Higher-order logarithmic contributions to the Lamb shift in hydrogen, deuterium, and He^+

Savely G. Karshenboim*
Ludwig-Maximilians-Universität, Fakultät für Physik, 80799 München, Germany;
Max-Planck-Institut für Quantenoptik, Garching 85748, Germany;
and Pulkovo Observatory, St. Petersburg 196140, Russia

Vladimir G. Ivanov
Pulkovo Observatory, St. Petersburg 196140, Russia

(Received 20 June 2018; published 31 August 2018)

We study here higher-order two-loop and three-loop logarithmic contributions to the Lamb shift in light hydrogenlike atoms. We have found the leading logarithmic contributions in order $\alpha^2(Z\alpha)^7 m$ and $\alpha^3(Z\alpha)^6 m$ for the arbitrary states. Those terms are double logarithmic for the ns states and single logarithmic for the np states and vanish for the states with $l \geqslant 2$. We have also obtained the leading (single-logarithmic) contribution to the specially normalized difference for the Lamb shift of the ns states $\Delta_L(n) = E_L(1s) - n^3 E_L(ns)$, which is important for a combined evaluation of the overall set of the experimental data available on various transitions in hydrogen and deuterium.

DOI: 10.1103/PhysRevA.98.022522

I. INTRODUCTION

The Rydberg constant is one of the most accurately determined fundamental constants because of the good shape of both experiment and theory. Quantum electrodynamics (QED) theory of light hydrogen-like atoms is the most advanced bound-state QED theory. With few exceptions, the theoretical expressions are expansions in various small parameters, such as α (which characterizes the number of QED loops), $Z\alpha$ (the Coulomb strength and relativistic parameter), and the recoil parameter m/M (the electron-to-nucleus mass ratio). One group of the exceptions includes some "exact" calculations. Certain terms of the expansion in α and m/M have been found exactly in $Z\alpha$, while some terms of the expansion in α and $Z\alpha$ have been found exactly in m/M. The other group of exceptions involves additional parameters, e.g., due to the nuclear structure.

In this paper we focus on pure QED nonrecoil contributions to the Lamb shift, i.e., the contributions at the limit $m/M = 0$. Such external-field contributions dominate in the uncertainty of the QED theory. They can be presented in terms of a series (see, e.g., [1,2])

$$\Delta E(nl) = \frac{\alpha}{\pi}\frac{(Z\alpha)^4 m}{n^3} \times\left(F^{(1)} + \frac{\alpha}{\pi}F^{(2)} + \left(\frac{\alpha}{\pi}\right)^2 F^{(3)} + \cdots\right), \quad (1)$$

where the one-, two-, and three-loop coefficient functions are defined as

$$F^{(1)}(nl) = \sum_{kp} A_{kp}(nl)\,(Z\alpha)^{k-4}\ln^p\frac{1}{(Z\alpha)^2}, \quad (2)$$

$$F^{(2)}(nl) = \sum_{kp} B_{kp}(nl)\,(Z\alpha)^{k-4}\ln^p\frac{1}{(Z\alpha)^2}, \quad (3)$$

and

$$F^{(3)}(nl) = \sum_{kp} C_{kp}(nl)\,(Z\alpha)^{k-4}\ln^p\frac{1}{(Z\alpha)^2}, \quad (4)$$

and we apply throughout the paper the relativistic units in which $\hbar = c = 1$.

Those F state-dependent functions can be introduced for the complete contributions of certain orders as well as for their specific classes. For example, in first order in α one can distinguish the one-loop electron self-energy (SE) contribution and the one-loop vacuum polarization (VP) one. Here, the functions F are the complete functions and the coefficients A, B, C stand for the complete coefficients if otherwise is not explicitly told. When we consider a partial individual contribution we use appropriate indexes, e.g., the self-energy contribution to A_{50} is denoted as $A_{50}^{\rm SE}$.

In the case of the one-loop SE contribution, numerical results are available for some states for any values of the nuclear charge Z including $Z = 1$ (hydrogen and deuterium) and $Z = 2$ (the helium ion) [3,4]. The one-loop VP contribution (without the so-called Wichmann-Kroll contribution) is known for an arbitrary state analytically [5,6]. For the two-loop SE result (for the diagrams without internal VP loops) numerical results are available only for some medium and high values of Z and for only for a few states [7,8]. Some numerical results for the diagrams with the vacuum polarizations are also known numerically [9] for the ground state. For the rest of the states and contributions the results are known only as a few first terms of the expansion in $Z\alpha$.

The purpose of this paper is twofold. First, we calculate the leading unknown logarithmic contributions, which

*savely.karshenboim@mpq.mpg.de

FIG. 1. Characteristic diagrams for the δ-function potential, responsible for $A_{50}^{\rm SE}$ and $A_{50}^{\rm VP}$.

are double-logarithmic ones for the contributions of interest, namely, in the order $\alpha^2(Z\alpha)^7 m$ and $\alpha^3(Z\alpha)^6 m$. Second, we note that it is possible to partly evaluate the subleading logarithms, which are the single-logarithmic ones. Namely, we express the coefficient for the single-logarithmic contribution for an ns state in terms of the related coefficient for the $1s$ state. We also find all the related single-logarithmic contributions for the np states. The latter are the leading ones of the np states, but have the same order as the subleading ones for the ns state. That allows us to reduce all the unknown single-logarithmic coefficients to one for two-loop diagrams and one for three-loop diagrams, which should reduce the final uncertainty of the result, facilitate the fitting of the existing two-loop numerical results for medium Z [7,8], and facilitate a comparison of the results for hydrogen [10,11] and deuterium [12] with the ones on the helium ion, which are expected in some time [13,14].

