Screened self-energy correction to the $2p_{3/2}$-$2s$ transition energy in Li-like ions.

V. A. Yerokhin,1,2 A. N. Artemyev,2,3 V. M. Shabaev,2,3 G. Plunien,3 and G. Soff3

1 Center for Advanced Studies, St. Petersburg State Polytechnical University,
   Polytekhnicheskaya 29, St. Petersburg 195251, Russia
2 Department of Physics, St. Petersburg State University,
   Oulianovskaya 1, Petrodvorets, St. Petersburg 198504, Russia
3 Institutfür Theoretische Physik, TU Dresden,
   Mommsenstraße 13, D-01062 Dresden, Germany

Abstract

We present an ab initio calculation of the screened self-energy correction for $(1s)^22p_{3/2}$ and $(1s)^22s$ states of Li-like ions with nuclear charge numbers in the range $Z = 12-100$. The evaluation is carried out to all orders in the nuclear-strength parameter $Z\alpha$. This investigation concludes our calculations of all two-electron QED corrections for the $2p_{3/2}$-$2s$ transition energy in Li-like ions and thus considerably improves theoretical predictions for this transition for high-$Z$ ions.

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**Introduction**

Recent progress in high-precision spectroscopy of highly charged ions has attracted significant attention to these systems. Accurate experimental determination of energy levels is nowadays possible for very heavy ions of the periodical table up to H-like uranium. Such systems provide a unique testing ground for quantum electrodynamics (QED) in a strong field of the nucleus. While the simplicity of the hydrogen isoelectronic sequence makes it ideal for theoretical investigations, the achieved experimental accuracy is by far better in few-electron systems. In particular, the Lamb shift in H-like uranium is presently known at the 3% level \[1\], whereas the \(2p_{3/2}-2s\) splitting in Li-like bismuth was measured to be

\[E_{2p_{3/2}} - E_{2s} = 2788.139(9) \text{ eV},\]  

where the QED correction, which is about 26 eV, can be (in principle) tested at the 0.15% level. Very high experimental accuracy is also achieved for \(2p_{3/2}-2s\) and \(2p_{1/2}-2s\) transitions in other heavy Li-like ions \[2, 3, 4, 5\].

In order to match the experimental accuracy for Li-like ions in theoretical investigations, rigorous calculations of all QED effects to second order in the fine structure constant \(\alpha\) are needed. Characteristic property of heavy ions is that the nuclear-strength parameter \(Z\alpha\) can not be used as an expansion parameter in theoretical considerations, which corresponds to the non-perturbative (in \(Z\alpha\)) regime of the bound-state QED. On the other hand, the electron-electron interaction in heavy ions can be accounted for by a rapidly-converging perturbation expansion in the parameter \(1/Z\). In our approach, we start in zeroth approximation with non-interacting electrons propagating in the external field of the nucleus (the Furry picture). Corrections to this approximation arise from exchanges by one, two, and more virtual photons. For corrections involving one and two virtual photons, we employ a rigorous QED treatment complete to all orders in the parameter \(Z\alpha\). Higher-order corrections can not be addressed within bound-state QED at present. This part should be, therefore, evaluated within the standard approach based on the no-pair Dirac-Breit Hamiltonian.

Such project was carried out for the \(2p_{1/2}-2s\) transition of Li-like ions in a series of our investigations \[6, 7, 8, 9, 10\]. Comparison of the total theoretical value obtained for the Li-like uranium \[7, 8\] with the corresponding experimental results \[2, 4\] probes QED effects of second order in \(\alpha\) on the level of about 17%. This is the strictest test of predictions of...
bound-state QED in the background of a strong external field at the moment. Our present
goal is to perform a similar project for the $2p_{3/2}-2s$ transition energy in Li-like ions. For one
specific ion, Li-like bismuth, analogous calculation was carried out previously by Sapirstein
and Cheng [11].

