nonrelativistic form of the bound-state propagator. There exists a closed-form Sturmian decomposition for all angular components [29, 30, 31],

\[
g_l(r_1, r_2, \nu) = \frac{4m}{a_0 \nu} \left( \frac{2r_1}{a_0 \nu} \right)^l \left( \frac{2r_2}{a_0 \nu} \right)^l e^{-(r_1+r_2)/(a_0 \nu)} \sum_{k=0}^{\infty} \left( \frac{2r_1}{a_0 \nu} \right)^k \left( \frac{2r_2}{a_0 \nu} \right)^k \frac{L_k^{2l+1}}{(k+1)_{2l+1}} \frac{(k+1)_{2l+1}}{(l+1+k-\nu)}.
\]  

(19)

Here, \( a = 1/(Z\alpha m) \) is the Bohr radius, and \( (k)_c \) is the Pochhammer symbol. The symbols \( L_k^{2l+1} \) denote the associated Laguerre polynomials. The radial integrals can usually be evaluated using standard techniques, which leaves the sum over \( k \) as a final problem in the calculation (note that \( k \) in this context is to be differentiated from the virtual photon energy which is also denoted by \( k \) in many calculations in this field of research). In B, we discuss some important properties of typical hypergeometric function encountered which result from an evaluation the sums. Convergence acceleration techniques are useful for accurate calculations of relativistic effects, because the \( k \)-sum is typically slowly convergent for high virtual photon energies.

The nonrelativistic Schrödinger–Coulomb Green function for the hydrogen atom [30] reads

\[
\langle r_1 \left| \frac{1}{H-z} \right| r_2 \rangle = \sum_{lm} g_l(r_1, r_2; \nu) Y_{lm}(\theta_1, \varphi_1) Y_{lm}^*(\theta_2, \varphi_2).
\]  

(20)

Here, \( z = E_S - k \) is an energy parameter that involves the Schrödinger energy \( E_S \) of the reference state. When the photon energy \( k \) assumes values in the range \((0, \infty)\), the argument \( z \) decreases monotonically from \( E_S < 0 \) to \(-\infty\). The basic idea is now to set \( t = \sqrt{E_S/z} \), so that \( t \) runs from a value \( t = 1 \) for \( k = 0 \) to a value \( t = 0 \) for \( k = \infty \). As a function of \( Z\alpha \) and the principal quantum number \( n \), the quantity \( t \) parameterizes the energy argument \( z \) as

\[
z \equiv z(t) = \frac{(Z\alpha)^2 m}{2 n^2 t^2},
\]  

(21a)

\[
t \equiv t(z) = \frac{Z\alpha}{n} \sqrt{\frac{m}{2z}}.
\]  

(21b)

Equation (3.126) of Ref. [22] specializes this transformation to the case \( n = 2 \). In Refs. [29, 30, 31], we encounter the notation

\[
\nu = nt = (Z\alpha) \sqrt{\frac{m}{2z}},
\]  

(22)

which enters into Eqs. (19) and (20). An expansion for large \( k \) then corresponds to an expansion for small \( t \) (see B).

3.3 Extraction of a finite part

In many cases, it is necessary, within bound-state calculations, to extract a nonlogarithmic, constant term from an integral that contains a variety of divergent contributions in the ultraviolet
domain. Here, we discuss possible algorithms which can be used for such calculations, and which may eventually be useful for an independent verification of the results reported here. For example, the finite parts which lead to the relativistic Bethe logarithms might be alternatively extracted using a discretized Schrödinger–Coulomb propagator on a lattice [32]. In this case, it is necessary to have a means for extracting nonlogarithmic terms numerically rather than analytically. We believe that an independent verification of the nonlogarithmic terms, using purely numerical methods, could be a very worthwhile cross-check of the analytic approach (up to the last stage of the calculation where the integrals are evaluated numerically) which was used in previous evaluations.

