Two–Loop Self–Energy Corrections to the Fine–Structure

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Abstract. We investigate two-loop higher-order binding corrections to the fine structure, which contribute to the spin-dependent part of the Lamb shift. Our calculation focuses on the so-called "two-loop self-energy" involving two virtual closed photon loops. For bound states, this correction has proven to be notoriously difficult to evaluate. The calculation of the binding corrections to the bound-state two-loop self-energy is simplified by a separate treatment of hard and soft virtual photons. The two photon-energy scales are matched at the end of the calculation. We explain the significance of the mathematical methods employed in the calculation in a more general context, and present results for the fine-structure difference of the two-loop self-energy through the order of α^8.

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1. Introduction

Ultra-precise measurements in atomic systems represent today of the most stringent available tests of fundamental quantum theories and a means for the determination of fundamental physical constants with unprecedented accuracy [1]. The theoretical description of the bound states at a level of accuracy which matches the current experimental precision, which has reached 1.8 parts in 10^{14} and whose accuracy is to be improved in the near future [2], demands a thorough understanding of the bound state including – among other effects – the relativistic, one-loop, two-loop and higher-order radiative, recoil, radiative-recoil, and nuclear-size corrections [3, 4].

We focus here on radiative corrections, which can be described – for atomic systems with low nuclear charge number – by a nonanalytic expansion in powers of the three parameters (i) α (the fine-structure constant), (ii) the product $Z\alpha$ (Z is the nuclear charge number), and (iii) the logarithm $\ln[(Z\alpha)^{-2}]$. The expansion in powers of α, which is the perturbation theory parameter in quantum electrodynamics (QED), corresponds to the number of loops in the diagrams. The bound-state effects are taken into account by the expansions in the two latter parameters. Higher-order terms in the expansions in powers of $Z\alpha$ and $\ln[(Z\alpha)^{-2}]$ are referred to as the "binding corrections". One of the historically most problematic sets of Feynman diagrams in the treatment of the Lamb shift for atomic systems has been the radiative correction due to two closed virtual-photon loops shown in fig. 1.

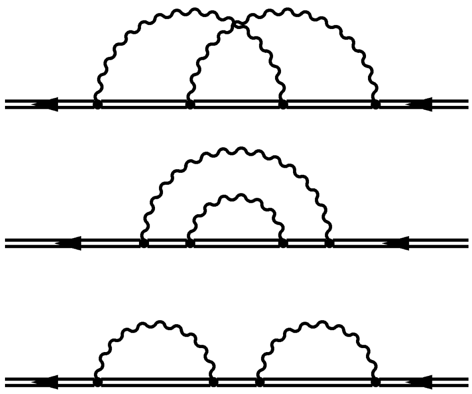


Figure 1. Feynman diagrams representing the two-photon electron self-energy. The double line denotes the bound electron propagator. The arrow of time is from right to left.

Let us recall at this point that even the evaluation of higher-order binding corrections to the one-loop self-energy, which *a priori* should represent a less involved calculational challenge, has represented a problem for analytic evaluations for over three decades [5–9]. The energy shifts of the bound states due to the radiative corrections are conveniently expressed by expansion coefficients corresponding to the powers of $Z\alpha$ and $\ln[(Z\alpha)^{-2}]$; the naming convention is that the power of $Z\alpha$ and the power of the logarithm are indicated as indices to the analytic coefficients [see also eq. (1)] below. Because the expansion in both the one-loop and the two-loop case starts with the fourth power of $Z\alpha$, the non-vanishing coefficients carry indices A_{kl} and B_{kl} for the one- and two-loop cases, respectively (with $k \geq 4$ – see [3] for a comprehensive review).

Logarithmic corrections with $l \geq 1$ can sometimes be inferred separately in a much simplified approach, e.g. by considering infrared divergent contributions to electron form factors. By contrast, the higher-order non-logarithmic coefficients represent a considerable calculational challenge. Realistically, i.e. with the help of current computer algebra systems [10,11], one can hope to evaluate non-logarithmic coefficients of sixth order in $Z\alpha$. Complete results for the one-loop higher-order correction A_{60} for S and P states have only been available recently [8,12,13,13]. Calculational difficulties have by now precluded a successful evaluation of the corresponding coefficient B_{60} for the two-loop effect. Ground-work for the evaluation of B_{60} was laid in [14]. Here, we are concerned with the evaluation of the fine-structure differences of the logarithmic and non-logarithmic coefficients B_{6L} (where $L = 0, 1, 2$), i.e. with the $n\mathrm{P}_{3/2}$–$n\mathrm{P}_{1/2}$ difference of these coefficients.

Using natural Gaussian units ($\hbar = c = \epsilon_0 = 1$), as it is customary for the current type of calculation, we write the two-photon self-energy in the $Z\alpha$-expansion for P states in terms of B-coefficients as

$$\Delta E_{\mathrm{SE}} = \left(\frac{\alpha}{\pi}\right)^2 (Z\alpha)^4 \, \frac{m}{n^3} \left[B_{40} \right.$$

$$\left. + (Z\alpha)^2 \left[B_{62} \ln^2(Z\alpha)^{-2} + B_{61} \ln(Z\alpha)^{-2} + B_{60}\right] + \mathcal{R} \right], \tag{1}$$

where the remainder $\mathcal{R}$ is of order $\mathcal{O}(Z\alpha)^3$. Relevant Feynman diagrams are shown in fig. 1.

Here, m denotes the electron mass (we write eq. (1) in the non-recoil limit, i.e. for an infinite nuclear mass). The double logarithmic B_{62}-coefficient is spin-independent, so that we have $\Delta_{\mathrm{fs}} B_{62} = 0$. In this paper, we evaluate the fine-structure differences

$$\Delta_{\mathrm{fs}} B_{61} = B_{61}(n\mathrm{P}_{3/2}) - B_{61}(n\mathrm{P}_{1/2}) \,,$$

$$\Delta_{\mathrm{fs}} B_{60} = B_{60}(n\mathrm{P}_{3/2}) - B_{60}(n\mathrm{P}_{1/2}) \,. \tag{2}$$

Throughout the paper, we will follow the convention that $\Delta_{\mathrm{fs}} X \equiv X(n\mathrm{P}_{3/2}) - X(n\mathrm{P}_{1/2})$ denotes the "fine-structure part" of a given quantity X. For $\Delta_{\mathrm{fs}} B_{61}$ and $\Delta_{\mathrm{fs}} B_{60}$, we provide complete results. It is perhaps worth noting that two-loop self-energy effects for bound states have represented a considerable challenge for theoretical evaluations. Our investigation represents a continuation of previous work on the two-loop problem (see e.g. [14–17]). It is probably a triviality to express that technical difficulties in the calculation and its description in the following sections of the paper cannot be avoided.

For the description of the self-energy radiative effects – mediated by hard virtual photons –, we use the modified Dirac hamiltonian

$$H_{\mathrm{D}}^{(m)} = \boldsymbol{\alpha} \cdot [\boldsymbol{p} - \mathrm{e}\, F_1(\Delta)\, \boldsymbol{A}] + \beta\, m + \mathrm{e}\, F_1(\Delta)\, \phi + F_2(\Delta)\, \frac{e}{2\,m}\, (\mathrm{i}\, \boldsymbol{\gamma} \cdot \boldsymbol{E} - \beta\, \boldsymbol{\sigma} \cdot \boldsymbol{B}) \,, \tag{3}$$

which approximately describes an electron subject to an external scalar potential $\phi \equiv \phi(\boldsymbol{r})$ and an external vector potential $\boldsymbol{A} \equiv \boldsymbol{A}(\boldsymbol{r})$. This modified hamiltonian is still local in coordinate space. The Dirac matrices in (3) are to be understood in the standard (Dirac) representation [19] (in the sequel, we will also use the non-covariant notation $\beta \equiv \gamma^0$ and $\alpha^i \equiv \gamma^0 \gamma^i$).

