# Theory of the Lamb shift in hydrogen and light hydrogen-like ions

Vladimir A. Yerokhin

Center for Advanced Studies, Peter the Great St. Petersburg Polytechnic University, Polytekhnicheskaya 29, St. Petersburg 195251, Russia

Krzysztof Pachucki

Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

Vojtěch Patkóš

Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 121 16 Prague 2, Czech Republic

Theoretical calculations of the Lamb shift provide the basis required for the determination of the Rydberg constant from spectroscopic measurements in hydrogen. The recent high-precision determination of the proton charge radius drastically reduced the uncertainty in the hydrogen Lamb shift originating from the proton size. As a result, the dominant theoretical uncertainty now comes from the two- and three-loop QED effects, which calls for further advances in their calculations. We review the present status of theoretical calculations of the Lamb shift in hydrogen and light hydrogen-like ions with the nuclear charge number up to Z = 5. Theoretical errors due to various effects are critically examined and estimated.

# I. INTRODUCTION

Hydrogen atom plays a special role in modern physics. As the simplest atomic system, hydrogen is often considered to be an ideal testing ground for exploring limits of the theory based on predictions of the bound-state quantum electrodynamics (QED). One of the important tests of theory is the comparison of the proton charge radius values obtained from the Lamb shift in electronic and muonic hydrogen. The 4.5  $\sigma$  discrepancy between these values, known as the proton radius puzzle [1, 2], attracted large attention of the scientific community. This discrepancy could indicate violation of the lepton universality and existence of interactions not accounted for in the Standard Model. Such a possibility is still open, although recent experiments on electronic hydrogen [3–6] hint at existence of unknown systematic effects in hydrogen measurements rather than at new physics.

Another important role of hydrogen is that comparison of theory and experiment for its transition energies is used [7] for determining the Rydberg constant, which is one of the most accurately known fundamental constants today. If one adopts the proton charge radius determined from the muonic hydrogen [2], the uncertainty of the Rydberg constant is defined by the currently available theory of the hydrogen Lamb shift.

Precise spectroscopy of light hydrogen-like ions may also provide determinations of the Rydberg constant in the foreseeable future. Such determinations will be independent on the proton radius and systematic effects in the hydrogen spectroscopy. Helium isotopes look most promising in this respect, because of high-precision results for nuclear radii expected soon from experiments on muonic helium [8]. We mention here the ongoing projects of measuring the 1S-2Stransition energy in He<sup>+</sup> pursued in Garching [9] and in Amsterdam [10], which require improved theoretical predictions for the helium Lamb shift.

Motivated by the needs outlined above, in the present work we summarize the presently available theory for the Lamb shift of hydrogen and light hydrogen-like ions with the nuclear charge up to Z = 5. This summary is intended as an update of the CODATA review of the hydrogen theory [7]. In particular, we perform a reanalysis of results available for the higherorder two-loop QED corrections, which presently define the theoretical uncertainty of the Lamb shift. Results for the nuclear recoil effect are significantly improved by taking into account recent nonperturbative calculations [11, 12]. The nuclear finite size and nuclear polarizability effects are reformulated, according to recent theoretical developments [13, 14].

Relativistic units  $m = \hbar = c = 1$  are used throughout this paper (where m is the electron mass). In these units the electron rest mass energy  $mc^2 = 1$ , so that all energy corrections appear to be dimensionless. In order to convert any energy correction in relativistic units to arbitrary units, it is sufficient to multiply it by  $2\mathcal{R}/\alpha^2$ , where  $\mathcal{R} = hcR_\infty$  is the Rydberg energy and  $R_\infty$  is the Rydberg constant. While m = 1 in our units, we will write m explicitly when it enters dimensionless ratios, such as m/M and  $m_r/m$ .

## **II. BINDING ENERGY**

We consider the binding energy  $E_{njl}$  of an electronic state with quantum numbers n, j, and l in a light hydrogen-like atom. If the atomic nucleus has a nonzero spin I, the energy level  $|njl\rangle$  is splitted by the interaction with the nuclear magnetic moment according to values of the total angular momentum F,  $|njlF\rangle$ . In this case, we define the binding energy  $E_{njl}$  as a centroid averaged over all hyperfine-structure (hfs) components,

$$E_{njl} = \frac{\sum_{F} (2F+1) E_{njlF}}{\sum_{F} (2F+1)} \,. \tag{1}$$

The interaction with the dipole nuclear magnetic moment, responsible for the hyperfine structure, does not contribute to  $E_{njl}$  in the first order. There is, however, a second-order hfs effect that shifts (slightly) the centroid energy  $E_{njl}$ . It manifests itself as a nuclear-spin dependent recoil correction and is addressed in Sec. IV. The goal of the present paper is to summarize the presently available theory for the binding energy  $E_{njl}$  of the 1*S*, 2*S*, and  $2P_{1/2}$  states of light hydrogen-like atoms. The hyperfine splitting of energy levels will not be discussed. For the *nS* states it was investigated in detail in Ref. [15]; a review of the hfs of the higher-*l* states is available in Ref. [16].

The binding energy of a light hydrogen-like atom is usually represented as a sum of three contributions,

$$E_{njl} = E_D + E_M + E_L , \qquad (2)$$

where  $E_D$  is the Dirac point-nucleus biding energy in the nonrecoil limit,  $E_M$  is the correction containing the dominant part of the nuclear recoil effect, and  $E_L$  is the Lamb shift. We note that the total recoil effect is thus distributed between  $E_M$  and  $E_L$  ( $E_M$  being the dominant part and smaller corrections being ascribed to the Lamb shift  $E_L$ ). This distribution is not unique and done differently in the literature.

The Dirac point-nucleus nonrecoil binding energy  $E_D$  is given by

$$E_D = \sqrt{1 - \frac{(Z\alpha)^2}{N^2}} - 1,$$
 (3)

where

$$N = \sqrt{(n_r + \gamma)^2 + (Z\alpha)^2},$$
 (4)

 $\gamma = \sqrt{\kappa^2 - (Z\alpha)^2}$ ,  $n_r = n - |\kappa|$  is the radial quantum number, n is the principal quantum number, and  $\kappa = (l-j)(2j+1)$  is the angular momentum-parity quantum number.

The leading recoil correction  $E_M$  is

$$E_M = \frac{m}{M} \frac{(Z\alpha)^2}{2N^2} - \left(\frac{m}{M}\right)^2 \frac{(Z\alpha)^2}{2n^2} \frac{m_r}{m},$$
 (5)

where M is the nuclear mass and  $m_r = mM/(m+M)$  is the reduced mass. All further recoil corrections are ascribed to the Lamb shift  $E_L$ . The first part of  $E_M$  comprises the complete m/M recoil effect to orders  $(Z\alpha)^2$  and  $(Z\alpha)^4$  and, in addition, corrections of order  $(Z\alpha)^6$  and higher that can be obtained from the Breit Hamiltonian. The second part of  $E_M$ is the nonrelativistic recoil correction of second and higher orders in m/M. In the nonrelativistic limit, the sum  $E_D + E_M$ reduces to the Schrödinger energy eigenvalue,

$$E_D + E_M = \frac{m_r}{m} \frac{(Z\alpha)^2}{2n^2} + \dots,$$
 (6)

where ... represents contributions of order  $(Z\alpha)^4$  and higher.

Our choice of  $E_M$  (and, therefore, our definition of the Lamb shift  $E_L$ ) follows Ref. [17] and differs slightly from the popular definition [18] based on the Barker-Glover formula [19] and, as a consequence, from the definition of the CODATA review [7] (*cf.* Eqs. (25) and (26) therein). The reason for this difference was the need for a simple and concise definition valid for an arbitrary nucleus, whereas the Barker-Glover formula is valid only for the spin-1/2 nucleus. Both definitions are equivalent through orders  $(m/M)(Z\alpha)^{2+n}$  and  $(m/M)^{2+n}(Z\alpha)^2$ , with  $n \ge 0$ . The difference is that our

present definition of Eq. (5) does not contain any contribution of order  $(m/M)^2(Z\alpha)^4$  (which depends on the nuclear spin) or any spurious higher-order terms. The correction of order  $(m/M)^2(Z\alpha)^4$  is included into the Lamb shift; it is given by the first line of Eq. (41).