In order to approach this problem, we first consider a model calculation inspired by the structure of the nonrelativistic integrand that leads to the Bethe logarithm in Eq. (37) below. It consists in the evaluation of the integral

\[ I = \int_0^\Lambda dk \frac{(Z\alpha)^2}{k + h(Z\alpha)^2} \]

\[ = (Z\alpha)^2\Lambda - (Z\alpha)^4 h \ln \left( \frac{\Lambda + (Z\alpha)^2h}{(Z\alpha)^2h} \right) \]

(23)

and in the extraction of the logarithmic and nonlogarithmic terms (\(\epsilon\) prescription), or in the calculation of just the nonlogarithmic term (numerical evaluation of generalized Bethe logarithms).

The first prescription would consist in expanding the integral for large \(\Lambda\), and dropping all linear, quadratic etc. terms for large \(\Lambda\). In this way, we obtain the result

\[ I \sim -(Z\alpha)^4 h \ln \left( \frac{\Lambda}{(Z\alpha)^2h} \right) . \]

(24)

Let us now consider a variation of the first prescription. We go to atomic units, i.e. scale all powers of \(Z\alpha\) out of the integrand via the transformation \(k \rightarrow (Z\alpha)^2k\). We then define \(\lambda = \Lambda/(Z\alpha)^2\) and obtain

\[ I = (Z\alpha)^4 \int_0^\lambda dk \frac{1}{k + h} \]

\[ = (Z\alpha)^4 h \left[ \lambda - \ln \left( \frac{h + \lambda}{h} \right) \right] \]

\[ \sim - (Z\alpha)^4 h \left[ \ln \left( \frac{\lambda}{h} \right) \right] , \]

(25)

where the last form is obtained after dropping the linear and (possibly further) quadratic terms; the final result is in full agreement with Eq. (24).

The second prescription is based on the identification \(\Lambda \rightarrow \epsilon\). We first expand the result in Eq. (23) in powers of \(Z\alpha\), which entails the replacement

\[ \frac{\epsilon + (Z\alpha)^2h}{(Z\alpha)^2h} \rightarrow \frac{\epsilon}{(Z\alpha)^2h} \]

(26)
in the argument of the logarithm in Eq. (23). We then expand in $\epsilon$ for small $\epsilon$, dropping the linear terms. We thus obtain the result
\[ I \sim -(Z\alpha)^4 h \ln \left( \frac{\epsilon}{(Z\alpha)^2 h} \right), \] (27)
which is equivalent to the result in Eq. (24) upon the identification $\Lambda \rightarrow \epsilon$. This illustrates that the expansion in small $\epsilon$ after the expansion in $Z\alpha$ is actually an expansion for $\epsilon \gg (Z\alpha)^2 m$, after dropping the linear terms. In particular, all of the above prescriptions lead to the result
\[ I \sim (Z\alpha)^4 h \ln ((Z\alpha)^2 h), \] (28)
for the nonlogarithmic term.

Let us now suppose that we can evaluate a general function $f(x)$ only numerically, but that we know its expansion for large $x$,
\[ f(x) = \sum_{n=-1,-1/2,0,1/2,...,m} a_n x^n + \mathcal{O}(x^{-3/2}), \quad x \rightarrow \infty, \] (29)
and we wish to evaluate the nonlogarithmic term $N$ that is generated by the integral
\[ \int_{0}^{A} dx \, f(x) \sim N. \] (30)
for large $\Lambda$. In the sense of Eq. (23), we would have $f(x) = x(Z\alpha)^2/[x + h(Z\alpha)^2]$ and and $N = (Z\alpha)^4 h \ln ((Z\alpha)^2 h)$. For the more general case [see Eq. (29)], we define
\[ d(x) = \sum_{n=-1,-1/2,0,1/2,...,m} a_n x^n \] (31)
and
\[ D(x) = a_{-1} \ln(x) + \sum_{n=-1/2,0,1/2,...,m} \frac{a_n x^{n+1}}{n+1}. \] (32)
For arbitrary $M$, the nonlogarithmic term $N$ may then be extracted according to
\[ N = \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_3, \] (33)
with
\[ \mathcal{I}_1 = \int_{0}^{M} dx \, f(x), \]
\[ \mathcal{I}_2 = \int_{M}^{\infty} dx \, [f(x) - d(x)], \]
\[ \mathcal{I}_3 = -D(M). \] (34)
The sign of the $\mathcal{I}_3$-term is determined by the necessity to subtract the integral $D(x)$ of the subtraction term $d(x)$ at the lower limit of integration $x = M$. This consideration effectively results in three minus signs. Analogous considerations have recently been used in Refs. [33, 34].
4 Numerical Results

