

## Two-Electron Lamb-Shift Calculations on Heliumlike Ions

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Complete second-order calculations of the two-electron contribution to the ground-state energy of heliumlike ions are presented and compared with recent experimental results. Calculations involve relativistic many-body effects and two-electron Lamb-shift (vacuum-polarization and self-energy) contributions as well as the recently presented nonradiative QED corrections. Agreement between experimental and theoretical results verifies the many-body part of the calculation. The accuracy of the results is not high enough to test the QED part of the calculations, but an improvement by half an order of magnitude would provide an experimental test of the QED effect for heavy ions beyond the first-order Lamb shift.

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The experimental situation concerning heavy-ion spectroscopy has improved drastically in recent years. Electron-beam ion trap (EBIT) and super-EBIT facilities together with storage rings with improved cooling facilities have made it possible to study highly charged ions with increasing precision. Also on the theoretical side corresponding progress has taken place.

Using the super-EBIT facility at Lawrence Livermore National Laboratory, Marrs, Schneider, and Stöhlker [1] have recently measured the two-electron contribution to the ground-state energy of some heavy heliumlike ions by comparing the ionization energy of heliumlike and hydrogenlike ions of the same elements. Data of this kind are particularly interesting for testing calculations of the tiny two-electron QED contribution, since the dominating one-body parts are completely eliminated. We shall present here such calculations and compare them with the experimental results of Marrs, Schneider, and Stöhlker.

QED corrections to the energy of heliumlike ions, correct to order  $(\alpha)^5 mc^2$  where  $\alpha$  is the fine-structure constant, were derived long ago by Araki and Sucher [2]. Considering the two-photon two-electron contribution only the leading terms in the  $Z\alpha$  expansion are included in their expressions. These terms are correct at the level  $(\alpha)^2(Z\alpha)^3 mc^2$ . However, for heavy highly charged ions where  $Z\alpha$  approaches unity, the  $Z\alpha$  expansion is no longer meaningful. Here, it is necessary to take into account the nuclear potential interaction to all orders by means of numerical techniques. The starting point is then single-electron states generated in the nuclear field, rather than free-electron states. This technique was first applied on self-energy calculations on hydrogenlike heavy ions [3]. We have recently developed a numerical technique for heavy ions with more than one electron and applied this to self-energy and vacuum-polarization calculations [4–7] as well as to calculations of the nonradiative QED effect [8]. Related calculations have also been performed by other groups using different numerical techniques [9,10].

The many-body contribution to the Lamb shift can to first approximation be regarded as a *screening* of the single-electron Lamb shift. This screening can be estimated by means of a modification of the nuclear potential [4,9,11]. In this way, however, it is not possible to treat the exchange effect and the effect due to transverse photons in an exact way. In order to reach high accuracy it is of importance to perform many-body Lamb-shift calculations without any approximations. We have for the first time performed such calculations, complete to second order, and the results will be presented here.

The two-photon contributions to the electron-electron interaction for two-electron systems are represented by the Feynman diagrams in Fig. 1. The first line represents the “nonradiative” diagrams, the “ladder” (a) and the “crossed-photon” (b) diagrams. The ladder diagram contains the leading many-body (second-order) contribution. The remaining part of that diagram together with the cross diagram represents the nonradiative QED effects first calculated for light elements by Araki and Sucher in the 1950s [2], and more recently by the Göteborg and Notre Dame groups for general nuclear charges [8,10]. The second line in Figs. 1(c) and 1(d) represents the two-electron vacuum polarization and the last line [1(e) and 1(f)] the two-electron—or *screened*—self-energy. We shall here be concerned with the calculation of the two-electron Lamb shift [diagrams 1(c)–1(f)].

The vacuum-polarization and self-energy calculations have been performed along the same line as in our recently published works [4–7]. In this Letter we use units where  $\hbar = \epsilon_0 = e = c = 1$ . The single-electron states are generated in the field of the nucleus by solving the Dirac equation with the nuclear potential  $u(r)$ ,

$$h^{\text{ext}}|i\rangle = [\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m + u(r)]|i\rangle = \epsilon_i|i\rangle.$$

This equation is solved by the method of discretization [12]. Finite nuclei are used with the experimentally determined radius and a uniform charge distribution.

