Extrapolation of the $Z\alpha$-expansion and two-loop bound-state energy shifts

U.D. Jentschura

Theoretische Quantendynamik, Fakultät Mathematik und Physik der Universität Freiburg,
Hermann-Herder-Straße 3, 79104 Freiburg, Germany

Abstract

Quantum electrodynamic (QED) effects that shift the binding energies of hydrogenic energy levels have been expressed in terms of a semi-analytic expansion in powers of $Z\alpha$ and $\ln[(Z\alpha)^{-2}]$, where Z is the nuclear charge number and α is the fine-structure constant. For many QED effects, numerical data are available in the domain of high Z where the $Z\alpha$ expansion fails. In this Letter, we demonstrate that it is possible, within certain limits of accuracy, to extrapolate the $Z\alpha$-expansion from the low-Z to the high-Z domain. We also review two-loop self-energy effects and provide an estimate for the problematic nonlogarithmic coefficient B_{60}.
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1. Introduction

The subject of the current Letter is the investigation of QED radiative corrections in bound hydrogenlike systems which provide one of the most stringent and accurate available tests of quantum field theory and are amenable to high-precision spectroscopy on which the determination of fundamental constants is based [1]. The purpose of this investigation is twofold: first, to demonstrate that the $Z\alpha$-expansion which is inherently valid only at small Z, can be extrapolated

by "deferred" Padé approximants to the domain of high Z, albeit with a certain loss of accuracy in the theoretical predictions. The second purpose is to provide a brief review of logarithmic two-loop higher-order binding corrections to the Lamb shift of hydrogenic states. The calculation of these effects has recently been completed [2,3], but results have been provided only for the total effect which is the sum of the two-loop self-energy, two-loop vacuum polarization and combined effects. For a comparison to numerical calculations which are currently being pursued [4], it is helpful to analyze the coefficients that relate to specific sets of gauge-invariant diagrams. This second purpose is actually a prerequisite for carrying out the extrapolation of the two-loop self-

E-mail address: jentschura@physik.uni-freiburg.de
(U.D. Jentschura).

energy from low to high Z, wherefore we commence this Letter with the endeavour of providing some "mini-review" of the two-loop hydrogenic energy shifts.

2. Brief review of two-loop hydrogenic energy shifts

We use natural Gaussian units with $\hbar = c = \epsilon_0 = 1$ and $e^2 = 4\pi\alpha$, as it is customary for QED bound-state calculations. The two-loop radiative shift of a hydrogenic S state, within the $Z\alpha$-expansion, reads

$$\Delta E_{\text{SE}}^{(2L)} = \left(\frac{\alpha}{\pi}\right)^2 (Z\alpha)^4 \frac{m}{n^3} H(Z\alpha), \tag{1}$$

where

$$H(Z\alpha) = B_{40} + (Z\alpha) B_{50}$$
$$+ (Z\alpha)^2 \big\{ B_{63} \ln^3 (Z\alpha)^{-2} + B_{62} \ln^2 (Z\alpha)^{-2}$$
$$+ B_{61} \ln(Z\alpha)^{-2} + B_{60} \big\} + \cdots, \tag{2}$$

and the ellipsis denotes higher-order terms.

This section is a brief review of the known two-loop coefficients B_{40}, B_{50}, B_{63}, B_{62} and B_{61}. The Feynman diagrams which contribute to the two-loop bound-state energy shifts are shown in Fig. 1.

For S states, the contributions to B_{40} can be evaluated by considering the form-factor approach described, e.g., in Sections VIII.B.1–VIII.B.3 of [5] or in Section 1 of [6]. Detailed information about the $F_1'(0)$ form factor slope and the magnetic form factor $F_2(0)$ attributable to the different sets of diagrams (2LSE) and (SVPE) shown in Fig. 1 are given in Eqs. (16), (17) and (18) of Ref. [6].

We recall the following n-independent results for the B_{40}-coefficients of S states,

$$B_{40}^{(2\text{LSE})}(nS)$$
$$= -\frac{163}{72} - \frac{85}{36}\zeta(2) + 9\ln(2)\zeta(2) - \frac{9}{4}\zeta(3)$$
$$= 1.409244, \tag{3a}$$

$$B_{40}^{(\text{SVPE})}(nS) = -\frac{7}{81} + \frac{5}{36}\zeta(2) = 0.142043, \tag{3b}$$