II. BRIEF OVERVIEW OF SOME KNOWN AND YET UNKNOWN HIGHER-ORDER LOGARITHMIC CONTRIBUTIONS

Let us briefly overview the highest known and unknown coefficients of the $Z\alpha$ expansion in Eqs. (2)–(4). The highest known one-loop coefficient is [15,16]

$$A_{71}(nl) = \tfrac{1}{2}\, A_{50}(1s)\, \delta_{l0}, \tag{5}$$

where we recall (see, e.g., [1,2]) that the coefficient A_{50} consists of two parts

$$A_{50}^{\rm SE}(nl) = \pi\left(\frac{139}{32} - 2\ln 2\right)\delta_{l0}, \quad A_{50}^{\rm VP}(nl) = \frac{5\pi}{48}\,\delta_{l0}, \tag{6}$$

which are both related to delta-function potentials (see Fig. 1) and therefore the related corrections to the energy are proportional to the squared value of the nonrelativistic hydrogenic wave function at the origin

$$|\psi_{nl}(0)|^2 = \frac{(Z\alpha m)^3}{\pi n^3}.$$

That is a rather often situation when a certain higher-order logarithmic coefficient is expressed through a lower-order δ-function-potential contribution. In the particular case of the $\alpha(Z\alpha)^7 m \ln[1/(Z\alpha)]$ term, the coefficient A_{50} determines a δ-function potential, the leading contribution to which is of order $\alpha(Z\alpha)^5 m$, while the higher-order term in Eq. (5) is due to the Dirac correction to the wave function at the origin (see [15] for details). A similar situation takes place in theory for the hyperfine interval in hydrogenlike atoms (see, e.g., [17–19]).

In the case of two-loop effects the logarithmic contributions in order $\alpha^2(Z\alpha)^6 m$ are known, while the leading unknown logarithmic terms are of the next order in $(Z\alpha)$. The leading logarithmic term for the ns states was found in [17] and for the np states in [20,21]:

$$\delta E_L(ns) = -\frac{8}{27}\,\frac{\alpha^2}{\pi^2}\,\frac{(Z\alpha)^6 m}{n^3}\ln^3\frac{1}{(Z\alpha)^2},$$
$$\delta E_L(np) = \frac{4}{27}\,\frac{n^2-1}{n^2}\,\frac{\alpha^2}{\pi^2}\,\frac{(Z\alpha)^6 m}{n^3}\ln^2\frac{1}{(Z\alpha)^2}. \tag{7}$$

The complete results for the logarithmic corrections for the ns and np states have been obtained in [22–24].

We have to mention that prior to a complete calculation of the subleading logarithmic coefficient $B_{62}(ns)$ in [22], it was possible to achieve the results [20,21] for the specific difference

$$\Delta_L(n) = E_L(1s) - n^3 E_L(ns), \tag{8}$$

where $E_L(nl_j)$ is the Lamb shift for the nl_j state. The specially normalized difference was introduced in [15,16]. The difference plays an important role in the evaluation of the actually measured atomic transitions in hydrogen and deuterium, which involves various ns states [25–27] (cf. [1]).

The two-loop logarithmic contributions in order $\alpha^2(Z\alpha)^7 m$ have not yet been calculated. They are the largest unknown two-loop logarithmic terms and their possible contributions should be compared with the uncertainty of a nonlogarithmic term in order $\alpha^2(Z\alpha)^6 m$.

In the meantime for the three-loop function $F^{(3)}$ only the leading term (with C_{40}) is known. The next-to-leading term (C_{50}) as well as the logarithmic contributions in order $\alpha^3(Z\alpha)^6 m$ remain unknown.

Following [1], the overall uncertainty of theory of the Lamb shift in light hydrogenic atoms is determined by the uncertainty in calculation of $B_{60}(ns)$ in [22,28,29] and the unknown contributions due to $B_{72}(ns)$, $C_{50}(ns)$, and $C_{63}(ns)$. It is also worth mentioning that combining the experimental results for different transitions in hydrogen and deuterium (in order to separate the contributions of the Rydberg constant and the proton charge radius) for the determination of a hydrogenic value of R_∞ one has to deal with the uncertainties of $B_{60}(np)$ as well as with the uncertainties due to B_{71}, and C_{62} for the p and d states and with the uncertainty due to the related coefficients for the difference in Eq. (8). The unknown coefficients $C_{50}(1s)$, $B_{72}(1s)$, and $C_{62}(1s)$, and the coefficient $B_{60}(1s)$ with a large uncertainty are involved when one is after a determination of the proton charge radius from hydrogen or after an application (in a hydrogenic theory) of a value of the charge radius obtained somewhere else. The purpose of the evaluation of this paper is to eliminate some of these uncertainties and to find the related contributions.