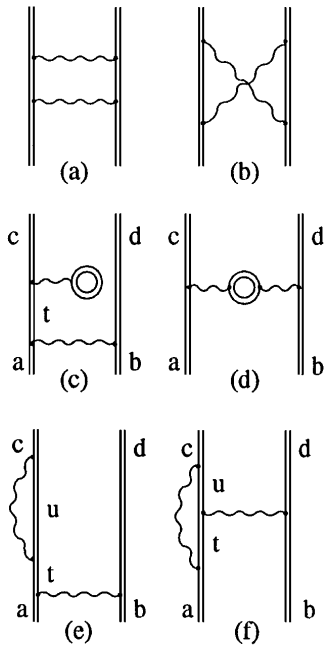


FIG. 1. Feynman diagrams representing the two-photon contribution to the electron-electron interaction for heliumlike ions. The first row, the “ladder” (a) and the “crossed-photon” (b) diagrams, represent the nonradiative part, and the remaining diagrams represent the two-electron Lamb shift, i.e., vacuum polarization (c) and (d) and self-energy (e) and (f), respectively.

We are primarily interested here in the Lamb-shift contributions for the ground state of the two-electron system, and in evaluating the energy contributions we shall therefore assume that all external orbital lines have the same energy,  $\epsilon_a = \epsilon_b = \epsilon_c = \epsilon_d$ .

Diagram 1(c) can be generated by perturbing the single-photon exchange,  $\langle cd|V_{12}|ab\rangle$ , by the vacuum-polarization

$$\begin{aligned} \langle c|\Sigma^1(\epsilon_c)|a\rangle &= -i\frac{2\alpha}{\pi} \sum_{l=0}^{\infty} (2l+1) \int \frac{dz}{2\pi} \int k^2 dk \frac{\langle c|\alpha'_l \alpha_{2\nu} \mathbf{C}^l(1) \cdot \mathbf{C}^l(2) j_l(kr_1) j_l(kr_2)|a\rangle}{[\epsilon_c - z - h^{\text{ext}}(1-i\eta)](z^2 - k^2 + i\epsilon)} \\ &= -\frac{\alpha}{\pi} \sum_{l=0}^{\infty} (2l+1) \int k dk \sum_u \frac{\langle c|\alpha^\nu \mathbf{C}^l j_l(kr)|u\rangle \cdot \langle u|\alpha_\nu \mathbf{C}^l j_l(kr)|a\rangle}{\epsilon_c - \epsilon_u - k \text{sgn}(\epsilon_u)}, \end{aligned} \quad (1)$$

by the interaction with the other electron [ $\text{sgn}(\epsilon_u) = \pm 1$  depending on the sign of  $\epsilon_u$ ]. Perturbing the incoming external orbital line  $|a\rangle$  leads to

$$\Delta E_e = \sum_t \frac{\langle c|\Sigma^1(\epsilon_c)|t\rangle \langle td|V_{12}|ab\rangle}{\epsilon_c - \epsilon_t}, \quad (2)$$

with  $\epsilon_t \neq \epsilon_c$ . This represents the contribution due to diagram 1(e), apart from the case  $\epsilon_t = \epsilon_c$ , which will be considered later. There is a similar contribution for the

potential (Uehling and Wickman-Kroll),  $V_{vp}$ ,

$$\Delta E_c = \sum_t \frac{\langle c|V_{vp}|t\rangle \langle td|V_{12}|ab\rangle}{\epsilon_c - \epsilon_t},$$

where  $\epsilon_t \neq \epsilon_c$ . The contribution for  $\epsilon_t = \epsilon_c$  from this diagram is completely canceled by the  $\langle S^2 \rangle^2$  term in Eq. (5) as discussed later.

The leading (Uehling) part of diagram 1(d) is evaluated in analogy with the Uehling part of the first-order vacuum polarization [5] by replacing the Feynman gauge photon propagator in the single-photon exchange

$$D_{F\nu\mu}(\mathbf{x}_2 - \mathbf{x}_1, \omega) = -g_{\nu\mu} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}_2 - \mathbf{x}_1)}}{\omega^2 - \mathbf{k}^2 + i\epsilon}$$

by the charge-renormalized propagator

$$\begin{aligned} D_{F\nu\mu}^{\text{ren}}(\mathbf{x}_2 - \mathbf{x}_1, \omega) &= -g_{\nu\mu} \frac{\alpha}{\pi} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \\ &\times \int_1^\infty dt \frac{e^{i\mathbf{k}\cdot(\mathbf{x}_2 - \mathbf{x}_1)}}{\omega^2 - \mathbf{k}^2 - 4t^2 + i\epsilon} \\ &\times \sqrt{t^2 - 1} \left( \frac{2}{3t^2} + \frac{1}{3t^4} \right). \end{aligned}$$

The remaining part of the diagram is evaluated in analogy with the Wichmann-Kroll part of the vacuum polarization by taking the difference between the bound state and the free-electron polarization operators in the photon line [5].

