Two-photon-exchange QED effects in the $1s2s$ ^1S and ^3S states of heliumlike ions

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A numerical calculation, based on full QED, of the energy shift due to the effect of two-photon exchange in the $1s2s$ ^1S and ^3S states in heliumlike ions is presented. At low Z, the QED effects are compared with the known analytical $(Z\alpha)^3$ contributions, and we find good agreement. The calculations have been performed in the range $Z=10$–92. Already in the medium-Z range, the effects beyond the leading $(Z\alpha)^3$ order are found to be dominant.

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I. INTRODUCTION

In this paper, we are concerned with accurate calculations of the energy of excited states of heliumlike systems, more specifically the $1s2s$ ^1S and ^3S states. For low Z there are very accurate calculations by Drake [1], using the so-called unified method. In this method the relativistic and quantum electrodynamic (QED) effects, beyond their very accurate nonrelativistic energy, are calculated to leading orders in the fine-structure constant α. All effects of order α^3, in atomic units, are included. For higher Z, effects scaling as $(Z\alpha)^4$ and higher become important. A large part of these effects are included in relativistic many-body perturbation theory (RMBPT). In this method one usually makes the *no-virtual-pair approximation* (NVPA), where the effects of negative energy states and retardation are neglected. To match the experimental accuracy that is possible to achieve today, it is necessary to also include the effects of QED to high order in the expansion parameter $Z\alpha$. In this paper, we give a complete description of the numerical calculations of the effect of the exchange of two virtual photons between the electrons in the $1s2s$ excited states of heliumlike ions. Other calculations of this effect for the $1s2s$ and $1s2p$ (not $J=1$) triplet states have recently been presented by Mohr and Sapirstein [2], and for the $1s2s$ singlet and triplet states by Andreev *et al.* [3]. A calculation of the quasidegenerate $1s2p$ $^1P_1$ and $^3P_1$ states has been performed by us in [4], using an extended model space, involving calculating matrix elements nondiagonal in energy, which is not possible with the commonly used S-matrix formulation by Sucher [5]. In this paper, however, we use the S-matrix formulation and the presented work is essentially a nontrivial generalization of a calculation in a previous paper concerning the ground state [6]. We are not considering here the remaining QED two-photon effects, the screened self-energy and vacuum polarization, although they are certainly as important as the considered two-photon exchange. Calculations of these effects have been made for the ground state of various heliumlike and lithiumlike systems [7–9]. The QED effect considered in this paper contains both negative energy states and retardation of the photons, both effects which scale as $(Z\alpha)^3$ and $(Z\alpha)^3\ln(Z\alpha)$. Our results are, in the low-Z region, compared with known analytical expressions for the $(Z\alpha)^3$ contributions. These analytical expressions contain the Bethe logarithm and to be able to make the comparison we have calculated the relevant $(Z\alpha)^3$ part associated with the two-photon exchange.

The outline of the paper is the following. In Sec. II a theoretical derivation of the expressions needed are performed both in the Feynman and Coulomb gauge. The numerical procedure and some numerical difficulties are presented in Sec. III. In Sec. IV, the numerical results are presented followed in Sec. V by a comparison with analytical results in the low-Z region and a discussion of the results.

II. FORMALISM

The exchange of two virtual photons between two electrons is represented by the two Feynman diagrams in Fig. 1, the ladder diagram (L) with uncrossed photons and the crossed photons diagram (X). The energy shift due to these effects are given by the formula derived in 1957 by Sucher [5]

$$\Delta E_A=\lim_{\gamma\to 0}\frac{1}{2}i\gamma\{4\langle\Phi_a^0|S^4_{\mathrm{lad},\gamma}|\Phi_a^0\rangle+4\langle\Phi_a^0|S^4_{\mathrm{cro},\gamma}|\Phi_a^0\rangle -2\langle\Phi_a^0|S^2_{\gamma}|\Phi_a^0\rangle^2\}, \tag{1}$$

where Φ_a^0, the reference state, is the two-electron state considered, constructed from orbitals that are solutions to the one-electron Dirac equation.

A. Feynman Gauge. Uncrossed photons

We consider first the uncrossed diagram in Fig. 1. The S-matrix element for this diagram is ($\hbar=1$)

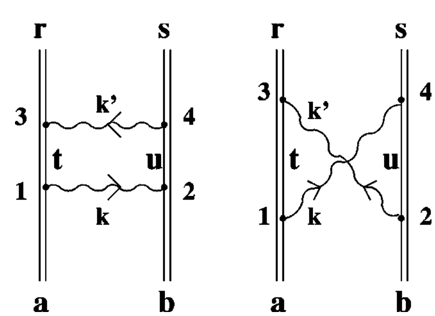

FIG. 1. The Feynman diagrams representing the two-photon exchange between two electrons with uncrossed and crossed photons.

$$\begin{aligned}\langle\Phi_a^0|S^4_{\mathrm{lad},\gamma}|\Phi_a^0\rangle\\ &=(ie)^4\int d^4x_1\int d^4x_2\int d^4x_3\int d^4x_4\\ &\times e^{-\gamma|t_3|}e^{-\gamma|t_1|}\Phi_r^\dagger(x_3)\alpha_3^\nu iS_F(x_3,x_1)\alpha_1^\mu\Phi_a(x_1)\\ &\times e^{-\gamma|t_4|}e^{-\gamma|t_2|}\Phi_s^\dagger(x_4)\alpha_4^{\nu'}iS_F(x_4,x_2)\alpha_2^{\mu'}\Phi_b(x_2)\\ &\times\frac{i}{c}D_{F\nu\nu'}(x_3-x_4)\frac{i}{c}D_{F\mu'\mu}(x_2-x_1),\end{aligned} \tag{2}$$

where the photon propagator in the Feynman gauge is defined by

$$\begin{aligned}D_{F\nu\mu}(x_2-x_1)&=-\frac{1}{\epsilon_0}g_{\nu\mu}\int\frac{d^4k}{(2\pi)^4}\frac{e^{-ik(x_2-x_1)}}{(k^2+i\epsilon)}\\ &=\int\frac{dz}{2\pi}e^{-iz(t_2-t_1)}D_{F\nu\mu}(\mathbf{x}_2-\mathbf{x}_1,z)\end{aligned} \tag{3}$$

and

$$D_{F\nu\mu}(\mathbf{x}_2-\mathbf{x}_1,z)=-\frac{c}{\epsilon_0}g_{\nu\mu}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}_2-\mathbf{x}_1)}}{(z^2-c^2\mathbf{k}^2+i\epsilon)}. \tag{4}$$

We have here defined the z parameter by $k=(z/c,\mathbf{k})$ and ϵ is a small positive number. The electron propagator is defined by

$$\begin{aligned}S_F(x_2,x_1)&=\sum_n\int\frac{dz}{2\pi}e^{-iz(t_2-t_1)}\frac{\Phi_n(\mathbf{x}_2)\Phi_n^\dagger(\mathbf{x}_1)}{z-e_n(1-i\eta)}\\ &=\int\frac{dz}{2\pi}e^{-iz(t_2-t_1)}S_F(\mathbf{x}_2,\mathbf{x}_1,z),\end{aligned} \tag{5}$$

where η is a small positive number. The time-dependent functions are given by

$$\Phi_n(x)=e^{-ie_nt}\Phi_n(\mathbf{x}). \tag{6}$$

We use here the Furry interaction picture [10], which implies that nuclear recoil is not included, with the single-electron states $\Phi_n(\mathbf{x})$ being solutions of the time-independent Dirac equation,

$$h_D\Phi_n(\mathbf{x})=e_n\Phi_n(\mathbf{x}) \tag{7}$$

where

$$h_D=c\boldsymbol{\alpha}\cdot\mathbf{p}+\beta mc^2+V. \tag{8}$$

V is here the Coulomb potential from the nucleus. For low Z we use a point nucleus but for higher Z an extended nucleus with homogeneous charge density is used. If the intermediate states are not degenerate with the reference state, the time integrations in Eq. (2) are trivial to perform leading to energy conservation at the vertices (in the limit where the adiabatic damping factor $\gamma\to 0$). The remainder of Eq. (2) reduces to a space integral M (the Feynman amplitude)

$$\begin{aligned}M=&\int d^3x_1\int d^3x_2\int d^3x_3\int d^3x_4\int\frac{dz}{2\pi}\\ &\times\Phi_r^\dagger(\mathbf{x}_3)iec\alpha_3^\nu iS_F(\mathbf{x}_3,\mathbf{x}_1,e_a-z)iec\alpha_1^\mu\Phi_a(\mathbf{x}_1)\\ &\times\Phi_s^\dagger(\mathbf{x}_4)iec\alpha_4^{\nu'}iS_F(\mathbf{x}_4,\mathbf{x}_2,e_b+z)iec\alpha_2^{\mu'}\Phi_b(\mathbf{x}_2)\\ &\times\frac{i}{c}D_{F\nu\nu'}(\mathbf{x}_3-\mathbf{x}_4,z')\frac{i}{c}D_{F\mu'\mu}(\mathbf{x}_2-\mathbf{x}_1,z),\end{aligned} \tag{9}$$

or, alternatively, by using the explicit representation of the photon and electron propagators, we obtain

$$\begin{aligned}M=&\left(\frac{e^2c^2}{\epsilon_0}\right)^2\sum_{t,u}\int\frac{dz}{2\pi}\\ &\times\langle rs|\alpha_4^\nu\alpha_{\nu3}\int\frac{d^3\mathbf{k}'}{(2\pi)^3}\frac{e^{i\mathbf{k}'\cdot(\mathbf{x}_3-\mathbf{x}_4)}}{(z'^2-\mathbf{k}'^2+i\epsilon)}|tu\rangle\\ &\times\langle tu|\alpha_2^\mu\alpha_{\mu1}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}_2-\mathbf{x}_1)}}{(z^2-\mathbf{k}^2+i\epsilon)}|ab\rangle\\ &\times\frac{1}{[e_a-z-e_t(1-i\eta)]}\frac{1}{[e_b+z-e_u(1-i\eta')]},\end{aligned} \tag{10}$$

where z and $z'=z+e_r-e_a$ are associated with the momentum k and k', respectively. Intermediate states t,u degenerate with the reference state are omitted in the summation. However, these states give rise to finite contributions, *the reference state contributions*, which are considered in the Appendix. We begin by evaluating the integral

$$\begin{aligned}I^L=&i\int_{-\infty}^{\infty}\frac{dz}{2\pi}\frac{1}{(p-z+i\eta_t)}\frac{1}{(p'+z+i\eta_u)}\\ &\times\frac{1}{[z'^2-(ck'-i\eta)^2]}\frac{1}{[z^2-(ck-i\eta)^2]}\end{aligned} \tag{11}$$

where η_t and η_u are small numbers with the same sign as e_t and e_u, respectively. (We have here used that $k=|\mathbf{k}|$ is positive.)

