

Lamb shift for states with $j = 1/2$

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The Lamb shift in the light hydrogenlike atoms is evaluated for the state-dependent part of the S states ($n^3 \Delta E_n - \Delta E_1$)/ n^3 and $P_{1/2}$ states by means of a recently proposed relativistic generalization of multipole expansion. We obtain the results for $Z = 1-5$ and $n = 2-10$, where Z is the charge of the nucleus and n is the principal quantum number of the state under consideration. The results are in an excellent agreement with the results obtained by means of $Z\alpha$ expansion truncated after the $\alpha(Z\alpha)^6$ term. The state-dependent part of the S states for $n = 2-4$ is evaluated also for the case of moderately strong Coulomb fields, $Z = 10-50$. It is argued that the present results for the state-dependent part of the S states for low Z are the most accurate results given so far in the literature. In the case of hydrogen the uncertainty is significantly less than 1 Hz. Finally, the extrapolation of the results to infinite n is performed.

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I. INTRODUCTION

Quantum electrodynamics (QED), the quantum field theory describing interactions of charged fermions and photons, is one of the most accurately tested physical theories. There are parameters that have to be taken from experiment, like the Rydberg constant, the fine structure constant, the ratios of electron to proton and electron to muon masses, and the nuclear parameters such as nuclear radii, magnetic moments of nuclei, etc. Testing QED then means to keep consistency in the determination of these parameters in various cases where both the experiment and the theory can be pushed to very high accuracy. These are most notably the g factors of bound electrons [1], the anomalous magnetic moments of electrons [2] and muons [3], and the Lamb shift in hydrogenlike atoms [4]. Summaries of various experiments and the information they provide can be found, for example, in Refs. [5,6]. Most importantly, these tests provide restrictions on the magnitude of the non-renormalizable electromagnetic interactions and give us information about nuclear structure.

It is customary [6–8] to write the Lamb shift of the general S state in the form

$$\Delta E_n = \frac{n^3 \Delta E_n - \Delta E_1}{n^3} + \frac{\Delta E_1}{n^3}, \quad (1)$$

where n is the principal quantum number of the state under consideration. The first and the second terms on the right-hand side are referred to as the state-dependent and the state-independent parts, respectively. The numerator of the state-dependent part is called the normalized difference. Various radiative corrections and nuclear structure effects affect mainly the state-independent part of the S states [5]. The Lamb shift of the state-dependent part of the S states and non- S states is given nearly completely by the self-energy effect in the one-loop approximation [9]. It is customary to express it in the form

$$\Delta E_n = \frac{\alpha}{\pi} \frac{(Z\alpha)^4}{n^3 s^3} F(n, l_j, Z\alpha), \quad (2)$$

where l and j are the orbital and total angular quantum numbers of the state under consideration, Z is the charge of the nucleus in units of elementary charge e , $\alpha = e^2/(4\pi)$ is the fine structure constant, and s is equal to 1 when the nucleus is considered to be infinitely heavy and to $1 + m_e/m_n$ when it is not. Apparently, m_e/m_n is the ratio of the electron and nucleus masses.

It is customary to write the dimensionless function $F(n, l_j, Z\alpha)$ for non- S states and $F(n, 0, Z\alpha) - F(1, 0, Z\alpha)$ for the S states in the form of series in $Z\alpha$ (see, e.g., Ref. [5]):

$$F(n, l_j, Z\alpha) = A_{40}(n, l_j, s) + (Z\alpha)^2 [A_{61}(n, l_j) \ln s (Z\alpha)^{-2} + G(Z\alpha, n, l_j)]. \quad (3)$$

For the S states

$$A_{40}(n, 0) - A_{40}(1, 0) = -\frac{4}{3} [\ln k_0(n, 0) - \ln k_0(1, 0)],$$

and for the $P_{1/2}$ states

$$A_{40}(n, 1_{1/2}, s) = -\frac{4}{3} \ln k_0(n, 1) - \frac{s}{6},$$

where $\ln k_0$ is the so-called Bethe logarithm. The extensive tabulation of the Bethe logarithms can be found in Ref. [10]. A general form of the coefficient A_{61} is given for example in Ref. [5]. The remainder $G(Z\alpha)$ has been determined either nonperturbatively [11,12] or perturbatively, (see, e.g., Eq. (5.5) of Ref. [11]):

$$G(Z\alpha) = A_{60} + A_{70}(Z\alpha) + (Z\alpha)^2 [A_{82} \ln^2 s (Z\alpha)^{-2} + A_{81} \ln s (Z\alpha)^{-2} + A_{80}] + \dots \quad (4)$$

