Two-loop QED corrections in few-electron ions

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Results of a calculation valid to all orders in the nuclear-strength parameter $Z\alpha$ are presented for the two-loop Lamb shift, notably for the two-loop self-energy correction, for the ground and first excited states of ions with the nuclear charge numbers $Z = 60-100$. A detailed comparison of the all-order calculation with earlier investigations based on an expansion in the parameter $Z\alpha$ is given. The calculation removes the largest theoretical uncertainty for the $2p_j-2s$ transition energies in heavy Li-like ions and is important for interpretation of experimental data.

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I. INTRODUCTION

Measurements of the $2p_j-2s$ transition energies in heavy Li-like ions [1, 2, 3, 4] have lately reached a fractional accuracy of 0.03% with respect to the total QED contribution. This corresponds to a 10% sensitivity of the experimental results to the two-loop QED effects. These measurements provide an excellent possibility for identification of the two-loop Lamb shift and for testing the bound-state QED theory up to second order in $\alpha$ in the strong-field regime. Adequate interpretation of experimental data requires theoretical investigations of the two-loop QED effects valid to all orders in the nuclear-strength parameter $Z\alpha$.

All-order calculations of the two-loop QED effects and, first of all, the two-loop self-energy correction are important also for low-$Z$ ions because of a very slow convergence of the corresponding $Z\alpha$ expansion. The higher-order (in $Z\alpha$) two-loop QED effects presently yield the second largest uncertainty in the theoretical prediction for the ground-state Lamb shift in hydrogen (after the proton charge distribution effect). Improved theoretical results for the $1s$ and $2s$ Lamb shift will be required in the near future for a more precise determination of the Rydberg constant, when an improved value for the proton charge radius is obtained from the muonic hydrogen experiment.

The complete set of two-loop one-electron QED corrections (also referred to as the two-loop Lamb shift) is graphically represented in Fig. 1. In this investigation, we will be mainly concerned with the two-loop self-energy correction represented by diagrams (a)-(c), which will be evaluated rigorously to all orders in $Z\alpha$. The other diagrams in Fig. 1 will be calculated as well; diagrams (d)-(g), rigorously and diagrams (h)-(k), within the free-loop approximation, i.e., keeping the leading term of the expansion of fermion loops in terms of the binding potential. In the one-loop case, the free-loop approximation corresponds to the Uehling potential and yields the dominant contribution even for high-$Z$ ions like uranium. We assume that the free-loop approximation is reasonably adequate in the two-loop case also.

II. TWO-LOOP SELF-ENERGY

The two-loop self-energy correction to the energy shift is conveniently represented in terms of the dimensionless function $F(Z\alpha)$ defined (in relativistic units $\hbar = c = 1$) by

$$\delta E = m \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^4}{n^3} F(Z\alpha),$$

where $n$ is the principal quantum number. The $Z\alpha$ expansion of the function $F$ reads

$$F(Z\alpha) = B_{40} + (Z\alpha) B_{50} + (Z\alpha)^2 \left[ L^3 B_{63} + L^2 B_{62} + L B_{61} + G^{\alpha\alpha}(Z\alpha) \right],$$

where $L = \ln[(Z\alpha)^{-2}]$ and $G^{\alpha\alpha}$ is a non-perturbative remainder whose expansion starts with a constant, $G^{\alpha\alpha}(Z\alpha) = B_{60} + Z\alpha (\cdots)$. The leading term in Eq. (2), $B_{40}$, is related to the free-electron form-factors and is known for a long time. Its first complete evaluation was reported in [6]. The next term $B_{50}$ was calculated only relatively recently by Pachucki [7] and by Eides and Shelyuto [8]. The result for the leading logarithmic contribution, $B_{63}$, was first reported in [9]. A considerable discussion about the correctness of the method of derivation followed this publication (see [10] and references therein). Finally, this result was rigorously re-derived by Pachucki in [11]. In that work, Pachucki also derived the remaining logarithmic terms for $ns$ states, $B_{62}(ns)$ and $B_{61}(ns)$. An additional contribution to the coefficient $B_{61}(1s)$ was recently identified and evaluated in [12]. The coefficient $B_{62}$ for $np$ states was calculated in [13]. The values of $B_{61}$ for states with $l \geq 1$ as well as the differences
B_{60}(ns) - B_{60}(1s) and B_{60}(np_j) - B_{60}(np_j) were recently presented in [12]. There are no complete results available at present for the coefficient B_{60} for single states. However, its non-relativistic part b_L (also termed as the two-loop Bethe logarithm) was calculated for 1s and 2s states in [14] and later for higher excited states in [15, 16]. This part presumably yields the dominant contribution to B_{60}; the uncertainty due to uncalculated terms was estimated in [14] to be 15% for the 1s and 2s states.