For the states under investigation, the $A_{60}$ coefficients are listed in Tables 1 and 2. For the $5F_{5/2}$ state, the result had previously been recorded as 0.002 403 158, and for $5F_{7/2}$, a value of 0.008 087 020 had been indicated (see Ref. [20]). The correction of this result, in the last decimal, is beyond current and projected levels of experimental accuracy. For the current brief review, we re-evaluate many of the integrals leading to the $A_{60}$ coefficients with an enhanced number of integration nodes. The two entries in question change by more than the previously indicated numerical accuracy. Results for $6F$, $7F$, $6G$, and $7G$ as reported in Tables 1 and 2 are obtained here. In Ref. [18], we already corrected a computational error for $3P_{1/2}$ as previously reported in Eq. (96) of Ref. [28], where a value of $-1.14768(1)$ had been given. As in previous calculations (see Refs. [13, 28]), certain remaining one-dimensional integrals involving (partial derivatives of) hypergeometric functions could only be evaluated numerically. For $n = 8$, we recall the results $A_{60}(8D_{3/2}) = 0.007 723 850$ and $A_{60}(8D_{5/2}) = 0.034 607 492$.

Table 1: A table of $A_{60}$ coefficients for higher excited atomic states with positive Dirac angular quantum number $\kappa$ (i.e., $j = l - 1/2$). All decimal figures shown are significant.

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<th>$n$</th>
<th>$A_{60}(nP_{1/2})$</th>
<th>$A_{60}(nD_{3/2})$</th>
<th>$A_{60}(nF_{5/2})$</th>
<th>$A_{60}(nG_{7/2})$</th>
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<tr>
<td>6</td>
<td>-1.226 702 391</td>
<td>0.006 749 745</td>
<td>0.002 531 636</td>
<td>0.000 827 468</td>
</tr>
<tr>
<td>7</td>
<td>-1.232 715 957</td>
<td>0.007 277 403</td>
<td>0.002 661 311</td>
<td>0.000 857 346</td>
</tr>
</tbody>
</table>

Table 2: Analog of Table 1 for states with negative $\kappa$.

<table>
<thead>
<tr>
<th>$n$</th>
<th>$A_{60}(nP_{3/2})$</th>
<th>$A_{60}(nD_{5/2})$</th>
<th>$A_{60}(nF_{7/2})$</th>
<th>$A_{60}(nG_{9/2})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>-0.503 373 465</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>-0.597 569 388</td>
<td>0.027 609 989</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>4</td>
<td>-0.630 945 795</td>
<td>0.031 411 862</td>
<td>0.007 074 961</td>
<td>-</td>
</tr>
<tr>
<td>5</td>
<td>-0.647 013 508</td>
<td>0.033 077 570</td>
<td>0.008 087 015</td>
<td>0.002 412 929</td>
</tr>
<tr>
<td>6</td>
<td>-0.656 154 893</td>
<td>0.033 908 493</td>
<td>0.008 610 109</td>
<td>0.002 748 250</td>
</tr>
<tr>
<td>7</td>
<td>-0.662 027 568</td>
<td>0.034 355 926</td>
<td>0.008 906 989</td>
<td>0.002 941 334</td>
</tr>
</tbody>
</table>

5 Conclusions

The challenges of bound-state quantum electrodynamic calculations are associated to the accuracy of the experimental verifications, to the significance of the theory for the determination
of the fundamental constants, and to the conceptual complexity of the calculations which is derived from the apparent simplicity of the physical systems under study. The latter aspect is developed to full extent only if an accurate understanding is required in higher orders of perturbation theory.