With the notation $p=e_a-e_t$, $p'=e_b-e_u$, $q=e_a-e_r$, $q'=e_b-e_s$, and with $+$ and $-$ denoting positive and negative intermediate states for t and u, respectively, we have

$$I^{L++}=\frac{1}{4ckck'(p+p')}\left\{-\frac{1}{(p-ck)(ck+ck'-q)}+\frac{1}{(q+p'-ck')(p'-ck)}-\frac{1}{(q+p'-ck')(ck+ck'-q)}+\frac{1}{(p-ck)(q'+p-ck')}-\frac{1}{(q'+p-ck')(ck+ck'-q')}-\frac{1}{(p'-ck)(ck+ck'-q')}\right\}, \tag{12}$$

$$I^{L--}=-\frac{1}{4ckck'(p+p')}\left\{-\frac{1}{(p'+ck)(ck+ck'-q)}+\frac{1}{(p-q+ck')(p+ck)}+\frac{1}{(p-q+ck')(ck+ck'-q)}+\frac{1}{(p'+ck)(p'-q'+ck')}+\frac{1}{(p+ck)(ck+ck'-q')}+\frac{1}{(p'-q'+ck')(ck+ck'-q')}\right\}, \tag{13}$$

$$I^{L+-}=\frac{1}{4ckck'(p+p')}\left\{-\frac{1}{(p-ck)(ck+ck'-q)}+\frac{1}{(p-ck)(p+q'-ck')}-\frac{1}{(p'+ck)(ck+ck'-q)}-\frac{1}{(p'+ck)(p'-q'+ck')}-\frac{1}{(p+q'-ck')(ck+ck'-q')}-\frac{1}{(p'-q'+ck')(ck+ck'-q')}\right\}, \tag{14}$$

$$I^{L-+}=\frac{1}{4ckck'(p+p')}\left\{-\frac{1}{(p-q+ck')(ck+ck'-q)}+\frac{1}{(p'-ck)(p'+q-ck')}-\frac{1}{(p'+q-ck')(ck+ck'-q)}+\frac{1}{(p+ck)(p-q+ck')}-\frac{1}{(p+ck)(ck+ck'-q')}-\frac{1}{(p'-ck)(ck+ck'-q')}\right\}. \tag{15}$$

The expressions that follow directly from the z integrals are not always suitable for implementation, since fictitious poles will appear. These poles cancel out but will make the implementation more difficult. The expressions given are rewritten such that no fictitious poles appear.

Multiplying the Feynman amplitude by the imaginary unit (i), yields the corresponding energy contribution

$$\Delta E^L_{tu}=\left(\frac{e^2c^2}{\epsilon_0}\right)^2\int\frac{d^3\mathbf{k}}{(2\pi)^3}\int\frac{d^3\mathbf{k}'}{(2\pi)^3}\times\langle rs|\alpha_3^{\nu}\alpha_{\nu 4}e^{i\mathbf{k}'\cdot(\mathbf{x}_3-\mathbf{x}_4)}|tu\rangle\times\langle tu|\alpha_1^{\mu}\alpha_{\mu 2}e^{i\mathbf{k}\cdot(\mathbf{x}_2-\mathbf{x}_1)}|ab\rangle I^L.$$

After the integration over the angular parts of k and k' this becomes

$$\Delta E^L_{tu}=\left(\frac{e^2}{2\pi^2\epsilon_0}\right)^2\int dk\int dk'\langle rs|\alpha_3^{\nu}\alpha_{\nu 4}\frac{\sin(k'r_{34})}{k'r_{34}}|tu\rangle\times\langle tu|\alpha_1^{\mu}\alpha_{\mu 2}\frac{\sin(kr_{12})}{kr_{12}}|ab\rangle(ck)^2(ck')^2I^L, \tag{16}$$

and by using the spherical-wave expansion

$$\frac{\sin(kr_{12})}{kr_{12}}=\sum_{l=0}^{\infty}(2l+1)j_l(kr_1)j_l(kr_2)\mathbf{C}^l(1)\cdot\mathbf{C}^l(2), \tag{17}$$

we obtain

$$\Delta E^L=\left(\frac{e^2}{2\pi^2\epsilon_0}\right)^2\sum_{l,l'}(2l+1)(2l'+1)\int dk\int dk'\times\sum_t\sum_u\langle r|\alpha^{\nu}\mathbf{C}^{l'}j_{l'}(k'r)|t\rangle\langle s|\alpha_{\nu}\mathbf{C}^{l'}j_{l'}(k'r)|u\rangle\times\langle t|\alpha^{\mu}\mathbf{C}^{l}j_{l}(kr)|a\rangle\langle u|\alpha_{\mu}\mathbf{C}^{l}j_{l}(kr)|b\rangle\times(ck)^2(ck')^2I^L. \tag{18}$$

Since the electrons are nonequivalent, antisymmetrization yields a direct integral $I_{\rm dir}(rs=ab)$ as well as an exchange integral $I_{\rm ex}(rs=ba)$. The angular integrations are performed using angular momentum graphs as described in [6] and give a total direct contribution D and a total exchange contribution E. The energy contribution to ${}^1S_0$ is $D+E$ and to ${}^3S_1$ $D-E$.

B. Feynman Gauge. Crossed photons

The Feynman amplitude for crossed-photon diagram (Fig. 1) can be evaluated in the same way as for uncrossed photons

$$M=\int d^3x_1\int d^3x_2\int d^3x_3\int d^3x_4\int\frac{dz}{2\pi}$$
$$\times\Phi_r^\dagger(\mathbf{x}_3)iec\alpha_3^\nu iS_F(\mathbf{x}_3,\mathbf{x}_1,e_a-z)iec\alpha_1^\mu\Phi_a(\mathbf{x}_1)$$
$$\times\Phi_s^\dagger(\mathbf{x}_2)iec\alpha_2^{\mu'}iS_F(\mathbf{x}_2,\mathbf{x}_4,e_b-z')iec\alpha_4^{\nu'}\Phi_b(\mathbf{x}_4)$$
$$\times\frac{i}{c}D_{F\nu\nu'}(\mathbf{x}_3-\mathbf{x}_4,z')\frac{i}{c}D_{F\mu'\mu}(\mathbf{x}_2-\mathbf{x}_1,z), \qquad (19)$$

where $z'=z+q'$. In the Feynman gauge this becomes

$$M=\left(\frac{e^2c^2}{\epsilon_0}\right)^2\sum_{t,u}\int\frac{dz}{2\pi}$$
$$\times\langle ru|\alpha_3^\nu\alpha_{\nu4}\int\frac{d^3\mathbf{k}'}{(2\pi)^3}\frac{e^{i\mathbf{k}'\cdot(\mathbf{x}_3-\mathbf{x}_4)}}{(z'^2-c^2\mathbf{k}'^2+i\epsilon)}|tb\rangle$$
$$\times\langle ts|\alpha_1^\mu\alpha_{\mu2}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}_2-\mathbf{x}_1)}}{(z^2-c^2\mathbf{k}^2+i\epsilon)}|au\rangle$$
$$\times\frac{1}{[e_a-z-e_t(1-i\eta)]}\frac{1}{[e_b-z'-e_u(1-i\eta')]}. \qquad (20)$$

The integration over z leads to the integral

$$I^X=i\int_{-\infty}^{\infty}\frac{dz}{2\pi}\frac{1}{[(p-z+i\eta_t)}\frac{1}{(p'-q'-z)+i\eta_u]}$$
$$\times\frac{1}{[(z'+q')^2-(ck'-i\eta)^2]}\frac{1}{[z^2-(ck-i\eta)^2]}. \qquad (21)$$