The self-energy contributions [1(e) and 1(f)] are quite similar to the corresponding contributions to the hyperfine interaction, recently calculated by Persson *et al.* [13]. These contributions can be obtained by perturbing the (unrenormalized) first-order self-energy,

modification of the outgoing orbital line. The corresponding modifications have to be made also in the mass counter term, used in renormalizing the first-order self-energy. This leads to an analogous expression, and the renormalization of Eq. (2) is then obtained simply by inserting the renormalized self-energy operator.

Perturbing the electron propagator by the interaction leads to a modification of the Hamiltonian and the orbital energy  $\epsilon_c$  in the denominator of Eq. (1). The modification of the Hamiltonian leads to

$$\Delta E_f = -\frac{\alpha}{\pi} \sum_{l=0}^{\infty} (2l+1) \int k dk \sum_{t,u} \frac{\langle c|\alpha^\nu \mathbf{C}^l j_l(kr)|u\rangle \langle ud|V_{12}|tb\rangle \cdot \langle t|\alpha_\nu \mathbf{C}^l j_l(kr)|a\rangle}{[\epsilon_c - \epsilon_u - k \text{sgn}(\epsilon_u)][\epsilon_a - \epsilon_t - k \text{sgn}(\epsilon_t)]} F, \quad (3)$$

where

$$F = 1 + [\text{sgn}(\epsilon_u) - \text{sgn}(\epsilon_t)] \frac{k}{\epsilon_c - \epsilon_a + \epsilon_u - \epsilon_t}.$$

This represents the contribution due to diagram 1(f).

The modification of the orbital energy leads to

$$\begin{aligned} \Delta E_{\text{ref}} &= \langle cd|V_{12}|ab\rangle \langle c| \left[ \frac{\partial}{\partial \omega} \Sigma^1(\omega) \right]_{\omega=\epsilon_c} |a\rangle \\ &= \frac{\alpha}{\pi} \sum_{l=0}^{\infty} (2l+1) \int k dk \sum_u \frac{\langle cd|V_{12}|ab\rangle \langle c|\alpha^{\nu} \mathbf{C}^l j_l(kr)|u\rangle \cdot \langle u|\alpha_{\nu} \mathbf{C}^l j_l(kr)|a\rangle}{[\epsilon_c - \epsilon_u - k \text{sgn}(\epsilon_u)]^2}. \end{aligned} \quad (4)$$

This is the finite contribution to diagram 1(e) when  $\epsilon_t = \epsilon_c$ . If the interaction is energy dependent, there is an additional term. This is not the case for the ground state considered here. There is no contribution from the mass counter term to the last two expressions.

The two expressions in Eqs. (3) and (4) are both infrared and ultraviolet divergent, but the divergences cancel when the two contributions are added. This cancellation is related to the Ward identity. The explicit cancellation of the ultraviolet divergencies are handled by the use of dimensional regularization [14]. The infrared divergency can explicitly be canceled by separating out for  $l=0$  the contribution  $e_c = e_u$  in Eq. (4) and the contribution  $e_c = e_a = e_u = e_t$  in Eq. (3).

The second-order contributions considered here can also be derived in a more formal way, using the  $S$ -matrix formalism and the Gell-Mann-Low-Sucher formula [15],

$$\Delta E = i\eta[2\langle S^{(4)}\rangle - \langle S^{(2)}\rangle^2], \quad (5)$$

in the limit where the adiabatic parameter  $\eta$  tends to zero. Here, the second term, representing products of disconnected first-order diagrams, is singular and cancels the corresponding singularity of the reference-state contribution (reducible part) of diagram 1(e). The remaining finite contribution from the reference state leads to the derivative term Eq. (4).

In Table I we present the vacuum-polarization and self-energy results for some heliumlike ions with nuclear charges ranging from 32 to 92. The results are separated into Coulomb and Breit parts for the photon connecting the two electrons. In Table II we collect the various contributions to the two-electron part of the energy and com-

pare with recent experimental results of Marrs, Schneider, and Stöhlker [1]. The all-order relativistic many-body result (RMBPT) is also calculated and the nonradiative QED contribution is taken from our recent publication [8]. In Table III we compare the results of several recent theoretical estimates of the two-electron energy contribution.

