Double–Logarithmic Two–Loop Self–Energy Corrections to the Lamb Shift

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Abstract Self-energy corrections involving logarithms of the parameter $Z\alpha$ can often be derived within a simplified approach, avoiding calculational difficulties typical of the problematic non-logarithmic corrections (as customary in bound-state quantum electrodynamics, we denote by Z the nuclear charge number, and by α the fine-structure constant). For some logarithmic corrections, it is sufficient to consider internal properties of the electron characterized by form factors. We provide a detailed derivation of related self-energy "potentials" that give rise to the logarithmic corrections; these potentials are local in coordinate space. We focus on the double-logarithmic two-loop coefficient B_{62} for P states and states with higher angular momenta in hydrogenlike systems. We complement the discussion by a systematic derivation of B_{62} based on nonrelativistic quantum electrodynamics (NRQED). In particular, we find that an additional double logarithm generated by the loop-after-loop diagram cancels when the entire gauge-invariant set of two-loop self-energy diagrams is considered. This double logarithm is not contained in the effective-potential approach.

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1 Introduction

Lamb-shift measurements and related theoretical calculations for bound atomic systems with increasing accuracy have historically provided accurate tests of quantum electrodynamics (QED), and the measurements have recently been improved in accuracy beyond previous limits [1–3]. In order to account for a theoretical description, corrections of various physical origin (one-loop self-energy and vacuum polarization, two-loop, and higher order radiative, recoil, radiative-recoil, nuclear-size corrections) have to be evaluated [4].

Here, we focus on logarithmic self-energy corrections which are evaluated within the $Z\alpha$-expansion [5]. Within the analytic treatment, self-energy radiative corrections can be taken into account by means of a nonanalytic expansions in powers of the fine-structure constant α, the product of $Z\alpha$ and the logarithm $\ln[(Z\alpha)^{-2}]$ (Z is the nuclear charge number). The expansion in powers of α corresponds to the loop-expansion in the framework of the usual perturbative treatment for QED. The higher order terms in powers of $Z\alpha$ and $\ln[(Z\alpha)^{-2}]$ are related to atomic-physics effects; they are referred to as the "binding corrections".

The purpose of this investigation is twofold: first, to illustrate how Lamb-shift "potentials" that give rise to the logarithmic corrections can be derived within the context of bound-state QED, and second, to provide a rigorous and detailed derivation of the B_{62} double-logarithmic two-loop self-energy coefficient for P states and states with higher angular momenta. The P-state coefficient B_{62} has already appeared in the literature [6]; however the derivation has been rather sketchy.

2 Modified Dirac Hamiltonian, One–Loop Corrections and A_{41}

It has been observed by many authors (e.g. [7–9]) that a rather important class of self-energy radiative effects for bound states can be described by a modified Dirac Hamiltonian ($\hbar = c = \epsilon_0 = 1$),

$$\begin{aligned} H_D^{(\mathrm{m})} &= \boldsymbol{\alpha}\,[\,\boldsymbol{p} - e\,F_1(\Delta)\,\boldsymbol{A}] + \beta\,m + e\,F_1(\Delta)\,\phi \\ &\quad + F_2(\Delta)\,\frac{e}{2m}\,(\mathrm{i}\,\boldsymbol{\gamma}\cdot\boldsymbol{E} - \beta\,\boldsymbol{\sigma}\cdot\boldsymbol{B})\,, \end{aligned} \tag{1}$$

which approximately describes an electron subject to an external scalar potential $\phi \equiv \phi(r)$ and an external vector potential $\boldsymbol{A} \equiv \boldsymbol{A}(\boldsymbol{r})$ (the vector potential vanishes for a point nucleus that gives rise to a static Coulomb potential; we may neglect the nuclear magnetic field and the hyperfine structure). We have

$$e\,\phi(r) = e\,A_0(r) = -\frac{Z\alpha}{r} \tag{2}$$

in coordinate space, which corresponds to $\phi(\boldsymbol{q}^2) = -4\pi Z\alpha/\boldsymbol{q}^2$ in momentum space. In this article, following the commonly accepted convention, the function $\phi(r)$ and its Fourier transform $\phi(\boldsymbol{q}^2)$ are denoted by the same symbol ϕ. We avoid possible ambiguities by denoting with $\boldsymbol{r}$ and r the arguments in coordinate space and with $\boldsymbol{q}$ or $\boldsymbol{p}$ those in momentum space. The argument $\Delta \equiv (\partial/\partial\boldsymbol{r})^2$ of the electron form factor F_1 in Eq. (1) 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 $\psi(\boldsymbol{r})$.

Equation (1) entails a replacement of the binding Coulomb potential as

$$e\,\phi(\boldsymbol{r}) \to e\,F_1(\Delta)\,\phi(\boldsymbol{r})$$

and leads to a correction to the Coulomb potential $\Delta V_{\rm C}(r)$ according to

$$\Delta V_{\rm C}(r) = [F_1(\Delta) - 1] \left(-\frac{Z\alpha}{r}\right) \tag{3}$$

in coordinate space, and

$$\Delta V_{\rm C}(\boldsymbol{q}^2) = [F_1(-\boldsymbol{q}^2)) - 1] \left(-\frac{4\pi\, Z\alpha}{\boldsymbol{q}^2}\right) \tag{4}$$

in momentum space. In first-order perturbation theory, this gives rise to the following perturbative correction which we write down in coordinate and momentum space,

$$\begin{aligned}
\Delta E_1 &= \langle\psi\,|\Delta V_{\rm C}(r)|\,\psi\rangle = \langle\psi\,|\,[F_1(\Delta) - 1]\,e\,\phi\,|\,\psi\rangle \\
&= \int {\rm d}^3 r\,\psi^+(\boldsymbol{r}) \left[[F_1(\Delta) - 1] \left(\frac{-Z\alpha}{r}\right)\right] \psi(\boldsymbol{r}) \\
&= \int \frac{{\rm d}^3 p}{(2\pi)^3} \int \frac{{\rm d}^3 p'}{(2\pi)^3}\,\psi^+(\boldsymbol{p}') \left[[F_1(-\boldsymbol{q}^2) - 1] \left(\frac{-4\pi Z\alpha}{\boldsymbol{q}^2}\right)\right] \psi(\boldsymbol{p})\,,
\end{aligned} \tag{5}$$

with $\boldsymbol{q} = \boldsymbol{p}' - \boldsymbol{p}$. An expansion of the electron form factor F_1 in terms of its argument gives rise to higher-order terms in the $Z\alpha$-expansion, because the atomic momentum is of the order of $Z\alpha$ in natural units. Therefore, within the $Z\alpha$-expansion, it is admissible to expand both the bound-state Dirac wavefunctions ψ in powers of $Z\alpha$ (the leading-order term is then the Schrödinger wavefunction), as well as the electron form factor in Eq. (5) in powers of its argument.