The coefficient A_{60} was calculated in Refs. [8,13]. Nonperturbative evaluation has been accomplished either by means of extrapolation of the partial wave expansion (PWE) [11] or by means of the relativistic generalization of multipole expansion (RME) [12],

In Ref. [12] a slight numerical disagreement between the results of the RME and both $Z\alpha$ expansion truncated after the $\alpha(Z\alpha)^6$ term and the PWE was noted for the normalized difference of the S states but not for the non- S states. The purpose of this paper is to clarify the situation with regard to the current state-of-the-art theoretical determination of the

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one-loop self-energy of the state-dependent part of the S states and the $P_{1/2}$ states.

II. THE METHOD

The RME can be applied to the calculation of the Lamb shift for the state-dependent part of the S states and for non- S states either exactly [14] or approximately [12].

The exact form of the RME has been used in Ref. [14] for the calculation of the state-independent part of the S states. Only minor modifications are needed to extend the method to the calculation of the state-dependent part of the S states. In particular, for the wave function of the reference state we use Eq. (A38) of Ref. [12]. The self-energy function in Eq. (2) is then expressed in the form of the series

$$F = \sum_{v=1}^{\infty} F_v, \quad (5)$$

where the ‘‘relativistic multipoles’’ F_v read (see Eq. (73) of Ref. [14])

$$\begin{aligned} & -2(Z\alpha)^4 F_v \\ &= \sum_{t=0}^v \left\langle \gamma_0 G_4^{2(v-t),t} + \gamma_\mu G_4^{2(v-t-1),t} \frac{(\Pi - \varepsilon)_\mu}{m} + \gamma_0 G_0^{2(v-t),t} \right. \\ & \left. + \gamma_0 G_i^{2(v-t)-1,t} \gamma_i \gamma_0 + \left(-\frac{1}{2}\right) \gamma_\mu [G_0^{2(v-t-3),t}, \gamma_0 \gamma_\mu] \right\rangle. \end{aligned} \quad (6)$$

Here, $\langle O \rangle = \langle \psi | \gamma_0 O | \psi \rangle$ and the wave function ψ of the reference state is a solution of the stationary Dirac equation $(\gamma_\mu \Pi_\mu - m)\psi = 0$ with the energy E . Furthermore, $\Pi = (E + \frac{Z\alpha}{R}, \vec{P})$ is the four-momentum of the electron in the external Coulomb field, γ 's are Dirac matrices, and the relativistic dot product is defined as $A_\mu B_\mu = A_0 B_0 - \vec{A} \cdot \vec{B}$. The operators $G_{4,v}^{2v,t}$ are the expansion of $G_{4,v}$ in the $2v$ space

and t time components of $\Pi - \varepsilon$, where

$$G_{4,v} = (-4) \int_0^{\Lambda^2} d\lambda \int \frac{d^4 k_F}{(k^2 - \lambda)^2} \frac{(1, k_v/m)}{k^2 - 2k_\mu \Pi_\mu + H}, \quad (7)$$

$H = (\gamma_\mu \Pi_\mu + m)(\gamma_\mu \Pi_\mu - m)$ stands for the second-order Hamilton operator, and $\varepsilon = (m, 0, 0, 0)$. The integration in Eq. (7) is over the four-momentum k of the virtual photon. The integral diverges logarithmically with the cutoff Λ . The finite result is obtained when the part contributing to the electromagnetic mass of the electron is subtracted.

The individual terms in Eq. (6) are arranged in such a way to contribute at the same order of naive counting in $Z\alpha$. The naive counting in $Z\alpha$ comes from the transition from natural to atomiclike units, $\vec{R} = \vec{r}/(EZ\alpha)$ and $\vec{P} = EZ\alpha\vec{p}$. Then obviously each additional time and space component of $\Pi - \varepsilon = (E - m + E(Z\alpha)^2/r, EZ\alpha\vec{p})$ contributes additional powers of $(Z\alpha)^2$ and $Z\alpha$, respectively. This naive counting is spoiled by a contribution from the high-energy virtual electron region where the typical electron momentum is of the order $p \sim (Z\alpha)^{-1}$ or higher. Special care then has to be taken to deal separately with this contribution to get accurate results [14]. However, in the case of the state-dependent part of the S states and for the non- S states this contribution is strongly suppressed [12]. The convergence of the series (5) is then very rapid. The first three terms contain the complete coefficient A_{60} . In the actual calculation the integration over the four-momentum of the virtual photon is done analytically and for the evaluation of the remaining expressions the spectral decomposition of the Hamilton operator H is used. The one-dimensional integrations over the continuous spectrum of hydrogen are the only ones to be performed numerically.