The summary of the results available for the Zα-expansion coefficients of the two-loop self-energy correction reads

\[
\begin{align*}
B_{40} & = \left[ -\frac{163}{72} - \frac{85}{216} \pi^2 + \frac{3}{2} \frac{\pi^2}{2} \ln 2 - \frac{9}{4} \zeta(3) \right] \delta_{l0} \\
& \quad - \left[ -\frac{31}{16} + \frac{5}{27} \pi^2 - 2 \frac{1}{2} \frac{\pi^2}{2} \ln 2 + \frac{3}{4} \zeta(3) \right] \frac{1}{\kappa (2I + 1)} , \\
B_{50} & = -24.2668 (31) \delta_{l0} , \\
B_{63} & = -\frac{8}{27} \delta_{l0} , \\
B_{62}(ns) & = \frac{16}{9} \left( \frac{13}{12} - \ln 2 + \frac{1}{4n^2} - \frac{1}{n} - \ln n + \psi(n) + C \right) , \\
B_{62}(np) & = \frac{4}{27} \frac{n^2 - 1}{n^2} , \\
B_{62}(nd) & = 0 , \\
B_{61}(ns) & = \left( \frac{15473}{2592} + \frac{1039}{432} \pi^2 - \frac{152}{27} \ln 2 - \frac{2}{3} \pi^2 \ln^2 2 + \frac{40}{9} \ln^2 2 + \zeta(3) + \frac{4}{3} N(ns) \right) \\
& \quad + \left( \frac{80}{27} - \frac{32}{9} \ln 2 \right) \left( \frac{1}{4n^2} - \frac{1}{n} \right) - \ln n + \psi(n) + C , \\
B_{61}(np_{1/2}) & = \frac{4}{3} N(np) + \frac{n^2 - 1}{n^2} \left( \frac{38}{81} - \frac{8}{27} \ln 2 \right) , \\
B_{61}(np_{3/2}) & = \frac{4}{3} N(np) + \frac{n^2 - 1}{n^2} \left( \frac{11}{81} - \frac{8}{27} \ln 2 \right) , \\
B_{61}(nd) & = 0 ,
\end{align*}
\]

FIG. 1: Two-loop one-electron QED corrections. Gauge-invariant subsets are referred to as SESE (a-c), SEVP (d-f), VPVP (g-i), S(VP)E (k).
\[ B_{60}(ns) = b_L(ns) + \frac{10}{9} N(ns) + \ldots, \]  
\[ B_{60}(np) = b_L(np) + \ldots, \]  
where \( \kappa \) is the Dirac angular-momentum quantum number, \( l \) is the orbital quantum number, \( l = |\kappa + 1/2| - 1/2 \), \( \zeta(n) \) is the Riemann zeta function, \( \psi(n) \) is the logarithmic derivative of the gamma function, \( C \) is the Euler constant, and \( (\ldots) \) denotes uncalculated terms. Complete results are available for the differences of the coefficients \( B_{60} \) [12]. In particular,

\[ B_{60}(2s) - B_{60}(1s) = b_L(2s) - b_L(1s) + 0.318486, \]  
\[ B_{60}(2p_{3/2}) - B_{60}(2p_{1/2}) = -0.361196. \]  
Accurate numerical values for the function \( N(nl) \) were obtained in [12, 17]. For the states with \( n = 1 \) and 2, they are given by