This integral becomes

$$I^{X++}=\frac{1}{4ckck'}\Bigg\{-\frac{1}{(q+p'-ck)(p-ck)(ck+ck'-q)}$$
$$+\frac{1}{(q+p'-ck)(p-ck)(p'-ck')}$$
$$-\frac{1}{(q'+p-ck')(p'-ck')(ck+ck'-q')}$$
$$+\frac{1}{(q'+p-ck')(p'-ck')(p-ck)}\Bigg\}. \qquad (22)$$

$$I^{X--}=-\frac{1}{4ckck'}\Bigg\{+\frac{1}{(p'-q'+ck)(p+ck)(ck+ck'-q')}$$
$$+\frac{1}{(p'-q'+ck)(p+ck)(p'+ck')}$$
$$+\frac{1}{(p-q'+ck')(p'+ck')(ck+ck'-q)}$$
$$+\frac{1}{(p-q+ck')(p'+ck')(p+ck)}\Bigg\}, \qquad (23)$$

$$I^{X+-}=-\frac{1}{4ckck'(p-ck)(p'+ck')(ck+ck'-q)}$$
$$-\frac{1}{4ckck'(p-p'+q')}\Bigg\{-\frac{1}{(p-ck)(p'+ck')}$$
$$+\frac{1}{(p'-q'+ck)(p'+ck')}$$
$$+\frac{1}{(p'-q'+ck)(ck+ck'-q')}$$
$$+\frac{1}{(p-ck)(p+q'-ck')}$$
$$-\frac{1}{(p+q'-ck')(ck+ck'-q')}\Bigg\}, \qquad (24)$$

$$I^{X-+}=-\frac{1}{4ckck'(p+ck)(p'-ck')(ck+ck'-q')}$$
$$-\frac{1}{4ckck'(p-p'-q)}\Bigg\{\frac{1}{(p+ck)(p'-ck')}$$
$$-\frac{1}{(p+ck)(p-q+ck')}$$
$$-\frac{1}{(p-q+ck')(ck+ck'-q)}$$
$$+\frac{1}{(p'-ck')(p'+q-ck)}$$
$$+\frac{1}{(p'+q-ck)(ck+ck'-q)}\Bigg\}, \qquad (25)$$

and the corresponding energy contribution

$$\Delta E^X_{tu} = \left(\frac{e^2c^2}{\epsilon_0}\right)^2 \int \frac{d^3\mathbf{k}}{(2\pi)^3} \int \frac{d^3\mathbf{k}'}{(2\pi)^3} \times \langle ru|\alpha_3^\nu \alpha_{\nu 4} e^{i\mathbf{k}'\cdot(\mathbf{x}_3-\mathbf{x}_4)}|tb\rangle \times \langle ts|\alpha_1^\mu \alpha_{\mu 2} e^{i\mathbf{k}\cdot(\mathbf{x}_2-\mathbf{x}_1)}|au\rangle I^X. \tag{26}$$

After the integration over the angular parts of the photon momenta we then get

$$\Delta E^X = \left(\frac{e^2}{2\pi^2\epsilon_0}\right)^2 \sum_{l,l'} (2l+1)(2l'+1) \int dk \int dk' \times \sum_t \sum_u \langle r|\alpha^\nu \mathbf{C}^{l'} j_{l'}(k'r)|t\rangle \langle u|\alpha_\nu \mathbf{C}^{l'} j_{l'}(k'r)|b\rangle \times \langle t|\alpha^\mu \mathbf{C}^l j_l(kr)|a\rangle \langle s|\alpha_\mu \mathbf{C}^l j_l(kr)|u\rangle \times (ck)^2 (ck')^2 I^X. \tag{27}$$

C. Coulomb gauge

In the Coulomb gauge we have to replace the interaction in the Feynman gauge

$$-\alpha_1^\mu \alpha_{\mu 2} \frac{e^2c^2}{\epsilon_0} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}_2-\mathbf{x}_1)}}{(z^2-c^2\mathbf{k}^2+i\epsilon)} \tag{28}$$

by the following three terms.

(a) Unretarded Coulomb interaction (scalar)

$$-\frac{e^2c^2}{\epsilon_0} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}_2-\mathbf{x}_1)}}{(-c^2\mathbf{k}^2+i\epsilon)}, \tag{29}$$

(b) Retarded Gaunt interaction (vector)

$$-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2 \frac{e^2c^2}{\epsilon_0} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}_2-\mathbf{x}_1)}}{(z^2-c^2\mathbf{k}^2+i\epsilon)}, \tag{30}$$

(c) Scalar retardation

$$-\left[c\boldsymbol{\alpha}_1\cdot\boldsymbol{\nabla}_1, \left[c\boldsymbol{\alpha}_2\cdot\boldsymbol{\nabla}_2, \frac{e^2c^2}{\epsilon_0} \int \frac{d^3\mathbf{k}}{(2\pi)^3} \times \frac{e^{i\mathbf{k}\cdot(\mathbf{x}_2-\mathbf{x}_1)}}{(z^2-c^2\mathbf{k}^2+i\epsilon)(-c^2\mathbf{k}^2+i\epsilon)}\right]\right]. \tag{31}$$

If the orbitals are generated in a local potential, we can replace $c\boldsymbol{\alpha}\cdot\boldsymbol{\nabla}$ in the commutators by the imaginary unit times the single-electron Dirac Hamiltonian h_D which generates the difference between the orbital energies (p or p') when acting on the orbitals. This gives the matrix element

$$\frac{e^2c^2}{\epsilon_0}(e_a-e_t)(e_b-e_u)\langle tu| \int \frac{d^3\mathbf{k}}{(2\pi)^3} \times \frac{e^{i\mathbf{k}\cdot(\mathbf{x}_2-\mathbf{x}_1)}}{(z^2-c^2\mathbf{k}^2+i\epsilon)(-c^2\mathbf{k}^2+i\epsilon)}|ab\rangle. \tag{32}$$

1. Coulomb-Coulomb

The combination of two unretarded Coulomb interactions leads, in the ladder case, to the z integral

$$I^L_{CC} = i\int_{-\infty}^{\infty} \frac{dz}{2\pi} \frac{1}{(p-z+i\eta_t)} \frac{1}{(p'+z+i\eta_u)} \times \frac{1}{(-c^2k^2+i\eta)} \frac{1}{(-c^2k'^2+i\eta)}. \tag{33}$$

If the intermediate energies e_t and e_u are both positive, the integral becomes $1/(p+p')$ and if both are negative $-1/(p+p')$. If e_t and e_u have different signs, the integral vanishes.

Considering crossed photons, the z integral will be

$$I^X_{CC} = i\int_{-\infty}^{\infty} \frac{dz}{2\pi} \frac{1}{(p-z+i\eta_t)} \frac{1}{(p'-q'-z+i\eta_u)} \times \frac{1}{(-c^2k^2+i\eta)} \frac{1}{(-c^2k'^2+i\eta)}. \tag{34}$$

In this case, the intermediate energies e_t and e_u must have different signs for a nonvanishing integral. The integral for positive e_t, negative e_u becomes $1/(-p+p'-q')$ and for negative e_t, positive e_u we have $1/(p-p'+q')$.

2. Coulomb-Gaunt

There are two ways of writing this interaction. The k photon may be Coulomb and the k'-photon Gaunt (denoted CG) and vice versa (GC). The z integrals become for uncrossed photons

$$I^L_{\mathrm{CG}} = i\int_{-\infty}^{\infty} \frac{dz'}{2\pi} \frac{1}{(p+q'-z'+i\eta_t)} \frac{1}{(p'+q+z'+i\eta_u)} \times \frac{1}{(z'^2-c^2k'^2+i\eta)} \frac{1}{(-c^2k^2+i\eta)}, \tag{35}$$

$$I^L_{\mathrm{GC}} = i\int_{-\infty}^{\infty} \frac{dz}{2\pi} \frac{1}{(p-z+i\eta_t)} \frac{1}{(p'+z+i\eta_u)} \times \frac{1}{(z^2-c^2k^2+i\eta)} \frac{1}{(-c^2k'^2+i\eta)}, \tag{36}$$

which yields

$$I^{L++}_{\mathrm{CG}} = -\frac{1}{p+p'}\left[\frac{1}{q'+p-ck'}\frac{1}{2ck'} + \frac{1}{q+p'-ck'}\frac{1}{2ck'}\right]\frac{1}{(-c^2k^2)}, \tag{37}$$

$$I_{\rm GC}^{L++}=-\frac{1}{p+p'}\left[\frac{1}{p-ck}\frac{1}{2ck}+\frac{1}{p'-ck}\frac{1}{2ck}\right]\frac{1}{(-c^2k'^2)}, \tag{38}$$

$$I_{\rm CG}^{L--}=-\frac{1}{p+p'}\left[\frac{1}{p-q+ck'}\frac{1}{2ck'}+\frac{1}{p'-q'+ck'}\frac{1}{2ck'}\right]\frac{1}{(-c^2k^2)}, \tag{39}$$

$$I_{\rm GC}^{L--}=-\frac{1}{p+p'}\left[\frac{1}{p+ck}\frac{1}{2ck}+\frac{1}{p'+ck}\frac{1}{2ck}\right]\frac{1}{(-c^2k'^2)}, \tag{40}$$

$$I_{\rm CG}^{L+-}=-\frac{1}{q'+p-ck'}\frac{1}{p'-q'+ck'}\frac{1}{2ck'}\frac{1}{(-c^2k^2)}, \tag{41}$$

$$I_{\rm GC}^{L+-}=-\frac{1}{p-ck}\frac{1}{p'+ck}\frac{1}{2ck}\frac{1}{(-c^2k'^2)}, \tag{42}$$

$$I_{\rm CG}^{L-+}=-\frac{1}{p-q+ck'}\frac{1}{p'+q-ck'}\frac{1}{2ck'}\frac{1}{(-c^2k^2)}, \tag{43}$$

$$I_{\rm GC}^{L-+}=-\frac{1}{p+ck}\frac{1}{p'-ck}\frac{1}{2ck}\frac{1}{(-c^2k'^2)}. \tag{44}$$