The one-loop (1L) self-energy correction for S states within the $Z\alpha$-expansion reads

$$\Delta E_{\rm SE}^{\rm (1L)} = \left(\frac{\alpha}{\pi}\right) (Z\alpha)^4 \frac{m}{n^3} \left(A_{41}\,\ln[(Z\alpha)^{-2}] + A_{40} + \mathcal{R}\right)\,, \tag{6}$$

where the remainder $\mathcal{R}$ is of the order of $\mathcal{O}(Z\alpha)$, m is the electron mass and n is the principal quantum number.

As indicated in Eq. (5), the form factor $F_1(\Delta)$ in momentum space assumes arguments according to the replacement $\Delta \to -\boldsymbol{q}^2 \equiv -(\boldsymbol{p}'-\boldsymbol{p})^2$ in momentum space. With the convention $q^2 = q^\mu q_\mu = (q^0)^2 - \boldsymbol{q}^2$, the evaluation of the radiative corrections to the binding Coulomb field is mediated by space-like virtual photons ($q^0 = 0$), and the momentum transfer can be written as: $q^2 = -\boldsymbol{q}^2 \equiv t$ (this is consistent with the conventions employed in [10, 11]).

The form factor $F_1(t)$ can be expanded in powers of α, which corresponds to the loop expansion. According to Eqs. (1.2) and (1.20) of [10], we have up to two-loop order:

$$F_1(t) = 1 + \left(\frac{\alpha}{\pi}\right) F_1^{(2)}(t) + \left(\frac{\alpha}{\pi}\right)^2 F_1^{(4)}(t) + \mathcal{O}(\alpha^3) \tag{7}$$

with

$$F_1^{(2)}(t) = B(t)\,\ln\frac{\lambda}{m} + \mathcal{F}_1^{(2)}(t)\,, \tag{8}$$

$$F_1^{(4)}(t) = \frac{1}{2}\,B^2(t)\ln^2\frac{\lambda}{m} + \ln\frac{\lambda}{m}\,B(t)\,\mathcal{F}_1^{(2)}(t) + \mathcal{F}_1^{(4)}(t)\,, \tag{9}$$

where the $\mathcal{F}$ are infrared finite (i.e. finite in the limit $\lambda \to 0$), and the definition of the function $B(t)$ [see Eq. (1.18a) of [10]] reads as follows,

$$B(t) = -\left[1 + \frac{t - 2\,m^2}{t(1-4m^2/t)^{1/2}}\ln\frac{(1-4m^2/t)^{1/2} - 1}{(1-4m^2/t)^{1/2} + 1}\right] = -\frac{t}{3m^2} + \mathcal{O}(t^2)\,. \tag{10}$$

In Eq. (8), λ denotes the fictitious photon mass. How should the problem of the infrared divergence of the form factors be interpreted in the context of bound-state QED? The free electron can emit an infinite number of infrared photons, because it may undergo transitions between free states with infinitesimal energy differences. However, this is not the case for a bound electron which has a discrete bound-state spectrum; energy levels are separated from each other by intervals of the order of $(Z\alpha)^2\,m$ (the energy level differences are determined by Schrödinger theory). This leads to an infrared cutoff in bound-state QED of the order of $\lambda \approx (Z\alpha)^2\,m$. Therefore, we may replace $\lambda \to (Z\alpha)^2\,m$ for the determination of leading logarithms of the Lamb shift. At some risk to over-simplification, one may therefore argue that the infrared catastrophe is avoided in a natural way for bound states. For the description of bound states, we have $\ln(\lambda/m) \approx -\ln[(Z\alpha)^{-2}]$ within logarithmic accuracy, i.e. neglecting non-logarithmic contributions which are given e.g. by A_{40} coefficients [see Eq. (6)].

The focus of the current article is on double-logarithmic corrections which are present from the first term on the right-hand side of Eq. (9). Note that single-logarithmic two-loop corrections are not being considered in this article. Corrections of this latter type are generated, for example, by the *second* term on the right-hand side of Eq. (9).

At this point, it may be helpful to point out that the cutoff of the infrared divergence of QED at the "bound-state photon mass" $\lambda \to (Z\alpha)^2\,m$ is consistent with the matching procedure that involves an explicit infrared cutoff ϵ which can be interpreted as an infrared cutoff for the bremsstrahlung spectrum [7,9,12]. The procedure is described in some detail in Eqs. (32) – (34) of [9]. This matching procedure offers an alternative interpretation for the infrared catastrophe: the infrared divergence crucially relies on transitions between asymptotically free electron states. Any infinitesimally small additional interaction of the electrons within that interferes with the emission of bremsstrahlung will avoid the infrared catastrophe and provide an infrared cutoff whose order-of-magnitude is determined by the energy scale of the additional external field.