\[ N(1s) = 17.85567203(1), \]  
\[ N(2s) = 12.03214158(1), \]  
\[ N(2p) = 0.003300635(1). \]  
The two-loop Bethe logarithms for these states are [14, 16]:

\[ b_L(1s) = -81.4(3), \]  
\[ b_L(2s) = -66.6(3), \]  
\[ b_L(2p) = -2.2(3). \]  
We note that the formulas (10), (11) for the two-loop self-energy correction were obtained from the full two-loop results in [12] by subtracting the contribution due to diagrams with closed fermion loops, which is [18]

\[ B_{60}(np, VP) = -\frac{8}{135} \frac{n^2 - 1}{n^2}. \]  
We now turn to our calculation of the two-loop self-energy correction to all orders in \( Z \alpha \). The starting point of our consideration is the Furry picture, where the interaction of an electron with the nucleus is taken into account to all orders right from the beginning. As a consequence of this choice, we have to deal with the bound-electron propagators, whose structure is much more complicated than that of the free-electron propagators. A method for the evaluation of the two-loop self-energy correction was developed for the ground state in our previous studies [19, 20]. In the present investigation, we extend it to the excited states. The general procedure for isolation and cancelation of ultraviolet and infrared divergences is similar to that for the complicated than that of the free-electron propagators. A method for the evaluation of the two-loop self-energy correction was developed for the ground state in our previous studies [19, 20]. In the present investigation, we extend it to the excited states. The general procedure for isolation and cancelation of ultraviolet and infrared divergences is similar to that for the single state, but the actual calculational scheme requires substantial modifications due to a more complicated pole and angular-momentum structure of expressions involved. Details of our calculation are cumbersome and will be published elsewhere; in this paper we concentrate on presentation and analysis of the results obtained and discuss their experimental consequences.

We performed our all-order calculations of the two-loop self-energy correction for the \( 1s, 2s, 2p_{1/2}, \) and \( 2p_{3/2} \) states of ions with \( Z = 60, 70, 83, 92 \) and 100. The results can be conveniently expressed in terms of the higher-order remainder \( G^{h.o.} \) defined by Eq. (2). The values of the remainder as a function of \( Z \) are plotted in Fig. 2 for the \( 1s \) and \( 2s \) states and in Fig. 3 for the \( 2p_{1/2} \) and \( 2p_{3/2} \) states. The results for the \( 1s \) state and \( Z < 60 \) are taken from our previous investigation [20] (the points with \( Z = 10 \) and 15 are omitted because of large numerical uncertainty). We present separate graphs for individual states and for the differences \( \Delta_{s}^{h.o.} = G^{h.o.}(2s) - G^{h.o.}(1s) \) and \( \Delta_{p}^{h.o.} = G^{h.o.}(2p_{3/2}) - G^{h.o.}(2p_{1/2}) \). On the ordinate axis of the graphs, the limiting values of the higher-order remainder at \( Z = 0 \) are indicated, as obtained within the \( Z \alpha \)-expansion approach. The status of these limiting values is different for single states and for the differences \( \Delta_{s}^{h.o.} \) and \( \Delta_{p}^{h.o.} \). For the single states, the limiting values represent incomplete results for the coefficients \( B_{60} \) given by Eqs. (12) and (14). The error bars indicated for the \( 1s \) and \( 2s \) states correspond to the 15% uncertainty suggested in [14]. For \( 2p \) states, the uncertainty is undefined, although it is believed to be significantly smaller than the two-loop Bethe logarithm. For the differences \( \Delta_{s}^{h.o.} \) and \( \Delta_{p}^{h.o.} \), the limiting values are known much better and given by Eqs. (15) and (16).

