Two-Photon Exchange Corrections to the $2p_{1/2}$-$2s$ Transition Energy in Li-Like High-Z Ions

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A rigorous QED calculation of the two-photon exchange corrections to the $2p_{1/2}$-$2s$ transition energy in Li-like high-Z ions is presented. The contribution due to an exchange by more than two photons is evaluated within the Breit approximation. The resulting theoretical value of the $2p_{1/2}$-$2s$ transition energy in Li-like uranium is found to be 280.44(20) eV.

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Measurements of the Lamb shift in high-Z Li-like ions are very promising for testing quantum electrodynamics (QED) up to second order in the fine structure constant α in the region of a strong nuclear field. The uncertainty of the best experimental results for the energy of the $2p_{1/2}$-$2s$ transition in Li-like uranium [1] and the $2p_{3/2}$-$2s$ transition in Li-like bismuth [2] is by an order of magnitude smaller than the second-order QED contribution to the transition energy. At present, the accuracy of theoretical predictions does not match the experimental precision. To achieve that level for high-Z ions, rigorous calculations of all Feynman diagrams of second order in α are needed without any expansion in the nuclear-strength parameter αZ. In our previous investigations [3,4] we calculated the two-electron self-energy and vacuum-polarization corrections for the $2p_{1/2}$-$2s$ transition in Li-like high-Z ions. In this Letter we report on the evaluation of the last unknown two-electron contribution of order α^2 for the transition under consideration, the two-photon exchange correction.

QED calculations of heavy few-electron ions are generally based on the Furry picture in which the nucleus is considered only as a source of the classical Coulomb field. From a physical point of view the use of the Furry picture appears to be quite natural since the mass of the nucleus (M) is much bigger than the electron mass (m). However, it is by no means a simple task to derive this picture starting from the free-particle QED and considering the infinite nuclear mass limit. In particular, projection operators arise if one uses the Bethe-Salpeter approach [5,6] or standard quasipotential methods [7]. It was shown in [8] (cf. also [9]) that the Dirac equation with the Coulomb potential can be derived from the free-particle QED by using a version of the quasipotential method with the heavy particle (nucleus) put on mass shell and by summing an infinite sequence of Feynman diagrams describing the electron-nucleus interaction to zeroth order in m/M. This may serve as a good justification for the application of the Furry picture from the point of view of free-particle QED.

Till recently, electron correlations in few-electron ions have been predominantly studied by traditional methods for solving the atomic many-body problem. We mention here only a few of the latest studies of Li-like high-Z ions based on the relativistic many-body perturbation theory [10,11] and the configuration-interaction method [12,13]. A first accurate QED calculation of an interelectronic-interaction effect has been carried out by Blundell and co-workers [14] and by Lindgren *et al.* [15] for the two-photon exchange diagrams for the ground state of He-like ions. A detailed analysis of the two-electron two-photon exchange correction was presented by Shabaev and Fokeeva [16] for the general case of the one-determinant two-electron wave function. In the present investigation we apply the formalism developed in Ref. [16] for the rigorous evaluation of the two-photon exchange contributions for the $2p_{1/2}$-$2s$ transition in Li-like high-Z ions. The corresponding Feynman diagrams are presented in Fig. 1. We refer to the diagram Fig. 1(a) as *ladder* contribution and to the diagrams Figs. 1(b) and 1(c) as *crossed* and *three-electron* contributions, respectively.

We begin with the ladder and the crossed corrections. The unperturbed wave function of a Li-like ion with one electron outside the closed $(1s)^2$ shell can be written as

$$u = \frac{1}{\sqrt{3!}} \sum_P (-1)^P \psi_a(P1)\psi_b(P2)\psi_v(P3), \qquad (1)$$

where P is the permutation operator, a and b denote the electrons in the $(1s)^2$ shell, and v indicates the valence electron. Only two electrons are involved in the photon exchange in Figs. 1(a) and 1(b), and therefore the