In combining the result (8) with the expansion of $B(t)$ in powers of t, we reproduce the well-known expression

$$F_1^{(2)}(t) = -\frac{t}{3m^2}\,\left[\ln\frac{\lambda}{m} + \frac{1}{8}\right] + \mathcal{O}(t^2)\,. \tag{11}$$

Together with the definition of the modified Coulomb potential in Eq. (4) and the bound-state "infrared-cutoff prescription" $\lambda \to (Z\alpha)^2\,m$, this leads to the following one-loop (1L) self-energy potential

$$\Delta V_{\rm C}^{(\rm 1L)}(\boldsymbol{q}^2) = \frac{\alpha}{\pi}\,\left[-\frac{-\boldsymbol{q}^2}{3m^2}\,(-\ln[(Z\alpha)^{-2}])\right]\,\left(-\frac{4\pi Z\alpha}{\boldsymbol{q}^2}\right) = \frac{4\alpha}{3m^2}\,(Z\alpha)\,\ln[(Z\alpha)^{-2}]\,, \tag{12}$$

in momentum space; this translates into a potential

$$\Delta V_{\rm C}^{(\rm 1L)}(r) = \frac{4\alpha}{3\pi}\,(Z\alpha)\,\ln[(Z\alpha)^{-2}]\,\frac{\delta^{(3)}(\boldsymbol{r})}{m^2} \tag{13}$$

in coordinate space. This potential can also be found as Eq. (2) of [13], given there without derivation. The first-order one-loop perturbation, evaluated according to Eq. (5), reads

$$\Delta E_1^{(\rm 1L)} = \langle\psi\,|\Delta V_{\rm C}^{(\rm 1L)}(r)|\,\psi\rangle = \frac{4\alpha}{3\pi}\,(Z\alpha)^4\,\frac{m}{n^3}\,\ln[(Z\alpha)^{-2}]\,\delta_{l0}\,. \tag{14}$$

This correction is nonvanishing only for S states ($l = 0$), and it reproduces the leading logarithmic A_{41} coefficient as given in Eq. (6). It may be interesting to point out that since $|\psi(r=0)|^2 = (Z\alpha)^3\,(m_{\rm r}^3/\pi)\,\delta_{l0}$, where $m_{\rm r}$ is the reduced mass of the system, the correction (14) also has the

correct reduced-mass dependence (this is of relevance for systems like positronium and pionium). In the limit of a large nuclear mass, we have of course $m = m_{\rm r}$.

Note that the potential (13) is local in coordinate space. In contrast, the nonrelativistic (NR) one-loop self-energy operator (as well as its relativistic counterpart which assumes a slightly more complicated form) may be expressed in the length-gauge form as [cf. Eq. (29) of [14])],

$$\Sigma^{(1{\rm L})}_{\rm NR}(\boldsymbol{r},\boldsymbol{r}') = -\frac{2\alpha}{3\pi} \int_0^\epsilon {\rm d}\omega\, \omega^3\, \boldsymbol{r}' \left\langle \boldsymbol{r}' \left| \frac{1}{H-E+\omega} \right| \boldsymbol{r} \right\rangle \boldsymbol{r}\,, \tag{15}$$

where ϵ is the upper cutoff for the photon energy originally introduced in [12]. The self-energy operator (15) involves *two* spatial coordinates. The locality of the potential (13) expresses the fact that the high-energy virtual photons which mediate the form-factor corrections in Eq. (1) act on a relativistic length scale given by the Compton wavelength of the electron which is smaller by one order of $Z\alpha$ than the atomic length scale given by the Bohr radius.

3 Effective Local Potential for Two–Loop Corrections and B_{62}

In combining the result (9) with the expansion of $B(t)$ in powers of t [see Eq. (10)] and the modified Coulomb potential in Eq. (4), and using the bound-state "infrared-cutoff prescription" $\lambda \to (Z\alpha)^2\, m$, we obtain the following two-loop (2L) self-energy potential

$$\begin{aligned} \Delta V^{(2{\rm L})}_{\rm C}(\boldsymbol{q}^2) &= \left(\frac{\alpha}{\pi}\right)^2 \frac{1}{2} \left(\frac{\boldsymbol{q}^2}{3\,m^2}\right)^2 \ln^2[(Z\alpha)^{-2}] \left(-\frac{4\pi\,Z\alpha}{\boldsymbol{q}^2}\right) \\ &= \left(\frac{\alpha}{\pi}\right)^2 \frac{1}{18} \ln^2[(Z\alpha)^{-2}] \frac{4\pi\,Z\alpha}{m^4} \left(-\boldsymbol{q}^2\right)\,. \end{aligned} \tag{16}$$

This correction has previously appeared as Eq. (3) of [6], without a detailed derivation. After Fourier transformation, we have

$$\Delta V^{(2{\rm L})}_{\rm C}(r) = \frac{2}{9} \left(\frac{\alpha}{\pi}\right)^2 \ln^2[(Z\alpha)^{-2}] \frac{\pi\,\Delta\delta^{(3)}(\boldsymbol{r})}{m^4}\,, \tag{17}$$

which is a highly singular potential in coordinate space. Its expectation value on S states diverges, giving rise to a further logarithm, and we will not discuss here the associated problems, which have recently attracted remarkable attention [15–22].

The first-order perturbation, evaluated according to Eq. (5), reads

$$\Delta E^{(2{\rm L})}_1 = \left(\frac{\alpha}{\pi}\right)^2 \frac{2}{9} \frac{\pi Z\alpha}{m^4} \ln^2\left[(Z\alpha)^{-2}\right]\, \Delta\left[|\phi_{n,l=1,m}(\boldsymbol{r})|^2\right]\Big|_{r=0}\,. \tag{18}$$

In Eq. (18), the Laplacian operator acts on a Schrödinger P wavefunction. The following analytic result

$$\Delta\left[|\phi_{n,l=1,m}(\boldsymbol{r})|^2\right]\Big|_{r=0} = \frac{2}{3\pi}\left[(Z\alpha)^5 m^5\right] \frac{n^2-1}{n^5}\,, \tag{19}$$

where n is the principal quantum number, has previously appeared in the literature (e.g. [6,8]). Within the current investigation, we would like to present a complete derivation of the analytic expression for this matrix element in the Appendix A. Finally, we rewrite the energy correction in the form

$$\Delta E^{(2{\rm L})}_1 = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^6 m}{n^3} \ln^2\left[(Z\alpha)^{-2}\right]\, \frac{4}{27}\, \frac{n^2-1}{n^2}\,. \tag{20}$$

This double-logarithmic correction originates solely from the two-loop F_1 form factor of the electron. This corresponds to the diagrams in Fig. 1 (a) and (b). To complete the gauge-invariant set, the loop-after-loop diagram in Fig. 1 (c) should also be taken into consideration.