The leading ($\sim 1/Z^0$) QED effect in Li-like ions is the one-loop self-energy and vacuum-
polarization corrections. Their calculation can be considered as well established at present
(see, e.g., review [12] and references therein). Other important QED effects are those of
order $1/Z$, the screened self-energy and vacuum-polarization corrections and the two-photon
exchange correction. The screened vacuum-polarization correction for $n = 1$ and $n = 2$ states
of Li-like ions was evaluated previously in Ref. [6]. The two-photon exchange correction was
obtained in Refs. [7, 8] for the $2s$ and $2p_{1/2}$ states and in Refs. [13, 14] for the $2p_{3/2}$ state. An
independent evaluation of the two-photon exchange correction for Li-like ions was performed
by Andreev et al. [15, 16]. A calculation of the screened self-energy correction was carried
out in Ref. [9] for the $2s$ and $2p_{1/2}$ states. The goal of the present investigation is to perform
an evaluation of the screened self-energy correction for the $2p_{3/2}$ state of Li-like ions, which
concludes the calculation of all QED corrections of order $1/Z$ for the $2p_{3/2}-2s$ transition.
The remaining QED effect that involves two virtual photons is the one-electron two-loop
QED correction. Its calculation to all order to $Z\alpha$ is presently performed for the $1s$ state
only [17, 18]. In this work, we present an estimation for this correction based on known
terms of the $Z\alpha$ expansion and on the full result for the $1s$ state.

The paper is organized as follows. In Sec. I we describe general formulas for the screened
self-energy correction for a Li-like ion. A brief discussion of the renormalization of the
formal expressions is given. In Sec. II we present the results of our numerical evaluation.
Various theoretical contributions to the $2p_{3/2}-2s$ transition energy are collected in Sec. III.
Theoretical predictions obtained for the total transition energy are compared with results
by other authors and experimental data. The relativistic units ($\hbar = c = m = 1$) are used
throughout the paper.

I. BASIC FORMULAS

The screened self-energy correction is graphically represented by Feynman diagrams
shown in Fig. I. The detailed derivation of formal expressions for this correction can be
found in Ref. [9], where it was obtained by the two-time Green function method developed by Shabaev (see Ref. [19] for the description of the method). Here, we present only the final expressions for the screened self-energy correction due to the interaction of the valence electron with the $(1s)^2$ shell.

The contribution of diagrams in Fig. 1(a) is conveniently divided into the reducible and irreducible parts. The reducible part is a contribution in which the energy of the total intermediate state of the system coincides with the initial (final) energy of the system, and the irreducible part is the remainder. The irreducible part can be expressed in terms of non-diagonal matrix elements of the one-loop self-energy operator $\Sigma$,

$$\Delta E_{\text{ir}} = 2 \sum_{\mu_c} \left[ \langle c | \Sigma(\varepsilon_c) | \delta c \rangle + \langle v | \Sigma(\varepsilon_v) | \delta v \rangle \right],$$  \hspace{1cm} (2)

where $c$ and $v$ label the core and the valence electron, respectively; $\mu_c$ is the momentum projection of the core electron, the factor of 2 accounts for two equivalent diagrams, the self-energy operator is defined by

$$\Sigma(\varepsilon, x_1, x_2) = 2i \alpha \int_{-\infty}^{\infty} d\omega D^{\mu\nu}(\omega, x_{12}) \alpha_\mu G(\varepsilon - \omega, x_1, x_2) \alpha_\nu,$$  \hspace{1cm} (3)