III. CALCULATION OF TWO- AND THREE-LOOP LOGARITHMIC CONTRIBUTIONS

The leading logarithmic contribution to the Lamb shift comes from the one-loop radiative correction

$$\delta E_L^{\rm lead}(nl) = \frac{\alpha}{\pi}\,\frac{(Z\alpha)^4 m}{n^3}\,A_{41}\,\ln\frac{1}{(Z\alpha)^2}. \tag{9}$$

That is a result for the energy of an electron bound by a Coulomb field of a pointlike nucleus. As it was demonstrated in [21] (following [17]), a perturbation of the Coulomb

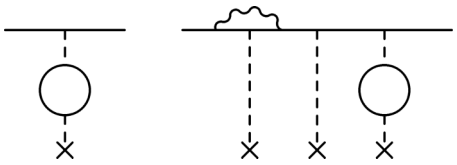

FIG. 2. δ-function potential in Eq. (10) and a characteristic diagram for calculation of the logarithmic contributions in Eq. (11).

potential with a δ-function potential due to the vacuum polarization

$$V_{\rm VP}(\mathbf{r}) = -\frac{4}{15}\,\frac{\alpha(Z\alpha)}{m^2}\delta(\mathbf{r}) \tag{10}$$

leads to the following higher-order logarithmic contributions [see Eqs. (16), (33), and (34) of [21]]

$$\begin{aligned}
\delta E_L(ns) &= \frac{8}{45}\,\frac{\alpha^2}{\pi^2}\,\frac{(Z\alpha)^6 m}{n^3}\ln^2\frac{1}{(Z\alpha)^2},\\
\delta E_L(np) &= -\frac{8}{135}\,\frac{n^2-1}{n^2}\,\frac{\alpha^2}{\pi^2}\,\frac{(Z\alpha)^6 m}{n^3}\ln\frac{1}{(Z\alpha)^2},\\
\delta \Delta_L(n) &= -\frac{8}{45}\,\frac{\alpha^2}{\pi^2}\,\frac{(Z\alpha)^6 m}{n^3}\ln\frac{1}{(Z\alpha)^2}\\
&\quad\times\left[\frac{n^2-1}{n^2}+4\left(\ln n-1+\frac{1}{n}-\sum_{k=1}^{n-1}\frac{1}{k}\right)\right].
\end{aligned} \tag{11}$$

The related diagrams are present in Fig. 2.

The statement of [21], reproduced in Eq. (11), can be generalized for an arbitrary δ-function potential

$$V_\delta(\mathbf{r}) = \frac{\pi\,\delta E_\delta(1s)}{(Z\alpha m)^3}\,\delta(\mathbf{r}), \tag{12}$$

where $\delta E_\delta(1s)$ is the shift of the ground-state energy due to the potential.

The related correction to Eq. (9) due to the potential in Eq. (12) now reads as

$$\begin{aligned}
\delta E_L(ns) &= -\frac{2}{3}\,\frac{\alpha}{\pi}\,\frac{(Z\alpha)^2\delta E_\delta(1s)}{n^3}\ln^2\frac{1}{(Z\alpha)^2},\\
\delta E_L(np) &= \frac{2}{9}\,\frac{n^2-1}{n^2}\,\frac{\alpha}{\pi}\,\frac{(Z\alpha)^2\delta E_\delta(1s)}{n^3}\ln\frac{1}{(Z\alpha)^2},\\
\delta \Delta_L(n) &= \frac{2}{3}\,\frac{\alpha}{\pi}\,\frac{(Z\alpha)^2\delta E_\delta(1s)}{n^3}\ln\frac{1}{(Z\alpha)^2}\\
&\quad\times\left[\frac{n^2-1}{n^2}+4\left(\ln n-1+\frac{1}{n}-\sum_{k=1}^{n-1}\frac{1}{k}\right)\right].
\end{aligned} \tag{13}$$

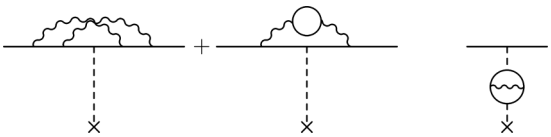

FIG. 3. Characteristic diagrams for the δ-function potential, responsible for $B_{40}^{\rm SE2}$ (the left and middle diagrams) and $B_{40}^{\rm VP2}$ (the right diagram).

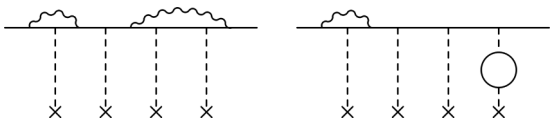

FIG. 4. Characteristic diagrams for calculation of the B_{72} contribution.

That generalized form can be applied to many other logarithmic contributions to the Lamb shift in a hydrogenlike atom.

In the meanwhile, we note that the terms related to $A_{50}^{\rm SE}$ and $A_{50}^{\rm VP}$ (see Fig. 1) and $B_{40}^{\rm SE2}$ and $B_{40}^{\rm VP2}$ (see Fig. 3) produce δ-function-like potentials, the contributions of which to the Lamb shift of an ns state are

$$\begin{aligned}
\delta E_{A50}^{\rm SE}(ns) &= \frac{\alpha}{\pi}\,A_{50}^{\rm SE}\,\frac{(Z\alpha)^5 m}{n^3},\\
\delta E_{A50}^{\rm VP}(ns) &= \frac{\alpha}{\pi}\,A_{50}^{\rm VP}\,\frac{(Z\alpha)^5 m}{n^3},\\
\delta E_{B40}^{\rm SE2}(ns) &= \frac{\alpha^2}{\pi^2}\,B_{40}^{\rm SE2}\,\frac{(Z\alpha)^4 m}{n^3},\\
\delta E_{B40}^{\rm VP2}(ns) &= \frac{\alpha^2}{\pi^2}\,B_{40}^{\rm VP2}\,\frac{(Z\alpha)^4 m}{n^3}.
\end{aligned} \tag{14}$$

In our notation the index SE2 stands for the complete two-loop self-energy including the diagrams with the one-loop vacuum polarization (see the middle Feynman graph in Fig. 3).