For crossed photons the z integrals become

$$I_{\rm CG}^{X}=i\int_{-\infty}^{\infty}\frac{dz'}{2\pi}\frac{1}{(p+q'+z'+i\eta_t)}\frac{1}{(p'+z'+i\eta_u)}\times\frac{1}{(z'^2-c^2k'^2+i\eta)}\frac{1}{(-c^2k^2+i\eta)}, \tag{45}$$

$$I_{\rm GC}^{X}=i\int_{-\infty}^{\infty}\frac{dz}{2\pi}\frac{1}{(p'+q-z+i\eta_u)}\frac{1}{(p-z+i\eta_t)}\times\frac{1}{(z^2-c^2k^2+i\eta)}\frac{1}{(-c^2k'^2+i\eta)}, \tag{46}$$

which leads to

$$I_{\rm CG}^{X++}=-\frac{1}{p+q'-ck'}\frac{1}{p'-ck'}\frac{1}{2ck'}\frac{1}{(-c^2k^2)}, \tag{47}$$

$$I_{\rm GC}^{X++}=-\frac{1}{p-ck}\frac{1}{p'+q-ck}\frac{1}{2ck}\frac{1}{(-c^2k'^2)}, \tag{48}$$

$$I_{\rm CG}^{X--}=-\frac{1}{p-q+ck'}\frac{1}{p'+ck'}\frac{1}{2ck'}\frac{1}{(-c^2k^2)}, \tag{49}$$

$$I_{\rm GC}^{X--}=-\frac{1}{p+ck}\frac{1}{p'-q'+ck}\frac{1}{2ck}\frac{1}{(-c^2k'^2)}, \tag{50}$$

$$I_{\rm CG}^{X+-}=-\frac{-2ck'+p-p'+q'}{2ck'(p+q'-ck')(p'+ck')(p-p'+q')}\times\frac{1}{(-c^2k^2)}, \tag{51}$$

$$I_{\rm GC}^{X+-}=-\frac{-2ck+p-p'+q'}{2ck(p-ck)(p'-q'+ck)(p-p'+q')}\times\frac{1}{(-c^2k'^2)}, \tag{52}$$

$$I_{\rm CG}^{X-+}=-\frac{-2ck'-p+p'+q}{2ck'(p-q+ck')(p'-ck')(p'-p+q)}\times\frac{1}{(-c^2k^2)}, \tag{53}$$

$$I_{\rm GC}^{X-+}=-\frac{-2ck-p+p'+q}{2ck(p'+ck)(p'+q-ck)(p'-p+q)}\times\frac{1}{(-c^2k'^2)}. \tag{54}$$

3. Coulomb-Scalar retardation

The z integrals are, for uncrossed and crossed photons, the same as for Coulomb-Gaunt and Gaunt-Coulomb [Eqs. (37–44) and (47–54), respectively]. There is also an additional factor from the scalar retardation interaction. For the Coulomb-Scalar case the resulting momentum expressions must be multiplied with the factor $-(p-q)(p'-q')/(ck')^2$ for ladder and $-(p-q)p'/(ck')^2$ for crossed. For the Scalar-Coulomb case the resulting momentum expressions must be multiplied with the factor $-pp'/(ck)^2$ for ladder and $-p(p'-q')/(ck)^2$ for crossed.

4. Gaunt-Scalar retardation

The z integrals are, for uncrossed and crossed photons, the same as in the Feynman gauge [Eqs. (12–15) and (22–25), respectively]. The additional factors from the scalar retardation interaction are the same as in the Coulomb-Scalar retardation case.

5. Scalar retardation-Scalar retardation

The z integral is, for uncrossed as well as crossed photons, the same as in the Feynman gauge [Eqs. (12–15) and (22–25), respectively] times $pp'(p-q)(p'-q')/[(ck)^2(ck')^2]$.

D. Unretarded contributions

In order to be able to compare the QED results with those of standard RMBPT calculations, we have performed the calculations also without retardation. This is easily done in the formalism presented here simply by setting $z=0$ in the photon propagators. Leaving out the effects of the virtual pairs then yields results which are equivalent to the corresponding RMBPT results.

III. NUMERICAL PROCEDURE

The basis functions used in this calculation are obtained by solving the single-particle Dirac equation in the nuclear potential, using the method of discretization, developed by Salomonson and Öster [11]. Analytical Bessel functions are used, and the radial integrations are performed numerically. Also the integrations over the photon momenta are performed numerically using the method of Gaussian quadrature. 100–200 grid points are used in the radial integrations and 100–140 points in the momentum integration. The angular factors needed are taken from Ref. [6].

A. Pole-integration

Since the k integration is performed along the real axis we have to perform principal-value integrals whenever a pole appears. Special care must be taken when integrating over these poles in order to maintain the numerical accuracy. For excited states both simple and double poles will appear. Consider now the case of a simple pole at $k=\omega$. The integral can then be written as

$$\int dk \frac{f(k)}{k-\omega}, \tag{55}$$

where the numerator $f(k)$ is a discrete-valued function in the chosen k grid. We use a Lagrange polynomial in $(k-k_i)$ to interpolate $f(k)$ to a continuous function. The integral above then reduces to a number of k integrals which look like

$$\int_{k_i}^{k_{i+1}} dk \frac{(k-k_i)^m}{k-\omega}. \tag{56}$$

These integrals are easily evaluated analytically and the principal-value integrals are obtained with high accuracy. For the case of double poles we have instead the integral

$$\int dk \frac{f(k)}{(k-\omega)^2}. \tag{57}$$

By rewriting the numerator as $f(k)=f(\omega)+[f(k)-f(\omega)]$, the double pole is isolated in the first term and the remainder is again of simple pole structure. The double pole can be integrated analytically and we obtain

$$\begin{aligned}\int_0^\infty dk \frac{f(k)}{(k-\omega)^2} &= \int_0^{\mathcal{K}} dk \frac{f(\omega)}{(k-\omega)^2} + \int_0^{\mathcal{K}} dk \frac{f(k)-f(\omega)}{(k-\omega)^2} \\ &\quad + \int_{\mathcal{K}}^\infty dk \frac{f(k)}{(k-\omega)^2} \\ &= \frac{f(\omega)\mathcal{K}}{\omega(\omega-\mathcal{K})} + \int_0^{\mathcal{K}} dk \frac{f(k)-f(\omega)}{(k-\omega)^2} \\ &\quad + \int_{\mathcal{K}}^\infty dk \frac{f(k)}{(k-\omega)^2},\end{aligned} \tag{58}$$

where the integration limit $\mathcal{K}$ is defined such that all possible poles lies in the interval $[0,\mathcal{K}]$. The reason for letting $\mathcal{K}$ be finite is that the second term converges slowly for large $\mathcal{K}$. The second term is calculated using the scheme for simple poles outlined above and the last term, together with all other pole free k integrations, is computed using Gauss-Legendre and Gauss-Laguerre quadrature.

B. Products of poles

Since we integrate over two momenta, k and k', and thus on two different real axes, there are cases when there are poles on both these axes simultaneously. We will then not just get a contribution from the principal integration, but also from the product of the two imaginary semicircle integrations, which when multiplied will yield a real contribution to the energy. For the case with two simple poles we have the expression

$$\int dk \int dk' \frac{f(k)}{k-\omega} \frac{g(k')}{k'-\omega'} h(k,k'). \tag{59}$$

It is convenient to separate out the matrix elements, which depend only on k or k'. The additional contribution will be

$$i\pi f(\omega) i\pi g(\omega') h(\omega,\omega'). \tag{60}$$

We only find contributions from poles which are on the same side of the real axis.

If one (or both) of the poles is a double pole one has to differentiate the expression with respect to the momentum that corresponds to the double pole. Considering

$$\int dk \int dk' \frac{f(k)}{(k-\omega)^2} \frac{g(k')}{(k'-\omega')^2} h(k,k'), \tag{61}$$

the contribution will in this case be

$$\begin{aligned}(i\pi)^2 \{ & f_k'(\omega) g_{k'}'(\omega') h(\omega,\omega') + f_k(\omega) g_{k'}'(\omega') h_k'(\omega,\omega') \\ & + f_k'(\omega) g_{k'}(\omega') h_{k'}'(\omega,\omega') \\ & + f_k(\omega) g_{k'}(\omega') h_{k,k'}''(\omega,\omega') \}.\end{aligned} \tag{62}$$

An extra difficult case is for the crossed exchange case when the intermediate states t,u both are $1s$. The term

$$\int dk\int dk'\frac{f(k)}{(k+k'-\omega)}\frac{g(k')}{(k'-\omega)^2}h(k,k') \qquad (63)$$

will have a pole in $k=0,k'=w$. The imaginary contribution from the k integration here comes from a *quarter circle*.

When differentiating the matrix elements one needs the derivatives of the spherical Bessel functions. We have chosen to use known recurrence relations to express these derivatives analytically.

The contributions from products of poles are very important, especially for the reference states (see the Appendix) and corresponding crossed diagrams. We also find that the sum of all contributions from products of poles are gauge invariant.

C. Canceling of singularities

Some of the reference state contributions are singular in the limit $k,k'\to 0$. These singularities occur when the matrix elements do not approach zero when $k,k'\to 0$, implying that the Bessel functions $j_L(kr)$ and $j_{L'}(k'r)$, which are involved in the matrix elements, do not approach zero, which will only be the case if $L=L'=0$. Singularities in the crossed integrals with the same matrix elements, will be cancelled by a corresponding singularity in one of the reference state contributions. There is a singularity in the crossed direct contribution when $t,u=1s,2s$. This singularity is cancelled by the reference state contribution in the ladder direct case when $t,u=1s,2s$. There is also a singularity in the crossed exchange contribution when $t,u=1s,1s$ or $t,u=2s,2s$. These expressions are canceled by the reference state contributions for the ladder exchange when $t,u=1s,2s$ and $t,u=2s,1s$, respectively.