The argument Δ of the electron form factors F_1 and F_2 in eq. (3) is to be interpreted as a Laplacian operator acting on all quantities to the right (but not on the wave function of the bound electron in evaluating $H_{\mathrm{D}}^{(m)}|\psi\rangle$). In momentum space, the action of the hamiltonian $H_{\mathrm{D}}^{(m)}$ is described by the convolution $\left[H_{\mathrm{D}}^{(m)}\psi\right](\boldsymbol{p}') = \int \mathrm{d}^3p/(2\pi)^3\, H_{\mathrm{D}}^{(m)}(\boldsymbol{p}' - \boldsymbol{p})\, \psi(\boldsymbol{p})$. The form factors – in momentum space – assume arguments according to the replacement $\Delta \to -\boldsymbol{q}^2 \equiv -(\boldsymbol{p}' - \boldsymbol{p})^2$. In eq. (3), radiative corrections are taken into account in the sense of an effective theory via the inclusion of the on-shell form factors F_1 and F_2. Although the bound electron is not an on-shell particle, the modified hamiltonian (3) can still approximately account for significant radiative systems with low nuclear charge number Z. Of course, the hamiltonian (3) cannot offer a complete description of the bound electron. Recoil effects cannot be described by a one-particle equation *in principle*, and vacuum-polarization effects are not contained in eq. (3). However, the effective description of self-energy radiative corrections mediated by hard virtual photons given by eq. (3) will turn out to be useful in the context of the current investigation.

Both of the form factors F_1 and F_2 entering in eq. (3) are infrared divergent, but this divergence is cut off in a natural way at the atomic binding energy scale $(Z\alpha)^2\, m$. The fact that on-shell form factors can describe radiative corrections to the fine structure – mediated by high-energy virtual photons – has been demonstrated explicitly in [18]. The modified Dirac hamiltonian (3) and the associated modified Dirac equation have been introduced – in the one-loop approximation – in ch. 7 of [19] [see for example eqs. (7-77) and (7-103) *ibid.*]. The low-energy part of the calculation is carried out using nonrelativistic approximations in the spirit of the simplified treatment introduced in the previous one- and two-loop calculations [8,12–14,20]. This approach was inspired, in part, by various attempts to formulate simplified low-energy ("nonrelativistic") approximations to quantum electrodynamics ("NRQED"), see e.g. [21,22]. Both the high-energy and the low-energy contributions are matched at the separation scale ϵ whose rôle in the calculation is illustrated by the mathematical model example discussed in app. Appendix A.

In a two-loop calculation, either of the two virtual photons may have a high or low energy as compared to the separation scale ϵ. *A priori*, this necessitates [14] a separation of the calculation into three different contributions: (i) both photon energies large, (ii) one photon with a large and one with a small energy, and (iii) both photons with small energies. For the particular problem at hand (the fine-structure differences of B_{61} and B_{60}), we are in the fortunate position that effects caused by hard virtual photons (i) are described by the modified Dirac hamiltonian (3), whereas the low-energy part discussed in sec. 4 below comprises both remaining contributions (ii) and (iii).

This paper is organized as follows: Two-loop form factors entering in eq. (3) are analyzed in sec. 2. The calculation is split into two parts: the high-energy part discussed in sec. 3 and the low-energy part, which is treated along ideas introduced in [22] in sec. 4. Results and conclusions are left to sec. 5.

2. Two-loop Form Factors

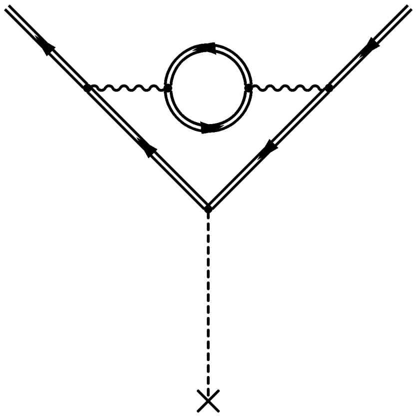
In order to analyze the modified Dirac hamiltonian (3) through two-loop order, we first have to investigate certain expansion coefficients of the electronic F_1 and F_2 form factors which are thoroughly discussed in the seminal papers [23, 24]. For the momentum transfer q^2 which is the argument of the two functions $F_1 \equiv F_1(q^2)$ and $F_2 \equiv F_2(q^2)$, we use the convention $q^2 = q_\mu q^\mu = (q^0)^2 - \boldsymbol{q}^2$. The variable t in [23, 24] is given as $t = q^2$. When we evaluate radiative corrections to the binding Coulomb field which is mediated by space-like virtual photons, we have $q^2 = -\boldsymbol{q}^2$ because for $q^0 = 0$. We use the conventions (see eq. (1.2) in [23]):

$$F_1(t) = 1 + \sum_{n=1}^{\infty} \left(\frac{\alpha}{\pi}\right)^n F_1^{(2n)}(t)\,, \quad F_2(t) = \sum_{n=1}^{\infty} \left(\frac{\alpha}{\pi}\right)^n F_2^{(2n)}(t)\,. \tag{4}$$

One and two-loop effects are denoted by upper indices 2 and 4, respectively. This notation is motivated by the observation that two-loop effects are of forth order in the quantum electrodynamic interaction Lagrangian $-e\,\bar{\psi}\,\gamma^\mu A_\mu\,\psi$ (in the Furry picture, which is used for the description of bound states, the Coulomb interaction is taken out of the interaction Lagrangian).

There are two different points of view regarding the choice of diagrams to be included in the two-loop form factors, depending on whether the self-energy vacuum polarization diagram fig. 2 is included in the calculation or not. We will discuss both cases and give results with and without the diagram shown in fig. 2 taken into account.

First, we discuss results obtained for F_1 *including* the combined self-energy vacuum polarization diagram. In this case, the known results for the slope $F_1'(0)$ and for $F_2(0)$, through two-loop order, read



(V)

Figure 2. Combined self-energy vacuum-polarization diagram (denoted "V" in the text).