The approximate form of the RME, given in Ref. [12], has been designed to obtain the complete contribution to the coefficient A_{60} in Eq. (4), but otherwise to simplify the calculation as much as possible. Part of the calculation, Eq. (53) of Ref. [12], can then be evaluated analytically. The

TABLE I. Results for the normalized difference of S states for low nuclear charges Z obtained by various methods. The results are displayed with more digits than the actual precision. This is due to the fact that these results are used for the fit of the coefficient A_{60} presented in Tables III and IV. See the text for additional discussion. The values in the first and the second rows for $n = 2-4$ are obtained by means of the approximate [12] and the exact [14] versions of the RME taken to the fourth order. The values in the third row for $n = 2-4$ are those from Ref. [11]. The values for $n = 5-10$ are obtained by means of the approximate version of the RME.

| $F(nS, Z\alpha) - F(1S, Z\alpha)$ | $Z = 1$ | $Z = 2$ | $Z = 3$ | $Z = 4$ | $Z = 5$ |
|-----------------------------------|----------------|-----------------|-----------------|-----------------|-----------------|
| $n = 2$ | 0.230029465820 | 0.230529879452 | 0.231225201100 | 0.232069031283 | 0.233029461830 |
| | 0.230031540204 | 0.230545207000 | 0.231273798798 | 0.232178312529 | 0.233233307638 |
| | 0.230031535(5) | 0.230545198(10) | 0.231273778(10) | 0.232178329(10) | 0.233233342(10) |
| $n = 3$ | 0.288818281298 | 0.289274182161 | 0.289907432678 | 0.290675208328 | 0.291547912919 |
| | 0.288820431261 | 0.289290056735 | 0.289957726374 | 0.290788217416 | 0.291758555864 |
| | 0.28882057(5) | 0.28929009(5) | 0.28995775(5) | 0.29078834(5) | 0.29175890(5) |
| $n = 4$ | 0.312592620143 | 0.312983954338 | 0.313526743305 | 0.314183551481 | 0.314928375433 |
| | 0.312594693655 | 0.312999260227 | 0.313575219113 | 0.314292437376 | 0.315131260560 |
| | 0.31259475(20) | 0.31299905(20) | 0.31357508(20) | 0.31429252(20) | 0.31513172(20) |
| $n = 5$ | 0.324554043015 | 0.324892894751 | 0.325362071652 | 0.325928532024 | 0.326569214448 |
| $n = 6$ | 0.331415782285 | 0.331713903742 | 0.332125927289 | 0.332622226171 | 0.333182029956 |
| $n = 7$ | 0.335715422925 | 0.335981642484 | 0.336348892487 | 0.336790224022 | 0.337286665250 |
| $n = 8$ | 0.338586906920 | 0.338827668208 | 0.339159185558 | 0.339556649207 | 0.340002525239 |
| $n = 9$ | 0.340599414943 | 0.340819470576 | 0.341121925461 | 0.341483711243 | 0.341888465247 |
| $n = 10$ | 0.342064311623 | 0.342267234662 | 0.342545642543 | 0.342877908997 | 0.343248641713 |

TABLE II. The self-energy of $P_{1/2}$ states for low nuclear charges Z obtained by means of the approximate version of the RME. The values in the second row for $n = 2$ are those from Ref. [11].