$G$ is the Dirac-Coulomb Green function $G(\varepsilon) = (\varepsilon - H(1 - i0))^{-1}$, $H$ is the Dirac-Coulomb Hamiltonian, $D^{\mu\nu}$ is the photon propagator, $\alpha^\mu = (1, \alpha)$ are the Dirac matrices, and $x_{12} = x_1 - x_2$. The modified wave functions $|\delta c\rangle$ and $|\delta v\rangle$ in Eq. (2) are the first-order perturbations of the initial wave functions $|c\rangle$ and $|v\rangle$ due to the electron-electron interaction:

$$|\delta c\rangle = \sum_n^{\varepsilon_n \neq \varepsilon_c} \frac{|n\rangle}{\varepsilon_c - \varepsilon_n} \sum_P (-1)^P \langle P c P v | I(\Delta) | cv \rangle,$$  \hspace{1cm} (4)

$$|\delta v\rangle = \sum_n^{\varepsilon_n \neq \varepsilon_v} \frac{|n\rangle}{\varepsilon_v - \varepsilon_n} \sum_P (-1)^P \langle P c P v | I(\Delta) | cn \rangle,$$  \hspace{1cm} (5)

where $I$ is the operator is the electron-electron interaction,

$$I(\omega) = e^2 \hat{\alpha}_\mu \hat{\alpha}_\nu D^{\mu\nu}(\omega),$$  \hspace{1cm} (6)

$P$ is the permutation operator $[\langle PcPv | = (cv), (vc)]$, and $\Delta = \varepsilon_{Pc} - \varepsilon_c$.

The reducible part is given by

$$\Delta E_{\text{red}} = \sum_{\mu_c} \left\{ \sum_P (-1)^P \langle P c P v | I(\Delta) | cv \rangle \left[ \langle c | \Sigma'(\varepsilon_c) | c \rangle + \langle v | \Sigma'(\varepsilon_v) | v \rangle \right] \\
+ \langle vc | I'(\Delta) | cv \rangle \left[ \langle c | \Sigma(\varepsilon_c) | c \rangle - \langle v | \Sigma(\varepsilon_v) | v \rangle \right] \right\},$$  \hspace{1cm} (7)
where $I'(\Delta) = d/(d\omega)I(\omega)|_{\omega=\Delta}$, $\Sigma'(\epsilon_i) = d/(d\epsilon)\Sigma(\epsilon)|_{\epsilon=\epsilon_i}$.

The contribution of the diagrams in Fig. 1(b) is referred to as the vertex part and is given by

$$\Delta E_{\text{ver}} = \sum_{\mu c} \sum_P (-1)^P \sum_{n_1n_2} \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \begin{pmatrix} \langle n_1 P | I(\Delta) | n_2 \rangle \langle P c n_1 | I(\omega) | n_1 c \rangle \\ (\epsilon_{P c} - \omega - u\epsilon_{n_1})(\epsilon_{c} - \omega - u\epsilon_{n_2}) \end{pmatrix} + \begin{pmatrix} \langle P c n_1 | I(\Delta) | c n_2 \rangle \langle P v n_2 | I(\omega) | n_1 v \rangle \\ (\epsilon_{P v} - \omega - u\epsilon_{n_1})(\epsilon_{v} - \omega - u\epsilon_{n_2}) \end{pmatrix},$$

(8)

where $u = 1 - i0$ ensures the correct position of poles of the electron propagators with respect to the integration contour.

The total self-energy correction to the interaction of the valence electron with the $(1s)^2$ shell is given by the sum of the irreducible, reducible, and vertex parts:

$$\Delta E_{\text{scr.se.}} = \Delta E_{\text{ir}} + \Delta E_{\text{red}} + \Delta E_{\text{ver}}.$$

(9)

The formulas presented so far are only the formal expressions and suffer from ultraviolet (UV) and infrared (IR) divergences that should be explicitly eliminated before the numerical calculation can be started. We note that the irreducible part given by Eq. (2) is expressed in terms of non-diagonal matrix elements of the one-loop self-energy operator and, therefore, can be calculated by a straightforward generalization of a scheme developed for the first-order self-energy correction. The method used for this in the present investigation is based on an expansion of the bound-electron propagator in terms of the interaction with the nuclear Coulomb field [20]; a detailed description of the numerical procedure is given in Ref. [21]. The second term in the reducible part (7) consists of the first-order self-energy corrections multiplied by a simple expression; the corresponding numerical evaluation is also reduced to a first-order calculation.