Another difference in definitions in the literature is associated with the off-diagonal hfs correction, which is small but relevant on the level of the experimental interest for the l > 0states [20]. In the old Lamb-shift measurements (in particular, Ref. [21]), this correction was subtracted from the experimental result. Reviews [7, 17] do not discuss it, thus excluding it from the definition of the Lamb shift. The review [16] includes this correction [see Eq. (30) therein] but ascribes it to the hyperfine splitting. A part of the off-diagonal hfs correction shifts the centroid energy  $E_{njl}$  and thus needs to be included into the definition of the Lamb shift. The corresponding contribution is given by Eq. (42).

We now turn to examining various effects that contribute to the Lamb shift  $E_L$ .

#### III. QED EFFECTS

### A. One-loop QED effects

The one-loop QED effects for the point nuclear charge are represented as

$$E_{\text{QED1}} = \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{n^3} \left(\frac{m_r}{m}\right)^3 \times \left[F_{\text{SE}}(Z\alpha) + F_{\text{VP}}(Z\alpha)\right], \quad (7)$$

where the functions  $F_{SE}(Z\alpha)$  and  $F_{VP}(Z\alpha)$  correspond to the one-loop self-energy and vacuum-polarization, respectively.

The  $Z\alpha$  expansion of the electron self-energy is given by

$$F_{\rm SE}(Z\alpha) = L A_{41} + A_{40} + (Z\alpha) A_{50} + (Z\alpha)^2 \left[ L^2 A_{62} + L A_{61} + G_{\rm SE,pnt}(Z\alpha) \right],$$
(8)

where  $L = \ln \left[ (m/m_r)(Z\alpha)^{-2} \right]$  and  $G_{\rm SE}(Z\alpha) = A_{60} + ...$ is the remainder that contains all higher-order expansion terms in  $Z\alpha$ . The coefficients of the  $Z\alpha$  expansion in Eq. (8) are well known. They are discussed, e.g., in review [22] and summarized in Table I. Numerical results for the remainder function are obtained by Jentschura and Mohr [23, 24] and listed in Table II. Results for Z = 0 correspond to the coefficient  $A_{60}$ ; they were taken from Ref. [25].

The  $Z\alpha$  expansion of the vacuum-polarization correction is given by

$$F_{\rm VP}(Z\alpha) = -\frac{4}{15} \,\delta_{\ell 0} + \frac{5}{48} \pi(Z\alpha) \,\delta_{\ell 0} + (Z\alpha)^2 \\ \times \left[ -\frac{2}{15} L \,\delta_{\ell 0} + G_{\rm Ueh}(Z\alpha) + G_{\rm WK}(Z\alpha) \right], \quad (9)$$

where  $G_{\text{Ueh}}(Z\alpha)$  and  $G_{\text{WK}}(Z\alpha)$  are the higher-order remainder functions induced by the Uehling and Wichmann-Kroll parts of the vacuum polarization, respectively. Numerical results for the remainder functions are listed in Table II. The Wichmann-Kroll part of the vacuum polarization was calculated with help of the approximate potential based on the analytical expansions of Whittaker functions from Ref. [26]. The uncertainty due to approximations in the potential is negligible at the level of current interest. In the limit  $Z \rightarrow 0$ , results for the higher-order remainders are (see review [22] for details)

$$G_{\text{Ueh}}(Z=0,1S) = \frac{4}{15} \left( \ln 2 - \frac{1289}{420} \right),$$
 (10)

$$G_{\text{Ueh}}(Z=0,2S) = -\frac{743}{900},$$
 (11)

$$G_{\text{Ueh}}(Z=0,2P_{1/2}) = -\frac{9}{140},$$
 (12)

$$G_{\rm WK}(Z=0) = \left(\frac{19}{45} - \frac{\pi^2}{27}\right)\delta_{\ell 0}.$$
 (13)

The vacuum-polarization induced by the  $\mu^+\mu^-$  virtual pairs is given by [27, 28]

$$E_{\mu \text{VP}} = \left(\frac{m}{m_{\mu}}\right)^2 \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{n^3} \left(\frac{m_r}{m}\right)^3 \left(-\frac{4}{15}\right) \delta_{\ell 0} \,, \quad (14)$$

where  $m_{\mu}$  is the muon mass.

The hadronic vacuum-polarization correction is of the same order as the muonic vacuum polarization and is given by [29]

$$E_{\rm hadVP} = 0.671 \,(15) \, E_{\mu \rm VP} \,.$$
 (15)

## B. Two-loop QED effects

The two-loop QED correction is expressed as

$$E_{\text{QED2}} = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^4}{n^3} \left(\frac{m_r}{m}\right)^3 F_{\text{QED2}}(Z\alpha), \quad (16)$$

where the function  $F_{\text{QED2}}$  is given by

$$F_{\text{QED2}}(Z\alpha) = B_{40} + (Z\alpha) B_{50} + (Z\alpha)^2 [B_{63} L^3 + B_{62} L^2 + B_{61} L + G_{\text{QED2}}(Z\alpha)], \quad (17)$$

and  $G_{\text{QED2}}(Z\alpha) = B_{60} + \dots$  is the remainder that contains all higher-order expansion terms in  $Z\alpha$ .

The two-loop QED correction is conveniently divided into three parts: the two-loop self-energy (SESE), the two-loop vacuum-polarization (VPVP), and the mixed self-energy and vacuum-polarization (SEVP),

$$F_{\text{QED2}} = F_{\text{SESE}} + F_{\text{SEVP}} + F_{\text{VPVP}} \,. \tag{18}$$

Coefficients of the  $Z\alpha$  expansion of the individual two-loop corrections for the states under consideration are summarized in Table III, for details see recent studies [25, 30–34] and

references to earlier works therein. We note that the analytical result for the  $B_{61}$  coefficient derived in Ref. [30] was incomplete; one missing piece was added later in Ref. [25] and another, in Ref. [34]. The listed value of  $B_{61}$  for the *S* states differs from that given in Refs. [7, 17] by  $-43/36 + 133\pi^2/864 = -0.134567...$ , which is the lightby-light contribution from Ref. [34]. Numerical values for the delta-function correction to the Bethe logarithm  $\mathcal{N}(nS)$  and  $\mathcal{N}(nP)$  that enter  $B_{61}$  can be found in Refs. [25, 35].