| $F(nP_{1/2}, Z\alpha)$ | $Z = 1$ | $Z = 2$ | $Z = 3$ | $Z = 4$ | $Z = 5$ |
|------------------------|-----------------------------------|-----------------------------------|-----------------------------------|-----------------------------------|-----------------------------------|
| $n = 2$ | -0.126396590783 -0.12639637(1) | -0.125817796170 -0.12581616(1) | -0.124997389529 -0.12499224(1) | -0.123980316789 -0.12396879(1) | -0.122796373009 -0.12277494(1) |
| $n = 3$ | -0.115459399418 | -0.114788732977 | -0.113837544810 | -0.112657636109 | -0.111283293768 |
| $n = 4$ | -0.110425885748 | -0.109722308269 | -0.108724094056 | -0.107485453354 | -0.106042257800 |
| $n = 5$ | -0.107646279274 | -0.106927238818 | -0.105906878620 | -0.104640528550 | -0.103164799693 |
| $n = 6$ | -0.105939357201 | -0.105211815014 | -0.104179256564 | -0.102897622308 | -0.101403928096 |
| $n = 7$ | -0.104813203259 | -0.104080478027 | -0.103040470861 | -0.101749491769 | -0.100244802453 |
| $n = 8$ | -0.104030209251 | -0.103294083916 | -0.102249182738 | -0.100952056447 | -0.0994401274440 |
| $n = 9$ | -0.103463424906 | -0.102724943512 | -0.101676645868 | -0.100375248328 | -0.0988582842162 |
| $n = 10$ | -0.103039788457 | -0.102299603440 | -0.101248846276 | -0.0999443520697 | -0.0984237340198 |

remaining part, Eq. (49) of Ref. [12], can be evaluated by using the spectral decomposition of the Hamilton operator H , much in the same way as in the case of the exact calculation.

III. RESULTS AND DISCUSSION

We applied the approximate form of the RME to the calculation of the one-loop self-energy for the normalized difference of the S states and for the $P_{1/2}$ states for $n = 2-10$ and for $Z = 1-5$ in the infinite nucleus mass limit, $s = 1$. The results obtained are for each $n = 2-10$ in the first rows of Tables I and II. As mentioned in the Introduction we noted in Ref. [12] a slight numerical disagreement for the normalized difference of the S states between the approximate RME calculation and the $Z\alpha$ expansion truncated after the $\alpha(Z\alpha)^6$ term. This we found puzzling since the approximate form of the RME calculation should contain all the terms of the $Z\alpha$ expansion up to the $\alpha(Z\alpha)^6$ term. To clarify this observation we subtracted from the results displayed in the Tables I and II the first two terms on the right-hand side of Eq. (3) and fitted the remainder function $G(Z\alpha)$ to the series (4). The results are displayed in Tables III, IV, and V. It is seen from Table III that the agreement between the value of the coefficient A_{60} obtained directly by $Z\alpha$ expansion [8,13] and from the fit of the RME calculation to the series (4) is excellent. This confirms that the approximate version of the RME really contains the complete A_{60} coefficient.

To clarify the situation further, we applied the exact form of the RME to the calculation of the state-dependent part of the S

states; see the results displayed for each $n = 2-4$ in the second row of Table I. As mentioned above, the convergence of the RME is very rapid (see the Table VI). For low Z the error of the RME is of the order $\alpha(Z\alpha)^7$, but the multiplicative factor is very small. Comparison between the first and second rows of Table IV then shows where the slight numerical disagreement between the approximate RME and both the $Z\alpha$ expansion truncated after the $\alpha(Z\alpha)^6$ term and the PWE comes from. The approximate version of the RME yields a value of the A_{70} coefficient that is too wrong for the normalized difference of the S states, but remarkably not for the P states (compare Tables IV and V).

We extrapolated the results for the A_{60} coefficients to infinite n . We did so by assuming that for large n the coefficients $A_{60}(n)$ behave as

$$A_{60}(n) = C_0 + \frac{C_1}{n} + \frac{C_2}{n^2} + \dots \quad (8)$$

The results are displayed in Table VII. To get more accurate values of the coefficients C one would need the values of the coefficients $A_{60}(n)$ for higher n . The extrapolation of the results for the A_{40} coefficients can be found in the second reference in Ref. [10].

We also applied the exact version of the RME to the calculation of the state-dependent part of the S states for the ions with higher nuclear charges Z (see Table VIII). On the basis of rapidity of convergence of the RME we believe that the results for $Z = 10$ are by 2 orders of magnitude more accurate than those obtained by means of the PWE [15,17]. The

TABLE III. Comparison between the values of the $A_{60}(nP_{1/2})$ and $\Delta A_{60}(nS) = A_{60}(nS) - A_{60}(1S)$ coefficients for $n = 2-10$ obtained either by fitting the results in the first rows in Tables I and II to the series (3) and (4) or by direct calculation.