The diagram in Fig. 1 (c) gives rise to a "second-order perturbation" involving to one-loop self energies as first-order perturbations (the "irreducible part" of the diagram), supplemented by a further term involving the derivative of the bound electron's Green function (the "reducible part"). The correction is known to read (see e.g. [23])

$$\left\langle \overline{\psi} \left| \Sigma_{\rm R}^{(1{\rm L})}(E) \left(\sum_{\psi' \neq \psi} \frac{|\psi'\rangle \langle \overline{\psi}'|}{E - E_{\psi'}} \right) \Sigma_{\rm R}^{(1{\rm L})}(E) \right| \psi \right\rangle + \left\langle \overline{\psi} \left| \Sigma_{\rm R}^{(1{\rm L})}(E) \right| \psi \right\rangle \left\langle \overline{\psi} \left| \frac{\rm d}{{\rm d}E} \Sigma^{(1{\rm L})}(E) \right| \psi \right\rangle , \quad (21)$$

where $\Sigma_{\rm R}^{(1{\rm L})}(E)$ is the renormalized relativistic one-loop self-energy operator, and E is the energy of the electron in the state $|\psi\rangle$. *Within the effective-potential approach*, the one-loop potential (13) describes the two one-loop self-energy insertions in the first term of (21). The potential (13) involves a Dirac delta-function in coordinate space that vanishes on P states, and consequently it can be argued that no further double-logarithmic corrections originate from this term (*but* see the discussion in Secs. 4 and 5).

The second term in (21), which involves the derivative of the self-energy operator with respect to its argument [see also Eq. (2.6) of [12] or Eq. (2) of [6]] and constitutes the reducible part of the diagram in Fig. 1 (c), does not give rise to any further double logarithm, either. The first factor $\left\langle \overline{\psi} \left| \Sigma_{\rm R}^{(1{\rm L})}(E) \right| \psi \right\rangle$ does not create any logarithm for P states in the order of $\alpha\,(Z\alpha)^4$. The second factor, which contains the derivative of the self-energy operator, is not separately gauge invariant, and consequently, there exists no "effective potential" which could be inserted for this term. This is in itself a rather unsatisfactory situation for the effective-potential approach. However, it is possible to analyze the logarithm which is generated by the nonrelativistic photon integration region in this term. Consider the nonrelativistic "velocity-gauge" form of (15) and differentiate with respect to the energy,

$$\left\langle \overline{\psi} \left| \frac{\rm d}{{\rm d}E} \Sigma^{(1{\rm L})}(E) \right| \psi \right\rangle_{\rm NR} = -\frac{2\alpha}{3\pi} \int_0^\epsilon {\rm d}\omega\, \omega \left\langle \phi \left| \frac{\boldsymbol{p}}{m} \left(\frac{1}{H - E + \omega} \right)^2 \frac{\boldsymbol{p}}{m} \right| \phi \right\rangle , \quad (22)$$

where ϕ is the nonrelativistic (Schrödinger) wavefunction, There is only a *single* logarithm $\ln[\epsilon/(Z\alpha)^2 m]$ generated in the integration region $\omega \in [(Z\alpha)^2\, m, \epsilon]$ which may be extracted by replacing $1/(H - E + \omega) \to 1/\omega$. The logarithmic term is proportional to the matrix element $\langle\phi|(\boldsymbol{p}^2/m^2)|\phi\rangle$, which is finite on P states. Consequently, no further double logarithms arise from the second term of (21).

The two-loop effect for P states is usually characterized by the following semi-analytic expansion in powers of $Z\alpha$ [cf. Eq. (6)],

$$\Delta E_{\rm SE}^{(2{\rm L})} = \left(\frac{\alpha}{\pi}\right)^2 (Z\alpha)^4 \frac{m}{n^3} \left(B_{40} + (Z\alpha)^2 \left[B_{62} \ln^2 (Z\alpha)^{-2} + B_{61} \ln (Z\alpha)^{-2} + B_{60} \right] + \mathcal{R} \right) , \quad (23)$$

where the remainder $\mathcal{R}$ is order $\mathcal{O}(Z\alpha)^3$. Using Eq. (20), one can immediately read off the two-loop double logarithmic spin-independent coefficient

$$B_{62}(n, l = 1) = \frac{4}{27} \frac{n^2 - 1}{n^2} . \quad (24)$$

We confirm the result obtained for this correction in Ref. [6].

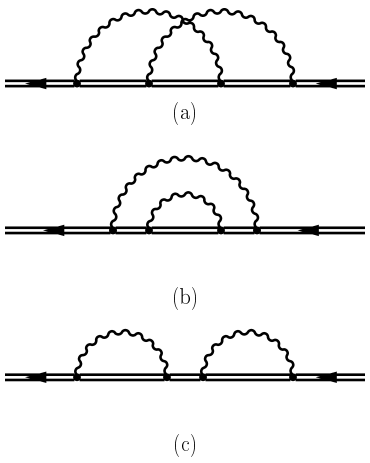

Figure 1: The crossed (a), rainbow (b) and the loop-after-loop diagram (c) which contribute to the two-loop self-energy for a bound electron. The propagator of the bound electron is denoted by a double line.

4 Double Logarithms and the Loop–After–Loop Diagram

In the previous section, we have seen that *within the effective-potential approach*, no double logarithm originates in the order $(Z\alpha)^6$ from the loop-after-loop diagram in Fig. 1 (c). This is because, within this approach, we insert the delta-like local potential (13) for the two one-loop self-energies in the first term of (21).

However, if we consider the diagram in Fig. 1 (c) within the Coulomb gauge and formulate the contribution due to low-energy virtual photons, then we obtain for the irreducible part the expression

$$\Delta E_{\rm LAL} = -\left\langle \phi_{n,1,m} \left| \Sigma^{(1{\rm L})}_{\rm NR} \, \left(\frac{1}{H-E}\right)' \, \Sigma^{(1{\rm L})}_{\rm NR} \right| \phi_{n,1,m} \right\rangle , \tag{25}$$

where the nonrelativistic self-energy operator is given by Eq. (15), and $\phi_{n,1,m}$ is the Schrödinger P wavefunction [see also Eq. (40)], the prime denotes the reduced Green function, and E is the energy of the nP state ("LAL" = loop-after-loop). The double-logarithmic term $\Delta E^{\rm 2log}_{\rm LAL}$ originating from (25) reads

$$\begin{aligned} \Delta E^{\rm 2log}_{\rm LAL} &= -\frac{4}{9} \left(\frac{\alpha}{\pi}\right)^2 \ln^2\left[\frac{\epsilon}{(Z\alpha)^2 m}\right] \\ &\quad \times \left\langle \phi_{n,1,m} \left| \frac{\boldsymbol{p}}{m} \, (H-E) \, \frac{\boldsymbol{p}}{m} \, \left(\frac{1}{H-E}\right)' \, \frac{\boldsymbol{p}}{m} \, (H-E) \, \frac{\boldsymbol{p}}{m} \right| \phi_{n,1,m} \right\rangle . \end{aligned} \tag{26}$$