The two-loop higher-order remainder  $G_{\text{QED2}}$  is only partly known up to now. Its  $Z\alpha$  expansion has the form

$$G_{\text{QED2}}(Z\alpha) = B_{60} + (Z\alpha) \left[ B_{72} L^2 + B_{71} L + \dots \right].$$
(19)

The dominant part of the coefficient  $B_{60}$  comes from the two-loop self-energy. It was calculated for the 1S and 2S states by Pachucki and Jentschura [31], with the result

$$B_{60}(1S, \text{SESE}) = -61.6(9.2),$$
 (20)

$$B_{60}(2S, \text{SESE}) = -53.2(8.0),$$
 (21)

where the uncertainty comes from omitted contributions. The complete *n* dependence of  $B_{60}(nS)$  was calculated in Refs. [25, 32]. For the *nP* states, the coefficient  $B_{60}$  was calculated in Ref. [36]. The results for the SESE and SEVP corrections and the  $2P_{1/2}$  state are

$$B_{60}(2P_{1/2}, \text{SESE}) = -1.5(3),$$
 (22)

$$B_{60}(2P_{1/2}, \text{SEVP}) = -0.016\,571\dots$$
 (23)

We use opportunity to correct a mistake in Ref. [36] for the VPVP correction (given by Eqs. (A3) and (A6) of that work). The corrected results are

$$B_{60}(nP_{1/2}, \text{VPVP}) = -\frac{713}{2025} \left(1 - \frac{1}{n^2}\right),$$
 (24)

$$B_{60}(nP_{3/2}, \text{VPVP}) = -\frac{401}{4050} \left(1 - \frac{1}{n^2}\right).$$
 (25)

The logarithmic coefficients  $B_{72}$  and  $B_{71}$  in Eq. (19) were recently investigated in Ref. [37]. The leading logarithmic coefficient  $B_{72}$  was derived as

$$B_{72}(\text{SESE}) = \left(-\frac{139}{48} + \frac{4}{3}\ln 2\right)\pi\,\delta_{\ell 0}\,,\qquad(26)$$

$$B_{72}(\text{SEVP}) = -\frac{5}{72} \pi \,\delta_{\ell 0} \,, \tag{27}$$

$$B_{72}(VPVP) = 0.$$
 (28)

The next coefficient  $B_{71}$  was obtained for the nP states, with the result

$$B_{71}(\text{SESE}, nP) = \left(\frac{139}{144} - \frac{4}{9}\ln 2\right) \pi \frac{n^2 - 1}{n^2} , \qquad (29)$$

$$B_{71}(\text{SEVP}, nP) = \frac{5}{216} \pi \frac{n^2 - 1}{n^2} , \qquad (30)$$

$$B_{71}(\text{VPVP}, nP) = 0.$$
(31)

Ref. [37] also reported the *n* dependence of  $B_{71}(nS)$ .

TABLE I: Coefficients of the  $Z\alpha$  expansion of the one-loop electron self-energy in Eq. (8).

Term		1S	2S	$2P_{1/2}$
$A_{41}$	$\frac{4}{3}\delta_{\ell 0}$	$\frac{4}{3}$	$\frac{4}{3}$	0
$A_{40} \\ A_{50}$	$ \begin{array}{c} -\frac{1}{3}  \ln \kappa_0(n,l) + \frac{1}{9}  \delta_{\ell 0} - \frac{1}{2\kappa(2l+1)} (1 - \delta_{\ell 0}) \\ \left(\frac{139}{32} - 2 \ln 2\right)  \pi  \delta_{\ell 0} \end{array} $	-2.867726964 9.291120908	-2.637915413 9.291120908	$-0.126644388(m/m_r)$ 0
$A_{62}$	$-\delta_{\ell 0}$	-1	-1	0
A <sub>61</sub>	$4\left(\frac{4}{3}\ln 2 + \ln \frac{2}{n} + \psi(n+1) - \psi(1) - \frac{001}{720} - \frac{1}{180n^2}\right)\delta_{\ell 0} + \left[\frac{n^2 - 1}{n^2}\left(\frac{2}{15} + \frac{1}{3}\delta_{j,1/2}\right) + 8\frac{3 - l(l+1)/n^2}{3(2l+3)l(l+1)(4l^2 - 1)}\right](1 - \delta_{\ell 0})$	5.419373685	5.930 118 296	0.572 222 222

TABLE II: Results for the higher-order remainder functions  $G_{SE}$ ,  $G_{Ueh}$ , and  $G_{WK}$  in Eqs. (8) and (9).

Ζ	1S	2S	$2P_{1/2}$
Self-energy:			
0	-30.92414946(1)	-31.84046509(1)	-0.99890440
1	-30.29024(2)	-31.18515(9)	-0.97345(19)
2	-29.770967(5)	-30.64466(5)	-0.94940(5)
3	-29.299170(2)	-30.15193(2)	-0.92637(2)
4	-28.859222(1)	-29.69127(1)	-0.90412(1)
5	-28.443372(1)	-29.255033(8)	-0.882478(8)
Vacuum-pola	rization, Uehling:		
0	-0.633573	-0.825556	-0.064286
1	-0.618724	-0.808872	-0.064006
2	-0.607668	-0.796118	-0.063768
3	-0.598207	-0.785075	-0.063567
4	-0.589838	-0.775230	-0.063399
5	-0.582309	-0.766322	-0.063262
Vacuum-pola	rization, Wichmann-Kroll:		
0	0.056681	0.056681	0
1	0.055721	0.055721	0.000002
2	0.054823	0.054824	0.000006
3	0.053978	0.053983	0.000012
4	0.053178	0.053188	0.000020
5	0.052418	0.052437	0.000030

Calculations of the SESE part of the higher-order remainder,  $G_{\text{SESE}}$ , were carried out to all orders in  $Z\alpha$  for hydrogenlike ions with  $Z \ge 10$  [38, 39]. The latest results were obtained in Ref. [40] for Z < 30 and in Ref. [41] for  $Z \ge 30$ . The extrapolation of the all-order 1S results down to Z = 1reported in Ref. [40] showed only a marginal agreement with the analytical value (20). A possible reason for this could be a large contribution from the unknown logarithmic coefficient  $B_{71}$ .

In the present work, we merge together the numerical and analytical results, in order to obtain the presumably best values for the higher-order remainder. Specifically, for the 1S state, we fit the numerical all-order data for  $Z \ge 15$  from Refs. [40, 41] to the form

$$G_{\text{SESE}}(1S) = B_{60} + B_{72}(Z\alpha) \ln^2 (Z\alpha)^{-2} + b_{71}(Z\alpha) \ln(Z\alpha)^{-2} + (Z\alpha) \operatorname{pol}(Z\alpha),$$
(32)

where  $B_{60}$  and  $B_{72}$  are given by Eqs. (20) and (26), and  $pol(Z\alpha)$  denotes a polynomial in  $Z\alpha$ .  $b_{71}$  and the coeffi-

cients of the polynomial are fitting parameters. The uncertainty was obtained by varying (i)  $B_{60}$  within its error bars (20), (ii) numerical data within their error bars, and (iii) the length of the polynomial and the number of data points included. The higher-order remainder for the 2S state was obtained by adding to  $G_{\rm SESE}(1S)$  the difference  $G_{\rm SESE}(2S) - G_{\rm SESE}(1S)$ , as fitted in Ref. [41]. For the  $2P_{1/2}$  state, we merged together the analytical results (22) and (29) and numerical data from Ref. [41]. The uncertainty was obtained by quadratically adding the error of the  $B_{60}$  coefficient and one half of the leading logarithmic  $B_{71}$  contribution. The obtained results for the higher-order SESE remainder are summarized in Table IV.

Calculations of the SEVP and VPVP corrections were performed in Ref. [42] to all orders in  $Z\alpha$ . Results for the higherorder remainder  $G_{\text{SEVP}}$  listed in Table IV were obtained from Tables I and IV of Ref. [42], after subtracting contributions of the leading  $Z\alpha$ -expansion coefficients and keeping in mind that the light-by-light (LBL) contribution was not included in numerical calculations and thus should not be subtracted. The uncertainty of the SEVP contribution comes from the missing LBL contribution. It was estimated for the S states as one half of the LBL  $B_{61}$  contribution, calculated in Ref. [34]. For the P states, we assume the uncertainty to be negligible.

The results for the higher-order remainder  $G_{\rm VPVP}$  listed in Table IV were obtained from Tables II and III of Ref. [42], after subtracting contributions of the leading  $Z\alpha$ -expansion coefficients summarized in Table III. The uncertainty due to omitted higher-order Källén-Sabry contributions is assumed to be negligible at the level of present interest.

For the 1S state of hydrogen, our result for the two-loop higher-order remainder is  $G_{\text{QED2}} = -92(13)$ , which is slightly lower than the value adopted by CODATA 2016 of -81(20) [7].