Let us briefly discuss possible extensions of this work in addition to the independent verification using a more numerically inspired approach, as outlined in Sec. 3.3. In Refs. [24, 35], calculations of the fine-structure splitting for P states are described which rely on a form-factor approach; this would be equivalent to using an effective operator for the high-energy part. Usually, NRQED-inspired calculations involve a high-energy part, which takes care of the contribution of the high-energy virtual photons, and which is given by effective operators, and a low-energy part, which is given by photons whose energy is of the order of the electron binding energy. The latter integration region is often referred to as the “ultrasoft scale” in the literature (see, e.g., Refs. [7, 8, 9, 36, 37]). The two scales (sometimes three, if one makes an additional distinction with regard to electron momenta) require a completely separate treatment and cannot be calculated on the same footing. Thus, the introduction of scale-separation parameters is required. These cancel at the end of the calculation. For the high-energy effective operators, this scale-separation parameter takes the role of an infrared cutoff, whereas for the low-energy contributions, the scale-separation parameter gives a natural scale for the failure of the nonrelativistic (“ultrasoft”) approximation to the virtual photons, i.e. it acts as an ultraviolet cutoff. This property is characteristic of QED bound-state calculations and is a feature that adds a certain twist to the analysis which is not present in usual quantum-field theoretic loop calculations.

A Mass renormalization and the leading-order result

In the first articles on the self-energy, the concepts of mass renormalization and covariant integration were developed and applied for the first time to the calculation of observable physical effects. The leading-order energy shift, of order $\alpha (Z\alpha)^4 m c^2$, is the sum of a Dirac $F_1$ form-factor contribution, an anomalous magnetic moment term ($F_2$ electron form factor), a vacuum-polarization term, and an effect mediated by low-energy virtual photons. The latter contribution can be interpreted as an “average virtual excitation energy”, as a “logarithmic sum” or, as it is most widely called, a “Bethe logarithm” $\ln k_0$. One may therefore point out that the leading order-$\alpha (Z\alpha)^4$-effect summarizes already the core of most properties of the electron mediated by the virtual interactions with the quantum fields. The self-energy of a bound electron is actually the difference of the self energies of a bound and a free electron, the latter being attributable to its mass, wherefore it can be reabsorbed into a redefined physical parameter entering the Lagrangian of QED.

Yet at the same time, it is important to remember that different energy scales enter the problem: (a) the atomic binding energy and (b) the relativistic electron rest mass energy scale. The separation is already explained in §123 of Ref. [5], and its extension to higher orders in the $Z\alpha$ expansion is discussed in this brief review.

The generalization of the $\alpha (Z\alpha)^4 m$-part of the result in Eq. (12) to an arbitrary non-S state, reads

$$E \sim \frac{\alpha}{\pi} \frac{(Z\alpha)^4 m}{n^3} \left( -\frac{1}{2\kappa (2l + 1)} - \frac{4}{3} \ln k_0(n, l) \right).$$

(35)
The $A_{40}$-coefficient for a non-S state thus reads (see, e.g., Refs. [38] and [39])

$$A_{40} = -\frac{1}{2\kappa (2l + 1)} - \frac{4}{3} \ln k_0(nl),$$

(36)

where $\kappa = 2(l - j)(j + 1/2)$, with the usual meaning for the bound-state angular momentum quantum numbers. The Bethe logarithm $\ln k_0(nl)$ is an inherently nonrelativistic quantity, whose expression in natural units reads

$$\ln k_0(nl) = \frac{n^3}{2(Z\alpha)^4 m} \left\langle \phi \left| \frac{p^i}{m} (H_S - E_n) \ln \left[ \frac{2 |H_S - E_n|}{(Z\alpha)^2 m} \right] \frac{p^i}{m} \right| \phi \right\rangle.$$

(37)

Here, $\phi$ is the nonrelativistic (Schrödinger) form of the bound-state wave function.