| State | $\Delta A_{60}(nS)$ | Results from Ref. [8] | $A_{60}(nP_{1/2})$ | Results from Ref. [13] |
|----------|---------------------|-----------------------|--------------------|------------------------|
| $n = 2$ | -0.916321 | -0.91631563 | -0.998909 | -0.998904402 |
| $n = 3$ | -0.778356 | -0.778351 | -1.148197 | -1.148189956 |
| $n = 4$ | -0.637779 | -0.637772 | -1.195698 | -1.195688142 |
| $n = 5$ | -0.531255 | -0.531243 | -1.216240 | -1.216224512 |
| $n = 6$ | -0.450999 | -0.450980 | -1.226761 | -1.226702391 |
| $n = 7$ | -0.389106 | -0.389074 | -1.232753 | -1.232715957 |
| $n = 8$ | -0.340155 | -0.340107 | -1.236423 | |
| $n = 9$ | -0.300565 | | -1.238792 | |
| $n = 10$ | -0.267929 | | -1.240403 | |

TABLE IV. Comparison between the coefficients $\Delta A_{60}(nS) - \Delta A_{80}(nS)$ for $n = 2-4$ obtained either from the RME or the PWE. The values in the first, second, and third rows for each n were obtained by fitting the results from the first, second, and third rows of Table I to the series (3) and (4), respectively.

| State | $\Delta A_{60}(nS)$ | $\Delta A_{70}(nS)$ | $\Delta A_{82}(nS)$ | $\Delta A_{81}(nS)$ | $\Delta A_{80}(nS)$ |
|---------|---------------------|---------------------|---------------------|---------------------|---------------------|
| $n = 2$ | -0.916321 | -3.1774 | 1.1211 | -0.709 | 6.21 |
| | -0.916307 | 2.9677 | 0.0129 | -0.305 | -1.30 |
| | -0.917815 | 3.6392 | -2.2 | 21 | -63 |
| $n = 3$ | -0.778356 | -3.8952 | 1.2297 | -0.725 | 7.04 |
| | -0.778348 | 2.4788 | 0.0914 | -0.506 | -0.35 |
| | -0.759911 | -3.4242 | 14.4 | -124 | 336 |
| $n = 4$ | -0.637779 | -4.1889 | 1.2306 | -0.698 | 7.20 |
| | -0.637773 | 1.9591 | 0.1434 | -0.624 | 0.35 |
| | -0.613998 | -7.3251 | 25.2 | -224 | 617 |

TABLE V. The same as in Table IV but for the coefficients $A_{60}(nP_{1/2}) - A_{80}(nP_{1/2})$ for $n = 2-5$. The inputs for fit are now the first and second rows of Table II.

| State | $A_{60}(nP_{1/2})$ | $A_{70}(nP_{1/2})$ | $A_{82}(nP_{1/2})$ | $A_{81}(nP_{1/2})$ | $A_{80}(nP_{1/2})$ |
|---------|--------------------|--------------------|--------------------|--------------------|--------------------|
| $n = 2$ | -0.998909 | 3.00826 | -0.0481 | -0.676 | -0.50 |
| | -0.999492 | 3.90196 | -0.7897 | 4.8 | -16 |
| $n = 3$ | -1.148197 | 3.56568 | -0.0572 | -0.793 | -0.62 |
| $n = 4$ | -1.195698 | 3.76163 | -0.0627 | -0.821 | -0.73 |
| $n = 5$ | -1.216240 | 3.85355 | -0.0683 | -0.810 | -0.87 |

TABLE VI. Contribution of individual multipoles to the normalized difference of S states for $n = 2-4$. "Lead" stands for first two multipoles, $F_1 + F_2$.