#### C. Higher-order QED effects

The  $Z\alpha$  expansion of the three-loop QED correction is given by

$$E_{\text{QED3}} = \left(\frac{\alpha}{\pi}\right)^3 \frac{(Z\alpha)^4}{n^3} \left(\frac{m_r}{m}\right)^3 \left[C_{40} + (Z\alpha)C_{50} + (Z\alpha)^2 \left(C_{62}L^2 + C_{61}L + \dots\right)\right],$$
(33)

The leading-order contribution  $C_{40}$  was obtained in Refs. [43, 44] and is given by

$$C_{40} = \left[ -\frac{568 a_4}{9} + \frac{85 \zeta(5)}{24} - \frac{121 \pi^2 \zeta(3)}{72} - \frac{84 071 \zeta(3)}{2304} - \frac{71 \ln^4 2}{27} - \frac{239 \pi^2 \ln^2 2}{135} + \frac{4787 \pi^2 \ln 2}{108} + \frac{1591 \pi^4}{3240} - \frac{252 251 \pi^2}{9720} + \frac{679 441}{93 312} \right] \delta_{\ell 0} + \left[ -\frac{100 a_4}{3} + \frac{215 \zeta(5)}{24} - \frac{83 \pi^2 \zeta(3)}{72} - \frac{139 \zeta(3)}{18} - \frac{25 \ln^4 2}{18} + \frac{25 \pi^2 \ln^2 2}{18} + \frac{298 \pi^2 \ln 2}{9} + \frac{239 \pi^4}{2160} - \frac{17101 \pi^2}{810} - \frac{28 259}{5184} \right] \frac{m/m_r}{\kappa(2\ell+1)} (1 - \delta_{\ell 0}),$$
(34)

where  $a_4 = \sum_{n=1}^{\infty} 1/(2^n n^4) = 0.517\,479\,061\ldots$ . For the next-order contribution  $C_{50}$ , there are only partial results up to now [45, 46]. Following Ref. [7], we do not include partial results and estimate the uncertainty due to absence of this term as  $C_{50} = \pm 30 \,\delta_{\ell 0}$ . The leading logarithmic contribution  $C_{62}$  was derived in Ref. [37] as

$$C_{62} = -\frac{2}{3} B_{40} \,, \tag{35}$$

where  $B_{40}$  is the leading-order two-loop coefficient summarized in Table III. Ref. [37] presented results also for the single-logarithmic contribution  $C_{61}$  for the nP states and the difference  $C_{61}(nS) - C_{61}(1S)$ .

## **IV. NUCLEAR RECOIL**

The dominant part of the nuclear recoil effect is accounted for by  $E_M$  in Eq. (5) and by the reduced-mass prefactors in previous formulas. Beyond that, there are a number of further recoil corrections. The first one is the nuclear recoil correction of order  $(Z\alpha)^{\geq 5}$  and of first order in m/M,

$$E_{\text{REC}} = \frac{m}{M} \frac{(Z\alpha)^5}{\pi n^3} \left[ \left(\frac{m_r}{m}\right)^3 \ln(Z\alpha)^{-2} D_{51} + \left(\frac{m_r}{m}\right)^3 D_{50} + (Z\alpha) D_{60} + (Z\alpha)^2 G_{\text{REC}}(Z\alpha) \right],$$
(36)

where  $G_{\text{REC}}(Z\alpha)$  is the higher-order remainder containing all higher orders in  $Z\alpha$ . Coefficients of the  $Z\alpha$  expansion in Eq. (36) are reviewed in Ref. [22] and summarized in Table V. The higher-order remainder  $G_{\text{REC}}$  has an expansion of the form

$$G_{\text{REC}}(Z\alpha) = D_{72} \ln^2 (Z\alpha)^{-2} + D_{71} \ln^2 (Z\alpha) + D_{70} + \dots$$
(37)

where  $D_{72} = -11/60 \,\delta_{\ell 0}$  [47, 48] and the next two coefficients were obtained by fitting numerical results in Refs. [11, 12]

$$D_{71}(1S) = 2.919(10), \quad D_{70}(1S) = -1.32(10), \quad (38)$$

$$D_{71}(2S) = 3.335(10), \quad D_{70}(2S) = -0.26(6), \quad (39)$$

$$D_{71}(2P_{1/2}) = 0.149(5), \quad D_{70}(2P_{1/2}) = -0.035(15).$$
  
(40)

Numerical, all-order in  $Z\alpha$  results for the higher-order remainder  $G_{\rm REC}$  are obtained in Refs. [11, 12] and summarized in Table VI. In the present review we do not include results for the finite nuclear size correction to  $E_{\rm REC}$  obtained in Refs. [11, 12], since this effect is partly included in calculations of nuclear polarizability summarized in the next section.

The relativistic recoil corrections of second order in the mass ratio is [18, 49, 50],

$$E_{\text{REC},2} = \left(\frac{m}{M}\right)^2 \frac{(Z\alpha)^4}{n^3} \left[\frac{3}{4n} - \frac{1}{2l+1} + \frac{1}{2}\,\delta_{\ell 0}\,\delta_{I,1/2} - (Z\alpha)\,\frac{2}{\pi}\,\left(1 + \frac{m}{M}\ln\frac{m}{M}\right)\,\delta_{\ell 0}\right].\tag{41}$$

The first part of this correction  $\propto (Z\alpha)^4$  depends on the nuclear spin I, which is the consequence of the choice of the definition of the point-like particle with a spin I. For I > 1 such a definition is not commonly established, so we ascribe an uncertainty of  $\pm \frac{1}{2} \delta_{\ell 0}$  relative to the square brackets in the above formula. This part agrees with the  $(Z\alpha)^4 (m/M)^2$  term

TABLE III: Coefficients of the  $Z\alpha$  expansion of the two-loop QED effects in Eq. (17).  $\zeta(n)$  denotes the Riemann zeta function,  $\psi(n)$  is the digamma function,  $\gamma_E$  is Euler's constant,  $\mathcal{N}(nL)$  is a delta-function correction to the Bethe logarithm, defined by Eq. (4.21a) of Ref. [25].