In order to obtain this result, the denominator of the Green function $H-E+\omega$ has been expanded in powers of $H-E$ within the integration region $\omega \in [(Z\alpha)^2\, m, \epsilon]$. Using the commutator relation

$$ABA = \frac{1}{2}\left([A,[B,A]] + A^2 B + B A^2\right), \tag{27}$$

with $A = \boldsymbol{p}/m$ and $B = H - E$, the matrix element can be rewritten in a much simpler fashion, and the double-logarithmic term becomes

$$\Delta E_{\rm LAL}^{\rm 2log} = -\frac{1}{9}\,\left(\frac{\alpha}{\pi}\right)^2\,\ln^2\left[\frac{\epsilon}{(Z\alpha)^2 m}\right]\,\frac{1}{m^4}\,\left\langle\phi_{n,1,m}\left|\,\boldsymbol{p}^2\,(H-E)\,\boldsymbol{p}^2\right|\,\phi_{n,1,m}\right\rangle\,. \tag{28}$$

We have

$$\left\langle\phi_{n,1,m}\left|\,\boldsymbol{p}^2\,(H-E)\,\boldsymbol{p}^2\right|\,\phi_{n,1,m}\right\rangle = \frac{(Z\alpha)^6 m^5}{n^3}\,\left(\frac{4}{5} - \frac{8}{15n^2}\right)\,, \tag{29}$$

Note that for S states, the above matrix element is divergent, and a regularization of the matrix element gives rise to an additional (triple) logarithm B_{63}. With the natural ultraviolet cutoff $\epsilon \approx m$ for nonrelativistic QED, we obtain from (28) and (29) the following double-logarithmic contribution,

$$\Delta E_{\rm LAL}^{\rm 2log}(n, l=1) = -\left(\frac{\alpha}{\pi}\right)^2\,\frac{(Z\alpha)^6\,m}{n^3}\,\ln^2[(Z\alpha)^{-2}]\,\left(\frac{4}{45} - \frac{8}{135n^2}\right)\,. \tag{30}$$

Note that the presence of an additional double-logarithmic term originating from the loop-after-loop diagram in Fig. 1 (c) in the Coulomb gauge does not imply that the result given in (24) for the total value of B_{62} is necessarily incomplete, but it means that additional double logarithms have to expected if, e.g., this diagram is treated numerically, and numerical and analytic results are compared. For S states, an additional contribution to the triple logarithm B_{63} originating from the loop-after-loop diagram was found in [15,18,19], but the result originally obtained in [6] for the *total* value of B_{63} was confirmed in [17, 22]. In the following section, we will derive the result (24) by an independent calculation which includes the entire gauge-invariant set of the diagrams in Fig. 1 in a rigorous way.

5 Derivation Based on NRQED

We start from the expression [see Eq. (16) of [22]],

$$\begin{aligned}
\Delta E_{\rm NRQED} \;=\; & -\left(\frac{2\,\alpha}{3\,\pi\,m^2}\right) \int_0^{\epsilon_1} {\rm d}\omega_1\,\omega_1 \int_0^{\epsilon_1} {\rm d}\omega_2\,\omega_2 \\
& \left\{ \left\langle p^i\,\frac{1}{H-E+\omega_1}\,p^j\,\frac{1}{H-E+\omega_1+\omega_2}\,p^i\,\frac{1}{H-E+\omega_2}\,p^j \right\rangle \right. \\
& +\frac{1}{2}\left\langle p^i\,\frac{1}{H-E+\omega_1}\,p^j\,\frac{1}{H-E+\omega_1+\omega_2}\,p^j\,\frac{1}{H-E+\omega_2}\,p^i \right\rangle \\
& +\frac{1}{2}\left\langle p^i\,\frac{1}{H-E+\omega_2}\,p^j\,\frac{1}{H-E+\omega_1+\omega_2}\,p^j\,\frac{1}{H-E+\omega_1}\,p^i \right\rangle \\
& +\left\langle p^i\,\frac{1}{H-E+\omega_1}\,p^i\,\left(\frac{1}{H-E}\right)'\,p^j\,\frac{1}{H-E+\omega_2}\,p^i \right\rangle \\
& -\frac{1}{2}\left\langle p^i\,\frac{1}{H-E+\omega_1}\,p^i \right\rangle \left\langle p^j\,\left(\frac{1}{H-E+\omega_2}\right)^2\,p^i \right\rangle \\
& -\frac{1}{2}\left\langle p^i\,\frac{1}{H-E+\omega_2}\,p^i \right\rangle \left\langle p^j\,\left(\frac{1}{H-E+\omega_1}\right)^2\,p^i \right\rangle \\
& -m\left\langle p^i\,\frac{1}{H-E+\omega_1}\,\frac{1}{H-E+\omega_2}\,p^i \right\rangle \\
& \left. -\frac{m}{\omega_1+\omega_2}\left\langle p^i\,\frac{1}{H-E+\omega_2}\,p^i \right\rangle - \frac{m}{\omega_1+\omega_2}\left\langle p^i\,\frac{1}{H-E+\omega_1}\,p^i \right\rangle \right\} . \qquad (31)
\end{aligned}$$

All of the matrix elements are evaluated on the reference state $|\phi\rangle$, which can be taken as the Schrödinger wave function.