The results of Drake [16] are obtained by means of accurately correlated nonrelativistic wave functions and the QED corrections are calculated using expressions, correct to order  $\alpha^3$ , derived by Araki and Sucher [2]. The results of Plante, Johnson, and Sapirstein [17] are relativistic many-body calculations, corrected for the Lamb shift using Drake's QED data [16]. The results of Indelicato, Gorceix, and Desclaux [18] are obtained by multiconfiguration Dirac-Fock calculations, using the "Welton" method [18] to approximate the Lamb shift.

The agreement between the various theoretical results is generally quite good, which indicates that the earlier estimates of the Lamb-shift contributions have been quite accurate. Drake's result suffers from the inaccuracy of the  $Z\alpha$  expansion for the QED and relativistic effects for heavy elements, which becomes particularly evident for Bi ( $Z = 83$ ). On the other hand, Drake uses correlated hydrogenic wave functions and thus includes also higher-order Coulomb correlation in the QED effects. The relative effect of correlation is largest for light elements, where the absolute effect is smaller. Therefore, the missing correlation effect in our QED values is estimated to be at most of the order of 0.1 eV for all elements. The very weak dependence of the nuclear structure on the results was investigated by calculating the first-order energy varying the nuclear parameters and using Fermi—and uniform—

TABLE I. Two-electron vacuum-polarization and self-energy contributions to the ground-state energy of some heliumlike ions (in eV).

Nuclear Charge	$R_{\text{rms}}$ (fm)	Vacuum polarization			Self-energy			Two-electron Lamb shift
		Coulomb	Breit	Total	Coulomb	Breit	Total	
32	4.07	0.0	0.0	0.0	-0.5	0.0	-0.5	-0.4
54	4.78	0.2	0.0	0.2	-1.6	-0.2	-1.8	-1.6
66	5.21	0.4	0.1	0.6	-2.8	-0.4	-3.2	-2.7
74	5.37	0.7	0.2	0.9	-3.8	-0.8	-4.6	-3.7
83	5.519	1.1	0.4	1.6	-5.3	-1.4	-6.7	-5.2
92	5.860	1.8	0.8	2.6	-7.4	-2.3	-9.7	-7.1

TABLE II. Various components of the two-electron contribution to the ground-state energy of some heliumlike ions and a comparison with experiment (in eV). The errors assigned for the “1st order RMBPT” values are due to a variation of the nuclear  $R_{\text{rms}}$  value by 1%. The “2nd order RMBPT” values include two Breit interactions but no retardation. The “ $\geq 3$ rd order RMBPT” values include only one Breit interaction.

Nuclear charge	1st order RMBPT	2nd order RMBPT	$\geq 3$ rd order RMBPT	Nonradiative QED	Lamb shift	Total theory	Experiment Marrs <i>et al.</i> [1]
32	567.61	-5.22	0.02	0.0	-0.4	562.0	562.5 $\pm$ 1.6
54	1036.56	-7.04	0.03	0.2	-1.6	1028.2	1027.2 $\pm$ 3.5
66	1347.45(1)	-8.59	0.03	0.4	-2.7	1336.6	1341.6 $\pm$ 4.3
74	1586.93(2)	-9.91	0.04	0.6	-3.7	1573.9	1568 $\pm$ 15
83	1897.56(4)	-11.77	0.04	0.9	-5.2	1881.5	1876 $\pm$ 14
92	2265.87(10)	-14.16	0.05	1.3	-7.1	2246.0	$\pm$

charge distribution models to describe the extended nucleus. The dominating numerical uncertainty comes from the uncertainty in the  $R_{\text{rms}}$  values. A 1% variation of the  $R_{\text{rms}}$  value gives a change of 0.01 eV for  $Z = 66$  and 0.1 eV for  $Z = 92$ . The nuclear uncertainties do not affect the QED contributions at the present level of accuracy.

The agreement between the experimental and theoretical results supports the accuracy of the experimental and many-body results, but the accuracy of the experimental results is not yet high enough to seriously test the QED part of the calculation. On the other hand, an improvement of only half an order of magnitude is required here in order to achieve—for the first time—an experimental test of QED contributions for heavy elements beyond the lowest-order Lamb shift.

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TABLE III. Comparison between various theoretical calculations (in eV).

$Z$	Ref. [17]	Ref. [18]	Ref. [16]	Present work
32	562.05	562.1	562.1	562.0
54	1028.4	1028.2	1028.8	1028.2
66	1337.2	1336.5	1338.2	1336.6
74	1574.8	1573.6	1576.6	1573.9
83		1880.8	1886.3	1881.5
92				2246.0

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