Term		1S	2S	$2P_{1/2}$
SESE				
$B_{40}$	$\left[-\frac{163}{72} - \frac{85}{216}\pi^2 + \frac{3}{2}\pi^2\ln 2 - \frac{9}{4}\zeta(3)\right]\delta_{\ell 0}$	1.409244	1.409244	$0.114722(m/m_r)$
	$-\left[-\frac{31}{16}+\frac{5}{12}\pi^2-\frac{1}{2}\pi^2\ln 2+\frac{3}{4}\zeta(3)\right]\frac{m/m_r}{\kappa(2l+1)}\left(1-\delta_{l0}\right)$			0
$B_{50}$	unknown 8 s	-24.26506(13)	-24.26506(13)	0
$B_{63}$ $B_{62}$	$-\frac{16}{27} \delta_{\ell 0} = \frac{16}{13} - \ln 2 + \frac{1}{12} - \frac{1}{12} - \ln n + \psi(n) + \gamma_E \delta_{\ell 0}$	-8/27 -0.639.669	-8/27 0 461 403	0 1/9
1002	9 (12 $m^2 + \frac{4n^2}{4n} - m^2 m m n + \psi(n) + \frac{1}{2})^{0} \delta_{n0} + \frac{4}{4\pi} \frac{n^2 - 1}{2} \delta_{\ell_1}$	0.000 000	0.101 100	1/0
$B_{61}$	$\frac{4}{3}\mathcal{N}(nL) + \left[\frac{15473}{2592} + \frac{1039}{432}\pi^2 - \frac{152}{27}\ln 2 - \frac{2}{3}\pi^2\ln 2 + \frac{40}{9}\ln^2 2 + \zeta(3)\right]$	48.388 913	40.932915	0.202220
	$+\left(\frac{80}{27}-\frac{32}{9}\ln 2\right)\left(\frac{3}{4}+\frac{1}{4n^2}-\frac{1}{n}-\ln n+\psi(n)+\gamma_E\right)\bigg]\delta_{\ell 0}$			
	$+\frac{n^2-1}{n^2}\left(\frac{11}{81}+\frac{1}{3}\delta_{j,1/2}-\frac{8}{27}\ln 2\right)\delta_{\ell 1}$			
SEVP				
$B_{40}$	$\left(-\frac{7}{81} + \frac{5\pi^2}{216}\right) \delta_{\ell 0}$	0.142043	0.142043	$-0.005229(m/m_r)$
_	$+\left(\frac{119}{36}-\frac{\pi}{3}\right)\frac{f(f+1)-b(r+1)-b/4}{l(l+1)(2l+1)}\frac{m}{m_r}\left(1-\delta_{\ell 0}\right)$			
$B_{50}$	unknown	1.305 370	1.305 370	0
$B_{63}$ $B_{62}$	$\frac{0}{\frac{8}{2}\delta_{\ell 0}}$	0 8/45	0 8/45	0
$B_{61}$	$\left[-\frac{259}{2100}+\frac{41\pi^2}{100}+\frac{16}{10}\ln 2-\frac{32}{30}\left(\frac{3}{2}+\frac{1}{10}-\frac{1}{10}-\ln n+\psi(n)+\gamma_{\rm F}\right)\right]\delta_{\ell 0}$	1.436241	0.995812	-0.044444
201	$\begin{bmatrix} 1080 + 432 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 45 & (4 + 4n^2 - n + 4n^2) + (4n^2 + 7n^2) \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 432 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 432 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 432 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 432 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 432 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 432 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 432 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 432 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 432 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 432 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 432 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{2}{45} \delta_{\ell 1} \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{1080 + 15 \\ -\frac{1080 + 15 } \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{1080 + 15 \\ -\frac{1080 + 15 } \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{1080 + 15 \\ -\frac{1080 + 15 } \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{1080 + 15 \\ -\frac{1080 + 15 } \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{1080 + 15 \\ -\frac{1080 + 15 } \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{1080 + 15 \\ -\frac{1080 + 15 } \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -\frac{1080 + 15 \\ -\frac{1080 + 15 } \end{bmatrix} = \begin{bmatrix} 1080 + 15 \\ -10$	11100 - 11	0.000012	0.011111
VPVP				
$B_{40}$	$-rac{82}{81}\delta_{\ell 0}$	-82/81	-82/81	0
$B_{50}$	$\left(\frac{7421-2625\pi}{6615}+\frac{52}{63}\ln 2\right)\pi\delta_{\ell 0}$	1.405241	1.405241	0
$B_{63}$	0	0	0	0

contained in Eq. (25) of the CODATA review [7]. The second part of this correction  $\propto (Z\alpha)^5$  is the Erickson formula (see the last line of Eq. (27) in Ref. [7]) expanded in m/M. This formula is derived for the spin-1/2 nucleus; its dependence on nuclear spin is not known. However, we assume the corresponding uncertainty to be negligible.

 $B_{62}$ 

 $B_{61}$ 

0

 $\frac{1097}{2025} \delta_{\ell 0}$ 

An additional recoil contribution arises for the P (and higher-l) states because of mixing of the fine-structure sublevels by the hyperfine-structure (hfs) interaction. This contribution is also known as the off-diagonal hfs shift. It depends on the nuclear spin I and the nuclear magnetic moment  $\mu$  and is given, for the nP states [16, 20], by

$$E_{\text{REC,hfs}}(nP) = \left(\frac{m}{m_p}\right)^2 \frac{\alpha^2 (Z\alpha)^2}{n^3} \times \left(\frac{\mu}{\mu_N}\right)^2 \frac{2I(I+1)}{81} (-1)^{j+1/2} \delta_{\ell 1} ,$$
(42)

where  $\mu_N=|e|/(2\,m_p)$  is the nuclear magneton and  $m_p$  is the proton mass. This correction shifts the  $2P_{1/2}$  centroid

energy by -1.88 kHz for hydrogen, by -0.47 kHz for deuterium, and by -4.36 kHz for <sup>3</sup>He. We note that this correction was not included in the definition of the energy levels in the CODATA review [7] and needed to be accounted for together with the hyperfine structure. Corrections to Eq. (42) are assumed to be suppressed by  $\alpha/\pi$ , which is included into uncertainty.

0

-0.541728

0

0

0

-0.541728

Furthermore, there is the radiative recoil correction [47, 51–53]

$$E_{\text{RREC}} = \frac{m}{M} \left(\frac{m_r}{m}\right)^3 \frac{\alpha (Z\alpha)^5}{\pi^2 n^3} \delta_{\ell 0} \left[ 6\,\zeta(3) - 2\pi^2 \ln 2 + \frac{35\pi^2}{36} - \frac{448}{27} + \frac{2}{3}\,\pi(Z\alpha)\ln^2(Z\alpha)^{-2} \right].$$
(43)

Following Ref. [54], we ascribe to this correction an uncertainty of  $10(Z\alpha)\ln(Z\alpha)^{-2}$  relative to the square brackets in the above equation.

Z	15	2S	$2P_{1/2}$
SESE			,
0	-61.6(9.2)	-53.2(8.0)	-1.5(3)
1	-75.9(12.6)	-61.2(12.6)	-1.37(31)
2	-82.6(9.9)	-67.6(9.9)	-1.28(31)
3	-86.8(8.0)	-71.7(8.0)	-1.20(33)
4	-89.7(6.7)	-74.4(6.7)	-1.13(34)
5	-91.6(5.8)	-76.3(5.8)	-1.06(35)
SEVP			
0			-0.01657
1	-12.9(1.6)	-11.3(1.6)	-0.016(6)
2	-11.8(1.4)	-10.2(1.4)	-0.015(5)
3	-11.0(1.2)	-9.4(1.2)	-0.011(2)
4	-10.5(1.2)	-8.9(1.1)	-0.007(2)
5	-10.0(1.1)	-8.4(1.1)	-0.004(1)
VPVP			
0			-0.26407
1	-2.76(2)	-3.37	-0.263
2	-2.70	-3.30	-0.261
3	-2.65	-3.24	-0.260
4	-2.61	-3.20	-0.259
5	-2.58	-3.16	-0.258

TABLE IV: Results for the two-loop higher-order remainder  $G_{\text{QED2}}$  in Eq. (17).

#### V. NUCLEAR SIZE AND POLARIZABILITY

It is customary in the literature to consider separately the finite nuclear size (fns) effect (also known as the elastic part of the nuclear structure) and the nuclear polarizability (also known as the inelastic nuclear structure). To a large extent, the separate treatment is due to the fact that the fns correction can be obtained numerically from the Dirac equation, whereas calculations of the nuclear polarizability are much more complicated. However, it was shown [13, 55, 56] that for light atoms, there is significant cancelation between the fns effects and the polarizability corrections. Moreover, it turned out that some of the nuclear model dependence of the individual corrections cancels out in the sum. Because of this, it is desirable to keep these contributions together and address them on the same footing. We thus consider the sum of the fns correction  $E_{\rm fns}$  and the polarizability correction  $E_{\rm pol}$ ,

$$E_{\rm nucl} = E_{\rm fns} + E_{\rm pol} = \sum_{i>4} E_{\rm nucl}^{(i)} ,$$
 (44)

where the upper index *i* indicates the order in  $Z\alpha$ .

## A. $(Z\alpha)^4$ nuclear contribution

The leading-order nuclear contribution comes solely from the finite nuclear size. It is given for an arbitrary hydrogenlike system by a simple formula,

$$E_{\rm nucl}^{(4)} = E_{\rm fns}^{(4)} = \frac{2}{3} \frac{(Z\alpha)^4}{n^3} \left(\frac{m_r}{m}\right)^3 R_C^2 \,\delta_{\ell 0} \,, \qquad (45)$$

where  $R_C$  is the root-mean-square (rms) charge radius of the nucleus

$$R_C^2 = \int d^3 r \ r^2 \ \rho(r) \,, \tag{46}$$

and  $\rho(r)$  is the nuclear charge distribution.