The coefficients A_{50} have been already defined above [see Eq. (6)]. The coefficients B_{40} have been also known for a while (see, e.g., [1,2])

$$\begin{aligned}
B_{40}^{\rm SE2}(ns) &= \left(-\frac{9}{4}\zeta(3)+\frac{3}{2}\pi^2\ln 2-\frac{10}{27}\pi^2-\frac{1523}{648}\right),\\
B_{40}^{\rm VP2}(nl) &= -\frac{82}{81}\,\delta_{l0}.
\end{aligned} \tag{15}$$

Those potentials are responsible for the leading logarithms in order $\alpha^2(Z\alpha)^7 m$ and $\alpha^3(Z\alpha)^6 m$. There are many subtypes of the two- and three-loop diagrams for the contributions in order $\alpha^2(Z\alpha)^7 m$ and $\alpha^3(Z\alpha)^6 m$, respectively. However, only those presented in the Figs. 4–6 produce the leading logarithmic contributions, discussed above.

Applying Eq. (13) to the potentials considered above, we arrive at the following expression for the two-loop logarithmic contributions (see Fig. 4):

$$\begin{aligned}
\delta E_L(ns) &= -\frac{2}{3}\,\frac{\alpha^2}{\pi^2}\,\frac{A_{50}^{\rm SE}\,(Z\alpha)^7 m}{n^3}\ln^2\frac{1}{(Z\alpha)^2},\\
\delta E_L(np) &= \frac{2}{9}\,\frac{n^2-1}{n^2}\,\frac{\alpha^2}{\pi^2}\,\frac{A_{50}^{\rm SE}\,(Z\alpha)^7 m}{n^3}\ln\frac{1}{(Z\alpha)^2},
\end{aligned}$$

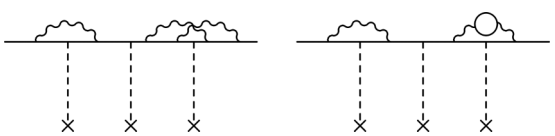

FIG. 5. Characteristic diagrams for calculation of the $C_{62}^{\rm SE:SE2}$ contribution.

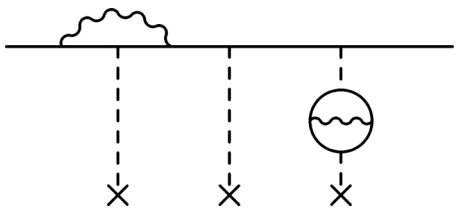

FIG. 6. Characteristic diagrams for calculation of the $C_{62}^{\mathrm{SE:VP2}}$ contribution.

$$\delta\Delta_L(n) = \frac{2}{3}\frac{\alpha^2}{\pi^2}\frac{A_{50}^{\mathrm{SE}}\,(Z\alpha)^7 m}{n^3}\ln\frac{1}{(Z\alpha)^2} \times\left[\frac{n^2-1}{n^2}+4\left(\ln n-1+\frac{1}{n}-\sum_{k=1}^{n-1}\frac{1}{k}\right)\right], \quad (16)$$

and

$$\delta E_L(ns) = -\frac{2}{3}\frac{\alpha^2}{\pi^2}\frac{A_{50}^{\mathrm{VP}}\,(Z\alpha)^7 m}{n^3}\ln^2\frac{1}{(Z\alpha)^2},$$
$$\delta E_L(np) = \frac{2}{9}\frac{n^2-1}{n^2}\frac{\alpha^2}{\pi^2}\frac{A_{50}^{\mathrm{VP}}\,(Z\alpha)^7 m}{n^3}\ln\frac{1}{(Z\alpha)^2},$$
$$\delta\Delta_L(n) = \frac{2}{3}\frac{\alpha^2}{\pi^2}\frac{A_{50}^{\mathrm{VP}}\,(Z\alpha)^7 m}{n^3}\ln\frac{1}{(Z\alpha)^2} \times\left[\frac{n^2-1}{n^2}+4\left(\ln n-1+\frac{1}{n}-\sum_{k=1}^{n-1}\frac{1}{k}\right)\right]. \quad (17)$$