Within the ϵ-method [9, 12, 24], we extract those divergent contributions from (31) that involve double logarithms $\alpha^2\,(Z\alpha)^6\,\ln^2[\epsilon/(Z\alpha)^2 m]$ (we may put $\epsilon = \epsilon_1 = \epsilon_2$ for simplicity). These logarithms correspond to the ultraviolet divergence of NRQED and are generated by the contributions of two infrared photons ($\omega_1 < \epsilon, \omega_2 < \epsilon$). The divergences in ϵ necessarily cancel at the end of the calculation due to contributions proportional to $\ln(m/\epsilon)\,\ln[\epsilon/(Z\alpha)^2 m]$ which are generated by intermediate integration regions ($\omega_1 > \epsilon, \omega_2 < \epsilon$), and by terms proportional to $\ln^2(m/\epsilon)$ originating from high-energy virtual photons ($\omega_1 > \epsilon, \omega_2 > \epsilon$). The latter terms correspond to the infrared divergent terms proportional to $\ln^2(\lambda/m)$ of the electron form factors. For a discussion of the related cancellations in the context of the ϵ method, we refer to [12] and the Appendix of [9]. For the double logarithms, the dependence on ϵ cancels between the low-energy, the intermediate and the high-energy regions according to $\ln^2[\epsilon/(Z\alpha)^2 m] + 2\ln(m/\epsilon)\,\ln[\epsilon/(Z\alpha)^2 m] + \ln^2(m/\epsilon) = \ln[(Z\alpha)^{-2}]$.

There are nine terms in curly brackets on the right-hand side of Eq. (31) which we would like to denote by $\mathcal{T}_1$ – $\mathcal{T}_9$. These fall quite naturally into six groups, giving rise to six double logarithms $\mathcal{L}_1$ – $\mathcal{L}_6$ according to the following correspondence:

- $\mathcal{T}_1 \to \mathcal{L}_1$,
- $\mathcal{T}_2 + \mathcal{T}_3 \to \mathcal{L}_2$,
- $\mathcal{T}_4 \to \mathcal{L}_3$,

- $\mathcal{T}_5 + \mathcal{T}_6 \to \mathcal{L}_4$,
- $\mathcal{T}_7 \to \mathcal{L}_5$,
- $\mathcal{T}_8 + \mathcal{T}_9 \to \mathcal{L}_6$.

After an integration in the logarithmic region $\omega_1 \in [(Z\alpha)^2 m, \epsilon_1]$ and $\omega_2 \in [(Z\alpha)^2 m, \epsilon_2]$, the logarithmic contributions can be expressed by matrix elements, evaluated on the reference state, according to the following formulas (again, we put for simplicity $\epsilon = \epsilon_1 = \epsilon_2$):

$$\mathcal{L}_1 = \left(\frac{\alpha}{\pi}\right)^2 \ln^2\left[\frac{\epsilon}{(Z\alpha)^2}\right] \frac{4\langle p^i\,(H-E)\,p^i\,\boldsymbol{p}^2\rangle}{9\,m^4}\,, \tag{32}$$

$$\mathcal{L}_2 = \left(\frac{\alpha}{\pi}\right)^2 \ln^2\left[\frac{\epsilon}{(Z\alpha)^2}\right] \frac{2\,\langle p^i\,p^j\,(H-E)\,p^j\,p^i\rangle - 4\langle p^i\,(H-E)\,p^i\,\boldsymbol{p}^2\rangle}{9\,m^4}\,, \tag{33}$$

$$\mathcal{L}_3 = \left(\frac{\alpha}{\pi}\right)^2 \ln^2\left[\frac{\epsilon}{(Z\alpha)^2}\right] \frac{-\langle \boldsymbol{p}^2\,(H-E)\,\boldsymbol{p}^2\rangle}{9\,m^4}\,, \tag{34}$$

$$\mathcal{L}_4 \propto \langle p^i\,(H-E)\,p^i\rangle = 0\,, \tag{35}$$

$$\mathcal{L}_5 = \left(\frac{\alpha}{\pi}\right)^2 \ln^2\left[\frac{\epsilon}{(Z\alpha)^2}\right] \frac{4\langle p^i\,(H-E)^2\,p^i\rangle}{9\,m^3}\,, \tag{36}$$

$$\mathcal{L}_6 = \left(\frac{\alpha}{\pi}\right)^2 \ln^2\left[\frac{\epsilon}{(Z\alpha)^2}\right] \frac{-4\langle p^i\,(H-E)^2\,p^i\rangle}{9\,m^3}\,. \tag{37}$$

All of these matrix elements are finite when evaluated on P states and on states with higher angular momenta. In deriving these results, use is made of the integrals I_1 – I_3 listed in Appendix B. In particular, I_1 is used in deriving $\mathcal{L}_1$, I_2 is used in deriving $\mathcal{L}_2$, and $\mathcal{L}_6$ can be derived using I_3. The double logarithm $\mathcal{L}_3$ corresponds to Eq. (28). Summing all contributions $\mathcal{L}_1$ – $\mathcal{L}_6$, we obtain

$$\begin{aligned}
\mathcal{L} &= \sum_{i=1}^{6} \mathcal{L}_i \\
&= \left(\frac{\alpha}{\pi}\right)^2 \ln^2\left[\frac{\epsilon}{(Z\alpha)^2}\right] \frac{2\,\langle p^i\,p^j\,(H-E)\,p^j\,p^i\rangle - \langle \boldsymbol{p}^2\,(H-E)\,\boldsymbol{p}^2\rangle}{9\,m^4} \\
&= \left(\frac{\alpha}{\pi}\right)^2 \ln^2\left[\frac{\epsilon}{(Z\alpha)^2}\right] \frac{2\pi\,\langle \Delta\delta^{(3)}(\boldsymbol{r})\rangle}{9\,m^4}
\end{aligned} \tag{38}$$

in agreement with formulas (17) and (18). Here, use is made of the equality

$$\langle p^i\,p^j\,(H-E)\,p^j\,p^i\rangle = \pi\,(Z\alpha)\,\langle \Delta\delta^{(3)}(\boldsymbol{r})\rangle + \frac{1}{2}\,\langle \boldsymbol{p}^2\,(H-E)\,\boldsymbol{p}^2\rangle\,, \tag{39}$$

which is valid for P states and states with higher angular momenta and can be derived using the commutator relation (27). We thereby confirm that the additional double logarithm $\mathcal{L}_3$ generated by the loop-after-loop diagram Fig. 1 (c) is cancelled by an additional contribution from $\mathcal{L}_2$ according to Eqs. (33) and (39).