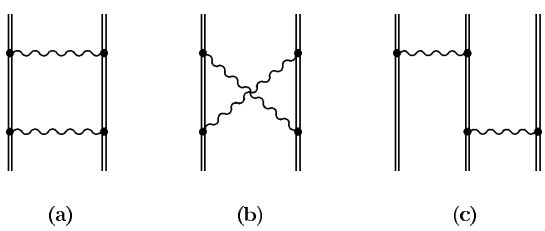

FIG. 1. Feynman diagrams representing the two-photon exchange corrections.

three-electron problem can be decomposed into three two-electron problems. The two-electron contribution with both electrons in the $(1s)^2$ shell is the same as for the ground state of a He-like ion and was investigated in Refs. [14,15]. It does not affect the $2p_{1/2}$-$2s$ transition energy. For the two remaining two-electron corrections we use a slightly modified version of the formulas derived in Ref. [16]. The reason for this modification is that only the one-determinant two-electron wave function was considered in Ref. [16]. In our case this holds true only if the angular momentum projections of the valence and the core electron carry the same sign. As a consequence, the intermediate states with opposite signs of the angular momentum projections of the valence and the core electron yield a nonzero contribution to the reducible part of the ladder diagram. It should be considered together with the corresponding term from the reducible part of the three-electron diagram.

The ladder and the crossed contributions are conveniently divided into the direct and the exchange parts according to the relative alignment of the ingoing and outcoming states. The numerical evaluation of the direct part was carried out similarly to that for the $(1s)^2$ state [14]. We rotate the contour of the integration over the photon energy in the complex plane from the real to the imaginary axis, separating some pole contributions which arise from intermediate discrete states n with $\varepsilon_n \leq \varepsilon_v$. While for the direct part a different structure of the pole terms is the only complication comparing to the $(1s)^2$ state, the evaluation of the exchange contribution is essentially different. In this case the energies of the two photons differ by $\Delta = \varepsilon_v - \varepsilon_c$ (c indicates the core electron). The branch points corresponding to the two photons are shifted by Δ with respect to each other and, therefore, the integration contour is squeezed at two points $\omega = 0$ and $\omega = \Delta$. For the numerical evaluation we employ the integration contour in the complex ω plane deformed in the following way: $(-\epsilon - i\infty, -\epsilon] + [-\epsilon, \Delta + \epsilon] + [\Delta + \epsilon, \Delta + \epsilon + i\infty)$, where ϵ is an arbitrary small positive constant. The numerical integration over the interval $[-\epsilon, \Delta + \epsilon]$ demands some care due to the presence of singularities close to the integration contour which arise from low-lying discrete states. They are treated using the standard identity

$$\int_{-\infty}^{\infty} dx \, \frac{f(x)}{x - x_0 + i0} = \text{v.p.} \int_{-\infty}^{\infty} dx \, \frac{f(x)}{x - x_0} - i\pi f(x_0), \tag{2}$$

and the principal-value integral is evaluated numerically.

The computation of the ladder and the crossed contributions is carried out as follows. The summation over the whole spectrum of the intermediate states is performed using the method of the B-spline basis set for the Dirac equation [17]. Typically, the basis set contains 50 positive and 50 negative energy states. The finite size of the nucleus is taken into account by using a homogeneously charged sphere distribution of the nuclear charge with rms radii given in Ref. [4]. The infinite partial-wave summation is terminated typically at $|\kappa| = 10$. The remainder of the sum is estimated by polynomial fitting in $1/|\kappa|$. Calculations performed both in Feynman and in Coulomb gauge exhibit an excellent agreement. The direct and the exchange parts are found to be separately gauge invariant on the level of numerical accuracy.