The three-loop logarithmic terms (see Fig. 5) are found to be

$$\delta E_L(ns) = -\frac{2}{3}\frac{\alpha^3}{\pi^3}\frac{B_{40}^{\mathrm{SE}}\,(Z\alpha)^6 m}{n^3}\ln^2\frac{1}{(Z\alpha)^2},$$
$$\delta E_L(np) = \frac{2}{9}\frac{n^2-1}{n^2}\frac{\alpha^3}{\pi^3}\frac{B_{40}^{\mathrm{SE}}\,(Z\alpha)^6 m}{n^3}\ln\frac{1}{(Z\alpha)^2},$$
$$\delta\Delta_L(n) = \frac{2}{3}\frac{\alpha^3}{\pi^3}\frac{B_{40}^{\mathrm{SE}}\,(Z\alpha)^6 m}{n^3}\ln\frac{1}{(Z\alpha)^2} \times\left[\frac{n^2-1}{n^2}+4\left(\ln n-1+\frac{1}{n}-\sum_{k=1}^{n-1}\frac{1}{k}\right)\right],$$

and

$$\delta E_L(ns) = -\frac{2}{3}\frac{\alpha^3}{\pi^3}\frac{B_{40}^{\mathrm{VP}}\,(Z\alpha)^6 m}{n^3}\ln^2\frac{1}{(Z\alpha)^2},$$
$$\delta E_L(np) = \frac{2}{9}\frac{n^2-1}{n^2}\frac{\alpha^3}{\pi^3}\frac{B_{40}^{\mathrm{VP}}\,(Z\alpha)^6 m}{n^3}\ln\frac{1}{(Z\alpha)^2},$$
$$\delta\Delta_L(n) = \frac{2}{3}\frac{\alpha^3}{\pi^3}\frac{B_{40}^{\mathrm{VP}}\,(Z\alpha)^6 m}{n^3}\ln\frac{1}{(Z\alpha)^2} \times\left[\frac{n^2-1}{n^2}+4\left(\ln n-1+\frac{1}{n}-\sum_{k=1}^{n-1}\frac{1}{k}\right)\right].$$

The related logarithmic coefficients are the coefficients B_{72}, B_{71}, C_{62}, C_{61}. In terms of those coefficients the results read as

$$B_{72}^{\mathrm{SESE}}(ns) = -\frac{2}{3}A_{50}^{\mathrm{SE}}, \quad B_{71}^{\mathrm{SESE}}(np) = \frac{2}{9}\frac{n^2-1}{n^2}A_{50}^{\mathrm{SE}},$$
$$B_{71}^{\mathrm{SESE}}(ns) = B_{71}^{\mathrm{SESE}}(1s) - \frac{2}{3}A_{50}^{\mathrm{SE}} \times\left[\frac{n^2-1}{n^2}+4\left(\ln n-1+\frac{1}{n}-\sum_{k=1}^{n-1}\frac{1}{k}\right)\right], \quad (18)$$

$$B_{72}^{\mathrm{SEVP}}(ns) = -\frac{2}{3}A_{50}^{\mathrm{VP}}, \quad B_{71}^{\mathrm{SEVP}}(np) = \frac{2}{9}\frac{n^2-1}{n^2}A_{50}^{\mathrm{VP}},$$
$$B_{71}^{\mathrm{SEVP}}(ns) = B_{71}^{\mathrm{SEVP}}(1s) - \frac{2}{3}A_{50}^{\mathrm{VP}} \times\left[\frac{n^2-1}{n^2}+4\left(\ln n-1+\frac{1}{n}-\sum_{k=1}^{n-1}\frac{1}{k}\right)\right], \quad (19)$$

$$C_{62}^{\mathrm{SE:SE2}}(ns) = -\frac{2}{3}B_{40}^{\mathrm{SE2}}, \quad C_{61}^{\mathrm{SE:SE2}}(np) = \frac{2}{9}\frac{n^2-1}{n^2}B_{40}^{\mathrm{SE2}},$$
$$C_{61}^{\mathrm{SE:SE2}}(ns) = C_{61}^{\mathrm{SE:SE2}}(1s) - \frac{2}{3}B_{40}^{\mathrm{SE2}} \times\left[\frac{n^2-1}{n^2}+4\left(\ln n-1+\frac{1}{n}-\sum_{k=1}^{n-1}\frac{1}{k}\right)\right], \quad (20)$$

and

$$C_{62}^{\mathrm{SE:VP2}}(ns) = -\frac{2}{3}B_{40}^{\mathrm{VP2}}, \quad C_{61}^{\mathrm{SE:VP2}}(np) = \frac{2}{9}\frac{n^2-1}{n^2}B_{40}^{\mathrm{VP2}},$$
$$C_{61}^{\mathrm{SE:VP2}}(ns) = C_{61}^{\mathrm{SE:VP2}}(1s) - \frac{2}{3}B_{40}^{\mathrm{VP2}} \times\left[\frac{n^2-1}{n^2}+4\left(\ln n-1+\frac{1}{n}-\sum_{k=1}^{n-1}\frac{1}{k}\right)\right]. \quad (21)$$

We recall that a δ-function potential perturbs the evaluation of the one-loop self-energy which explains our notation. For example, the one-loop VP potential (A_{50}^{VP}) leads to a two-loop SEVP contribution (B_{72}^{SEVP}). The logarithmic contributions of order $\alpha^2(Z\alpha)^7 m$ and $\alpha^3(Z\alpha)^6 m$ vanish for the states with $l \geqslant 2$.

IV. NUMERICAL RESULTS

The numerical values of the leading logarithmic coefficients derived above are

$$B_{72}(ns) \simeq -6.41, \quad B_{71}(2p) \simeq 1.60,$$
$$B_{71}(1s) - B_{71}(2s) \simeq -15.9, \quad C_{62}(ns) \simeq -0.36,$$
$$C_{61}(2p) \simeq 0.09, \quad C_{61}(1s) - C_{61}(2s) \simeq -1.43. \quad (22)$$

TABLE I. Higher-order perturbative results for the Lamb shift for the $1s$ and $2s$ states in hydrogen and deuterium atoms and in helium ions. The numerical values correspond to the contribution in the units of $(\alpha/\pi)^2(Z\alpha)^6 m/n^3$. The values of B_{60} are taken from [28]. The value of C_{50} is estimated as $\pm 30\delta_{l0}$ following [1]. The effective contribution of C_{63}, estimated in [1] as ± 2.2 for hydrogen and deuterium and ± 1.4 for the He^+ ions in those units, is eliminated since it has been found here to be $C_{63} = 0$. The result for B_{72} and C_{62} are obtained in this paper.