Characterizing the comparison presented in Fig. 2 we observe that our all-order results do not seem to agree well with the theoretical results to order \( \alpha^2(Z \alpha)^6 \) for \( 1s \) and \( 2s \) states separately whereas a rather good agreement is found for the difference \( \Delta_{s}^{h.o.} \). For the \( 2p_{3} \) states presented in Fig. 3 the situation is even less definite, due to smaller numerical values of the higher-order remainder function. But we again observe that agreement for the differences \( \Delta_{s}^{h.o.} \) is much better than for the single states. It should be mentioned that the agreement observed for the differences is a valuable evidence in favor of reliability of our all-order results. The reason is that numerical evaluations for different single states are completely independent and individual contributions, e.g., to the functions \( F(1s) \) and \( F(2s) \) are even of different orders of magnitude. It is thus very unlikely that a contribution appears in numerical evaluations that vanishes identically in the difference, which is contrary to the situation in the \( Z \alpha \)-expansion calculations.
FIG. 2: The higher-order remainder function $G^{\cdot\cdot}(1s)$ for the $1s$ and $2s$ states (dots and squares on the left graph, respectively) and for the difference $\Delta_{h.o.}(1s)$ (the right graph).

FIG. 3: The higher-order remainder function $G^{\cdot\cdot}(2p_{1/2})$ for the $2p_{1/2}$ state (the left upper graph), $2p_{3/2}$ state (the right upper graph), and for the difference $\Delta_{h.o.}(2p_{3/2})$ (the lower graph).
TABLE I: Individual contributions to the $2p_{3/2}$-$2s$ and $2p_{1/2}$-$2s$ transition energies in Li-like bismuth and uranium, in eV.

|                  | $2p_{3/2}$-$2s$, $Z = 83$ | $2p_{1/2}$-$2s$, $Z = 92$ |
|------------------|----------------------------|----------------------------|
| Dirac value      | 2792.21 (3)                | −33.27 (9)                 |
| One-photon exchange | 23.82                    | 368.83                     |
| Two-photon exchange | −1.61                    | −13.37                     |
| Three-photon exchange | −0.02 (2)               | 0.15 (7)                   |
| One-loop QED      | −27.48                    | −42.93                     |
| Screened QED      | 1.15 (4)                  | 1.16 (3)                   |
| Two-loop QED      |                           |                            |
| SESE             | 0.15                      | 0.30                       |
| SEVP             | −0.10                     | −0.19                      |
| VPVP (g)         | 0.02                      | 0.04                       |
| VPVP (h,i)       | 0.07 (3)                  | 0.10 (5)                   |
| S(VP)E           | −0.01 (2)                 | −0.02 (5)                  |
| Recoil           | −0.07                     | −0.07                      |
| Nuclear polarization |                        | 0.04 (2)                   |
| Total theory     | 2788.12 (7)               | 280.76 (14)                |
| Experiment       | 2788.14 (4) [2]          | 280.645 (15) [4]          |
                                        |                           | 280.516 (99) [3]          |
                                        |                           | 280.59 (10) [1]           |

Assuming correctness of both the all-order and the $Z\alpha$-expansion calculation, we can surmise two possible explanations of the situation observed. The first possibility is that uncalculated contributions to the coefficients $B_{00}$ for single states are larger than previously expected and, when calculated, they will shift the limiting values $G^{h,\alpha}(Z = 0)$ in Figs. 4 and 5 considerably. The second possibility is that remarkably large logarithmic terms appear in the $Z\alpha$ expansion to order $\alpha^2(Z\alpha)^2$ and induce a very rapidly varying structure in the $Z$ dependence of the remainder $G^{\alpha,\alpha}(Z)$ in the low-$Z$ region. The both scenarios will have a significant influence on the theoretical values of the higher-order two-loop QED effects for the 1s and 2s states in hydrogen.