as follows. From eq. (1.11) of [23], we have:

$$m^2 F_1'(0) = \frac{\alpha}{\pi}\,\left[-\frac{1}{3}\,\ln\left(\frac{\lambda}{m}\right) - \frac{1}{8}\right] + \left(\frac{\alpha}{\pi}\right)^2\,\left[-\frac{4819}{5184} - \frac{49}{72}\,\zeta(2) + 3\,\zeta(2)\,\ln 2 - \frac{3}{4}\,\zeta(3)\right]\,, \tag{5}$$

where the forth-order coefficient has the numerical value

$$m^2 F_1'^{(4)}(0) = 0.469\,941\,487\,460\,. \tag{6}$$

According to eq. (1.7) in [23], the value of $F_2(0)$, through two-loop order, reads

$$F_2(0) = \frac{1}{2}\,\frac{\alpha}{\pi} + \left(\frac{\alpha}{\pi}\right)^2\,\left[\frac{197}{144} + \frac{1}{2}\,\zeta(2) - 3\,\zeta(2)\,\ln 2 + \frac{3}{4}\,\zeta(3)\right]\,, \tag{7}$$

where the two-loop coefficient has the numerical value

$$F_2^{(4)}(0) = -0.328\,478\,965\,579\,. \tag{8}$$

We now turn to the discussion of the slope $F_2'^{(4)}(0)$. In view of eq. (1.20) of [23] (see also [25]), we have (up to two-loop order)

$$F_2(t) = \frac{\alpha}{\pi}\,\mathcal{F}_2^{(2)}(t) + \left(\frac{\alpha}{\pi}\right)^2\,\left[\ln\frac{\lambda}{m}\,B(t)\,\mathcal{F}_2^{(2)}(t) + \mathcal{F}_2^{(4)}(t)\right]\,, \tag{9}$$

where the coefficients $\mathcal{F}$ are by definition infrared safe and

$$\mathcal{F}_2^{(2)}(0) = \frac{1}{2}\,, \quad B(t) = -\frac{t}{3\,m^2} - \frac{t^2}{20\,m^2} + \mathcal{O}(t^3)\,. \tag{10}$$

Equations (9) and (10) uniquely determine the infrared divergent contribution to $F_2'^{(4)}(0)$. An analytic expressions for $\mathcal{F}_2^{(4)}(t)$, t spacelike, has recently been obtained [26] in terms of harmonic polylogarithms [27, 28]. As a byproduct, an analytic expression for the the slope $\mathcal{F}_2'^{(4)}(0)$ was found. The result reads

$$m^2\, F_2'^{(4)}(0) = -\frac{1}{6}\ln\left(\frac{\lambda}{m}\right) + m^2\,\mathcal{F}_2'^{(4)}(0)\,,$$

$$m^2\,\mathcal{F}_2'^{(4)}(0) = \frac{1751}{2160} + \frac{13}{20}\,\zeta(2) - \frac{23}{10}\,\zeta(2)\,\ln 2 + \frac{23}{40}\,\zeta(3)\,. \tag{11}$$

A numerical result for $\mathcal{F}_2'^{(4)}(0)$, complementing the above analytic expression, can easily be derived in combining eq. (1.20), eq. (1.30), and eq. (3.2) in [23], as will be explained in the sequel. The dispersion relation (1.30) in [23] reads,

$$\mathrm{Re}\, F_2(t) = -\frac{4m^2}{t-4m^2}\, F_2(0) + \frac{1}{\pi}\,\frac{t}{t-4m^2}\, P\int\limits_{4m^2}^{\infty} \frac{\mathrm{d}t'}{t'-t}\,\frac{t'-4m^2}{t'}\,\mathrm{Im}F_2(t')\,, \tag{12}$$

where P denotes the Cauchy principal value. Equation (12) applies also if we single out the two-loop effect and differentiate at zero momentum transfer, and we obtain for the slope $F_2'^{(4)}(0)$ the relation

$$m^2\, F_2'^{(4)}(0) = \frac{1}{4}\, F_2^{(4)}(0) + \frac{1}{4\,\pi}\, P\int\limits_{4m^2}^{\infty} \mathrm{d}t'\,\frac{4m^2-t'}{t'^2}\,\mathrm{Im}F_2'^{(4)}(t') = \frac{1}{4}\, F_2^{(4)}(0) + \mathcal{T}\,, \tag{13}$$

where $F_2^{(4)}(0)$ is given in eq. (8). The second term on the right-hand side, denoted by $\mathcal{T}$, can be evaluated using the result for $\mathrm{Im}\, F_2^{(4)}(x)$ presented in eq. (3.2) in [23]; it reads

$$\mathcal{T} = -\int\limits_0^1 \mathrm{d}x\,\frac{(1-x)^3}{x\,(1+x)}\,\mathrm{Im}\, F_2^{(4)}(x) = -\frac{1}{6}\,\ln\left(\frac{\lambda}{m}\right) + 0.030\,740\,507\,833(1)\,. \tag{14}$$

Here, the last error is due to numerical integration, and use is made of the natural variable [23]

$$x = \frac{1-\sqrt{1-4m^2/t}}{1+\sqrt{1-4m^2/t}}\,. \tag{15}$$

In combining the result of eq. (8) with eqs. (13) and (14), the result $m^2\,\mathcal{F}_2'^{(4)}(0) = -0.051\,379\,233\,561(1)$ is obtained which is in agreement with (11).

Now we will provide results for the form factors obtained *excluding* the self-energy vacuum-polarization graph V shown in fig. 2. These results refer to the pure two-photon self-energy diagrams shown in fig. 1. The two-loop self-energy diagrams independently form a gauge-invariant set. They represent a historically problematic correction, and are the main subject of our investigation. The combined self-energy vacuum-polarization diagram, according to eqs. (1.9) and (1.10) in [24] – taking into account the subtracted dispersion relation (1.30) of [23] – leads to the following corrections:

$$F_1'^{(4),V}(0) = -\frac{1099}{1296} + \frac{77}{144}\,\zeta(2) = 0.031\,588\,972\,474\,,$$

$$F_2^{(4),V}(0) = \frac{119}{36} - 2\,\zeta(2) = 0.015\,687\,421\,859\,,$$

$$F_2'^{(4),V}(0) = \frac{311}{216} - \frac{7}{8}\,\zeta(2) = 0.000\,497\,506\,323\,. \tag{16}$$

For the pure self-energy graphs, which we would like to denote by the symbol S, we therefore obtain the following results,

$$m^2\, F_1^{\prime(4),S}(0) = -\frac{47}{576} - \frac{175}{144}\,\zeta(2) + 3\,\zeta(2)\,\ln 2 - \frac{3}{4}\,\zeta(3) = 0.438\,352\,514\,986\,, \tag{17}$$

$$F_2^{(4),S}(0) = -\frac{31}{16} + \frac{5}{2}\,\zeta(2) - 3\,\zeta(2)\,\ln 2 + \frac{3}{4}\,\zeta(3) = -0.344\,166\,387\,438\,, \tag{18}$$

$$\begin{aligned} m^2\, F_2^{\prime(4),S}(0) &= -\frac{1}{6}\,\ln\left(\frac{\lambda}{m}\right) - \frac{151}{240} + \frac{61}{40}\,\zeta(2) - \frac{23}{10}\,\zeta(2)\,\ln 2 + \frac{23}{40}\,\zeta(3) \\ &= -\frac{1}{6}\,\ln\left(\frac{\lambda}{m}\right) - 0.051\,876\,739\,885 \equiv -\frac{1}{6}\,\ln\left(\frac{\lambda}{m}\right) + \mathcal{F}_2^{\prime(4),S}(0)\,. \end{aligned} \tag{19}$$

where the latter equality defines $\mathcal{F}_2^{\prime(4),S}(0)$ in analogy with eqs. (9) and (11).