Atom, state	B_{60}	$B_{72}\,(Z\alpha)$ $\ln^2(Z\alpha)^2$	$C_{50}/Z/\pi$	$C_{62}(\alpha/\pi)$ $\ln^2(Z\alpha)^2$
H/D, $1s$	−61.6(9.2)	−4.5	±9.5	−0.08
H/D, $2s$	−53.2(8.0)	−4.5	±9.5	−0.08
He^+, $1s$	−61.6(9.2)	−6.7	±4.8	−0.06
He^+, $2s$	−53.2(8.0)	−6.7	±4.8	−0.06

We have also found that in contrast to the expectation of [1],

$$C_{63}(nl) = 0.$$

Due to a possible nonzero value of such a coefficient, an additional theoretical uncertainty was introduced in [1] (see Table I for detail). It was claimed there that such a cubic three-loop logarithmic C_{63} term, similar to the B_{63} two-loop one, may be present. We note that the insertion of an additional radiative correction into the two-loop diagrams for the B_{63} contributions [17] softens one of the logarithmic integrations at low-q area. The same happens for the would-be leading C_{62} contributions to $\Delta_L(n)$ and $E_L(2p)$, which also vanish. (The situation is very similar to the absence of the two-loop logarithmic contribution in order $\alpha^2(Z\alpha)^4 m$, where the insertion of the radiative correction into the one-loop logarithmically infrared divergent vertex softens the one-loop logarithmic divergence.) Therefore the three-loop logarithms presented above are of the leading order for $\alpha^3(Z\alpha)^6 m$ and we state that they present a complete result for the leading contributions.

Only one of the listed in Eq. (22) two- and three-loop coefficients was studied previously. The result of [23] reads $B_{71}(1s) - B_{71}(2s) = -16(8)$. They analytically computed the same value for the contribution, but considered it as a partial one and assigned the uncertainty of 50% for the other contributions of the same order. However, the contributions above to $\alpha^2(Z\alpha)^7 m$ results are the complete contributions in the leading order. Later, the result of $-16(8)$ was applied in [1] for the evaluation of the set of the spectroscopic data on hydrogen and deuterium.

TABLE II. Higher-order perturbative results for the Lamb shift for the $2p_{1/2}$ state in hydrogen, deuterium, and the helium ion. They correspond to the contribution in the units of $(\alpha/\pi)^2(Z\alpha)^6 m/8$. The value of B_{60} is taken from [30]. The result for B_{71} and C_{61} are obtained in this paper.

Atom	B_{60}	$B_{71}\,(Z\alpha)$ $\ln(1/(Z\alpha)^2)$	$C_{50}/Z/\pi$	$C_{61}(\alpha/\pi)$ $\ln[1/(Z\alpha)^2]$
H/D,	−1.6(3)	0.12	0	0.0021
He^+	−1.6(3)	0.20	0	0.0018

The numerical importance of the higher-order logarithmic contributions is summarized in Tables I and II. Using the tables one can compare the new results with the uncertainties of the calculations of the B_{60} and C_{50} contributions for the lowest states in the Lamb shift in the hydrogen and deuterium atoms and in the helium ion. The elimination of other various uncertainties (including our finding above that $C_{63} = 0$) makes two uncertainties, namely, those of B_{60} and C_{50}, strongly dominant. If one of them will be improved, that should allow us to benefit from a comparison of hydrogen-atom and helium-ion experimental results.

Considering the leading logarithmic contributions as an estimation of the complete contributions in the related orders, $\alpha^2(Z\alpha)^7 m$ and $\alpha^3(Z\alpha)^6 m$, we assign them an uncertainty of 50%.

We note that for the $1s$ state the calculation of the B_{60} coefficient has a relatively large uncertainty as well as the potential contribution of the C_{50} term. In contrast to that the latter vanishes for the np states and the difference in Eq. (8). The accuracy for the B_{60} coefficient for those quantities is also higher. The results for $B_{60}(1s) - B_{60}(ns)$ are available for $n = 2, 3, 4, 5, 6$, [23] and, in particular,

$$B_{60}(1s) - B_{60}(2s) = -15.1(4).$$

That makes the calculation of the logarithmic contributions in the orders $\alpha^2(Z\alpha)^7 m$ and $\alpha^3(Z\alpha)^6 m$ an important progress for those np states and the difference $\Delta_L(n)$.

Concerning the three-loop contributions, we recall that C_{40} is known for the np states (see, e.g., [1,2]) and vanishes for the difference $\Delta_L(n)$; the related C_{50} contributions vanish both for the p state and $\Delta_L(n)$. Therefore the C_{61} contributions, found here, have been leading unknown contributions for those values.