| Term | State | $Z = 1$ | $Z = 2$ | $Z = 3$ | $Z = 4$ | $Z = 5$ |
|-------|-----------|---------------------------|---------------------------|---------------------------|---------------------------|---------------------------|
| | $2s - 1s$ | | | | | |
| Lead | | 0.229991606931 | 0.230390709933 | 0.230936267290 | 0.231594004269 | 0.232342252851 |
| F_3 | | 0.000039870858 | 0.000154033610 | 0.000336061748 | 0.000581009986 | 0.000884923162 |
| F_4 | | 6.241492×10^{-8} | 4.634566×10^{-7} | 1.469760×10^{-6} | 3.298274×10^{-6} | 6.131626×10^{-6} |
| Total | | 0.2300315402(3) | 0.230545207(2) | 0.231273799(6) | 0.23217831(1) | 0.23323331(3) |
| | $3s - 1s$ | | | | | |
| Lead | | 0.288771400893 | 0.289100037681 | 0.289541947085 | 0.290067435815 | 0.290657954914 |
| F_3 | | 0.000048953133 | 0.000189443771 | 0.000413949977 | 0.000716666402 | 0.001092933279 |
| F_4 | | 7.723537×10^{-8} | 5.752828×10^{-7} | 1.829313×10^{-6} | 4.115199×10^{-6} | 7.667670×10^{-6} |
| Total | | 0.2888204313(3) | 0.289290057(2) | 0.289957726(8) | 0.29078822(2) | 0.29175856(3) |
| | $4s - 1s$ | | | | | |
| Lead | | 0.312542251722 | 0.312795865525 | 0.313129873756 | 0.313519935279 | 0.313951042166 |
| F_3 | | 0.000052358450 | 0.000202772029 | 0.000443363221 | 0.000768038994 | 0.001171895758 |
| F_4 | | 8.348329×10^{-8} | 6.226729×10^{-7} | 1.982136×10^{-6} | 4.463102×10^{-6} | 8.322636×10^{-6} |
| Total | | 0.3125946937(3) | 0.312999260(3) | 0.313575219(8) | 0.31429244(2) | 0.31513126(3) |

TABLE VII. The fit of the coefficients $\Delta A_{60}(n)$ for the S states and $A_{60}(n)$ for the $P_{1/2}$ states to the functions $A_{60}(n) = \sum_{i=0}^k C_i/n^i$ for different values of k . For each k the first row stands for the S states and the second for the $P_{1/2}$ states. The numbers in brackets for each coefficient C_i and k stand for the difference between the results for k and $k - 1$. This serves as an estimate of the uncertainty of the result.

| k | C_0 | C_1 | C_2 | C_3 | C_4 |
|-----|--------------|-------------|----------|-----------|-------|
| 3 | 0.0644(386) | -3.670(733) | 3.5 | | |
| | -1.2425(121) | -0.088(231) | 1.1 | | |
| 4 | 0.0654(11) | -3.699(29) | 3.72(26) | -0.76 | |
| | -1.2428(2) | -0.081(6) | 1.04(6) | 0.17 | |
| 5 | 0.0656(1) | -3.703(4) | 3.78(6) | -1.07(31) | 0.65 |
| | -1.2429(1) | -0.076(5) | 0.97(7) | 0.57(39) | -0.83 |

TABLE VIII. The results for the normalized difference $ns - 1s$, $n = 2-4$, for strong Coulomb fields, $Z = 10-50$ obtained by means of the RME and other methods. “Lead” stands for the first two multipoles, $F_1 + F_2$. “Other” stands for the results taken from Ref. [15] for $Z = 10$ and $n = 2$, from Ref. [16] for $Z > 10$ and $n = 2$, and from Ref. [17] for $n = 3$ and 4.

| Term | State | $Z = 10$ | $Z = 20$ | $Z = 30$ | $Z = 40$ | $Z = 50$ |
|-------|-----------|--------------|-------------|--------------|--------------|--------------|
| | $2s - 1s$ | | | | | |
| Lead | | 0.23701763 | 0.2488452 | 0.2619688 | 0.2750076 | 0.286348 |
| F_3 | | 0.00319454 | 0.0112895 | 0.0241665 | 0.0433987 | 0.072537 |
| F_4 | | 0.00004031 | 0.0002495 | 0.0007118 | 0.0014503 | 0.002181 |
| Total | | 0.2402525(2) | 0.260384(1) | 0.28685(1) | 0.3199(7) | 0.361(1) |
| Other | | 0.2402825(6) | 0.260392(2) | 0.2868234(7) | 0.3196008(7) | 0.3600634(7) |
| | $3s - 1s$ | | | | | |
| Lead | | 0.29422885 | 0.3026260 | 0.3109028 | 0.3174785 | 0.320080 |
| F_3 | | 0.00396535 | 0.0140854 | 0.0301636 | 0.0540166 | 0.089915 |
| F_4 | | 0.00005088 | 0.0003186 | 0.0009121 | 0.0018445 | 0.002654 |
| Total | | 0.2982451(2) | 0.317030(1) | 0.34198(1) | 0.3733(9) | 0.413(1) |
| Other | | 0.2982(2) | 0.3170(2) | 0.3420(2) | 0.3731(2) | 0.4114(2) |
| | $4s - 1s$ | | | | | |
| Lead | | 0.31643820 | 0.3216252 | 0.3255893 | 0.3267328 | 0.322514 |
| F_3 | | 0.00426010 | 0.0151522 | 0.0324072 | 0.0578502 | 0.095876 |
| F_4 | | 0.00005539 | 0.0003475 | 0.0009926 | 0.0019940 | 0.002808 |
| Total | | 0.3207537(2) | 0.337125(1) | 0.35899(1) | 0.3866(9) | 0.421(1) |
| Other | | 0.3207(2) | 0.3371(2) | 0.3590(2) | 0.3863(2) | 0.4199(2) |