D. Numerical singularities

Considering crossed exchange, there is a contribution of the form

$$\int dk\int dk'\frac{kk'M(k,k')}{(k+k'-\omega)(k'-\omega)^2}, \qquad (64)$$

which becomes singular when $k'\to\omega$ and $k\to 0$, if the matrix elements $M(k,k')$ do not approach zero. This makes the principal integration very difficult numerically, a problem which is solved by subtracting the most singular part. More explicitly this is done by expanding the numerator

$$kk'=[(k+k'-\omega)-(k'-\omega)]k' \qquad (65)$$

and the matrix-elements $M(k,k')$ around the pole. In the numerical evaluation we subtract the most singular part, which involves the second term in Eq. (65) and is given by

$$-M(0,w)\int_0^{\mathcal{K}}dk\int_0^{\mathcal{K}}dk'\frac{(k'-\omega)\omega}{(k+k'-\omega)(k'-\omega)^2}. \qquad (66)$$

One of the k integrations can be performed analytically which yields

$$-M(0,w)\int_{-\omega}^{\omega}\frac{1}{x}\ln\left(1+\frac{x}{\mathcal{K}}\right)dx+\int_{\omega}^{\mathcal{K}-\omega}\frac{1}{x}\left[\ln\left(1+\frac{x}{\mathcal{K}}\right)-\ln\left(\frac{x}{\mathcal{K}}\right)\right]dx. \qquad (67)$$

Here the x integration can be performed to arbitrary accuracy using Gaussian quadrature and then this semianalytically evaluated term is readded.

E. Extrapolation

The calculation procedure discussed above is executed for different numbers of radial grid points N for each given partial wave (L value). The values obtained are then grid extrapolated to $N=\infty$. We evaluate several partial waves, the maximum number of L depending on the convergence properties of the given contribution, and finally we extrapolate to $L=\infty$. We typically use three grids in the range of 100–200 radial grid points and evaluate partial wave terms up to $L=20$. For $Z=10$, however, we use up to $L=30$ partial waves, since for such low Z the effects are so small that the accuracy has to be high to give relevant results. It is also necessary to use a large number of partial waves for the singlet state, since it converges slowly, which can be seen in Tables I and II.

IV. RESULTS

The results of our calculations are given in Tables I–III. It should be noted that we have used *point* nucleus for $Z=10,14,18$ and *extended* nucleus for $z=24,30,60,92$. When possible, we compare our values with recent calculations by Mohr and Sapirstein [2]. We have performed the calculations in both the Feynman and Coulomb gauges, and the total results are found to be gauge invariant. The A0-A0, A0-ALF, and ALF-ALF parts, where A0 stands for the scalar part and ALF for the vector part of the interaction, are also separately gauge invariant. Furthermore, these parts as well as the total values are gauge invariant for each partial wave limit for the exchanged photons, $l,l'\leqslant L$ in Eqs. (18) and (27)

V. ANALYSIS

The various energy contributions to heliumlike ions of order $(Z\alpha)^3$ and $(Z\alpha)^3\ln(\alpha)$ have been evaluated analytically by Kabir and Salpeter [12], Araki [13], Sucher [5], Ermolaev [14] and others, and the results of Sucher are summarized in Table IV. Araki gives the following total contributions in the three cases (we are omitting the factor α^3 below):

TABLE I. Full two-photon-exchange calculation for $Z=10$ using Coulomb gauge (in μhartree). The calculation is performed with a point nucleus. "Unretarded" represents results without retardation and without virtual pairs (negative-energy states) and is equivalent to RMBPT; "no-virtual pairs" (NVP) represents results with retardation but without virtual pairs;

$Z=10$	^1S	^3S
Coulomb-Coulomb		
Unretarded=NVP	-115180.10	-47627.57
Virtual pairs	4.86	0.04
Total	-115175.24	-47627.53
Coulomb-Breit		
Unretarded	-815.00	-10.37
No-virtual pairs	-791.42	-11.36
Virtual pairs	-19.09	0.05
Total	-810.51	-11.31
QED=Total-Unretarded	4.49	-0.94
Breit-Breit		
Unretarded	-10.10	-0.14
No-virtual pairs	-7.33	-0.12
Virtual pairs	-5.67	-0.34
Total	-13.00	-0.46
QED=Total-Unretarded	-2.90	-0.32
Total		
Unretarded	-116005.55	-47638.07
No-virtual pairs	-115978.85	-47639.05
Virtual pairs	-19.90	-0.25
A0-A0	-115170.83	-47584.02
A0-ALF	-803.53	-54.66
ALF-ALF	-24.40	-0.62
GRAND TOTAL	-115998.77	-47639.30
QED=Total-Unretarded ($L=10$)	7.67	-1.23
QED=Total-Unretarded	6.45	-1.23

$$-\frac{4}{3}\langle\delta(\mathbf{r}_{12})\rangle,\quad \text{Coulomb-Coulomb}$$

$$\frac{4}{3}\left(\frac{8}{3}-2\ln\alpha\right)\langle\delta(\mathbf{r}_{12})\rangle-\frac{4}{3}\langle\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\delta(\mathbf{r}_{12})\rangle-\frac{8}{3}Q$$
$$-\frac{2}{3\pi}M',\quad \text{Coulomb-Breit}$$

$$\left(\frac{17}{3}-\frac{8}{3}\ln 2+2\ln\alpha\right)\langle\delta(\mathbf{r}_{12})\rangle+\frac{1}{3}\langle\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\delta(\mathbf{r}_{12})\rangle$$
$$-2Q,\quad \text{Breit-Breit} \tag{68}$$

which gives the *total contribution*

TABLE II. Full two-photon-exchange calculation for $Z=30$ using Coulomb gauge (in μhartree). The calculation is performed with an extended nucleus (RMS=3.955). "Unretarded" represents results without retardation and without virtual pairs (negative-energy states) and is equivalent to RMBPT; "no-virtual pairs" (NVP) represents results with retardation but without virtual pairs;

$Z=30$	^1S	^3S
Coulomb-Coulomb		
Unretarded=NVP	-120895.80	-49433.33
Virtual pairs	99.73	3.11
Total	-120796.12	-49430.22
Coulomb-Breit		
Unretarded	-7056.69	-98.20
No-virtual pairs	-6712.45	-120.12
Virtual pairs	-379.43	3.49
Total	-7091.88	-116.63
QED=Total-Unretarded	-35.05	-18.42
Breit-Breit		
Unretarded	-396.63	-10.21
No-virtual pairs	-274.22	-8.18
Virtual pairs	11.35	7.05
Total	-262.88	-1.13
QED=Total-Unretarded	133.95	9.08
TOTAL		
Unretarded	-128349.12	-49541.73
No-virtual pairs	-127882.47	-49561.62
Virtual pairs	-268.35	13.66
A0-A0	-121057.69	-49031.91
A0-ALF	-6669.60	-517.23
ALF-ALF	-423.59	1.19
GRAND TOTAL	-128150.88	-49547.95
QED=Total-Unretarded ($L=10$)	205.01	-6.44
QED=Total-Unretarded	198.24	-6.22
RMBPT [a]		-49541.34
Grand Total[a]		-49550.08
QED[a]		-8.74

[a]From Ref. [2].

$$\left(\frac{71}{9}-\frac{8}{3}\ln 2-\frac{2}{3}\ln\alpha\right)\langle\delta(\mathbf{r}_{12})\rangle-\langle\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\delta(\mathbf{r}_{12})\rangle-\frac{14}{3}Q$$
$$-\frac{2}{3\pi}M', \tag{69}$$

where Q is the principal part of the logarithmically diverging quantity $\mathbf{r}_{12}^{-3}$ [1] and M' is a part of the Bethe logarithm [15]. These results agree with those given by Sucher.

TABLE III. Full two-photon-exchange calculation compared with MBPT and other calculations. The values are in hartree.

	$2\ ^1S_0$	2^3S_1	
$Z=10$			
2γ	-0.11599877	-0.04763930	
RMBPT	-0.11600497	-0.04763807	
QED	0.00000620	-0.00000123	
$Z=14$			
2γ	-0.11742901	-0.04786237	
RMBPT	-0.11744606	-0.04785964	
QED	0.0001690	-0.00000273	
$Z=18$			
2γ	-0.11934461	-0.04816257	
RMBPT	-0.11938138	-0.04815795	
QED	0.0000379	-0.00000462	
$Z=24$ (RMS $=3.655$)			
2γ	-0.12315605	-0.04876184	
RMBPT	-0.12324940	-0.04875490	
QED	0.00009343	-0.00000694	
$Z=30$ (RMS $=3.955$)			
2γ	-0.1276 [a]	-0.04954 [a]	
2γ	-0.12815090	-0.04954795	-0.04955508 [b]
RMBPT	-0.12834910	-0.04954173	-0.04954134 [b]
QED	0.00019810	-0.00000622	-0.00000874 [b]
$Z=60$ (RMS $=4.915$)			
2γ	-0.1753732	-0.0568096	-0.056799 [b]
RMBPT	-0.1777315	-0.0570252	-0.057023 [b]
QED	0.0023583	0.0002156	0.000224 [b]
$Z=92$ (RMS $=5.86$)			
2γ	-0.3008 [a]	-0.07416 [a]	
2γ	-0.3018243	-0.0743067	-0.074246 [b]
RMBPT	-0.3149504	-0.0762391	-0.076230 [b]
QED	0.0131261	0.0019323	0.001984 [b]

[a]Corresponding values from Ref. [3].
[b]From Ref. [2].

The self-energy and vacuum-polarization contributions have been evaluated by Araki with the following results:

$$\Delta E_{\mathrm{se}}=\frac{4}{3}\left(\frac{5}{6}-\ln 2-2\ln\alpha\right)[Z\langle\delta(\mathbf{r}_1)\rangle+Z\langle\delta(\mathbf{r}_2)\rangle-2\langle\delta(\mathbf{r}_{12})\rangle]-\frac{2}{3}\langle\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\rangle\langle\delta(\mathbf{r}_{12})\rangle-\frac{2}{3\pi}M'', \tag{70}$$

$$\Delta E_{\mathrm{vp}}=\frac{4}{15}\langle\delta(\mathbf{r}_{12})\rangle-\frac{4}{15}Z[\langle\delta(\mathbf{r}_1)\rangle+\langle\delta(\mathbf{r}_2)\rangle], \tag{71}$$

where M'' is a second part of the Bethe logarithm. The $\langle\delta(\mathbf{r}_{12})\rangle$ parts of the self-energy and vacuum-polarization contributions come from the vertex diagram and the inter-electronic vacuum-polarization diagram, respectively. The $\langle\delta(\mathbf{r}_1)\rangle,\langle\delta(\mathbf{r}_2)\rangle$ parts consists of one electron self-energy and vacuum polarization effects, as well as higher-order coulomb-screening effects.