In the tables mentioned we use direct perturbative results for B_{60}. We have already mentioned the existence of exact in $Z\alpha$ calculations of the pure self-energy two-loop contributions at medium values of the nuclear charge Z. Fitting those results, one may obtain an alternative estimation of the B_{60} contribution. Unfortunately, the perturbative results of the $Z\alpha$ expansion and the results of the fits [7] do not well agree (see, e.g., a discussion in [1]).

Tables III–V demonstrate that the understanding of the two-loop logarithmic terms is crucial for the appropriate fitting of the numerical data. Note, the B coefficients in those three tables are not the same as in the two previous ones. The coefficients in Tables I and II correspond to complete

TABLE III. Numerical results at lowest available Z [7] and leading $\alpha^2(Z\alpha)^7 m$ logarithmic contribution to $F^{(2)}$ for the $1s$ state (SESE contribution).

Z	$F^{(2)}_{\rm SESE}(1s)$ [7]	$B^{\rm SESE}_{60}(Z\alpha)^2$ [28]	$B^{\rm SESE}_{72}\,(Z\alpha)^3 \ln^2(Z\alpha)^2$
10	0.172(36)	−0.328(2)	−0.066
12	0.004(38)	−0.472(2)	−0.099
15	−0.212(12)	−0.738(4)	−0.159
17	−0.336(10)	−0.948(5)	−0.206
20	−0.501(5)	−1.312(6)	−0.285
25	−0.728(6)	−2.05(1)	−0.435

TABLE IV. Numerical results at lowest available Z [8] and leading $\alpha^2(Z\alpha)^7 m$ logarithmic contribution to $F^{(2)}(1s) - F^{(2)}(2s)$ for the $\Delta_L(2)$ (SESE contribution).

Z	$(F^{(2)}(1s) - F^{(2)}(2s))_{\rm SESE}$ [8]	$B_{60}^{\rm SESE}(Z\alpha)^2$ [23]	$B_{71}^{\rm SESE}(Z\alpha)^3 \ln[1/(Z\alpha)^2]$
30	0.00(2)	−0.69(2)	−0.489
40	0.07(1)	−1.22(3)	−0.940
50	0.175(8)	−1.92(5)	−1.503

TABLE V. Numerical results at lowest available Z [8] and leading $\alpha^2(Z\alpha)^7 m$ logarithmic contribution to $F^{(2)}$ for $2p_{1/2}$ (SESE contribution).

Z	$F_{\rm SESE}^{(2)}(2p_{1/2})$ [8]	$B_{60}^{\rm SESE}(Z\alpha)^2$ [30]	$B_{71}^{\rm SESE}(Z\alpha)^3 \ln[1/(Z\alpha)^2]$
30	0.18(2)	−0.07(1)	0.049
40	0.19(1)	−0.13(3)	0.094
50	0.198(7)	−0.20(4)	0.152

two-loop results, while those in Tables III–V are for the SESE contribution. In [22] and subsequent papers on perturbative calculations of contribution in order $\alpha^2(Z\alpha)^6 m$, that contribution is referred to as "pure self-energy' or the (self-energy) contribution without any closed electron loops.

The logarithmic contributions found above are larger than the computational uncertainties for all the available numerical results. They are important to improve the quality of fitting the numerical data obtained for medium values of the nuclear charge Z in [7,8]. In the case of the $1s$ state (see Table III) the leading logarithmic contribution is compared with the uncertainty of the numerical evaluations for the Lamb shift at the lowest available values of Z [7].

Tables IV and V do the same comparison for the difference $\Delta_L(n)$ and the Lamb shift in the $2p_{1/2}$ state. The lowest values of Z here are essentially larger than in the case of the $1s$ state; however, the numerical coefficients of the expansion are expected to have essentially smaller values (see, e.g., a discussion in [15,31]), which still could make an extrapolation to low Z possible.

V. CONCLUSIONS

Concluding, we have obtained the leading logarithmic contributions in orders $\alpha^2(Z\alpha)^7 m$ and $\alpha^3(Z\alpha)^6 m$ to the Lamb shift of the ns and np states as well as to the difference $\Delta_L(n) = E_L(1s) - n^3 E_L(ns)$ of the Lamb shift for the ns states. The obtained results can be used in different ways. One may combine all the available coefficients to build an accurate theory for the Lamb shift in hydrogen, deuterium, and the helium ion. Or one may compare the experimental results for the hydrogen atom and the helium ion, once the latter have been achieved. (The helium-ion experiments are in progress [13,14].) One may also use the logarithmic results to fit the numerical data at medium Z. In one way or the other, the calculation of the logarithmic contributions presented here eliminates some contributions to the uncertainty of the QED theory of the Lamb shift in low-Z hydrogenlike atoms and in particular in hydrogen, deuterium, and the helium ions.

We note that for the two-loop self-energy contribution for the $1s$ state at medium-Z atoms (see Table III), the B_{72} logarithmic contribution is below but still comparable with the uncertainty of the B_{60} term, while for the $2p_{1/2}$ state the B_{71} term is larger than such an uncertainty for the result for B_{60} (see Table V). In all cases, the logarithmic contributions obtained here are larger than the uncertainty of the available numerical data for medium Z from [7,8]. Fitting them without knowledge of the logarithmic coefficients found in this paper should lead to systematic errors in determination of B_{60}. The straightforward fitting procedure applied on the numerical exact (in $Z\alpha$) data (at medium Z) is not in a good agreement with the perturbative results (at low Z) as discussed, e.g., in [1]. More sophisticated fitting, with inclusion of the presently established logarithms, should help us understand to what extent the perturbative results and exact results agree or disagree.