3. High–Energy Part

Based on the modified Dirac hamiltonian (3), corrections to the energy of the bound Dirac particle can be inferred. We will refer to the energy corrections attributable to the F_1 and F_2 form factors as E_1 and E_2, respectively. For E_1, we have

$$E_1 = \left\langle \left[F_1(-\boldsymbol{q}^2) - 1\right]\, e\,\phi \right\rangle_{\rm fs}\,, \tag{20}$$

where the index fs refers to the fine-structure terms, i.e. to the result obtained by subtracting the value of the matrix element for a $n\mathrm{P}_{3/2}$ state from the value of the same matrix element evaluated on a $n\mathrm{P}_{1/2}$ state. A matrix element $\langle A\rangle_{\rm fs}$ of a given operator A is evaluated as

$$\langle A\rangle_{\rm fs} \equiv \left\langle \psi^+_{\rm nP_{3/2}} \middle| A \middle| \psi_{\rm nP_{3/2}} \right\rangle - \left\langle \psi^+_{\rm nP_{1/2}} \middle| A \middle| \psi_{\rm nP_{1/2}} \right\rangle\,,$$

where ψ^+ denotes the hermitian conjugate of the Dirac wave function ψ (not the Dirac adjoint $\bar{\psi} = \psi^+\gamma^0$). The Dirac wave functions ψ are expanded in powers of $(Z\alpha)$ up to the order relevant for the current investigation. This expansion avoids potential problems associated with the logarithmic divergence of the Dirac wave function at the origin.

For E_1, up to the order of $(Z\alpha)^6$, we have

$$E_1 = 4\pi Z\alpha\, F_1^{\prime(4)}(0)\, \left\langle \delta^{(3)}(\boldsymbol{r}) \right\rangle_{\rm fs}\,. \tag{21}$$

For P states, the nonrelativistic (Schrödinger) wave function – the leading term in the $Z\alpha$-expansion of the Dirac wave function – vanishes at $\boldsymbol{r} = 0$, but the first relativistic correction gives a finite contribution, resulting in

$$\langle \delta^{(3)}(\boldsymbol{r})\rangle_{\rm fs} = -\frac{n^2-1}{4\,n^5}\,(Z\alpha)^5\, m^3\,. \tag{22}$$

This leads – again up to the order of $(Z\alpha)^6$ – to the following result for E_1,

$$E_1 = \left(\frac{\alpha}{\pi}\right)^2\, \frac{(Z\alpha)^6}{n^3}\, \left[-F_1^{\prime(4)}(0)\,\frac{n^2-1}{n^2}\right]\, m^3\,. \tag{23}$$

Observe that the derivative of the F_1 form factor has a physical dimension of $1/m^2$ in natural units, giving the correct physical dimension for E_1. The correction due to F_2 in (3) reads,

$$E_2 = \langle F_2(-\boldsymbol{q}^2)\,\frac{e}{2m}\,\mathrm{i}\,\boldsymbol{\gamma}\cdot\boldsymbol{E}\rangle_{\rm fs}\,. \tag{24}$$

A particle in an external binding Coulomb field feels an electric field $\boldsymbol{E} = \mathrm{i}\,(Ze)\,\boldsymbol{q}/\boldsymbol{q}^2$ – in momentum space – or $\boldsymbol{E} = -(Ze)\,\boldsymbol{r}/(4\pi r^3)$ in coordinate space. Vacuum polarization corrections to $\boldsymbol{E} = -(Ze)\,\boldsymbol{r}/(4\pi r^3)$ lead to higher-order effects. The correction E_2 splits up in a natural way into two contributions E_{2a} and E_{2b} which are associated with $F_2(0)$ and the slope $F_2'(0)$, respectively. E_{2a} reads

$$E_{2a} = \frac{Z\alpha}{2m}\,F_2^{(4)}(0)\,\left\langle -\mathrm{i}\,\frac{\boldsymbol{\gamma}\cdot\boldsymbol{r}}{r^3}\right\rangle_{\mathrm{fs}}\,. \tag{25}$$

The evaluation of the matrix element leads to

$$\left\langle -\mathrm{i}\,\frac{\boldsymbol{\gamma}\cdot\boldsymbol{r}}{r^3}\right\rangle_{\mathrm{fs}} = \left\{\frac{(Z\alpha)^3}{n^3} + \left[\frac{487}{360} + \frac{5}{4n} - \frac{23}{10n^2}\right]\frac{(Z\alpha)^5}{n^3}\right\}\,m^2\,. \tag{26}$$

For the purpose of the current investigation, the $(Z\alpha)^6$-component of E_{2a} is selected only:

$$E_{2a} = \left(\frac{\alpha}{\pi}\right)^2\,\frac{(Z\alpha)^6}{n^3}\,\left[F_2^{(4)}(0)\,\left(\frac{487}{720} + \frac{5}{8n} - \frac{23}{20n^2}\right)\right]\,m\,. \tag{27}$$

The matrix element E_{2b} can be expressed as

$$E_{2b} = \frac{4\pi Z\alpha}{2m}\,F_2'^{(4)}(0)\,\langle\boldsymbol{\gamma}\cdot\boldsymbol{q}\rangle_{\mathrm{fs}}\,. \tag{28}$$

A transformation into coordinate space leads to

$$\langle\boldsymbol{\gamma}\cdot\boldsymbol{q}\rangle_{\mathrm{fs}} = \mathrm{i}\,\left[\frac{\partial}{\partial\boldsymbol{x}}\left(\psi^+(\boldsymbol{x})\boldsymbol{\gamma}\psi(\boldsymbol{x})\right)\right]_{x=0,\mathrm{fs}} = -\frac{n^2-1}{n^5}\,(Z\alpha)^5\,m^4\,. \tag{29}$$

As a function of the principal quantum number n, the result for E_{2b} reads:

$$E_{2b} = \left(\frac{\alpha}{\pi}\right)^2\,\frac{(Z\alpha)^6}{n^3}\,\left[-2\,F_2'^{(4)}(0)\,\frac{n^2-1}{n^2}\right]\,m^3\,. \tag{30}$$

This result involves the infrared divergent slope of the F_2 form factor [see eqs. (11) and (19)]. We are thus faced with the problem of matching the infrared divergence of the slope of the F_2 form factor, expressed in terms of the fictitious photon mass λ, with the usual (energy matching parameter) ϵ introduced originally in [8]. This can be done in two ways: (i) by matching the infrared divergence of the rate of soft bremsstrahlung, calculated with a fictitious photon mass λ, to a result of the same calculation, carried out with an explicit infrared cut-off ϵ for the photon energy. This way of calculation is described on pp. 361–362 of [19]. It leads to the result

$$\ln\frac{\lambda}{2\,\epsilon} = -\frac{5}{6}\,. \tag{31}$$

The matching procedure (ii) consists in a comparison of the result of the application of the formalism considered above, and its application to the high-energy part of the ground state Lamb shift, which is in leading order given by the infrared divergence of the F_1 form factor, and the result obtained by direct calculation of this high-energy part in a non-covariant formalism with an explicit energy cut-off ϵ, as it has been carried out in [8]. This second matching procedure leads to the following result – in agreement with (31) –,

$$\ln\frac{m}{\lambda} - \frac{3}{8} = \ln\frac{m}{2\epsilon} + \frac{11}{24}\,. \tag{32}$$