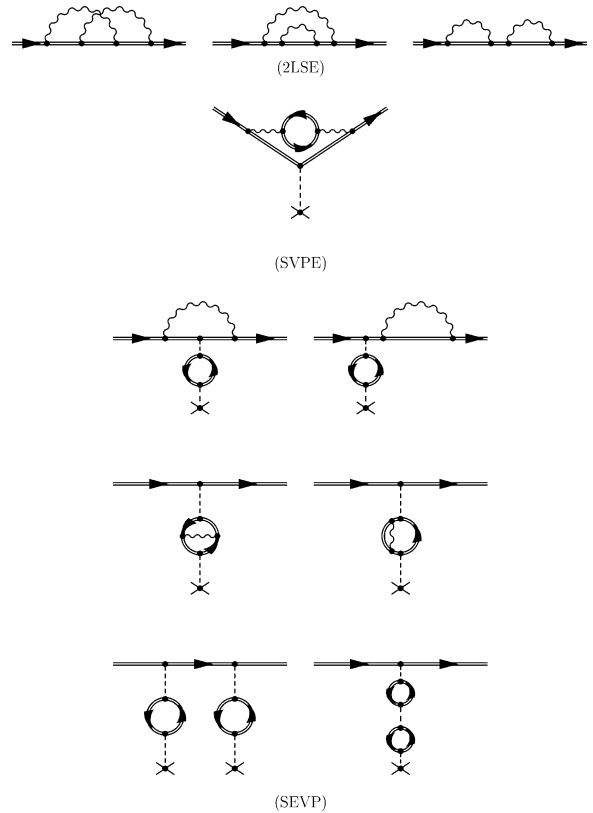$$B_{40}^{(\text{SEVP})}(nS) = -\frac{82}{81} = -1.012346, \tag{3c}$$

Fig. 1. The Feynman diagrams that contribute to the two-loop QED energy shifts of hydrogenic bound states fall quite naturally into three separately gauge invariant categories: (i) the two-loop self-energy effects (2LSE), which are historically the most problematic, (ii) the vacuum-polarization insertion into the virtual photon line of the one-loop self-energy (SVPE), and (iii) diagrams involving both the self-energy and the one-loop vacuum polarization on the one hand and pure two-loop vacuum-polarization corrections on the other hand, summarized here as the set (SEVP). The double line denotes the bound-state electron propagator, i.e., including all Coulomb interactions.

$$B_{40}(nS) = -\frac{2179}{648} - \frac{20}{9}\zeta(2) + 9\ln(2)\zeta(2) - \frac{9}{4}\zeta(3)$$
$$= 0.538941. \tag{3d}$$

Note that the distribution of B_{40}-contributions among the different sets of diagrams in Fig. 1 [notably (2LSE) and (SVPE)] is different from the separation into a "self-energy" correction (Eq. (A.24) of [1]) and a "magnetic moment contribution" (Eq. (A.25) of [1]). We also recall that the first treatment of the leading two-loop self-energy coefficient B_{40} was completed in [7].

The evaluation of the relativistic correction B_{50} due to the two-loop self-energy has represented a considerable challenge [8,9]. Diagrams involving a closed fermion loop were studied in [10,11]. It might be useful to point out that the contribution of the diagram (SVPE) is the sum of the contribution labeled E_{II} and E_{V} in Ref. [10]. The coefficients read:

$$B_{50}^{(2\mathrm{LSE})}(n\mathrm{S}) = -24.2668(31), \tag{4a}$$

$$B_{50}^{(\mathrm{SVPE})}(n\mathrm{S}) = -0.1571, \tag{4b}$$

$$B_{50}^{(\mathrm{SEVP})}(n\mathrm{S}) = 2.8677, \tag{4c}$$

$$B_{50}(n\mathrm{S}) = -21.5562(31). \tag{4d}$$

These results are in agreement with the data presented in Eqs. (A.28), (A.29) of [1].

The coefficients of sixth order in $Z\alpha$ have recently been analyzed in [2] (see also the references therein). The triple logarithm B_{63} originates exclusively from the set (2LSE). The diagrams of the set (SEVP) have been calculated in Section VII of [2], and the results for the double and single logarithms originating from these diagrams can be obtained by adding the contributions labeled E_{VP}^1 and E_{VP}^2 in Ref. [2], and the additional logarithm implicitly contained in Eq. (40) ibid. which is proportional to $B_{40}^{(\mathrm{SEVP})}$. The diagram (SVPE) generates only a single logarithm given by $B_{40}^{(\mathrm{SVPE})}/2$ (again consider Eq. (40) of Ref. [2]). In total, the results read as follows:

$$B_{63}(n\mathrm{S}) = B_{63}^{(2\mathrm{LSE})}(n\mathrm{S}) = -\frac{8}{27} = -0.296296. \tag{5}$$