As a byproduct of the current investigation, we obtain the rigorous result that B_{62} vanishes for states with higher angular momenta $l \geq 2$. This is because the expectation value of the

effective potential (17), when evaluated on hydrogenic D, F, G,... states, vanishes: states with higher angular momenta behave as r^l for small r, where l is the angular momentum. We thereby confirm a statement made in [6] [following Eq. (5) *ibid.*] where it was pointed out that a formula analogous to (18) holds for all states with $l \neq 1$ [see the text following Eq. (5) *ibid.*].

6 Results and Conclusions

The results of the current investigation can be summarized as follows: In Sec. 2, we attempt to clarify the derivation and physical origin of effective potentials [6] used for the approximate description of self-energy corrections in leading logarithmic accuracy, and to provide a more detailed derivation of known double-logarithmic corrections to the Lamb shift. In Sec. 3, restricting the discussion to P states and states with higher angular momenta, we rederive, within the effective-potential approach, known results [6] for the leading spin-independent double logarithm for P states as given by the B_{62} coefficient [see Eq. (24)]. In Sec. 4, we show that nonvanishing double logarithms have to be expected from the loop-after-loop diagram if this non-gauge invariant term is treated separately (e.g., within a numerical evaluation). By contrast, within the effective-potential approach, the double logarithm for this diagram *vanishes* (see the entry in column 2, row 4 of Table 1 of [6]). In Sec. 5, we show that a rigorous derivation of B_{62} based on the entire gauge-invariant set of diagrams in Fig. 1 confirms the result (24) for the *total* value of B_{62}. In particular, the additional double logarithm originating from the loop-after-loop diagram cancels when the contributions of all diagrams are added, and B_{62} vanishes for all states with angular momenta $l > 1$.

A reliable understanding of the problematic two-loop corrections is important for the determination of fundamental constants from precision spectroscopy [25]. We would also like to stress that analytic calculations, even in the low–Z region, could be supplemented by accurate numerical evaluations in the near future. Recently, a complete evaluation of the two-loop self-energy effect for high–Z has been reported [26]. A comparison of the numerical to the analytic results represents a crucial test for both methods [27]. In order to provide for a reliable comparison of numerical vs. analytic results, it is helpful to thoroughly analyze and understand the logarithmic terms from each one of the diagrams in Fig. 1. As outlined in Sec. 5 of [9], the most accurate theoretical predictions for the energy levels can be obtained using a combination of analytic and numerical results.

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A Appendix A: Analytic Evaluation of a Matrix Element

In this appendix, we discuss the derivation of the expression (19)

$$\Delta \left[\left| \phi_{n,l=1,m}(\boldsymbol{r}) \right|^2 \right] \Big|_{r=0}$$

for hydrogenic P states. In Eq. (18), the Laplacian operator acts on nonrelativistic, Schrödinger wavefunctions, which are given by

$$\phi_{n,l=1,m}(\boldsymbol{r}) = R_{n1}(r) Y_{1m}(\theta,\phi)\,, \tag{40}$$

where $R_{n1}(r)$ is the radial component, $Y_{1m}(\theta,\phi)$ is the spherical harmonics with the polar-coordinates r, θ and ϕ and with quantum numbers $(n, l = 1, m)$. Since the quantum number $l = 1$ than the magnetic quantum number can be $m = 0$ and $m = 1, -1$. For the sake of simplicity we consider the $m = 0$ case,

$$Y_{1m=0}(\theta,\phi) = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta. \tag{41}$$

The Laplacian in (18) can be written in polar-coordinates as

$$\Delta \equiv \Delta_r + \Delta_{\theta,\phi} \equiv \left(\frac{1}{r^2}\,\frac{\partial}{\partial r}\,r^2\,\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\,\left(\sin\theta\,\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right), \tag{42}$$

where Δ_r corresponds to the radial component and $\Delta_{\theta,\phi}$ stands for the angular-dependent part of the Laplacian operator. One easily obtains

$$\Delta\left[|\phi_{n,l=1,m=0}(\boldsymbol{r})|^2\right] = \Delta_r R_{n1}^2\,\frac{3}{4\pi}\,\cos^2\theta + R_{n1}^2\,\frac{3}{4\pi}\,\frac{2}{r^2}(1-3\cos^2\theta). \tag{43}$$

The final result (19) should be independent of the angle θ, i.e. independent of the spatial direction in which the origin is approached, and independent of the magnetic quantum number. Therefore, we may postulate that the θ-dependent terms in (43) mutually cancel. Alternatively, we observe that since (19) should be independent of the angle θ, so that so that we may set $\theta = \pi/2$. Reading off the θ-independent part of (43), the following result can be obtained:

$$\Delta\left[|\phi_{n,1,0}(\boldsymbol{r})|^2\right]\Big|_{r\to0} = \frac{3}{4\pi}\,\left(\frac{2}{r^2}R_{n1}^2\right)\Big|_{r\to0}. \tag{44}$$

The radial component of the Schrödinger wavefunction for hydrogenlike P states (R_{n1}) is defined by the associated Laguerre polynomials (L^3_{n+1}) which read

$$\begin{aligned} R_{n1}(r) &= -\left(\frac{(n-2)!}{(n+1)!^3\,(2n)!}\right)^{1/2}\left(\frac{2}{na_B}\right)^{5/2} r\,\exp\left(\frac{-r}{na_B}\right)\,L^3_{n+1}\left(\frac{2r}{na_B}\right), \\ L^3_{n+1}(\rho) &= \frac{\partial^3}{\partial\rho^3}\sum_{j=0}^{n+1}(-1)^j\binom{n+1}{j}\frac{(n+1)!}{j!}\,\rho^j, \end{aligned} \tag{45}$$

where the Bohr radius is $a_B = 1/(Z\alpha m)$. Using this relation, it is straightforward to obtain

$$\Delta\left[|\phi_{n,1,0}(\boldsymbol{r})|^2\right]\Big|_{r\to0} = \frac{2}{3\pi}\left[(Z\alpha)^5 m^5\right]\,\frac{n^2-1}{n^5}, \tag{46}$$

which is equivalent to Eq. (19).