So, we are led to the replacement

$$-\ln\frac{\lambda}{m} \to \ln\frac{m}{2\epsilon} + \frac{5}{6} \tag{33}$$

A comparison with the results in eqs. (11), (19), and (36) reveals that the logarithmic divergence for the fine-structure difference is given by a term

$$-\frac{n^2-1}{3n^2}\,\ln\frac{m}{2\epsilon}\,, \tag{34}$$

so that we may anticipate at this stage the result for $\Delta_{\rm fs} B_{61}$,

$$\Delta_{\rm fs} B_{61} = -\frac{n^2-1}{3n^2}\,. \tag{35}$$

Based on (30) and (33), we can express E_{2b} in terms of ϵ and $\mathcal{F}_2'^{(4)}(0)$,

$$E_{2b} = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^6}{n^3}\left[-\frac{1}{3}\,\frac{n^2-1}{n^2}\,\ln\frac{m}{2\epsilon} - \left(\frac{5}{18} + 2\,\mathcal{F}_2'^{(4)}(0)\,m^2\right)\,\frac{n^2-1}{n^2}\right]\,m\,. \tag{36}$$

There is a third correction due to the effect of *two* one-loop corrections on the electron vertices. Because we are only interested in the fine structure, we isolate the terms which are proportional to the spin-orbit coupling, and we obtain

$$E_3 = \left\langle [2F_2(0)]\;H_{\rm fs}\;\left(\frac{1}{E-H}\right)'\;[2F_2(0)]\;H_{\rm fs}\right\rangle_{\rm fs}\,, \tag{37}$$

where

$$H_{\rm fs} = \frac{Z\alpha}{4m^2r^3}\,\boldsymbol{\sigma}\cdot\boldsymbol{L}\,, \tag{38}$$

and $1/(E-H)'$ is the nonrelativistic, spin-independent reduced Schrödinger–Coulomb Green function [29, 30]. The only spin-dependence in (37) occurs in the coupling $\boldsymbol{\sigma}\cdot\boldsymbol{L}$, and it can be taken into account by an overall factor,

$$\left\langle(\boldsymbol{\sigma}\cdot\boldsymbol{L})^2\right\rangle_{\rm fs} = -3\,. \tag{39}$$

We are therefore led to consider the "spin-independent version" of the matrix element which occurs in eq. (37) and obtain the following result,

$$\left\langle\frac{Z\alpha}{4m^2r^3}\left(\frac{1}{E-H}\right)'\frac{Z\alpha}{4m^2r^3}\right\rangle_{\rm nP} = \left(-\frac{227}{8640} - \frac{1}{96n} + \frac{1}{80n^2}\right)\frac{(Z\alpha)^6\,m}{n^3}\,. \tag{40}$$

The spin-dependence can be easily restored by considering eq. (39). The index "nP" in eq. (40) means that the matrix element is evaluated with the nonrelativistic, spin-independent (Schrödinger) wave function. Alternatively, on may evaluate with either the $\rm nP_{1/2}$ or the $\rm nP_{3/2}$ Dirac wave function and expand up to the leading order in $(Z\alpha)$.

The evaluation of (40) can proceed e.g. by solving the differential equation which defines the correction to the wave function induced by $H_{\rm fs}$, and subsequent direct evaluation of the resulting standard integrals using computer algebra [10, 11]. The final result for E_3 reads,

$$E_3 = \left(\frac{\alpha}{\pi}\right)^2\frac{(Z\alpha)^6}{n^3}\left[\frac{227}{2880} + \frac{1}{32n} - \frac{3}{80n^2}\right]\,m\,. \tag{41}$$

This concludes the discussion of the high-energy part. The final result for the high-energy part is

$$E_{\rm H} = E_1 + E_{2a} + E_{2b} + E_3\,, \tag{42}$$

where E_1, E_{2a}, E_{2b}, E_3 are given in eqs. (23), (27), (36), (41), respectively.

4. Low–Energy Part

The low-energy part consists essentially of two contributions. Both effects, denoted here E_4 and E_5, can be obtained by a suitable variation of the low-energy part of the *one-loop* self energy, by considering the spin-dependent effects introduced by a *further* one-loop electron anomalous magnetic moment interaction. The first of the two terms, E_4, is caused by spin-dependent higher-order effects in the one-loop self-energy, which receive additional corrections due to the anomalous magnetic moment of the electron. The second term, E_5, is due to an anomalous magnetic moment correction to the electron transition current, which can also be seen as a correction to the radiation field of the electron due to its anomalous magnetic moment.

The leading-order low-energy part (see [8]) reads

$$E_{\mathrm{L}} = -\frac{2\alpha}{3\pi m} \int_0^{\epsilon} \mathrm{d}\omega\, \omega \left\langle \phi \left| \boldsymbol{p}\, \frac{1}{H-(E-\omega)}\, \boldsymbol{p} \right| \phi \right\rangle . \tag{43}$$

In order to isolate the fine-structure effects, we should now consider corrections to the wave function, to the current, to the hamiltonian and to the energy of the bound state due to the spin-dependent relativistic (spin-orbit) hamiltonian

$$\mathcal{H} = F_2(0)\, \frac{e}{2m}\, \mathrm{i}\, \boldsymbol{\gamma} \cdot \boldsymbol{E} = \frac{\alpha(Z\alpha)}{4\pi m}\, \frac{-\mathrm{i}\, \boldsymbol{\gamma} \cdot \boldsymbol{r}}{r^3} . \tag{44}$$

The above hamiltonian $\mathcal{H}$ is the last term in the modified Dirac hamiltonian [right-hand side of eq. (3)], approximated for a particle bound in a Coulomb field with the F_2 form factor evaluated at zero momentum. The electric field $\boldsymbol{E}$ in (44) corresponds to the binding Coulomb interaction. The hamiltonian (44) describes the modification of the spin-orbit interaction due to the anomalous magnetic moment of the electron.

The nonrelativistic limit of $\mathcal{H}$ is the spin-orbit coupling H_{fs} given in eq. (38), multiplied by a factor $2F_2^{(2)}(0) = \alpha/\pi$ (the additional factor 2 finds an explanation in [31]). The resulting hamiltonian

$$H_{\mathrm{eff}} = \frac{\alpha}{\pi}\, H_{\mathrm{fs}} = \frac{\alpha}{\pi}\, \frac{Z\alpha}{4m^2 r^3}\, \boldsymbol{\sigma} \cdot \boldsymbol{L} . \tag{45}$$

takes into account magnetic vertex corrections in the framework of an effective theory. Denoting the variation of the expression (43) mediated by H_{eff} with the symbol δ_{eff} – in the spirit of the notation introduced in [14] –, we obtain the contribution

$$E_{4a} = \delta_{\mathrm{eff}} \left\{ -\frac{2\alpha}{3\pi m} \int_0^{\epsilon} \mathrm{d}\omega\, \omega \left\langle \phi \left| \boldsymbol{p}\, \frac{1}{H-(E-\omega)}\, \boldsymbol{p} \right| \phi \right\rangle \right\} . \tag{46}$$

Following the notation introduced in [12,13], the contribution E_{4a} is the sum of the fine-structure effects created by the wave-function-correction $F_{\delta\phi}$, the first relativistic correction to the energy $F_{\delta E}$, and the correction due to the relativistic hamiltonian $F_{\delta H}$, each multiplied by a factor α/π. That is to say, the final result for E_4 is

$$E_{4a} = \left(\frac{\alpha}{\pi}\right)^2 (Z\alpha)^4\, \frac{m}{n^3}\, \left(\Delta_{\mathrm{fs}} F_{\delta\phi} + \Delta_{\mathrm{fs}} F_{\delta E} + \Delta_{\mathrm{fs}} F_{\delta H}\right) . \tag{47}$$