The total result for B_{62} as well as its n-dependence were obtained in Refs. [2,12–14]. Here, we give the formulas for the particular sets of diagrams shown in Fig. 1, for the case $n = 1$ as well as the difference to a state of general n:

$$B_{62}^{(2\mathrm{LSE})}(1\mathrm{S}) = \frac{16}{27} - \frac{16}{9}\ln(2) = -0.639669, \tag{6a}$$

$$
\begin{aligned}
B_{62}^{(2\mathrm{LSE})}(n\mathrm{S}) \\
= B_{62}^{(2\mathrm{LSE})}(1\mathrm{S}) + \frac{16}{9}\left(\frac{3}{4} + \frac{1}{4n^2} - \frac{1}{n} - \ln(n)\right. \\
\left. + \Psi(n) + C\right),
\end{aligned} \tag{6b}
$$

$$B_{62}^{(\mathrm{SVPE})}(n\mathrm{S}) = 0, \tag{6c}$$

$$B_{62}^{(\mathrm{SEVP})}(n\mathrm{S}) = \frac{8}{45} = 0.177778, \tag{6d}$$

$$B_{62}(1\mathrm{S}) = \frac{104}{135} - \frac{16}{9}\ln 2 = -0.461891, \tag{6e}$$

$$
\begin{aligned}
B_{62}(n\mathrm{S}) = B_{62}(1\mathrm{S}) + \frac{16}{9}\left(\frac{3}{4} + \frac{1}{4n^2} - \frac{1}{n} - \ln(n)\right. \\
\left. + \Psi(n) + C\right),
\end{aligned} \tag{6f}
$$

where Ψ denotes the logarithmic derivative of the gamma function, and $C = 0.577216\ldots$ is Euler's constant. The formulas for B_{61} are a little more involved,

$$
\begin{aligned}
&B_{61}^{(2\mathrm{LSE})}(1\mathrm{S}) \\
&= \frac{127069}{32400} + \frac{875}{72}\zeta(2) + \frac{9}{2}\zeta(2)\ln 2 - \frac{9}{8}\zeta(3) \\
&\quad - \frac{152}{27}\ln 2 + \frac{40}{9}\ln^2 2 + \frac{4}{3}N(1\mathrm{S}) \\
&= 49.731651,
\end{aligned} \tag{7a}
$$

$$
\begin{aligned}
&B_{61}^{(2\mathrm{LSE})}(n\mathrm{S}) \\
&= B_{61}^{(2\mathrm{LSE})}(1\mathrm{S}) + \frac{4}{3}\left[N(n\mathrm{S}) - N(1\mathrm{S})\right] \\
&\quad + \left(\frac{80}{27} - \frac{32}{9}\ln 2\right) \\
&\quad \times \left(\frac{3}{4} + \frac{1}{4n^2} - \frac{1}{n} - \ln(n) + \Psi(n) + C\right),
\end{aligned} \tag{7b}
$$

$$B_{61}^{(\mathrm{SVPE})}(n\mathrm{S}) = -\frac{7}{162} + \frac{5}{72}\zeta(2) = 0.071022, \tag{7c}$$

$$B_{61}^{(\mathrm{SEVP})}(1\mathrm{S}) = -\frac{401}{2025} + \frac{16}{15}\ln 2 = 0.541332, \tag{7d}$$

$$
\begin{aligned}
&B_{61}^{(\mathrm{SEVP})}(n\mathrm{S}) \\
&= B_{61}^{(\mathrm{SEVP})}(1\mathrm{S}) - \frac{32}{45}\left(\frac{3}{4} + \frac{1}{4n^2} - \frac{1}{n} - \ln(n)\right. \\
&\quad \left. + \Psi(n) + C\right),
\end{aligned} \tag{7e}
$$

$$B_{61}(1S) = \frac{39751}{10800} + \frac{110}{9}\zeta(2) + \frac{9}{2}\zeta(2)\ln 2$$
$$- \frac{9}{8}\zeta(3) - \frac{616}{135}\ln 2 + \frac{40}{9}\ln^2 2 + \frac{4}{3}N(1S)$$
$$= 50.344005, \tag{7f}$$

$$B_{61}(nS)$$
$$= B_{61}(1S) + \frac{4}{3}\big[N(nS) - N(1S)\big]$$
$$+ \left(\frac{304}{135} - \frac{32}{9}\ln 2\right)$$
$$\times \left(\frac{3}{4} + \frac{1}{4n^2} - \frac{1}{n} - \ln(n) + \Psi(n) + C\right). \tag{7g}$$

The results for $N(nS)$ taken from [3] read

$$N(1S) = 17.855672(1),$$
$$N(2S) = 12.032209(1),$$
$$N(3S) = 10.449810(1),$$
$$N(4S) = 9.722413(1),$$
$$N(5S) = 9.304114(1),$$
$$N(6S) = 9.031832(1),$$
$$N(7S) = 8.840123(1),$$
$$N(8S) = 8.697639(1). \tag{8}$$

The slightly shifted results for $N(1S)$ also explains a discrepancy in an intermediate step of the calculation of radiative corrections to the muonium hyperfine splitting [15,16].