### III. TWO-LOOP LAMB SHIFT IN LI-LIKE IONS

The best opportunity for experimental identification of the two-loop QED effects in the strong binding field is presently offered by measurements of the $2p_{1/2}$-2s transition energies in Li-like ions. In this work, we present results of our calculations of all two-loop corrections depicted in Fig. 1 for the $2p_{3/2}$-2s transition in Bi$^{82+}$ and the $2p_{1/2}$-2s transition in U$^{92+}$, for which most accurate experimental data are available. Numerical results for individual subsets of diagrams defined in Fig. 1 are presented in Table II under the entry “Two-loop QED”. The SESE subset represents the two-loop self-energy correction, which is the main result of our investigation. The SEVP(d-f) diagrams and the VPVP(g) diagram were calculated to all orders in $Z\alpha$ without any approximations involved, whereas the VPVP(h,i) and S(VP)E diagrams were evaluated within the free-loop approximation, i.e., keeping the first nonvanishing contribution in the expansion of the fermion loops in terms of the binding potential. The error bars specified for these corrections are estimations of uncertainty due to the approximation employed. They were obtained by multiplying the contribution of diagrams (h,i) by a factor of $(Z\alpha)^2$ and that of diagram (k) – by a factor of 3 $(Z\alpha)$. The factor of 3 $(Z\alpha)$ in the latter estimation arises as a ratio of the leading-order contribution beyond the free-loop approximation for the diagram (k), $-0.386\,\left(\alpha/\pi\right)^2(Z\alpha)^5$ [21], and the leading-order contribution within this approximation, $0.142\,\left(\alpha/\pi\right)^2(Z\alpha)^4$ [22]. The finite nuclear size effect was taken into account in our evaluation of the diagrams (d)-(i), whereas the other diagrams were calculated for the point nuclear model. In the case of uranium, our results for the diagrams with closed fermion loops are in good agreement with those reported previously [23][24][25][26].

We now explain the other theoretical contributions to the transition energies presented in Table II. The entry labeled “Dirac value” represents the transition energies as obtained from the Dirac equation with the nuclear potential induced by the standard two-parameter Fermi nuclear-charge distribution. Numerical values for the nuclear-charge root-mean-square (rms) radii were taken from [27], $<r^2>^{1/2} = 5.851(7)$ Fm for uranium and $5.521(3)$ Fm for bismuth. The dependence of the Dirac value on the nuclear model was conservatively estimated by comparing the results obtained within the Fermi and the homogeneously-charged-sphere models, as first suggested in [28]. We have checked that a wide class of more general models for the nuclear-charge distribution yields results well within the error bars obtained in this way.

The next 3 lines contain the corrections due to the one-, two-, and three-photon exchange, respectively. QED values for the two-photon exchange correction were taken from our previous evaluations [29][30]. The results for the three-photon exchange...
correction were obtained in this work within many-body perturbation theory (MBPT), with retaining the Breit interaction to the first order only. For uranium, we report good agreement with the previous evaluations of this effect \cite{31,32}. The error ascribed to the three-photon exchange correction is due to incompleteness of the MBPT treatment. It was estimated by calculating the third-order MBPT contribution with two and more Breit interactions for each state involved in the transition, adding these contributions quadratically, and multiplying the result by a conservative factor of 2.

The entry labeled “One-loop QED” represents the sum of the first-order self-energy and vacuum-polarization corrections calculated on hydrogenic wave functions \cite{33}. The next line (“Screened QED”) contains the results for the screened self-energy and vacuum-polarization corrections \cite{34,35,36}. The uncertainty ascribed to this entry is the estimation of higher-order screening effects; it was obtained by multiplying the correction by the ratio of the entries “Screened QED” and “One-loop QED”. The last two lines contain the values for the relativistic recoil correction \cite{37,38} and the nuclear polarization correction \cite{39,40}.

The comparison presented in Table I demonstrates that our total results agree well within the error bars specified with the experimental data for bismuth and uranium. The theoretical accuracy is significantly better in the former case, which is the consequence of the fact that the finite nuclear size effect is smaller and the nuclear radius is known better. Our result for the $2p_{3/2}$-$2s$ transition in bismuth can also be compared with the value of 2787.96 eV obtained by Sapirstein and Cheng \cite{41}. The difference of 0.16 eV between the results is mainly due to the two-loop Lamb shift contribution (0.12 eV) which is not accounted for in Ref. \cite{41}. We conclude that inclusion of the two-loop Lamb shift is necessary for adequate interpretation of the experimental result in the case of bismuth, whereas for uranium the two-loop Lamb shift is significantly screened by the uncertainty due to the nuclear charge distribution. Comparison of the theoretical and experimental results for bismuth yields the first identification of the two-loop QED effects in the region of strong binding field, which is a step toward the test of the strong-field regime of bound-state QED at the two-loop level.

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