ACKNOWLEDGMENTS

The authors are grateful to A. Czarnecki, K. Eikema, V. Korobov, A. Ozawa, K. Pachucki, Th. Udem, and V. Yerokhin for useful and stimulating discussions. The work was in part supported by Deutsche Forschungsgemeinschaft (DFG) (under Grant No. KA 4645/1-1).

[1] P. J. Mohr, D. B. Newell, and B. N. Taylor, Rev. Mod. Phys. **88**, 035009 (2016); P. J. Mohr, B. N. Taylor, and D. B. Newell, *ibid.* **84**, 1527 (2012).

[2] M. I. Eides, H. Grotch, and V. A. Shelyuto, *Theory of Light Hydrogenic Bound States* (Springer, Berlin, 2007).

[3] U. D. Jentschura, P. J. Mohr, and G. Soff, Phys. Rev. Lett. **82**, 53 (1999); Phys. Rev. A **63**, 042512 (2001).

[4] U. D. Jentschura and P. J. Mohr, Phys. Rev. A **69**, 064103 (2004); **72**, 014103 (2005).

[5] S. G. Karshenboim, Can. J. Phys. **76**, 169 (1998); JETP **89**, 850 (1999).

[6] E. Yu. Korzinin, V. G. Ivanov, and S. G. Karshenboim, Eur. Phys. J. D **41**, 1 (2007).

[7] V. A. Yerokhin, Phys. Rev. A **80**, 040501(R) (2009); Eur. Phys. J. D **58**, 57 (2010).

[8] V. A. Yerokhin, Phys. Rev. A **97**, 052509 (2018).

[9] V. A. Yerokhin, P. Indelicato, and V. M. Shabaev, Phys. Rev. A **71**, 040101 (2005); JETP **101**, 280 (2005); Can. J. Phys. **85**, 521 (2007).

[10] C. G. Parthey, A. Matveev, J. Alnis, B. Bernhardt, A. Beyer, R. Holzwarth, A. Maistrou, R. Pohl, K. Predehl, T. Udem, T. Wilken, N. Kolachevsky, M. Abgrall, D. Rovera, C. Salomon, P. Laurent, and T. W. Hänsch, Phys. Rev. Lett. **107**, 203001 (2011).

[11] A. Matveev, C. G. Parthey, K. Predehl, J. Alnis, A. Beyer, R. Holzwarth, T. Udem, T. Wilken, N. Kolachevsky, M. Abgrall,

D. Rovera, C. Salomon, P. Laurent, G. Grosche, O. Terra, T. Legero, H. Schnatz, S. Weyers, B. Altschul, and T. W. Hänsch, Phys. Rev. Lett. **110**, 230801 (2013).
[12] C. G. Parthey, A. Matveev, J. Alnis, R. Pohl, T. Udem, U. D. Jentschura, N. Kolachevsky, and T. W. Hänsch, Phys. Rev. Lett. **104**, 233001 (2010).
[13] M. Herrmann, M. Haas, U. D. Jentschura, F. Kottmann, D. Leibfried, G. Saathoff, C. Gohle, A. Ozawa, V. Batteiger, S. Knünz, N. Kolachevsky, H. A. Schüssler, T. W. Hänsch, and Th. Udem, Phys. Rev. A **79**, 052505 (2009); Th. Udem (private communication).
[14] R. K. Altmann, S. Galtier, L. S. Dreissen, and K. S. E. Eikema, Phys. Rev. Lett. **117**, 173201 (2016); K. S. E. Eikema (private communication).
[15] S. G. Karshenboim, JETP **79**, 230 (1994).
[16] S. G. Karshenboim, Z. Phys. D **39**, 109 (1997).
[17] S. G. Karshenboim, JETP **76**, 541 (1993).
[18] T. Kinoshita and M. Nio, Phys. Rev. Lett. **72**, 3803 (1994).
[19] S. G. Karshenboim, Z. Phys. D **36**, 11 (1996).
[20] S. G. Karshenboim, J. Phys. B **29**, L29 (1996).
[21] S. G. Karshenboim, JETP **82**, 403 (1996).
[22] K. Pachucki, Phys. Rev. A **63**, 042503 (2001).
[23] U. D. Jentschura, A. Czarnecki, and K. Pachucki, Phys. Rev. A **72**, 062102 (2005).
[24] U. D. Jentschura, J. Phys. A **36**, L229 (2003).
[25] S. G. Karshenboim, Can. J. Phys. **77**, 241 (1999).
[26] B. de Beauvoir, C. Schwob, O. Acef, J.-J. Zondy, L. Jozefowski, L. Hilico, F. Nez, L. Julien, A. Clairon, and F. Biraben, Eur. Phys. J. D **12**, 61 (2000); **14**, 398(E) (2001).
[27] S. G. Karshenboim, Phys. Rev. A **91**, 012515 (2015).
[28] K. Pachucki and U. D. Jentschura, Phys. Rev. Lett. **91**, 113005 (2003).
[29] U. D. Jentschura, Phys. Rev. A **70**, 052108 (2004).
[30] U. D. Jentschura, Phys. Rev. A **74**, 062517 (2006).
[31] S. G. Karshenboim, Phys. At. Nucl. **58**, 262 (1995).