There is a further correction to the nonrelativistic effective coupling to the radiation field due to the "anomalous spin-orbit hamiltonian" (44). The correction, in the nonrelativistic limit, can be derived by considering a Foldy–Wouthuysen transformation which by definition diagonalizes the hamiltonian (44) in spinor space and also leads to corrections to the current according to

$$\alpha^i \to U\, \alpha^i U^{-1} , \quad U = \exp\left(-\mathrm{i}\frac{\beta\mathcal{H}}{2m}\right) . \tag{48}$$

Here, β and α^i are standard Dirac matrices [19], i is a spatial index, and $\mathcal{H}$ is given in (44). The calculation is carried out along ideas introduced in [12] and leads to the result

$$\delta \boldsymbol{j}_{4b} = \frac{\alpha}{\pi}\, \frac{Z\alpha}{2mr^3}\, \boldsymbol{\sigma} \times \boldsymbol{r} , \tag{49}$$

as a relativistic correction to the electron current which is simply α^i in the relativistic formalism and p^i/m in the leading nonrelativistic approximation. Again, following the notation introduced in [12,13], the resulting additional contribution is

$$E_{4b} = \left(\frac{\alpha}{\pi}\right)^2 (Z\alpha)^4\, \frac{m}{n^3}\, \Delta_{\mathrm{fs}} F_{\delta y} . \tag{50}$$

The sum of (47) and (50) is just the $(Z\alpha)^6$–component of the fine-structure difference of the one-loop self energy from [12, 13], multiplied by an additional factor α/π. It can also be written as

$$E_4 = E_{4a} + E_{4b} = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^6\, m}{n^3} \left[-\frac{n^2-1}{3n^2} \ln\frac{2\epsilon}{(Z\alpha)^2\, m} + \frac{n^2-1}{n^2} \Delta_{\rm fs}\ell_4(n)\right] , \qquad (51)$$

where $\Delta_{\rm fs}\ell_4(n)$ could be interpreted as a relativistic generalization of a Bethe logarithm, which is n-dependent. However, a significant numerical fraction of the n-dependence can be eliminated if the factor $(n^2-1)/n^2$ is taken out of the final result. The evaluation of $\Delta_{\rm fs}\ell_4(n)$ has recently been performed in [32] with improved numerical methods (see e.g. [33]), and the following results have been obtained:

$$\begin{aligned} \Delta_{\rm fs}\ell_4(2) &= 0.512\ 559\ 768(1)\,, \\ \Delta_{\rm fs}\ell_4(3) &= 0.511\ 978\ 815(1)\,, \\ \Delta_{\rm fs}\ell_4(4) &= 0.516\ 095\ 539(1)\,, \\ \Delta_{\rm fs}\ell_4(5) &= 0.519\ 976\ 941(1)\,, \end{aligned} \qquad (52)$$

where the uncertainty is due to numerical integration.

There is, as stated above, a further correction due to the explicit modification of the transition current due to the anomalous magnetic moment; it can be obtained through the replacement

$$\alpha^i \to \alpha^i + F_2(0)\, \frac{{\rm i}\,\beta\,\sigma^{i\nu}}{2m}\, q_\nu \qquad (53)$$

and must be considered in addition to the correction (48). A careful consideration of the nonrelativistic limit of this correction to the current, including retardation effects, leads to the result

$$\delta \boldsymbol{j}_5 = \frac{\alpha}{2\pi}\, \frac{Z\alpha}{2mr^3}\, \boldsymbol{\sigma}\times\boldsymbol{r}\,. \qquad (54)$$

Consequently, we find that the correction is effectively $F_2(0)$ times the retardation corrections to the transition current $F_{\delta y}$ found in [12, 13]. We obtain

$$E_5 = \left(\frac{\alpha}{\pi}\right)^2 (Z\alpha)^4\, \frac{m}{n^3}\, \frac{\Delta_{\rm fs}F_{\delta y}}{2}\,. \qquad (55)$$

In analogy with E_4, this correction can favorably be rewritten as

$$E_5 = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^6\, m}{n^3} \left[\frac{n^2-1}{n^2} \Delta_{\rm fs}\ell_5(n)\right] , \qquad (56)$$

On the basis of [12, 13, 32], we obtain

$$\begin{aligned} \Delta_{\rm fs}\ell_5(2) &= \ -0.173\ 344\ 868(1)\,, \\ \Delta_{\rm fs}\ell_5(3) &= \ -0.164\ 776\ 514(1)\,, \\ \Delta_{\rm fs}\ell_5(4) &= \ -0.162\ 263\ 216(1)\,, \\ \Delta_{\rm fs}\ell_5(5) &= \ -0.161\ 165\ 602(1)\,. \end{aligned} \qquad (57)$$

The final result for the low-energy part is

$$E_{\rm L} = E_4 + E_5\,, \qquad (58)$$

with E_4 and E_5 being given in eqs. (51) and (56), respectively.

We can now understand why it was possible to join the two contributions with "mixed" and "low-and-low" energy virtual photons (ii) and (iii), which were discussed in sec. 1, into a joint "low-energy part". The reason is simple: The effective hamiltonian (45) has no infrared divergence, because it involves the low-energy limit of the magnetic form factor F_2, which is infrared safe in one-loop order according to eq. (9). Because the main contribution to the quantity $F_2(0)$ is caused by hard virtual photons, it is also justified to say that the contribution of "low-and-low" energy virtual photons vanishes at the order of interest for the current calculation (fine-structure difference). In higher-loop order, the further infrared divergence acquired by F_2 would lead to an infrared divergence in the effective hamiltonian constructed in analogy with eq. (45); this infrared divergence would have to be attributed to a "mixed" contribution.

5. Results and Conclusions

We have obtained analytic results for higher-order correction to the two-loop self-energy of P states in hydrogen-like systems. In our calculation, we have analyzed the electron form factors through two-loop order in sec. 2, and we have split the calculation into a high-energy part with two hard virtual photons discussed in sec. 3, and a low-energy part with at least one soft virtual photon analyzed in sec. 4. The final result for the contribution to the fine-structure energy difference is obtained by adding the high-energy contributions $E_1 - E_3$ given in eqs. (23), (27), (36), (41), and the low-energy effects E_4 and E_5 from eqs. (51) and (56). The dependence on ϵ cancels out in the final result which is the sum of the high-energy part $E_{\rm H}$ given in eq. (42) and the low-energy part $E_{\rm L}$ defined in eq. (58). This is also evident when considering explicitly the eqs. (36) and (51). The final results for the analytic coefficients of order $\alpha^2(Z\alpha)^6$ read

$$\Delta_{\rm fs} B_{61} = -\frac{n^2-1}{3n^2}\,. \tag{59}$$

[see also eq. (35)] and

$$\begin{aligned}\Delta_{\rm fs} B_{60} = {} & \left(\frac{227}{2880} + \frac{1}{32n} - \frac{3}{80n^2}\right) + F_2^{(4),S}(0)\left(\frac{487}{720} + \frac{5}{8n} - \frac{23}{20n^2}\right) \\ & + \frac{n^2-1}{n^2}\left[-\left(F_1'^{(4),S}(0) + 2\,\mathcal{F}_2'^{(4),S}(0)\right) m^2 - \frac{5}{18} + \Delta_{\rm fs}\ell_4(n) + \Delta_{\rm fs}\ell_5(n)\right]\,,\end{aligned} \tag{60}$$