results for $Z = 20$ obtained by the RME are of similar (for $n = 2$) or greater (for $n = 3$ and 4) accuracy than those obtained by the PWE [16,17]. It can be seen from Table VIII that for $Z > 20$ we are out of the perturbative region. Obviously, the convergence of the method slows down. Nonetheless, for the higher excited states the accuracy of both the RME and the PWE is similar up to $Z = 40$.

Finally, we compared the PWE results obtained in Ref. [11] for $Z < 6$ and nS states, $n = 2-4$, to both the $Z\alpha$ expansion and the RME. We tried to fit the results obtained in Ref. [11], presented here for each n in the third rows of Table I, to the series (4), see for each n the third rows in Table IV. This fit clearly shows that the accuracy of the results obtained in Ref. [11] is not sufficient for reliable extraction of the coefficients of the expansion (4). First, the agreement between the value of the coefficient A_{60} obtained directly and the value obtained by the fit is not impressive at all and it goes down with increasing the excitation. Second, with near certainty we can exclude the possibility that the coefficient A_{70} behaves as that displayed for given n in the third rows of Table IV. The known coefficients in Eqs. (3) and (4) always change only mildly with increasing the excitation even for low excitations [18].

On the other hand, comparison between the second and the third rows for each n in Table I shows that the agreement between the exact form of the RME and the PWE is good and estimates of the error made in Ref. [11] are correct.

To clarify this observation we tried to fit the exact RME results to the series (4) with less and less digits. We found that the results displayed for each n in the second rows of Table IV are relatively stable up to nine digit accuracy of the RME result. If less accuracy is allowed then the results of the fit blow up, much in the same way as in the third rows of Table IV. For this reason, the results displayed for each n in

the first two rows of Table I are presented to more digits than is the actual accuracy of our results. Compare for each n the second rows in Table I with the results displayed in Table VI under the heading “Total.”

This analysis shows that for reliable extraction of the coefficients of the series (4) from the numerical results a rather high accuracy of the latter is required.

IV. CONCLUSIONS

The approximate version of the RME given in Ref. [12] can be used for the extraction of the A_{60} coefficient. The nonperturbative information contained in it for the state-dependent part of the S states is, in contrast to the non- S states, not useful. It yields a value of the A_{70} coefficient that is too wrong.

The accuracy of the exact version of the RME for determination of the one-loop self-energy for the normalized difference of the S states for $Z < 20$ exceeds the accuracy of any other method. In the case of hydrogen the uncertainty of this calculation is significantly less than 1 Hz. This is more than enough to match the accuracy of the experiment [4]. We find it remarkable to achieve such an accuracy with four one-dimensional numerical integrations [14]. Further extension of the RME to the calculation of two-loop corrections (e.g., Ref. [8]) and few-electron atoms (e.g., Ref. [20]) thus seems to be highly desirable.

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- [18] There is a possibility that the remainder function $G(Z\alpha)$ does not behave according to Eq. (4). However, this is not very likely. First, the integrals appearing in the RME do not have for the normalized difference of the S states and the P states nonanalyticity in $Z\alpha$ worse than that given by Eqs. (3) and (4). This is nicely illustrated by the results displayed in Tables IV and V. See also the Appendix of Ref. [19] for a somewhat incomplete elaboration of this point. Second, once the renormalization of the electron mass is made, every term of the RME yields automatically the finite results [14]. Further, the RME is a convergent expansion even for the state-independent part of the S states [14]. For the state-dependent part of the S states the situation can only be better. Therefore, nothing essential is missed by the RME and there is no reason to expect that Eq. (4) is incorrect.
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