3. Extrapolation of the $Z\alpha$-expansion

We start our consideration with the one-loop self-energy which is the dominant radiative correction in hydrogenlike bound systems. We write the (real part of the) one-loop self-energy shift $\Delta E_{\text{SE}}^{(1L)}$ as

$$\Delta E_{\text{SE}}^{(1L)} = \frac{\alpha}{\pi}(Z\alpha)^4 \frac{m}{n^3} F(Z\alpha), \tag{9}$$

where $F(Z\alpha)$ is a dimensionless quantity which depends on the principal quantum number n, the total electron spin + angular momentum j and the electron orbital angular momentum l, and of course on the parameter $Z\alpha$.

The semi-analytic expansion of $F(Z\alpha)$ about $Z\alpha = 0$ for P states and states with higher angular momenta gives rise to the expression [21],

$$F(Z\alpha) = A_{40} + (Z\alpha)^2\big[A_{61}\ln(Z\alpha)^{-2} + A_{60}\big] + \cdots$$
$$(l \geqslant 1), \tag{10}$$

where the ellipsis again denotes omitted higher-order terms. The A_{60} coefficient has proven to be by far the most difficult to evaluate [22–26], and for 2P states, results have become available recently [17,18].

The semi-analytic expansion (10) is generally assumed to converge to the function $F(Z\alpha)$ for low Z, at least in an asymptotic sense. This is confirmed by recent numerical evaluations [27,28] for S and P states and the successful consistency check with available analytic results [17,26]. In many cases, an asymptotic expansion valid a priori for small expansion parameter $Z\alpha$ can be extrapolated to large coupling, if it is combined with a suitable convergence acceleration or resummation method (the latter in the case of a divergent input series [29]). The logarithms in Eq. (10) make a power series expansion about $Z\alpha = 0$ impossible. However, an extrapolation is still possible if we expand about $Z\alpha = \alpha \neq 0$ and use the fact that the nonperturbative function $F(Z\alpha)$, in the range of small Z, is very well represented by the first terms in its asymptotic expansion, as suggested by Fig. 1 of Ref. [27]. The logarithms in (10), when expanded about $Z\alpha = \alpha$, give rise to an infinite power series in the variable $g = (Z - 1)\alpha$. We proceed as follows: for all radiative corrections studied in the sequel, we start from the semi-analytic expansion and take into account all known coefficients. We then expand in g and evaluate the diagonal [2/2]-Padé approximant to the resulting power series (for the definition and a comprehensive discussion of Padé approximants we refer to [30]). This could be characterized a "deferred" approximant which is evaluated only after one has "advanced" to the point $Z = 1$ from the "starting point" $Z = 0$ (or equivalently $Z\alpha = 0$). Formally, the semi-analytic $Z\alpha$-expansion is performed about the point $Z = 0$. In re-expanding the perturbation series about a different point in the complex plane, we follow ideas outlined in [31] which were originally applied to the problem of calculating the autoionization width of atomic resonances in an external electric field.

The choice of the [2/2]-Padé approximant is motivated by the paradigm of finding a compromise between the necessity to harvest the information contained in the logarithms, which give rise to power series terms of arbitrarily high order, and at the same time to avoid spurious singularities which may be incurred when the degree of the Padé approximant is increased to an excessively high order. The [2/2]-deferred Padé approximant about $Z = 1$ to the function F (see also Eq. (3) of [32]) has five parameters $p_0, \ldots, p_2, q_1, \ldots, q_2$,

$$[2/2]_F(g) = \frac{\sum_{i=0}^{2} p_i g^i}{1 + \sum_{j=1}^{2} q_j g^j}, \tag{11}$$

which are determined by the requirement that the power series expansion of $[2/2]_F(g)$ about $g = 0$ reproduce the power series expansion of $F(Z\alpha)$ with $Z\alpha = \alpha + g$, also about $g = 0$, up to the order $\mathcal{O}(g^4)$. As discussed in [30], this condition alone defines the Padé approximant uniquely. The "one" in the denominator of (11) is the so-called Baker convention.