Adding these quantities to the total two-photon exchange above Eq. (69), gives $(M'+M''=M)$

$$\left[\frac{89}{15}+\frac{14}{3}\ln\alpha-\frac{5}{3}\langle\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\rangle\right]\langle\delta(\mathbf{r}_{12})\rangle+\frac{4}{3}\left(\frac{19}{30}-\ln(2\alpha^2)\right)\times[Z\delta(\mathbf{r}_1)+Z\delta(\mathbf{r}_2)]-\frac{14}{3}Q-\frac{2}{3\pi}M. \tag{72}$$

With $\langle\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\rangle=-3$ for singlet states, this agrees with the results of Drake [16].

To leading order in a 1/Z expansion, Q is

$$Q(^1S)=-[\ln(Z)+C(^1S)]\frac{2Z^3}{81\pi}, \tag{73}$$

$$Q(^3S)=-C(^3S)\frac{2Z^3}{81\pi}, \tag{74}$$

where we have evaluated the constants to be

$$C(^1S)=\frac{1}{2}\ln 3-142\ln 2+\frac{1947}{20}\approx-0.527\,59, \tag{75}$$

$$C(^3S)=-\frac{1}{2}\ln 3-141\ln 2+\frac{1963}{20}\approx-0.133\,06, \tag{76}$$

which is in agreement with Drake [1]. Similarly M' is in leading order given by

$$-\frac{2}{3\pi}M'(^1S)=\left(-\frac{16}{3}\ln Z+D(^1S)\right)\frac{2Z^3}{81\pi}, \tag{77}$$

$$-\frac{2}{3\pi}M'(^3S)=D(^3S)\frac{2Z^3}{81\pi}, \tag{78}$$

where $D(^1S)$ and $D(^3S)$ are constants that have to be evaluated numerically. We have evaluated these constants along the lines in Appendix C in Ref. [6]. The values achieved are $D(^1S)\approx-2.273\,67$ and $D(^3S)\approx-0.010\,80$, and are expected to be accurate to the number of digits given. We have chosen to factor out $2Z^3/81\pi$, which is the value of $\langle\delta(\mathbf{r}_{12})\rangle$ for the singlet state, using hydrogenic functions.

The total theoretical contributions are given in Tables V and VI, as well as numerical values from the average of several least-square fits, shown in Figs. 2 and 3. The fits are performed using different polynomials and do not include the $Z=60$ and $Z=92$ values, since other effects as, for instance the extended nucleus, affects the fits too much. Our calculated zeroth-order nonrelativistic values are $-114\,510$ har-

TABLE IV. Coefficients (in hartree units) for the $(Z\alpha)^3$ contributions for electron-electron interaction in heliumlike ions, evaluated by Sucher (Ref. [5]). The entries for both ^1S and ^3S should be multiplied by $2/81\pi$, which is the value of $\langle \delta(\mathbf{r}_{12})\rangle/Z^3$ for the singlet state. We have chosen to keep the separation of terms depending on $\langle \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\rangle$, which has the value of -3 for singlet states and 0 for triplet states. For ^3S, $\langle \delta(\mathbf{r}_{12})\rangle = 0$ and we only have contributions from the Q and M' parts.

Contribution	^1S	^3S
Coulomb-Coulomb		
No pair=RMBPT	$-\left(\frac{\pi}{2}+\frac{5}{3}\right)$	
Single pair	2	
Double pair	$\left(\frac{\pi}{2}-\frac{5}{3}\right)$	
Total Coul-Coul	$-\frac{4}{3}$	
Coulomb-Breit		
Unretarded=RMBPT	$-\frac{4}{3}\left(\frac{\pi}{2}+1\right)\langle\sigma_1\times\sigma_2\rangle$	
No pair	$\frac{8}{3}C(^1S)+D(^1S)+\frac{32}{9}-\frac{4}{3}\left(\frac{\pi}{2}+1+\frac{1}{2}\ln 2\right)\langle\sigma_1\times\sigma_2\rangle-\frac{8}{3}\ln(Z\alpha)$	$\frac{8}{3}C(^3S)+D(^3S)$
Single pair	$\frac{4}{3}(1+\ln 2)\langle\sigma_1\times\sigma_2\rangle$	
Double pair	$\frac{4}{3}\left(\frac{\pi}{2}-1-\frac{1}{2}\ln 2\right)\langle\sigma_1\times\sigma_2\rangle$	
Total Coul-Breit	$\frac{8}{3}C(^1S)+D(^1S)+\frac{32}{9}-\frac{4}{3}\langle\sigma_1\times\sigma_2\rangle-\frac{8}{3}\ln(Z\alpha)$	$\frac{8}{3}C(^3S)+D(^3S)$
Breit-Breit		
Unretarded=RMBPT	$4-2\pi$ [b]	
No pair	$-\frac{3\pi}{4}+1+\frac{1}{2}\ln 2+\frac{1}{3}\left(-\frac{\pi}{4}+1+\frac{1}{2}\ln 2\right)\langle\sigma_1\times\sigma_2\rangle$	
Single pair	$1+3\ln 2+\frac{1}{3}(1-\ln 2)\langle\sigma_1\times\sigma_2\rangle$	
Double pair	$2C(^1S)+\frac{3\pi}{4}+\frac{11}{3}-\frac{37}{6}\ln 2+\frac{1}{3}\left(\frac{\pi}{4}-1+\frac{1}{2}\ln 2\right)\langle\sigma_1\times\sigma_2\rangle$ $+2\ln(Z\alpha)$	$2C(^3S)$
Total Breit-Breit	$2C(^1S)+\frac{17}{3}-\frac{8}{3}\ln 2+\frac{1}{3}\langle\sigma_1\times\sigma_2\rangle+2\ln(Z\alpha)$	$2C(^3S)$
TOTAL		
Unretarded=RMBPT	$\frac{19}{3}-\frac{\pi}{2}$ [a]	
No pair	$\frac{8}{3}C(^1S)+D(^1S)+\frac{26}{9}-\frac{5\pi}{4}+\frac{1}{2}\ln 2-\left(\frac{3\pi}{4}+1+\frac{1}{2}\ln 2\right)\langle\sigma_1\times\sigma_2\rangle$ $-\frac{8}{3}\ln(Z\alpha)$	$\frac{8}{3}C(^3S)+D(^3S)$
Single pair	$3(1+\ln 2)+\left(\frac{5}{3}+\ln 2\right)\langle\sigma_1\times\sigma_2\rangle$	
Double pair	$2C(^1S)+\frac{5\pi}{4}+2-\frac{37}{6}\ln 2+\left(\frac{3\pi}{4}-\frac{5}{3}-\frac{1}{2}\ln 2\right)\langle\sigma_1\times\sigma_2\rangle$ $+2\ln(Z\alpha)$	$2C(^3S)$
GRAND TOTAL	$\frac{14}{3}C(^1S)+D(^1S)+\frac{71}{9}-\frac{8}{3}\ln 2-\langle\sigma_1\times\sigma_2\rangle-\frac{2}{3}\ln(Z\alpha)$	$\frac{14}{3}C(^3S)+D(^3S)$

[a]This expression is taken from Ref. [18]. Here the $\langle \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\rangle$ term is not separated out.
[b]This expression is deduced from the other unretarded values in this column.

TABLE V. Coefficients for $(Z\alpha)^n$ from the least-squares fit of the numerical data for the $1s2s\ ^1S$ state. The $(Z\alpha)^3$ coefficients are compared with theoretical predictions of Sucher (Ref. [5]). "Unretarded" represents results without retardation and without virtual pairs (negative-energy states); "no-virtual pairs" (NVP) represents results with retardation but without virtual pairs.

Contribution	$(Z\alpha)^2$ Numerical	$(Z\alpha)^3\ ^1S$ Numerical	$(Z\alpha)^3\ ^1S$ Sucher [5]	$(Z\alpha)^4\ ^1S$ Numerical
Coulomb-Coulomb	0.116(2)			
Unretarded=NVP		-0.025(2)	-0.02545	-0.06(1)
Virtual pairs		0.015(1)	0.01497	-0.04(1)
Total		-0.010(1)	-0.01048	-0.11(1)
Coulomb-Breit	0.158(1)			
Unretarded		0.081(2)	0.08082	-0.11(2)
No-virtual pairs		0.091(2)	0.09073	-0.19(1)
Virtual pairs		-0.058(3)	-0.06063	0.12(1)
Total		0.031(2)	0.03046	0.06(2)
QED=Total-Unretarded		-0.049(2)	-0.05037	0.06(2)
Breit-Breit				
Unretarded		-0.019(2)	-0.01795	-0.10(1)
No-virtual pairs		-0.013(1)	-0.01235	-0.11(2)
Virtual pairs		0.026(1)	0.02620	0.10(1)
Total		0.014(1)	0.01390	-0.08(2)
QED=Total-Unretarded		0.032(1)	0.03180	0.04(3)
TOTAL				
Unretarded		0.036(2)	0.03743	-0.33(2)
No-virtual pairs		0.051(2)	0.05294	-0.33(2)
Virtual pairs		-0.017(3)	-0.01946	0.01(1)
GRAND TOTAL	0.274(4)	0.033(2)	0.03380	0.23(2)
QED=Total-Unretarded		-0.003(1)	-0.00360	0.06(2)