The higher-order nuclear contributions are specific for each nucleus. We start our consideration with hydrogen, which is a special case since proton is the only non-composite (onenucleon) nucleus.

# B. $(Z\alpha)^5$ nuclear contribution for hydrogen

If we assume that the nucleus has a fixed charge density distribution, then the  $(Z\alpha)^5$  nuclear correction is given by the two-Coulomb exchange amplitude. The resulting fns correction is [57]

$$E_{\rm fns}^{(5)} = -\frac{1}{3} \, \frac{(Z\alpha)^5}{n^3} \left(\frac{m_r}{m}\right)^3 \, R_Z^3 \, \delta_{\ell 0} \,, \tag{47}$$

where  $R_Z$  is the third Zemach moment

$$R_Z^3 = \int d^3 r_1 \int d^3 r_2 \,\rho(r_1) \,\rho(r_2) \,|\vec{r_1} - \vec{r_2}|^3 \,. \tag{48}$$

The numerical value for the proton is  $R_{pZ} \equiv R_Z(H) = 1.41(2)$  fm, which is the average of two results derived from the electron-positron scattering [58, 59].

A more detailed consideration shows, however, that a nucleus cannot generally be treated as a rigid body, because it is polarized by the surrounding electron. This gives rise to the so-called nuclear polarizability contribution. The proton polarizability correction is usually calculated as the forward two-photon exchange amplitude, expressed via dispersion relations in terms of the inelastic scattering amplitude, which in turn is accessible in experiments.

The recent evaluation of the proton  $(Z\alpha)^5$  nuclear contribution [14] yields the result of -0.1092 (120) kHz for the hydrogen 1S state, which agrees with the previous (elastic + polarizability) value adopted by CODATA [7] of -0.10(1) kHz. The result [14] can be conveniently parameterized in terms of the effective proton radius  $R_{pF}$ , which is introduced in analogy with Eq. (47),

$$E_{\rm nucl}^{(5)}(\mathbf{H}) = -\frac{1}{3} \, \frac{(Z\alpha)^5}{n^3} \, \left(\frac{m_r}{m}\right)^3 \, R_{pF}^3 \, \delta_{\ell 0} \,, \qquad (49)$$

with

$$R_{pF} = 1.947 \,(75) \,\,\mathrm{fm} \,. \tag{50}$$

We note that for the proton there is no cancelation between the elastic and polarizability contributions, in contrast to the composite nuclei.

TABLE V: Coefficients of the  $Z\alpha$  expansion of the nuclear recoil correction in Eq. (36).

Term		1S	2S	$2P_{1/2}$
$D_{51}$	$rac{1}{3}\delta_{\ell 0}$	$\frac{1}{3}$	$\frac{1}{3}$	0
$D_{50}$	$-\frac{8}{3}\ln k_0 + \frac{14}{3}\left[1 - \frac{1}{42} - \frac{1}{2n} + \ln \frac{2}{n} + \psi(n+1) - \psi(1)\right]\delta_{\ell 0}$	2.165 899 582	2.890 835 841	-0.308844332
	$-rac{7}{3}\left[l(l+1)(2l+1) ight]^{-1}(1-\delta_{\ell 0})$			
$D_{60}$	$\left(4\ln 2 - \frac{7}{2}\right)\pi\delta_{\ell 0} + 2\pi\left[3 - \frac{l(l+1)}{n^2}\right]\left[(4l^2 - 1)(2l+3)\right]^{-1}(1 - \delta_{\ell 0})$	-2.285 229 926	-2.285 229 926	1.047 197 551

TABLE VI: Numerical results for the recoil higher-order remainder function in Eq. (36).

Z	1S	2S	$2P_{1/2}$
1	9.720(3)	14.899(3)	1.5097(2)
2	10.390(1)	15.010(1)	1.30739(5)
3	10.4803(9)	14.7806(9)	1.19204(2)
4	10.4155(6)	14.4926(6)	1.11268(2)
5	10.2944 (4)	14.2013 (4)	1.053 21 (2)

#### C. $(Z\alpha)^5$ nuclear contribution for composite nuclei

For compound nuclei consisting of several nucleons, the Zemach fns correction (47) cancels out in a sum with the corresponding nuclear structure contribution [13]. However, it survives in the contribution induced by the interaction with individual nucleons. In the result, we write the total nuclear structure correction  $E_{\rm nucl}^{(5)}$  (known also as the two-photon exchange correction) for a composite nuclei as

$$E_{\rm nucl}^{(5)} = E_{\rm pol}^{(5)} - \frac{1}{3} \, \frac{\alpha^2 (Z\alpha)^3}{n^3} \left[ Z \, R_{pF}^3 + (A - Z) \, R_{nF}^3 \right] \delta_{\ell 0} \,, \tag{51}$$

where the first term  $E_{\text{pol}}^{(5)}$  is the intrinsic nuclear polarizability and the second term is the contribution of individual nucleons. In the above equation,  $R_{pF}$  is the effective proton radius given in Eq. (50),  $R_{nF}$  is an analogous effective radius for the neutron, and A is the mass number. We extract  $R_{nF}$  from the calculation of Tomalak (Table II of Ref. [14]), with the result

$$R_{nF} = 1.43\,(16)\,\,\mathrm{fm}\,.\tag{52}$$

The nuclear polarizability correction  $E_{\rm pol}^{(5)}$  is dominated by the electric dipole excitations and is given by [13, 56, 60]

$$E_{\rm pol}^{(5)} = -\alpha^2 \phi^2(0) \frac{2}{3} \left\langle \phi_N \middle| \vec{d} \frac{1}{H_N - E_N} \left[ \frac{19}{6} + 5 \ln \frac{2(H_N - E_N)}{m} \right] \vec{d} \middle| \phi_N \right\rangle \\ - \frac{\pi}{3} \alpha^2 \phi^2(0) \sum_{i,j=1}^{Z} \langle \phi_N || \vec{R}_i - \vec{R}_j |^3 |\phi_N \rangle \\ + \text{ many small corrections }, \qquad (53)$$

where  $\vec{d}$  is the electric dipole operator divided by the elementary charge,  $H_N$  and  $E_N$  are the nuclear Hamiltonian and its eigenvalue,  $\phi_N$  and  $\phi$  are the nuclear and electronic wave functions, and  $\vec{R_i}$  is the position vector of *i*th proton in the nucleus. The second term in Eq. (53) is the remainder of the Zemach fns correction (47) for a composite nuclei.

For atoms with  $Z \leq 5$ , the nuclear polarizability correction has been investigated only for deuterium, helium, and some neutron-rich isotopes of Li and Be. For deuteron, the twophoton nuclear polarizability was calculated in Ref. [55] and recently reanalysed in Ref. [13],

$$E_{\rm pol}^{(5)}({\rm D}) = -21.78 \; \frac{\delta_{\ell 0}}{n^3} \; h \, {\rm kHz} \pm 1\% \,.$$
 (54)

For helium, the nuclear polarizability correction was calculated in Ref. [61], with the result

$$E_{\rm pol}^{(5)}({}^{4}{\rm He}) = -32.1 \; \frac{\delta_{\ell 0}}{n^{3}} \, h \, {\rm kHz} \pm 10\% \,, \qquad (55)$$

$$E_{\rm pol}^{(5)}({}^{3}{\rm He}) = -55.2 \frac{\delta_{\ell 0}}{n^{3}} h \, {\rm kHz} \pm 10\% \,.$$
 (56)

For stable isotopes with Z = 3, 4, and 5, we use the following estimate

$$E_{\rm pol}^{(5)} \approx -\frac{E_{\rm fns}}{1000} \pm 100\%$$
, (57)

which was obtained in Ref. [17] basing on an analysis of available results throughout the whole Z sequence.