Because we do not observe a factorially divergent alternating-sign pattern in the g-expansion, we do not employ the delta transformation [29, Chapter 8] which has proven to be superior to Padé approximants in a number of applications where factorial divergence is observed (e.g., [32]). We rely on the robust Padé approximants, while stressing that it may be possible to find better extrapolation algorithms that harvest the analytic structure of (10) and give rise to logarithmic terms *naturally*. As yet, we have been unable to find such algorithms.

Figs. 2, 3 show that the extrapolated semi-analytic expansions have a somewhat better agreement with medium and high-Z numerical data than the known terms of the $Z\alpha$-expansion alone. We observe that the high-Z results for the energy correction given by the irreducible set of two-loop self-energy insertions into the bound electron propagator (see Ref. [4]) can only be made consistent with our extrapolated $Z\alpha$-expansion if we assume that the coefficient $B_{60}(1S_{1/2})$ is negative and rather large in magnitude.

4. Conclusions

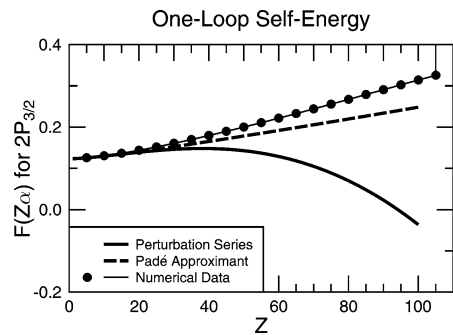We have presented a "mini-review" of recent two-loop self-energy calculations [2,3,12] in Section 2,

Fig. 2. Extrapolation of the semi-analytic $Z\alpha$-expansion of the one-loop self-energy (10) to the range of high nuclear charge via "deferred" [2/2]-Padé-approximants for the $2P_{3/2}$-state as described in the text. The analytic coefficients A_{40}, A_{61} and A_{60} in Eq. (10) are taken from Refs. [17,18]. The extrapolated semi-analytic $Z\alpha$-expansions are closer to the numerical data for high Z than the "raw" $Z\alpha$-expansion. Numerical data at high Z are taken from Refs. [19,20].
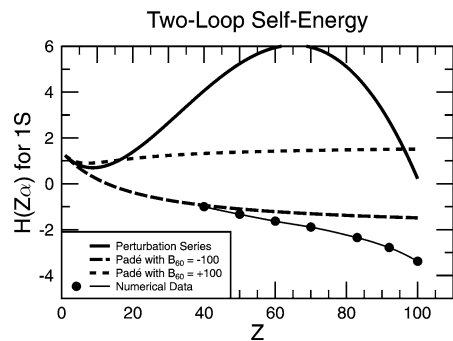

Fig. 3. Extrapolation of the two-loop self-energy. Analytic data are taken from Section 2 (see the (2LSE)-parts of Eqs. (3)–(8)). Numerical data are found in Ref. [4]. Much better agreement between numerical and analytic data is achieved for negative B_{60}.

clarifying the distribution of sixth-order (in $Z\alpha$) two-loop binding corrections to the Lamb shift over the set of diagrams shown in Fig. 1. Results for the two-loop coefficients, including excited S states, are provided in Eqs. (3)–(8). The distribution of the logarithmic corrections over distinct sets of diagrams needs to be clarified in order to allow for an accurate comparison to numerical calculations which are currently being pursued [4]. In Section 3, we present a crude extrapolation scheme for the extrapolation of the $Z\alpha$-expansion from low Z to high Z. The scheme follows ideas outlined in [31] and is based upon an expansion in the variable g where g is defined as $Z\alpha = \alpha + g$. The "deferred" Padé approximant is then evaluated in terms of

the variable g, i.e., after the coupling parameter $Z\alpha$ has acquired the value $\alpha \neq 0$, "starting" from $Z\alpha = 0$. This deferment circumvents the problems introduced by the logarithms in Eqs. (2) and (10); however, we stress here that it would be highly desirable to find better extrapolation algorithms that harvest the analytic structure of (2) and (10) and give rise to logarithmic terms *naturally*. Although the extrapolation scheme has problems (in some cases, we observe spurious poles in the Padé approximant at medium-Z values), we have observed rather consistent improvement over the "raw" $Z\alpha$-expansion with this scheme for a number of states and QED effects which we studied using the "deferred" Padé-extrapolation scheme. Details will be presented elsewhere. Based on our extrapolations of the two-loop effect in Fig. 3, we would like to advance the tentative estimate $B_{60}(1S_{1/2}) \approx -100(50)$.

Acknowledgements

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