It took 50 years [1, 2, 3, 4, 40] to advance our understanding from the order $\alpha(Z\alpha)^4 m_e c^2$ to the order $\alpha(Z\alpha)^6 m_e c^2$. For a successful calculation of the higher-order relativistic corrections, it has been essential to master the much more involved analytic, covariant integrations in the high-energy part, and to advance our understanding of relativistic and retardation corrections to the current. Also, the possibility of handling very involved analytic intermediate expressions by computer algebra has become an essential ingredient of the modern calculations.

Finally, let us remark that for low-lying states, it is possible to evaluate the one-loop effect numerically to very high accuracy [41, 42, 43], even for low nuclear charge numbers. For very highly excited states, however, first exploratory work has revealed that the numerical difficulties associated with the renormalization are still rather prohibitive in the context of an accurate numerical evaluation, because it entails a loss of more than twelve decimals for higher excited states. In addition, the wave functions become much more complex, and this inhibits a fast convergence of the numerical integrations, leading to the temporary conclusion that analytic calculations are still preferable for higher excited states, in the domain of low nuclear charge numbers.

B Asymptotics

We here discuss the asymptotics of two hypergeometric functions that are often encountered in bound-state calculations of the kind [13, 18, 21, 28] considered in the current brief review. The first of these functions is

$$\Phi_1(n, t) = 2F_1(1, -nt, 1 - nt, \xi) = -nt \sum_{k=0}^{\infty} \frac{\xi^k}{k - nt},$$

(38)

which develops singularities at $t = k/n$. These correspond to lower-lying states and their equidistant spacing is a consequence of the energy parameterization discussed in Sec. 3.2. For given $n$, there are typically $n - 1$ lower-lying states accessible by dipole decay, and thus $n - 1$ singularities at $t = m/n$, for $m = 1, \ldots, n - 1$, as $t$ is in the range $(0, 1)$. The argument $\xi$ of the hypergeometric typically reads

$$\xi = \left( \frac{1 - t}{1 + t} \right)^2.$$

(39)
The small-\(t\) asymptotics read
\[
\Phi_1(n, t) = 1 + nt \ln(4t) - \left[2n + n^2 \zeta(2)\right] t^2 \\
+ \left\{n + 4n^2 \left[1 - \ln(4t)\right] - n^3 \zeta(3)\right\} t^3
\]
\[
+ \left[-\frac{2}{3} n + 4n^2 + 4n^3 \zeta(2) - n^4 \zeta(4)\right] t^4 + \mathcal{O}\left[t^5 \ln(t)\right].
\] (40)

The other function which is often encountered reads
\[
\Phi_2(n, t, \zeta) = {}_2F_1(1, -nt, 1 - nt, \zeta) = -nt \sum_{k=0}^{\infty} \frac{(-\zeta)^k}{k - nt},
\] (41)
where
\[
\zeta = \frac{1}{1 + t}.
\] (42)

Its asymptotics are given by
\[
\Phi_2(n, t) = 1 + nt \ln(2) + \left[\frac{1}{2} n^2 \zeta(2) - n\right] t^2 \\
+ \left[\frac{n}{2} - 2n^2 \ln(2) + \frac{3}{4} n^3 \zeta(3)\right] t^3
\]
\[
+ \left[-\frac{1}{3} n + n^2 - n^3 \zeta(2) + \frac{7}{8} n^4 \zeta(4)\right] t^4 + \mathcal{O}\left[t^5 \ln(t)\right].
\] (43)

Numerical algorithms useful for different \(t\)-ranges are discussed in Table 3. For a description of the combined nonlinear-condensation transformation (CNCT), the reader is referred to Refs. \[44, 45\].

**Table 3: Numerical algorithms used in the calculation of the functions \(\Phi_1\) and \(\Phi_2\).**

<table>
<thead>
<tr>
<th>(0 &lt; t &lt; 0.05)</th>
<th>(0.05 &lt; t &lt; 1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\Phi_1(n, t, \xi))</td>
<td>CNCT</td>
</tr>
<tr>
<td>(\Phi_2(n, t, \zeta))</td>
<td>(\delta) transformation</td>
</tr>
</tbody>
</table>

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References