# **D.** $(Z\alpha)^6$ nuclear contribution

The  $(Z\alpha)^6$  nuclear contribution arises from the threephoton exchange between electron and the nucleus. The corresponding fns correction is known in the nonrecoil limit and is given for the nS and  $nP_{1/2}$  ( $\kappa = 1$ ) states by [13, 57]

$$E_{\rm fns}^{(6)} = \frac{(Z\alpha)^6}{n^3} R_C^2 \left\{ -\frac{2}{3} \left[ \frac{9}{4n^2} - 3 - \frac{1}{n} + 2\gamma_E - \ln\frac{n}{2} + \Psi(n) + \ln\left(mR_{C2} Z \alpha\right) \right] \delta_{\ell 0} + \frac{1}{6} \left( 1 - \frac{1}{n^2} \right) \delta_{\kappa 1} \right\},$$
(58)

where  $R_{C2}$  is the effective nuclear charge radii that encodes the high-momentum contribution (for exact definition see Ref. [13]). The effective nuclear radii  $R_{C2}$  has the numerical value close to  $R_C$  and depends on the model of the nuclear charge distribution. We use the result obtained in Ref. [13] for the exponential model,

$$R_{C2}/R_C = 1.068\,497\,,\tag{59}$$

which does not depend on nuclear charge. It was shown in Ref. [13] that the dependence on  $R_{C2}$  in Eq. (58) cancels out in the sum with the corresponding nuclear polarizability correction, so the model dependence of  $R_{C2}$  does not contribute to the uncertainty.

The  $(Z\alpha)^6$  nuclear polarizability is practically unknown for the electronic atoms. The only available results are estimates from Ref. [13] for hydrogen

$$E_{\rm pol}^{(6)}({\rm H}) = 0.393 \, \frac{\delta_{\ell 0}}{n^3} \, h \, {\rm kHz} \pm 100\% \,, \qquad (60)$$

and deuterium

$$E_{\rm pol}^{(6)}({\rm D}) = -0.541 \, \frac{\delta_{\ell 0}}{n^3} \, h \, \text{kHz} \pm 75\% \,. \tag{61}$$

It is remarkable that for hydrogen, the three-photon nuclear polarizability dominates over the two-photon polarizability. The reason for this is that  $E_{\rm pol}^{(6)} \propto (Z\alpha)^6 R_C^2$  whereas  $E_{\rm nucl}^{(5)}({\rm H}) \propto (Z\alpha)^5 R_C^3$ , so that the two-photon exchange is effectively suppressed by a parameter  $mR_C/(Z\alpha) \ll 1$ . For all atoms other than hydrogen, the two-photon exchange is dominated by the electric dipole polarizability  $\propto (Z\alpha)^5 R_C^2$  and, therefore, the three-photon polarizability is smaller than the two-photon one, as usually expected. We estimate the uncertainty due to the unknown three-photon nuclear polarizability for nuclei with Z = 2 - 5 to be 10% of the corresponding two-photon polarizability.

#### E. Radiative fns correction

The leading radiative fns correction is of order  $\alpha(Z\alpha)^5$  and nonzero only for S states (see review [22] for details),

$$E_{\rm fns,rad}^{(5)} = \frac{2}{3} \frac{\alpha (Z\alpha)^5}{n^3} \left(\frac{m_r}{m}\right)^3 R_C^2 \left(4\ln 2 - 5\right) \delta_{\ell 0} \,. \tag{62}$$

The next-order radiative fns correction for the S states is known only partially [35, 62, 63],

$$E_{\rm fns,rad}^{(6)}(nS) = \frac{2}{3} \frac{\alpha (Z\alpha)^6}{\pi n^3} R_C^2 \left[ -\frac{2}{3} \ln^2 (Z\alpha)^{-2} + \ln^2 (mR_C) \right]$$
(63)

In the above formula we keep only the squared logarithms and do not include some higher-order terms derived in Ref. [62], because the term  $\propto \ln(Z\alpha)^{-2}$  is not known and expected to

be of similar magnitude as the omitted terms. The result for the P states [35, 62, 63] is

$$E_{\rm fns,rad}^{(6)} \left( nP_{1/2} \right) = \frac{1}{6} \frac{\alpha \left( Z\alpha \right)^6}{\pi \, n^3} \, R_C^2 \left( 1 - \frac{1}{n^2} \right) \\ \times \left[ \frac{8}{9} \, \ln(Z\alpha)^{-2} - \frac{8}{9} \ln 2 + \frac{166}{135} + \frac{4n^2}{n^2 - 1} \mathcal{N}(nP) \right].$$
(64)

The uncertainty of Eqs. (63) and (64) was evaluated by comparing with results of the more complete treatment [63].

## F. Nuclear self-energy

The nuclear self-energy correction was derived in Ref. [64], with the result

$$E_{\text{NSE}} = \left(\frac{m}{M}\right)^2 \frac{4Z(Z\alpha)^5}{3\pi n^3} \\ \times \left[\ln\left(\frac{M}{m(Z\alpha)^2}\right) \delta_{\ell 0} - \ln k_0(n,l)\right].$$
(65)

It should be noted that there is some ambiguity associated with this correction since the nuclear self-energy contributes not only to the Lamb shift but to the nuclear charge radius and the nuclear magnetic moment. Specifically, addition of an arbitrary constant in the brackets of Eq. (65) is equivalent to changing the definition of the nuclear charge radius. This implies that the presently used definition of the nuclear charge radius (through the slope of the Sachs form-factor) is ambiguous on the level of a constant in the brackets of Eq. (65). This issue was pointed out in Ref. [64] (together with the suggestion for a rigorous definition of the nuclear charge radius) but did not attracted attention of the community up to now. In order to quantify this ambiguity, we ascribe to  $E_{\rm NSE}$  an uncertainty of 0.5 in the square brackets, as in Ref. [54]. The numerical value of this uncertainty is 0.2 kHz for the hydrogen 1S state, which can be disregarded at present but might become relevant in the future.

### VI. NUMERICAL RESULTS

In order to obtain numerical results for the Lamb shift and the transition energies, we need to specify values of fundamental constants and nuclear parameters. In the present review we use the charge radii of the proton and the deuteron as derived from the muonic atoms [2, 65] ( $R_p = 0.84087$  (39) fm and  $R_d = 2.12562$  (78) fm) and the corresponding value of the Rydberg constant from Ref. [16],

$$c R_{\infty} = 3\,289\,841\,960\,248.9\,(3.0)\,\text{kHz}\,.$$
 (66)

It should be mentioned that the exact values of  $R_p$ ,  $R_d$ , and  $R_\infty$  are under debates at present. In particular, the Rydberg constant of Eq. (66) differs from the value recommended by

CODATA 2014 [7] by  $5.5 \sigma$ . On the level of the present experimental accuracy, this controversy is relevant only for hydrogen and deuterium and can be disregarded for heavier atoms.

The nuclear charge radii for elements with Z > 1 are taken as follows. For <sup>3</sup>He and <sup>4</sup>He, we use values by Sick [66, 67]; for <sup>6</sup>Li and <sup>7</sup>Li isotopes, values from Ref. [68]; for other atoms, values from Ref. [69]. The nuclear masses are taken for hydrogen from Ref. [70], for deuterium and helium isotopes from Ref. [7], and for all other nuclei from Ref. [71]. Nuclear magnetic moments are taken from Ref. [72]. The fine-structure constant is [7]

$$\alpha = 1/137.035\,999\,139\,(31)\,. \tag{67}$$

The individual contributions to the Lamb shift for two experimentally most interesting cases, H and He<sup>+</sup>, are listed in Table VII. The results for the QED and the leading fns correction are presented in the nonrecoil limit (i.e., with  $m_r \rightarrow 1$ ). The contribution due to the reduced mass in all formulas is summed up and tabulated separately as the relativistic reduced mass (RRM) correction. The uncertainty of the fns correction is due to the uncertainty of the nuclear charge radius  $R_C$ , whose values are specified in the table. The total results for the Lamb shift  $E_L$  are given with two uncertainties. The first one is the theoretical uncertainty, whereas the second one comes from the uncertainty of the nuclear charge radius.