The calculation of the remaining part of Eq. (7) and the vertex part (8) is more difficult. These two contributions should be considered together since they contain UV and IR divergences that cancel each other in the sum. In order to separate UV divergences in a covariant way, we separate from the reducible and vertex parts the contribution of free-electron propagators. This contribution is treated in momentum space within the dimensional regularization and the divergences are separated by using the standard technique of free-particle QED. The remainder does not contain any UV divergences and is treated in coordinate space. IR divergences still present in the remainder are separated, regularized
by introducing a finite photon mass, and canceled analytically. The general procedure for handling divergent terms and the proof of their cancellation is described in our previous investigation [21].

II. NUMERICAL CALCULATION AND RESULTS

The calculation of the screened self-energy correction for the \((1s)^2 2p_{3/2}\) state resembles that for other \(n = 2\) states described in our previous work [9]. A higher value of the total momentum of the valence electron \((j_v = 3/2)\) in the present case makes final expressions more lengthy and their numerical evaluation more time consuming. Significant complications appear when performing angular integrations in momentum space for the vertex part with free electron propagators. For this purpose, we developed a generalization of the angular-integration procedure described in Ref. [9] to arbitrary states, using our experience in calculating similar angular integrals for the one-electron two-loop self-energy diagrams [18].

The actual calculation was carried out in the Feynman gauge and taking into account the finite size of the nucleus. The homogeneously-charged spherical-shell model was employed for the nuclear-charge distribution. Our numerical results for the screened self-energy correction due to the interaction of the valence electron with the \((1s)^2\) shell for the \(2s\) and \(2p_{3/2}\) states of Li-like ions are presented in Table II in terms of the dimensionless function \(F(\alpha Z)\) defined as

\[
\Delta E = m \alpha^2 (\alpha Z)^3 F(\alpha Z).
\]

(10)

The results listed for the \(2s\) state are very close to those obtained in our previous investigation [9]. In the present work, we slightly improve the numerical accuracy and extend our calculation to \(Z = 12, 14, \) and 16. In the table, we compare our results with those by Sapirstein and Cheng [11] obtained for one specific case \(Z = 83\). We observe a certain deviation of their numerical values from our results. A similar disagreement is present also for the \(2p_{1/2}\) state [9]. This discrepancy is not resolved at present. We note, however, that our results for \(n = 2\) states of He-like ions [22] (which are strongly related to the correction considered here) agree well with the known terms of the \(Z \alpha\) expansion and that our results for the ground state of He-like ions [23] are in excellent agreement with an independent calculation by Sunnergren [24].
TABLE I: Screened self-energy correction due to the interaction of the valence electron with the 
\((1s)^2\) shell for the 2s and \(2p_{3/2}\) states of Li-like ions, in units of \(F(Z\alpha)\). \(\langle r^2\rangle^{1/2}\) is the root-mean-
square radius expressed in Fermi.

| \(Z\) | \(\langle r^2\rangle^{1/2}\) | 2s       | 2p_{3/2} |
|------|----------------|--------|---------|
| 12   | 3.057          | −0.69667(7) | −0.2104(10) |
| 14   | 3.123          | −0.6491(6)  | −0.1986(9)  |
| 16   | 3.363          | −0.6093(5)  | −0.1884(6)  |
| 18   | 3.427          | −0.5755(5)  | −0.1797(3)  |
| 20   | 3.478          | −0.5466(4)  | −0.1723(3)  |
| 30   | 3.928          | −0.4492(2)  | −0.1480(2)  |
| 40   | 4.270          | −0.3968(2)  | −0.1353(2)  |
| 50   | 4.655          | −0.3693(2)  | −0.1288(2)  |
| 60   | 4.914          | −0.3590(2)  | −0.1261(2)  |
| 70   | 5.317          | −0.3628(1)  | −0.1259(1)  |
| 80   | 5.467          | −0.38103(5) | −0.1276(1)  |
| 83   | 5.533          | −0.38956(3) | −0.1284(1)  |
|      | −0.3908\textsuperscript{a} | −0.1350\textsuperscript{a} |
| 90   | 5.802          | −0.41585(2) | −0.1306(1)  |
| 92   | 5.860          | −0.42526(2) | −0.1314(1)  |
| 100  | 5.886          | −0.47372(2) | −0.1347(1)  |