Now we discuss the three-electron correction represented by Fig. 1(c). It is conveniently divided into the irreducible and the reducible parts. The reducible part is defined as the contribution in which the energy of the intermediate three-electron state coincides with the energy of the initial state of the atom. The irreducible part is the remainder. The expressions for them are obtained using the two-time Green function method [16,18]. The irreducible contribution is given by

$$\Delta E_{\text{ir}}^{\text{3el}} = \sum_{PQ} (-1)^{P+Q} {\sum_n}' \times \frac{I_{P2P3nQ3}(\varepsilon_{Q3} - \varepsilon_{P3}) I_{P1nQ1Q2}(\varepsilon_{P1} - \varepsilon_{Q1})}{\varepsilon_{Q1} + \varepsilon_{Q2} - \varepsilon_{P1} - \varepsilon_n}, \tag{3}$$

where P and Q denote the permutation operators over the outgoing and the incoming electrons, respectively; $I_{abcd}(\omega) = \langle ab|I(\omega)|cd\rangle$, $I(\omega) = e^2 \alpha^\mu \alpha^\nu D_{\mu\nu}(\omega)$, $\alpha^\mu = (1, \boldsymbol{\alpha})$ are the Dirac matrices, and $D_{\mu\nu}(\omega)$ is the photon propagator. The prime in the sum indicates that terms with vanishing denominator should be omitted in the summation. This expression holds if all three electrons have different energies and also for the case under consideration with two electrons of the same energy. However, the expression for the reducible contribution is different for these two cases. The reducible part of the three-electron correction for the state $(1s)^2 v$ can be written as

$$\Delta E_{\text{red}}^{\text{3el}} = \sum_{\mu_a} \Big[I'_{vaav}(\Delta) (I_{ab;ab} - I_{bv;bv}) + \frac{1}{2} I'_{bv\overline{v}a}(\Delta) I_{a\overline{v};bv} + \frac{1}{2} I'_{a\overline{v}vb}(\Delta) I_{vb;\overline{v}a} \Big], \tag{4}$$

where $I_{ab;cd} = I_{abcd}(\varepsilon_b - \varepsilon_d) - I_{bacd}(\varepsilon_a - \varepsilon_d)$, a and b denote the electrons in the $(1s)^2$ shell, μ_a is the angular momentum projection of the a electron, $\mu_b = -\mu_a$, v indicates the valence $2s$ or $2p_{1/2}$ electron, $\overline{v}$ is the valence electron with the opposite sign of the angular momentum projection, $I'(\Delta) = dI(\omega)/d\omega|_{\omega=\Delta}$. In the derivation of Eq. (4) some terms containing the $\overline{v}$ electron are canceled with the corresponding first four terms in Eq. (47) of Ref. [16]. The numerical evaluation of the three-electron contribution is relatively simple and is carried out using the same technique as for the two-electron corrections. The calculation is performed both in Feynman

TABLE I. Various contributions to the two-photon exchange correction to the energy shift of the ground state of Li-like high-Z ions, in atomic units.

Z	ΔE^{2el}_{dir}	ΔE^{2el}_{exch}	ΔE^{3el}	ΔE_{total}
80	−0.2435	0.0249	−0.1910	−0.4096
83	−0.2525	0.0245	−0.1981	−0.4261
90	−0.2775	0.0237	−0.2174	−0.4712
92	−0.2858	0.0235	−0.2237	−0.4860

TABLE II. Various contributions to the two-photon exchange correction to the energy shift of the $2p_{1/2}$ state of Li-like high-Z ions, in atomic units.

Z	ΔE^{2el}_{dir}	ΔE^{2el}_{exch}	ΔE^{3el}	ΔE_{total}
80	−0.3631	−0.0161	−0.3862	−0.7654
83	−0.3763	−0.0225	−0.4113	−0.8101
90	−0.4154	−0.0403	−0.4796	−0.9352
92	−0.4290	−0.0462	−0.5022	−0.9774

as well as in Coulomb gauge. The numerical results are found to be gauge invariant with a very high accuracy.