We observe that for the hydrogen Lamb shift, the theoretical uncertainty is twice larger than the uncertainty due to the proton charge radius (as extracted from muonic hydrogen). The two largest theoretical uncertainties come from (i) the two-loop self-energy and (ii) the three-loop QED correction. As compared to the previous CODATA review [7], the main change is due to our reanalysis of the two-loop QED effects; it shifted the theoretical value by one half of the previous uncertainty and improved the accuracy by a factor of 1.5.

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For helium, the uncertainty of the Lamb shift is presently dominated by the uncertainty from the nuclear radius. But this is likely to change once the results of the muonic helium experiment are evaluated [5, 8].

Table VIII presents theoretical results for the 2S-1S and  $2S-2P_{1/2}$  transition energies in hydrogen and light hydrogenlike ions. Theoretical predictions are given with two uncertainties. The first one is the theoretical uncertainty, whereas the second one is induced by uncertainties of nuclear radii and masses. The uncertainty due to the Rydberg constant  $R_{\infty}$ is not included. Theoretical predictions are compared with available experimental results for the  $2S-2P_{1/2}$  Lamb shift in hydrogen, helium and lithium. We do not present a comparison with the hydrogen 1S-2S experimental results [73, 74] since the value of the Rydberg constant (66) is derived from the comparison of theory and these experiments. For the same reason we do not include the uncertainty due to Rydberg constant in the theoretical predictions.

In summary, theoretical calculations of the Lamb shift in hydrogen and light hydrogen-like ions are required for the determination of the Rydberg constant. In the present work we summarized the present status and recent developments of theoretical calculations of QED and nuclear effects, critically evaluating uncertainties of all contributions.

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TABLE VII: Individual contributions to the Lamb shift  $E_L$ , in MHz. Abbreviations are as follows: "SE" is the one-loop self-energy, "Ue" is the Uehling one-loop vacuum polarization, "WK" is the Wichmann-Kroll one-loop vacuum-polarization, "Ue( $\mu$ had)" is the Uehling muon and hadronic vacuum polarization, "SESE" is the two-loop self-energy, "SEVP" is the electron self-energy with vacuum-polarization insertions, "VPVP" is the two-loop vacuum-polarization, "QED(ho)" is the three-loop QED correction, "RRM" is the relativistic reduced mass correction (see text), "REC" is the recoil correction  $E_{REC}$ , "REC(ho)" is the sum of higher-order recoil corrections  $E_{REC,2}$ ,  $E_{REC,hfs}$ , and  $E_{RREC}$ , "FNS" is the leading-order fns correction  $E_{nucl}^{(4)}$ , "NUCL5" is the  $(Z\alpha)^5$  nuclear correction  $E_{nucl}^{(5)}$ , "NUCL6" is the  $(Z\alpha)^6$  nuclear correction  $E_{nucl}^{(6)}$ , "FNS(rad)" is the radiative fns correction  $E_{fns,rad}$ , "NSE" is the nuclear self-energy correction  $E_{NSE}$ .

	1S	2S	$2P_{1/2}$		
$Z = 1, {}^{1}\text{H}, R_{C} = 0.84087(39) \text{ fm}, M/m = 1836.152673346(81)$					
SE	8396.453556(1)	1072.958455	-12.858661(1)		
Ue	-215.170186	-26.897303	-0.000347		
WK	0.002415	0.000302	0		
$Ue(\mu had)$	-0.00848(8)	-0.00106(1)	0		
SESE	2.3350(13)	0.292 48 (16)	0.027253(4)		
SEVP	0.28839(16)	0.036015(20)	-0.001241		
VPVP	-1.895224	-0.236911	-0.000003		
QED(ho)	0.00183(96)	0.00023(12)	-0.000216		
RRM	-12.765917	-1.633931	0.011741		
REC	2.402830	0.340469	-0.016656		
REC(ho)	0.01316(74)	-0.003227(92)	-0.001335(4)		
FNS	1.1076(10)	0.13845(13)	0		
NUCL5	-0.000109(1)	-0.000014	0		
NUCL6	0.00107(39)	0.000140(49)	0.000001		
FNS(rad)	-0.000135(1)	-0.000017	0		
NSE	0.00463(16)	0.000585(20)	0.000001(20)		
Total	8172.7704(18)(10)	1044.99466(23)(13)	-12.839463(21)(0)		
$Z = 2$ , <sup>4</sup> He <sup>+</sup> , $R_C$	w = 1.6810 (40)  fm,  M/m = 7294.299	9 541 36 (24)			
SE	111054.17069(1)	14257.03560(2)	-204.79417(2)		
Ue	-3415.09945	-426.95277	-0.022109		
WK	0.15206	0.01901	0.000002		
$Ue(\mu had)$	-0.1357(12)	-0.01697(15)	0		
SESE	32.569(64)	4.0959(80)	0.44050(25)		
SEVP	4.9568 (88)	0.6179(11)	-0.020086		
VPVP	-30.04728	-3.756393(1)	-0.000210		
QED(ho)	0.029(31)	0.0036(38)	-0.003468		
RRM	-41.91519	-5.39365	0.046950		
REC	17.67628	2.53338	-0.130835		
REC(ho)	-0.121(10)	-0.0200(13)	0.000549		
FNS	70.82(34)	8.853(42)	0		
NUCL5	-0.0346(32)	-0.00433(40)	0		
NUCL6	0.1520(35)	0.02066(43)	0.000354		
FNS(rad)	-0.01743(39)	-0.002179(50)	0.000007		
NSE	0.01875(65)	0.002372(82)	0.000005(82)		
Total	107693.18(7)(34)	13837.035(9)(42)	-204.48251(26)(0)		

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TABLE VIII: Theoretical transition energies of light hydrogen-like atoms (in GHz), in comparison with available experimental results.

Ζ		$R_C$ [fm]	M/m	2S-1S	$2S - 2P_{1/2}$
1	$^{1}\mathrm{H}$	0.84087 (39)	1 836.152 673 346 (81)	2466061.4131869(18)(10)	$1.05783412(23)(13)\ 1.057847(9)^a$
1	$^{2}$ D	2.12562 (78)	3 670.482 967 85 (13)	2466732.4075345(17)(52)	1.05921991(21)(65)
2	$^{4}\text{He}^{+}$	1.6810 (40)	7 294.299 541 36 (24)	9868561.00631(7)(34)	14.041517(9)(42)
					$14.04113(17)^{b}$
2	<sup>3</sup> He <sup>+</sup>	1.973 (16)	5 495.885 279 22 (27)	9868118.3826(1)(16)	14.04396(1)(20)
3	<sup>6</sup> Li <sup>2+</sup>	2.589 (39)	10 961.898 642 0 (83)	22 206 430.550 (1)(26)	$62.7342(1)(32) \\62.765(21)^c$
3	$^{7}Li^{2+}$	2.444 (42)	12786.392271(11)	22206719.625(1)(26)	62.7231(1)(33)
4	${}^{9}\text{Be}^{3+}$	2.519(12)	16 424.205 51 (16)	39482224.239(4)(24)	179.7719(5)(30)
5	${}^{11}B^{4+}$	2.406 (29)	20 063.737 33 (78)	61 697 635.70 (1)(14)	404.523 (1)(17)

<sup>a</sup> Experiment by Lundeen and Pipkin [75]; the original result is shifted by 1.88 kHz due to the off-diagonal hfs correction, in order to comply with the present definition of the Lamb shift,

<sup>b</sup> Experiment by van Wijngaarden et al. [76],

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