\textsuperscript{a} Ref. [11].

III. 2P_{3/2}-2S TRANSITION ENERGY IN LI-LIKE IONS

In this section we collect all presently available theoretical contributions to the \(2p_{3/2}-2s\) 
transition energy in Li-like bismuth, thorium, and uranium. Individual corrections for these 
ions are presented in Table II. The Dirac values including the finite-nuclear-size effect were 
obtained by solving the Dirac equation and employing the two-parameter Fermi model for 
the nuclear-charge distribution. Parameters of the Fermi model were expressed in terms 
of the root-mean-square (rms) radii, which numerical values are listed in the table. The 
uncertainty of the nuclear-size effect was evaluated by averaging two errors obtained by
varying the rms radius within the error bars given in the table and by varying the model of the nuclear-charge distribution (the Fermi and the homogeneously-charged-sphere models were employed). The one-photon exchange correction was evaluated utilizing the Fermi model for the nuclear-charge distribution. The one-loop self-energy correction was taken from a tabulation in Ref. [25] for the $2s$ state and from Ref. [26] for $2p_{3/2}$ state. The Uehling part of the one-loop vacuum-polarization correction was calculated in this work for the Fermi nuclear model. The Wichmann-Kroll part of this correction was taken from a tabulation in Ref. [27]. The two-photon exchange correction was evaluated within framework of QED in our previous investigation [13]. Numerical values for the screened self-energy correction are taken from Table I. The screened vacuum-polarization correction was calculated in Ref. [6].

Rigorous calculation of the two-loop QED correction is a challenging problem, which is presently accomplished for the $1s$ state and for $Z \geq 40$ only [17, 18]. For excited states, one has to rely on the $Z\alpha$ expansion, which reads

$$\Delta E_{2\text{loop}} = \frac{m}{\pi^2} \frac{\alpha^2 (Z\alpha)^4}{n^3} \left\{ B_{40} + (Z\alpha)B_{50} + (Z\alpha)^2 \left[ L^3 B_{63} + L^2 B_{62} + L B_{61} + G^{h.o.}(Z\alpha) \right] \right\},$$

where $L = \ln[(Z\alpha)^{-2}]$, $G^{h.o.}(Z\alpha) = B_{60} + (Z\alpha)(\cdots)$ is the higher-order remainder. For $ns$ states, results for all coefficients up to $B_{60}$ are available, whereas for $np$ states calculations were performed for the coefficients up to $B_{62}$ only. (Details can be found in a review [28], references therein, and more recent studies [29, 30].) Great care should be taken employing the $Z\alpha$ expansion for the evaluation of the total two-loop correction for middle- and high-$Z$ ions, due to a very slow convergence of this expansion. In order to estimate the two-loop QED correction for the $2s$ state, we separate the $1s$ higher-order remainder $G^{h.o.}(Z\alpha)$ from the numerical data of Ref. [18] and use it as an estimation of the corresponding contribution for the $2s$ state, with an uncertainty of 50%. For $p$ states, no analytical calculations for $B_{61}$ coefficient exist up to now. We thus separate from the $1s$ numerical results of Ref. [18] the function

$$\tilde{G}^{h.o.}(Z\alpha) = L B_{61} + G^{h.o.}(Z\alpha),$$

(12)
divide it by a factor of 8, and take the result as an uncertainty for the higher-order contribution for $p$ states.