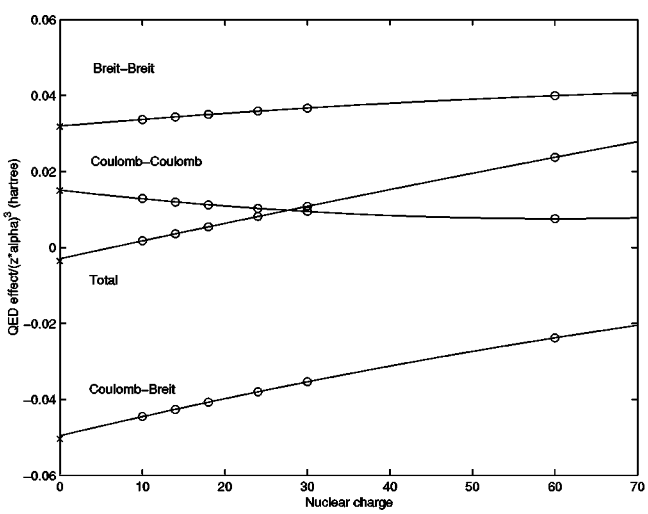

FIG. 2. Contributions to the total QED effect of the two-photon exchange for the $1s2s\ ^1S$ state, divided by $(Z\alpha)^3$. The $(Z\alpha)^3\ln(Z\alpha)$ parts have been subtracted. The curves represent only effects beyond RMBPT, although there are also $(Z\alpha)^3$ contributions in RMBPT. The points and slopes at the origin represent the $(Z\alpha)^3$ and $(Z\alpha)^4$ coefficients, respectively. The crosses represent the analytical results by Sucher [5]. The Coulomb-Coulomb curve only has contributions from virtual pairs.

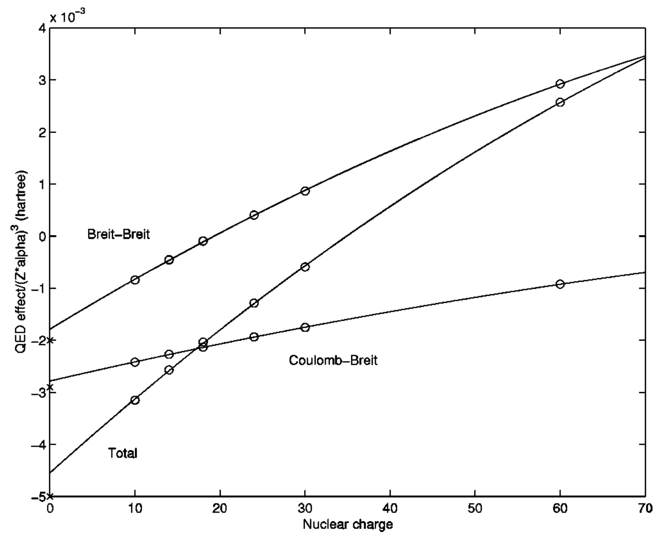

FIG. 3. Contributions to the total QED effect of the two-photon exchange for the $1s2s\ ^3S$ state, divided by $(Z\alpha)^3$. The points and slopes at the origin represents the $(Z\alpha)^3$ and $(Z\alpha)^4$ coefficients, respectively. The crosses represent the analytical results by Sucher [5].

TABLE VI. Coefficients for $(Z\alpha)^n$ from the least-squares fit of the numerical data for the $1s2s\ ^3S$ state. The $(Z\alpha)^3$ coefficients are compared with theoretical predictions of Sucher (Ref. [5]). "Unretarded" represents results without retardation and without virtual pairs (negative-energy states); "no-virtual pairs" represents results with retardation but without virtual pairs. We have omitted the Coulomb-Coulomb part since there are no $(Z\alpha)^3$ contributions here [there is however a $(Z\alpha)^2$ contribution].

Contribution	$(Z\alpha)^2$ Numerical	$(Z\alpha)^3\ ^3S$ Numerical	$(Z\alpha)^3\ ^3S$ Sucher [5]	$(Z\alpha)^4\ ^3S$ Numerical
Coulomb-Breit	-0.002(1)			
Unretarded				
No-virtual pairs		-0.0029(1)	-0.0029	0.002(2)
Virtual pairs				
Total				
QED=Total-Unretarded		-0.0029(1)	-0.0029	0.006(1)
Breit-Breit				
Unretarded				
No-virtual pairs				
Virtual pairs		-0.0019(2)	-0.0021	0.17(2)
Total				
QED=Total-Unretarded		-0.0019(2)	-0.0021	0.02(2)
TOTAL				
Unretarded				
No-virtual pairs		-0.0029(1)	-0.0029	-0.07(3)
Virtual pairs		-0.0019(2)	-0.0021	0.02(1)
GRAND TOTAL	-0.043(2)	-0.0048(3)	-0.0050	-0.05(4)
QED=Total-Unretarded		-0.0048(3)	-0.0050	0.03(2)

tree for the singlet state and $-47\,409$ hartree for the triplet state. The values are in agreement with previous calculations by Safronova [17].

We find good agreement between our numerical values and the theoretical ones by Sucher.

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APPENDIX: THE REFERENCE STATE CONTRIBUTIONS

Consider the two-photon electron exchange contributions given by the energy shift formula in Eq. (1). The intermediate states degenerate with the initial state, called *reference states*, lead to divergent expressions in the ladder diagram. However, these divergencies are canceled by the squared second-order *S*-matrix contribution, and the remaining finite contributions, called the *reference state contributions*, are derived in this section. Furthermore, the reference state contributions also contains singularities, when k or k' goes to zero, which are canceled by similar singularities in the crossed interaction, see Sec. III C. The procedure presented here is a generalization to retarded interactions of the procedure in [6]. There is no reference state divergency in the crossed photon interaction. Contrary to [6], we treat the reference states in the crossed photon interaction as any other intermediate state, and do not add the corresponding contributions to the ladder reference states contribution.

For simplicity the Feynman gauge is used below. The ladder contribution to the energy shift is given by Eq. (2). For simplicity we define a function

$$g_{srba}(z)=\int d^3\mathbf{x}_1\int d^3\mathbf{x}_2\frac{-c}{\epsilon_0}\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot(\mathbf{x}_2-\mathbf{x}_1)}}{(z^2-c^2\mathbf{k}^2+i\epsilon)}\times\Phi_s^\dagger(\mathbf{x}_2)\alpha_\mu\Phi_r(\mathbf{x}_2)\Phi_b^\dagger(\mathbf{x}_1)\alpha^\mu\Phi_a(\mathbf{x}_1). \qquad \text{(A1)}$$

There will be four different cases to be calculated. For the overall direct case D $(rs=ab)$, we may have internal direct D_d $(tu=ab)$ or internal exchange D_e $(tu=ba)$ (see Fig. 1).

Similarly we define for overall exchange $(rs=ba)E_d$ and E_e, here referring to direct and exchange of the first interaction. Considering the overall direct, internal direct part of $\langle\Phi_a^0|S_{lad,\gamma}^4|\Phi_a^0\rangle$, we have

$$D_d$$

$$=c^2e^4\int_{-\infty}^{\infty}\frac{dz_1}{2\pi}\int_{-\infty}^{\infty}\frac{dz_2}{2\pi}\int_{-\infty}^{\infty}\frac{dz_3}{2\pi}\int_{-\infty}^{\infty}\frac{dz_4}{2\pi}\,\frac{1}{[z_3-e_a(1-i\eta)]}$$
$$\times\frac{1}{[z_4-e_b(1-i\eta)]}\sum_{lad}g_{s'r'b'a'}(z_2)g_{srba}(z_1)$$
$$\times\int_{-\infty}^{\infty}dt_4e^{-i(z_4+z_2-e_b)t_4}e^{-\gamma|t_4|}$$
$$\times\int_{-\infty}^{\infty}dt_3e^{-i(z_3-z_2-e_a)t_3}e^{-\gamma|t_3|}$$
$$\times\int_{-\infty}^{\infty}dt_2e^{-i(z_1-z_4+e_b)t_2}e^{-\gamma|t_2|}$$
$$\times\int_{-\infty}^{\infty}dt_1e^{-i(e_a-z_3-z_1)t_1}e^{-\gamma|t_1|}. \tag{A2}$$

By using the integral identity

$$f_\gamma(z_2,z_1)=\int_{-\infty}^{\infty}dz\frac{1}{[z-e_0(1-i\eta)]}$$
$$\times\frac{\gamma}{(e_0-z-z_2)^2+\gamma^2}\,\frac{\gamma}{(e_0-z+z_1)^2+\gamma^2}$$
$$=\frac{\pi\gamma}{(z_2+z_1)^2+4\gamma^2}\,\frac{(z_2-z_1-4i\gamma)}{(z_2-i\gamma)(z_1+i\gamma)}, \tag{A3}$$

we can perform the z_3 and z_4 integrations, yielding the following expression:

$$D_d=\frac{c^2e^4}{\pi^4}\int dz_1\int dz_2f_\gamma(z_2,z_1)f_\gamma(z_1,z_2)$$
$$\times\sum_{lad}g_{s'r'b'a'}(z_2)g_{srba}(z_1). \tag{A4}$$

Using the same technique and introducing $\omega=e_b-e_a$, the other three cases become

$$D_e=\frac{c^2e^4}{\pi^4}\int dz_1\int dz_2f_\gamma(z_2+\omega,-\omega-z_1)$$
$$\times f_\gamma(-\omega-z_1,z_2+\omega)\sum_{lad}g_{s'r'b'a'}(z_2)g_{srba}(z_1), \tag{A5}$$

$$E_d=\frac{c^2e^4}{\pi^4}\int dz_1\int dz_2f_\gamma(z_2-\omega,z_1)f_\gamma(z_1,z_2-\omega)$$
$$\times\sum_{lad}g_{s'r'b'a'}(z_2)g_{srba}(z_1), \tag{A6}$$

$$E_e=\frac{c^2e^4}{\pi^4}\int dz_1\int dz_2f_\gamma(z_2,-\omega-z_1)f_\gamma(-\omega-z_1,z_2)$$
$$\times\sum_{lad}g_{s'r'b'a'}(z_2)g_{srba}(z_1). \tag{A7}$$