B Appendix B: Double–Logarithmic Integrals

In this Appendix, we provide the results for certain integrals which may be used in order to extract the double-logarithmic contributions of order $(Z\alpha)^6\,\ln^2[\epsilon/(Z\alpha)^2]$ from the NRQED two-loop self-energy (31). We have two photon energies ω_1 and ω_2 and denote arbitrary matrix elements of the various occurrences of the operator $H - E$, scaled by $(Z\alpha)^2$, by the symbols

A_1, A_2 and A_3, respectively. The symbol $\sim$ in this Appendix is meant to indicate that only the double-logarithmic terms of order $(Z\alpha)^6$ are selected. We have,

$$
\begin{aligned}
I_1 &= \int_0^{\epsilon_1} \mathrm{d}\omega_1\, \omega_1 \int_0^{\epsilon_2} \mathrm{d}\omega_2\, \omega_2\, \frac{(Z\alpha)^2}{\omega_1 + A_1\,(Z\alpha)^2}\, \frac{1}{\omega_1+\omega_2 + A_2\,(Z\alpha)^2}\, \frac{(Z\alpha)^2}{\omega_2 + A_3\,(Z\alpha)^2} \\
&\sim -\frac{1}{2}\,(Z\alpha)^6\, \ln\frac{\epsilon_1}{(Z\alpha)^2}\, \ln\frac{\epsilon_2}{(Z\alpha)^2}\, (A_1 + A_3)\,, \qquad (47)
\end{aligned}
$$

$$
\begin{aligned}
I_2 &= \int_0^{\epsilon_1} \mathrm{d}\omega_1\, \omega_1 \int_0^{\epsilon_2} \mathrm{d}\omega_2\, \omega_2\, \frac{(Z\alpha)^2}{\omega_1 + A_1\,(Z\alpha)^2}\, \frac{1}{\omega_1+\omega_2 + A_2\,(Z\alpha)^2}\, \frac{(Z\alpha)^2}{\omega_2 + A_3\,(Z\alpha)^2} \\
&\sim \frac{1}{2}\,(Z\alpha)^6\, \ln\frac{\epsilon_1}{(Z\alpha)^2}\, \ln\frac{\epsilon_2}{(Z\alpha)^2}\, (A_1 + A_3 - A_2)\,, \qquad (48)
\end{aligned}
$$

$$
\begin{aligned}
I_3 &= \int_0^{\epsilon_1} \mathrm{d}\omega_1\, \omega_1 \int_0^{\epsilon_2} \mathrm{d}\omega_2\, \omega_2\, \frac{1}{\omega_1+\omega_2}\, \frac{(Z\alpha)^2}{\omega_2 + A\,(Z\alpha)^2} \\
&\sim -\frac{1}{2}\,(Z\alpha)^6\, \ln\frac{\epsilon_1}{(Z\alpha)^2}\, \ln\frac{\epsilon_2}{(Z\alpha)^2}\, A^2\,. \qquad (49)
\end{aligned}
$$

References

[1] M. Niering, R. Holzwarth, J. Reichert, P. Pokasov, T. Udem, M. Weitz, T. W. Hänsch, P. Lemonde, G. Santarelli, M. Abgrall, P. Laurent, C. Salomon, and A. Clairon, Phys. Rev. Lett. **84**, 5496 (2000).

[2] M. C. George, L. D. Lombardi, and E. A. Hessels, Phys. Rev. Lett. **87**, 173002 (2001).

[3] A. van Wijngaarden, F. Holuj, and G. W. F. Drake, Phys. Rev. A **63**, 012505 (2001).

[4] M. I. Eides, H. Grotch, and V. A. Shelyuto, Phys. Rev. **342**, 63 (2001).

[5] J. Sapirstein and D. R. Yennie, in *Quantum Electrodynamics*, edited by T. Kinoshita (World Scientific, Singapore, 1990), pp. 560–672.

[6] S. G. Karshenboim, J. Phys. B **29**, L29 (1996).

[7] C. Itzykson and J. B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, NY, 1980).

[8] K. Pachucki, J. Phys. B **32**, 137 (1999).

[9] U. D. Jentschura and K. Pachucki, J. Phys. A **35**, 1927 (2002).

[10] E. Remiddi, Nuovo Cim. A **11**, 825 (1972).

[11] E. Remiddi, Nuovo Cim. A **11**, 865 (1972).

[12] K. Pachucki, Ann. Phys. (N. Y.) **226**, 1 (1993).

[13] V. G. Ivanov and S. G. Karshenboim, Phys. Lett. A **210**, 313 (1996).

[14] U. D. Jentschura, G. Soff, and P. J. Indelicato, QED Effects and Breit Hamiltonian for Spinless Particles, e-print hep-th/0111284 (J. Phys. B, in press, 2002).

[15] S. Mallampalli and J. Sapirstein, Phys. Rev. Lett. **80**, 5297 (1998).

[16] I. Goidenko, L. Labzowsky, A. Nefiodov, G. Plunien, and G. Soff, Phys. Rev. Lett. **83**, 2312 (1999).

[17] A. V. Manohar and I. W. Stewart, Phys. Rev. Lett. **85**, 2248 (2000).

[18] V. A. Yerokhin, Phys. Rev. A **62**, 012508 (2000).

[19] V. A. Yerokhin, Phys. Rev. Lett. **86**, 1990 (2001).

[20] A. V. Manohar, J. Soto, and I. W. Stewart, Phys. Lett. B **486**, 400 (2001).

[21] A. V. Manohar and I. W. Stewart, Nucl. Phys. Proc. Suppl. **94**, 130 (2001).

[22] K. Pachucki, Phys. Rev. A **63**, 042503 (2001).

[23] P. J. Mohr, G. Plunien, and G. Soff, Phys. Rep. **293**, 227 (1998).

[24] U. D. Jentschura and K. Pachucki, Phys. Rev. A **54**, 1853 (1996).

[25] P. J. Mohr and B. N. Taylor, Rev. Mod. Phys. **72**, 351 (2000).

[26] V. A. Yerokhin and V. M. Shabaev, Phys. Rev. A **64**, 062507 (2001).

[27] U. D. Jentschura, P. J. Mohr, and G. Soff, Phys. Rev. Lett. **82**, 53 (1999).