The relativistic recoil correction was evaluated to all orders in $Z\alpha$ in Refs. [31, 32]. The three-photon exchange correction was calculated for $Z = 83$ in Ref. [11] by utilizing many-
body perturbation theory. For two other cases, \( Z = 90 \) and 92, we use the result for \( Z = 83 \) with a 100% uncertainty. For \( Z = 83 \), a 50% uncertainty is assumed, which corresponds to neglected QED effects. Finally, the \textit{nuclear-polarization} correction was calculated in Refs. [33, 34].

The total theoretical values for the transition energy in Table III are compared with the experimental data [35, 36, 37] and with the previous theoretical evaluations [11, 38, 39, 40, 41]. We note that in all previous calculation except the one of Ref. [11], two-electron QED effects (effects of the “screening” of QED corrections) were accounted for only approximately or partly. A treatment which is closest to the approach presented in this work is that by Sapirstein and Cheng [11], where all two-electron QED corrections were evaluated for \( Z = 83 \). Difference between our total result and that of Ref. [11] is mainly due to the estimate of the two-loop QED correction that is included in the present compilation but was not accounted for in Ref. [11].

Summarizing, we have presented an evaluation of the screened self-energy correction to the \( 2p_{3/2}-2s \) transition energy of Li-like ions with \( Z \geq 12 \). This concludes our calculation of all two-electron QED corrections for this transition and considerably improves the corresponding theoretical predictions. It is demonstrated that the largest theoretical uncertainty for high-\( Z \) ions stems now from the two-loop QED correction, which calculation to all orders in \( Z \alpha \) is needed in order to approach the experimental accuracy.

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| Individual contributions to the $2p_{3/2}-2s$ transition energy in Li-like ions, in eV. |
|---------------------------------|---------------------------------|---------------------------------|
| $\langle r^2 \rangle^{1/2}$ [Fm] | $Z = 83$                       | $Z = 90$                       |
|                                  | 5.533(20)                      | 5.802(4)                       |
|                                  | 5.860(2)                       |                                |
| Dirac value (extended nucleus)   | 2792.164(79)                   | 4076.681(65)                   |
| One-photon exchange             | 23.821                         | -14.459                        |
| Self-energy                     | -35.903                        | -51.120                        |
| Vacuum-polarization             | 8.421                          | 13.561                         |
| Two-photon exchange             | -1.605                         | -0.956                         |
| Screened self-energy            | 1.579                          | 2.199                          |
| Screened vacuum polarization     | -0.431                         | -0.680                         |
| Two-loop QED                    | 0.21(19)                       | 0.30(23)                       |
| Recoil                          | -0.066                         | -0.086                         |
| Three-photon exchange           | -0.024(12)                     | -0.02(2)                       |
| Nuclear polarization            | 0.005(5)                       | 0.02(2)                        |
| Total theory                    | 2788.17(21)                    | 4025.44(24)                    |
| Experiment                      | 2788.14(4)$^a$                 | 4025.23(14)$^b$                |
| Other calculations:             |                                 | 4459.37(21)$^c$                |
| Indelicato and Desclaux, 1990 [38] | 2788.2                        | 4026.3                         |
| Kim et al., 1991 [39]           | 2787.84                        | 4024.96                        |
| Blundell, 1993 [40]             |                                 | 4025.10                        |
| Chen et al., 1995 [41]          |                                 | 4024.98$^d$                     |
| Sapirstein and Cheng, 2001 [11] | 2787.96                        | 4459.13$^d$                     |

$^a$ Ref. [35], $^b$ Ref. [36], $^c$ Ref. [37], $^d$ corrected for the right value of the nuclear-polarization correction [33, 34].

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FIG. 1: Feynman diagrams representing the screened self-energy correction. Double line indicates that the electron propagates in the field of the nucleus.