In order to handle the divergent part of the ladder diagram, we focus on the squared one-photon counter part which has to be subtracted in order to obtain the finite ladder contribution. Following standard rules, we can write the direct O_d and exchange O_e one-photon counter parts of $\langle\Phi_a^0|S_{red,\gamma}^2|\Phi_a^0\rangle$ as

$$O_d=-i\frac{ce^2}{2\pi}\int_{-\infty}^{\infty}dz\frac{4\gamma^2}{(z^2+\gamma^2)^2}g_{srba}(z), \tag{A8}$$

$$O_e=-i\frac{ce^2}{2\pi}\int_{-\infty}^{\infty}dz\frac{4\gamma^2}{((z+\omega)^2+\gamma^2)^2}g_{srba}(z). \tag{A9}$$

The contribution from the D_d diagram will be $4D_d-2O_d^2$ and for the D_e diagram $4D_e-2O_e^2$. The two exchange diagrams E_d and E_e yield the contributions $4E_d-2O_dO_e$ and $4E_e-2O_eO_d$, respectively.

Consider the sum

$$f_\gamma(z_2,z_1)+f_\gamma(z_1,z_2)$$
$$=\frac{\pi\gamma}{(z_2+z_1)^2+4\gamma^2}\times\left\{\frac{(z_2-z_1-4i\gamma)}{(z_2-i\gamma)(z_1+i\gamma)}\right.$$
$$\left.+\frac{(z_1-z_2-4i\gamma)}{(z_1-i\gamma)(z_2+i\gamma)}\right\}$$
$$=-\frac{2\pi\gamma^2i}{(z_1^2+\gamma^2)(z_2^2+\gamma^2)}, \tag{A10}$$

and the square of the sum

$$\frac{1}{2}[f_\gamma(z_2,z_1)+f_\gamma(z_1,z_2)]^2=\frac{-2\pi^2\gamma^4}{(z_1^2+\gamma^2)^2(z_2^2+\gamma^2)^2}. \tag{A11}$$

By using this identity we can rewrite the squared one-photon counter parts as

$$O_d^2=\frac{-c^2e^4}{4\pi^2}\int_{-\infty}^{\infty}dz_1\int_{-\infty}^{\infty}dz_2\frac{4\gamma^2}{(z_2^2+\gamma^2)^2}\frac{4\gamma^2}{(z_1^2+\gamma^2)^2}\times\sum_{lad}g_{s'r'b'a'}(z_2)g_{srba}(z_1)$$
$$=\frac{c^2e^4}{\pi^4}\int_{-\infty}^{\infty}dz_1\int_{-\infty}^{\infty}dz_2[f_\gamma(z_2,z_1)+f_\gamma(z_1,z_2)]^2\times\sum_{lad}g_{s'r'b'a'}(z_2)g_{srba}(z_1),\tag{A12}$$

$$O_e^2=\frac{-c^2e^4}{4\pi^2}\int_{-\infty}^{\infty}dz_1\int_{-\infty}^{\infty}dz_2\frac{4\gamma^2}{[(-z_2-w)^2+\gamma^2]^2}\times\frac{4\gamma^2}{[(z_1+w)^2+\gamma^2]^2}\sum_{lad}g_{s'r'b'a'}\times(-z_2-w)g_{srba}(z_1+w)$$
$$=\frac{c^2e^4}{\pi^4}\int_{-\infty}^{\infty}dz_1\int_{-\infty}^{\infty}dz_2[f_\gamma(-z_2-w,z_1+w)+f_\gamma(z_1+w,-z_2-w)]^2\sum_{lad}g_{s'r'b'a'}\times(-z_2-w)g_{srba}(z_1+w),\tag{A13}$$

$$O_dO_e=\frac{-c^2e^4}{4\pi^2}\int_{-\infty}^{\infty}dz_1\int_{-\infty}^{\infty}dz_2\frac{4\gamma^2}{[(-z_2-w)^2+\gamma^2]^2}\times\frac{4\gamma^2}{[(z_1)^2+\gamma^2]^2}\sum_{lad}g_{s'r'b'a'}(-z_2-w)g_{srba}(z_1)$$
$$=\frac{c^2e^4}{\pi^4}\int_{-\infty}^{\infty}dz_1\int_{-\infty}^{\infty}dz_2[f_\gamma(-z_2-w,z_1)+f_\gamma(z_1,-z_2-w)]^2\times\sum_{lad}g_{s'r'b'a'}(-z_2-w)g_{srba}(z_1),\tag{A14}$$

$$O_eO_d=\frac{-c^2e^4}{4\pi^2}\int_{-\infty}^{\infty}dz_1\int_{-\infty}^{\infty}dz_2\frac{4\gamma^2}{[(-z_2)^2+\gamma^2]^2}\times\frac{4\gamma^2}{[(z_1+w)^2+\gamma^2]^2}\times\sum_{lad}g_{s'r'b'a'}(-z_2)g_{srba}(z_1+w)$$
$$=\frac{c^2e^4}{\pi^4}\int_{-\infty}^{\infty}dz_1\int_{-\infty}^{\infty}dz_2[f_\gamma(-z_2,z_1+w)+f_\gamma(z_1+w,-z_2)]^2\times\sum_{lad}g_{s'r'b'a'}(-z_2)g_{srba}(z_1+w).\tag{A15}$$

Considering the D_d diagram, it can be rewritten as

$$D_d=\frac{c^2e^4}{\pi^4}\int dz_1\int dz_2f_\gamma(z_2,z_1)f_\gamma(z_1,z_2)\times\sum_{lad}g_{s'r'b'a'}(z_2)g_{srba}(z_1)$$
$$=\frac{c^2e^4}{\pi^4}\int dz_1\int dz_2\left\{\frac{1}{2}[f_\gamma(z_2,z_1)+f_\gamma(z_1,z_2)]^2-\frac{1}{2}[f_\gamma^2(z_2,z_1)+f_\gamma^2(z_1,z_2]\right\}\times\sum_{lad}g_{s'r'b'a'}(z_2)g_{srba}(z_1),\tag{A16}$$

and the squared one-photon counter term can then be subtracted, giving

$$4D_d-2O_d^2=\frac{-c^2e^4}{\pi^4}\int dz_1\int dz_2 2\times[f_\gamma^2(z_2,z_1)+f_\gamma^2(z_1,z_2)]\times\sum_{lad}g_{s'r'b'a'}(z_2)g_{srba}(z_1).\tag{A17}$$

Thus, we can in this case write the finite reference state contribution as

$$\Delta E_{D_d}^{\mathrm{ref}}=\lim_{\gamma\to0}\frac{1}{2}i\gamma(4D_d-2O_d^2)$$
$$=\lim_{\gamma\to0}\frac{1}{2}i\gamma\frac{-c^2e^4}{\pi^4}\int dz_1\int dz_2 2\times[f_\gamma^2(z_2,z_1)+f_\gamma^2(z_1,z_2)]\times\sum_{lad}g_{s'r'b'a'}(z_2)g_{srba}(z_1),\tag{A18}$$

or since $f_\gamma(-z_2,-z_1)=f_\gamma(z_1,z_2)$ and $g_{srba}(z)=g_{srba}(-z)$. Equation (A18) can be rewritten as

$$\Delta E_{D_d}^{\mathrm{ref}}=\lim_{\gamma\to0}\frac{1}{2}i\gamma\frac{-e^4}{\pi^4}\int dz_1\int dz_2 4f_\gamma^2(z_2,z_1)\times\sum_{lad}g_{s'r'b'a'}(z_2)g_{srba}(z_1).\tag{A19}$$

The other three cases can be done in the same fashion.

To obtain expressions which are appropriate for numerical calculations, the z_1 and z_2 integrations are performed analytically. This yields the momentum expressions to be used in the ladder energy contribution, Eq. (18),

$$I_{D_d}^{\rm ref}=-\frac{c^2k^2+c^2kk'+c^2k'^2}{2c^6k^3k'^3(ck+ck')}, \tag{A20}$$

$$I_{D_e}^{\rm ref}=-\frac{c^2k^2+c^2kk'+c^2k'^2+2(ck+ck')\omega+\omega^2}{4c^2kk'(ck+ck')(\omega+ck)^2(\omega+ck')^2} -\frac{c^2k^2+c^2kk'+c^2k'^2-2(ck+ck')\omega+\omega^2}{4c^2kk'(ck+ck')(\omega-ck)^2(\omega-ck')^2}, \tag{A21}$$

$$I_{E_d}^{\rm ref}=-\frac{1}{4}\left\{\frac{1}{c^3k^2k'(\omega-ck')^2}+\frac{1}{c^4k^3k'(ck+ck'-\omega)} +\frac{1}{c^3k^2k'(\omega+ck')^2}+\frac{1}{c^4k^3k'(ck+ck'+\omega)}\right\}, \tag{A22}$$

$$I_{E_e}^{\rm ref}=-\frac{1}{4}\left\{\frac{1}{c^3k'^2k(\omega-ck)^2}+\frac{1}{c^4k'^3k(ck+ck'-\omega)} +\frac{1}{c^3k'^2k(\omega+ck)^2}+\frac{1}{c^4k'^3k(ck+ck'+\omega)}\right\}. \tag{A23}$$

They replace the expression Eq. (12), which is only valid if the intermediate states are not degenerate with the initial state.

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