where explicit numerical results for $F_1'^{(4),S}(0)$, $F_2^{(4),S}(0)$ and $\mathcal{F}_2'^{(4),S}(0)$ can be found in eqs. (17), (18) and (19), respectively. This result refers to the pure self-energy diagrams in fig. 1. The result reads numerically for the principal quantum numbers $n = 2$–5,

$$\Delta_{\rm fs} B_{60}(2) = -\,0.361\,196\,470(1)\,, \tag{61}$$

$$\Delta_{\rm fs} B_{60}(3) = -\,0.411\,156\,068(1)\,, \tag{62}$$

$$\Delta_{\rm fs} B_{60}(4) = -\,0.419\,926\,624(1)\,, \tag{63}$$

$$\Delta_{\rm fs} B_{60}(5) = -\,0.419\,832\,876(1)\,. \tag{64}$$

If it is desired to add in the combined self-energy vacuum-polarization diagram from fig. 2, then the form-factor results from eqs. (6), (8) and (11) instead of the pure self-energy results given in eqs. (17), (18) and (19) have to be used in evaluating (60). When including the combined self-energy vacuum-polarization diagram from fig. 2, there is no further low-energy contribution, so that the alternative set of numerical values for the form factors from eqs. (6), (8) and (11) fully takes into account the additional effect of the diagram in fig. 1 on the fine-structure in the order of $\alpha^2\,(Z\alpha)^6$.

It is perhaps worth mentioning that for the one-loop self-energy, analytic coefficients are known only up to the order of $\alpha\,(Z\alpha)^6$ [12], but the remaining uncertainty is removed by recent non-perturbative numerical calculations [9,32,34]. For the two-loop effect, the $(Z\alpha)$-expansion converges more rapidly than for the one-loop effect in absolute frequency units because of the additional radiative factor α/π which decreases the overall size of the effect.

It is hoped that the analytic calculations for low nuclear charge number Z will be supplemented in the future by an accurate numerical treatment of the two-loop self-energy problem (see also related recent work in the high-Z region, refs. [35–37]). This presupposes that the considerable numerical problems in the domain of small nuclear charge could be solved by adequate numerical methods, and that the further problem of the increased computational demand of the two-loop effect in comparison to the one-loop problem [9, 34] can be tackled – possibly by massively parallel computer architectures. Note, however, that the most accurate theoretical predictions could only be reached in combining numerical and analytic results. The reason is the following: All numerical calculations are performed in the non-recoil limit which is the limit of infinite nuclear mass. This is not quite sufficient for an accurate theoretical treatment because the self-energy effect for a bound-state depends genuinely on the ratio of the orbiting particle to the nuclear mass – an effect beyond the recoil correction. For example, the argument of the logarithms in (1) should be replaced according to $\ln[(Z\alpha)^{-2}] \to \ln[\sigma\,(Z\alpha)^{-2}]$, where $\sigma = m/m_{\rm r}$ and $m_{\rm r}$ is the reduced mass [3]. The possibility to include these tiny, but important effects depends crucially on a reliable knowledge of the analytic coefficients *in combination* with an accurate numerical treatment of the problem.

The analytic results can be used to obtain improved theoretical predictions for the hydrogenic fine structure as compared to the previous order–α^7–calculations [12, 13], because they remove the principal theoretical uncertainty in the order of α^8 due to the problematic two-loop self-energy which is represented diagrammatically in fig. 1. A compilation of the other corrections relevant at the order of α^8, including but not limited to the vacuum polarization effects, whose evaluation is rather straightforward, will be presented elsewhere. Our calculation illustrates the usefulness of the simplified effective treatments of two-loop effects in the analytic approach based on the modified Dirac hamiltonian (3) and the "ϵ method" (see [8, 12, 13, 20] and app. Appendix A). This aspect highlights, as we believe, the need for systematic, simplified treatments of higher-order radiative corrections in bound systems.

In this paper, we primarily address spin-dependent effects in one-electron (hydrogenlike) systems. However, the same effects also contribute to the fine-structure splitting in two-electron (heliumlike) systems. There is currently remarkable interest in improved measurements of the fine-structure splitting in helium and heliumlike atomic systems with low nuclear charge [39]. The effects addressed in this paper contribute to the fine-structure splitting in helium on the level of 100 Hz, which is not much smaller than the current experimental accuracy of about 1 kHz, and allows for an estimate of uncalculated yet higher-order contributions.

The results of this paper are a step in a systematic study of the higher-order binding corrections to the two-loop Lamb shift of S and P states. The scheme of calculation permits not the only a simplified treatment of the problem via a separation into appropriate energy regions for the two virtual photons, but also a clear identification of the spin-independent and the spin-dependent contributions to the self-energy. The results will therefore be directly applicable to the total coefficients for P states once the spin-independent parts (the two-loop Bethe logarithms) are calculated. These are currently under study.

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Appendix A. The "ϵ Method"

We discuss here, by way of example, the ϵ method employed in the analytic calculation of self-energy effects in bound systems. This method is very suitable [12, 13] for the separation of the two different energy scales for virtual photons: the nonrelativistic domain, in which the virtual photon assumes values of the order of the atomic binding energy, and the relativistic domain, in which the virtual photon assumes values of the order of the electron rest mass. Different approximation schemes and different asymptotic expansions are adequate for the two different domains. Without these approximations and expansions, the analytic evaluation of either the high- or the low-energy part would not be feasible. At the same time, the model example discussed in this appendix is meant to illustrate the usefulness of the "ϵ method" in a more general context.

We will consider here a model problem with only one "virtual photon". The separation into high-and low-energy photons necessitates the temporary introduction of a parameter ϵ; the dependence on ϵ cancels when the high- and the low-energy parts are added together. We have,

$$\text{nonrelativistic domain} \ll \epsilon \ll \text{electron rest mass} \tag{A.1}$$

$$(Z\alpha)^2\, m_{\rm e} \qquad\qquad \ll \epsilon \ll m_{\rm e}\,, \tag{A.2}$$

where α is the fine structure constant, and Z is the nuclear charge. The high-energy part is associated with photon energies $\omega > \epsilon$, and the low-energy part is associated with photon energies $\omega < \epsilon$.

In order to illustrate the procedure, we discuss a simple, one-dimensional example: the evaluation of

$$I(\beta) = \int_0^1 \sqrt{\frac{\omega^2+\beta^2}{1-\omega^2}}\, {\rm d}\omega\,. \tag{A.3}$$

where the integration variable ω might be interpreted as the "energy" of a "virtual photon". The integral I can be expressed in terms of special functions,

$$I(\beta) = \beta\, E\left(-\frac{1}{\beta^2}\right) = \beta\, \frac{\pi}{2}\, {}_2F_1\left(-\frac{1}{2}, \frac{1}{2}; 1; -\frac{1}{\beta^2}\right)\,, \tag{A.4}$$

where E is the complete elliptic integral of the second kind, and ${}_2F_1$ denotes a hypergeometric function. An alternative integral representation reads $I(\beta) = \int_0^{\pi/2} \sqrt{\beta^2 + \sin^2(\omega)}\, {\rm d}\omega$.