The results for the two-photon exchange contributions to the energy shifts of the $2s$ and $2p_{1/2}$ states of some Li-like high-Z ions are presented in Tables I and II, respectively. ΔE^{2el}_{dir} and ΔE^{2el}_{exch} denote the direct and the exchange parts of the two-electron correction, and ΔE^{3el} indicates the three-electron contribution. We estimate the total numerical error to be less than 0.0001 a.u. In the case of the ground state of Li-like bismuth our calculation can be compared with the preliminary results reported by Sapirstein [19]. An excellent agreement is found for the three-electron correction (−5.3902 eV in this work and −5.390 eV in Ref. [19]). For the two-electron contribution we have −6.204 eV which should be compared to −6.367 eV of Ref. [19] in which not all terms have been included. It is of interest to compare the rigorous QED treatment with results of many-body perturbation theory. For this reason, we evaluated the contribution of diagrams Figs. 1(a) and 1(c) within the Breit approximation, keeping only the Coulomb and unretarded Breit parts of the photon propagators and neglecting negative energy states. This approximation yields −13.54 eV for uranium comparing to the total result of −13.37 eV.

We now turn to the experimental consequences of our results. Until now, the two-photon exchange correction represented the main source of uncertainty of the theoretical predictions for the $2p_{1/2}$-$2s$ transition energy in Li-like high-Z ions. In our previous investigation [4] the correction due to the exchange by two and more photons was evaluated to be −13.20(40) eV for uranium, utilizing the results of the relativistic configuration-interaction calculations [12,13]. The rigorous QED treatment of the two-photon exchange contribution presented in this Letter yields −13.37 eV for uranium. The correction due to the exchange by three and more photons is suppressed roughly by a factor of $1/Z$ compared to the two-photon exchange contribution, and therefore it is not negligible on the level of the experimental accuracy. We evaluate it within the Breit approximation as the difference between the relativistic configuration-interaction result obtained with hydrogenlike wave functions and the sum of the zeroth-, first-, and second-order (in $1/Z$) contributions calculated with the same hydrogenlike basis. The exchange with any number of Coulomb photons but not more than one unretarded Breit photon is included in the consideration. For the corresponding energy shift in uranium we obtain 0.14 eV. This has also been confirmed by a direct calculation of the $1/Z^3$ correction by perturbation theory within the Breit approximation. Taking into account that the accurate relativistic treatment of this correction can be accomplished only within QED, we assume the precision of this result to be about 50%.

In Table III we summarize all the contributions calculated up to now for the $2p_{1/2}$-$2s$ transition energy in Li-like uranium and compare the total theoretical prediction to the experimental value. All corrections are calculated with an rms radius of the nucleus of 5.860(2) fm [20]. From Table III it can be deduced that the difference between experiment and theory of 0.15(9) eV should be ascribed predominantly to the one-electron second-order QED correction. Corresponding calculations for the ground state of hydrogenlike ions are currently in progress [21].

In summary, with this paper we conclude the series of our investigations on the two- and three-electron corrections of order α^2. We have evaluated all these contributions to the $2p_{1/2}$-$2s$ transition energy in Li-like high-Z ions. In this Letter we have presented a rigorous QED

TABLE III. Various contributions to the $2p_{1/2}$-$2s$ transition in Li-like uranium, in eV.

Correction	Value	Reference
One-electron extended nucleus	−33.35(6)	Yerokhin *et al.* [4]
One-photon exchange	368.83	Yerokhin *et al.* [4]
First-order self-energy	−55.87	Mohr and Soff [22]
First-order vacuum polarization	12.94	Persson *et al.* [23]
Two-photon exchange	−13.37	This work
Three- and more photon exchange	0.14(7)	This work
Two-electron self-energy	1.52	Yerokhin *et al.* [4]
Two-electron vacuum polarization	−0.36	Artemyev *et al.* [3]
Nuclear recoil	−0.07	Artemyev *et al.* [24]
Nuclear polarization	0.03(1)	Plunien *et al.* [25] Nefiodov *et al.* [26]
One-electron second-order QED	±0.20	Not yet calculated
Total theory	280.44(20)	
Experiment	280.59(9)	Schweppe *et al.* [1]

calculation of the two-photon exchange diagrams and an evaluation of the correction due to the exchange by three and more photons within the Breit approximation. While the total accuracy of the theoretical prediction is significantly improved, a rigorous calculation of the second-order one-electron QED effects is still required.

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