The purpose of the calculation is to derive a semi-analytic expansion of $I(\beta)$ in powers of β and $\ln\beta$. The fine structure constant α takes the rôle of the expansion parameter β in actual self-energy calculations. We discuss first the "high-energy part" of the calculation. It is given by the expression

$$I_{\rm H}(\beta) = \int_\epsilon^1 \sqrt{\frac{\omega^2+\beta^2}{1-\omega^2}}\, {\rm d}\omega\,. \tag{A.5}$$

For $\omega > \epsilon$, we may expand

$$\sqrt{\omega^2+\beta^2} = \omega + \frac{\beta^2}{2\,\omega} + \frac{\beta^4}{8\,\omega^3} + \mathcal{O}(\beta^6)\,, \tag{A.6}$$

but this expansion is not applicable in higher orders to the domain $0 < \omega < \epsilon$ because of the appearance of inverse powers of ω (analogous to an "infrared divergence" in QED).

The separation parameter ϵ acts an infrared regulator. After expanding in β [see Eq. (A.6)], the resulting integrals in each order of β can be evaluated analytically. Subsequently, we expand every term in the β-expansion in powers of ϵ up to the order ϵ^0, i.e. we keep only the divergent and constant terms in ϵ. The result is

$$\begin{aligned} I_{\rm H}(\beta,\epsilon) = 1 &+ \beta^2 \left\{\frac{1}{2}\,\ln\left(\frac{2}{\epsilon}\right) + \mathcal{O}(\epsilon)\right\} \\ &+ \beta^4 \left\{-\frac{1}{16\,\epsilon^2} - \frac{1}{16}\,\ln\left(\frac{2}{\epsilon}\right) + \frac{1}{32} + \mathcal{O}(\epsilon)\right\} \\ &+ \beta^6 \left\{\frac{1}{64\,\epsilon^4} + \frac{1}{64\,\epsilon^2} + \frac{3}{128}\,\ln\left(\frac{2}{\epsilon}\right) - \frac{7}{512} + \mathcal{O}(\epsilon)\right\} \\ &+ \mathcal{O}(\beta^8)\,. \end{aligned} \tag{A.7}$$

Here, the "$\mathcal{O}$"-symbol identifies a contribution for which $\mathcal{O}(x)/x \to$ const. as $x \to 0$, whereas the "o"-symbol identifies the weaker requirement ${\rm o}(x) \to 0$ as $x \to 0$; this is consistent with the standard notation (see e.g. [38]).

The contribution $I_{\rm H}(\beta)$ corresponds to the "high-energy part" in analytic self-energy calculations, where the propagator of the bound electron is explicitly expanded in powers of the fine structure constant α. Now we turn to the "low-energy part". The expression for the low-energy part $(0 < \omega < \epsilon)$ reads

$$I_{\rm L}(\beta) = \int_0^\epsilon \sqrt{\frac{\omega^2+\beta^2}{1-\omega^2}}\, {\rm d}\omega\,. \tag{A.8}$$

The expansion (A.6) is not applicable in this energy domain; we therefore have to keep the numerator of the integrand $\sqrt{\omega^2+\beta^2}$ in unexpanded form. However, we can expand the denominator $\sqrt{1-\omega^2}$ of the integrand in powers of ω; because $0 < \omega < \epsilon$ (with ϵ small), this expansion in ω is in fact an expansion in β – although the situation is somewhat problematic in the sense that every term in the ω-expansion gives rise to terms of arbitrarily high order in the β-expansion [see also Eq. (A.10) below].

The term $\sqrt{\omega^2+\beta^2}$ is analogous to the Schrödinger–Coulomb propagator in the self-energy calculation which has to be kept in unexpanded form, whereas the expansion

$$\frac{1}{\sqrt{1-\omega^2}} = 1 + \frac{\omega^2}{2} + \frac{3}{8}\,\omega^4 + \mathcal{O}(\omega^6) \tag{A.9}$$

corresponds to the expansion into the $(Z\alpha)$-expansion in the low-energy part.

Every term in the expansion (A.9) gives rise to arbitrarily high-order corrections in β, but it starts with the power $\omega^n \to \beta^{n+2}$. For example, we have for the leading term of order $\omega^0 = 1$ from Eq. (A.9),

$$\begin{aligned} \int_0^\epsilon \sqrt{\omega^2+\beta^2}\,\mathrm{d}\omega &= \beta^2 \left\{ \ln\left(\frac{2}{\beta}\,\epsilon\right) + \frac{1}{4} + \mathcal{O}(\epsilon) \right\} \\ &+ \beta^4 \left\{ \frac{1}{16\,\epsilon^2} + \mathcal{O}(\epsilon) \right\} + \beta^6 \left\{ -\frac{1}{64\,\epsilon^4} + \mathcal{O}(\epsilon) \right\} + \mathcal{O}(\beta^8)\,. \end{aligned} \tag{A.10}$$

Note that the terms generated in the orders β^4 and β^6 are needed to cancel divergent contributions in respective orders of β from the high-energy part given in Eq. (A.6). The term of order ω^2 from (A.9) results in

$$\begin{aligned} \frac{1}{2}\int_0^\epsilon \omega^2\,\sqrt{\omega^2+\beta^2}\,\mathrm{d}\omega &= \beta^4 \left\{ -\frac{1}{16}\,\ln\left(\frac{2}{\beta}\,\epsilon\right) + \frac{1}{64} + \mathcal{O}(\epsilon) \right\} \\ &+ \beta^6 \left\{ -\frac{1}{64\,\epsilon^2} + \mathcal{O}(\epsilon) \right\} + \mathcal{O}(\beta^8)\,. \end{aligned} \tag{A.11}$$

Altogether, we obtain for the low-energy part,

$$\begin{aligned} I_{\mathrm{L}}(\beta,\epsilon) &= \beta^2 \left\{ \frac{1}{2}\,\ln\left(\frac{2}{\beta}\,\epsilon\right) + \frac{1}{4} + \mathcal{O}(\epsilon) \right\} \\ &+ \beta^4 \left\{ \frac{1}{16\,\epsilon^2} - \frac{1}{16}\,\ln\left(\frac{2}{\beta}\,\epsilon\right) + \frac{1}{64} + \mathcal{O}(\epsilon) \right\} \\ &+ \beta^6 \left\{ -\frac{1}{64\,\epsilon^4} - \frac{1}{64\,\epsilon^2} + \frac{3}{128}\,\ln\left(\frac{2}{\beta}\,\epsilon\right) - \frac{5}{512} + \mathcal{O}(\epsilon) \right\} \\ &+ \mathcal{O}(\beta^8\,\ln\beta)\,. \end{aligned} \tag{A.12}$$

When the high-energy part (A.7) and the low-energy part (A.12) are added, the dependence on ϵ cancels, and we have

$$\begin{aligned} I(\beta) &= I_{\mathrm{H}}(\beta,\epsilon) + I_{\mathrm{L}}(\beta,\epsilon) \\ &= 1 + \beta^2 \left\{ \frac{1}{2}\,\ln\left(\frac{4}{\beta}\right) + \frac{1}{4} \right\} \\ &\quad + \beta^4 \left\{ -\frac{1}{16}\,\ln\left(\frac{4}{\beta}\right) + \frac{3}{64} \right\} \\ &\quad + \beta^6 \left\{ \frac{3}{128}\,\ln\left(\frac{4}{\beta}\right) - \frac{3}{128} \right\} + \mathcal{O}(\beta^8\,\ln\beta)\,. \end{aligned} \tag{A.13}$$

In order to illustrate the analogy with the self-energy calculation presented here, we would like to point out that the dependence on ϵ cancels out in the final result which is the sum of the high-energy part E_{H} given in eq. (42) and the low-energy part E_{L} in eq. (58).

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