Contribution of the diagrams of screened self-energy to the Lamb shift of the ground state of a two-electron multiply-charged ion

V. A. Erokhin and V. M. Shabaev

Physics Research Institute, St. Petersburg State University, 198904 St. Petersburg, Russia
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We calculate the contribution of the diagrams of screened self-energy to the ground-state energy of a two-electron ion within a broad range of nuclear-charge values: $Z=20-100$. The calculations are done for the case of a point nucleus. The entire contribution is represented as the sum of the irreducible, reducible, and vertex contributions. The irreducible contribution is written in the form of off-diagonal self-energy and is calculated via a partial-wave expansion of the mass operator. The vertex and reducible contributions are calculated together, which makes it possible to avoid explicit renormalization. The total contribution of the diagrams of the screened self-energy of the ground state of U^{90+} amounts to -9.54 eV. The results of the calculations for low-Z ions are found to be in good agreement with the contribution of the screened self-energy calculated in the lowest order in αZ. © *1996 American Institute of Physics.*
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1. INTRODUCTION

Considerable progress achieved in the experimental studies of multiply-charged ions[1,2] has placed the problem of a consistent quantum-mechanical calculation of the diagrams representing the screened self-energy at the foreground of atomic physics. In our recent paper,[3] we calculated these diagrams for the ground state of a two-electron multiply-charged ion in the following interval of nucleus-charge numbers: $Z=60-92$. In the present paper we broaden this interval to $Z=20-110$ and provide a detailed description of the calculation procedure.

Figure 1 depicts the diagrams of screened self-energy under discussion. The first formal calculation expressions for these diagrams were derived in Refs. 4 and 5 by the Gell-Mann and Low method.[6] Derivation of these expressions and the analysis of other second-order diagrams in α have shown that while being fairly simple formally, the Gell-Mann and Low method leads to serious difficulties. First, the presence of an adiabatic parameter λ, which violates energy conservation at the diagram vertices, severely complicates the derivation of computational formulas for the contribution of reducible diagrams, i.e., diagrams for which the energy of an intermediate state coincides with that of the initial state. Second, in view of the fact that the adiabatic matrix $S_\lambda(\infty,-\infty)$ used by this method contains a noncovariant procedure for interaction turn-on ($H_I^{(\lambda)}(t)=\exp(-\lambda|t|)H_I(t)$), ultraviolet divergences remain even after renormalization. In the case of a single level, we can expect the expression for the shift in the level's energy to be finite. However, for degenerate states we must build a secular operator, which generally may not be ultraviolet-finite. (We can only expect the eigenvalues of this operator to be finite.) This leads to a serious problem of renormalizing the secular operator in the Gell-Mann–Low method. It has been solved only to within second-order terms in α.[4,5]

The same difficulties emerge in the method of the operator of evolution over a finite time interval.[7,8] The solution was found within a variant of the method of quantum-electrodynamics Green's functions developed in Ref. 9 (the most simple and detailed description of this approach can be found in Refs. 10 and 11). The method is based on applying the formalism of Szökefalvi-Nagy and Kato[12] to two-time Green's functions.[5,13,14] In Sec. 2 we use it to derive the calculation expressions for the diagrams of screened self-energy in a general covariant gauge. The details of the numerical calculations and the results are given in Sec. 3.

Throughout the paper we use the relativistic system of units ($\hbar=c=m=1$).

2. DERIVATION OF THE FORMULAS

The energy shift $\Delta E_n=E_n-E_n^{(0)}$ of an isolated level due to the interaction with a quantized electromagnetic field is given by the following formula:[9]

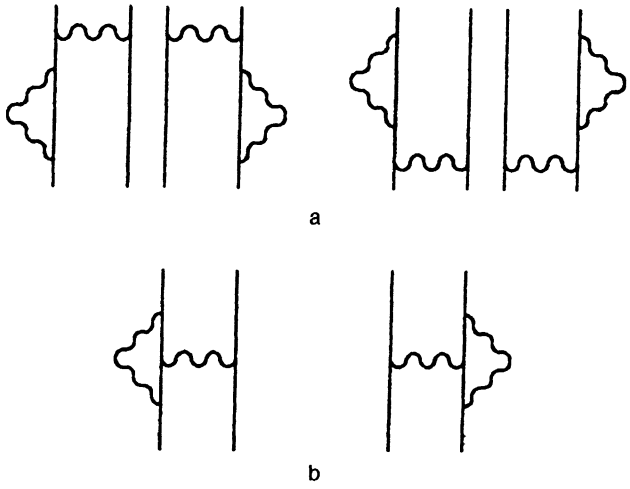

FIG. 1. The diagrams of the screened self-energy.

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$$\Delta E_n=\frac{(2\pi i)^{-1}\oint_\Gamma dE(E-E_n^{(0)})\Delta g_{nn}(E)}{1+(2\pi i)^{-1}\oint_\Gamma dE\Delta g_{nn}(E)}, \tag{1}$$

where the contour Γ surrounds only the unperturbed level $E=E_n^{(0)}$ (the contour is assumed to be traversed counterclockwise), and $\Delta g_{nn}(E)=g_{nn}(E)-g_{nn}^{(0)}(E)$, with $g_{nn}(E)$ the Fourier transform of the two-time Green's function,

$$\begin{aligned} g_{nn}(E)\delta(E-E')=\frac{2\pi}{i}\frac{1}{N!}\int_{-\infty}^{\infty}dp_1^0\cdots dp_N^0 dp_1'^0\cdots dp_N'^0 \\ \times\delta(E-p_1^0-\cdots-p_N^0) \\ \times\delta(E'-p_1'^0-\cdots-p_N'^0) \\ \times\langle u_n|G(p_1'^0,\ldots,p_N'^0;p_1^0,\ldots,p_N^0) \\ \times\gamma_1^0\cdots\gamma_N^0|u_n\rangle, \end{aligned} \tag{2}$$

$$\begin{aligned} G(p_1'^0,\ldots,p_N'^0;\,p_1^0,\ldots,p_N^0) \\ =\frac{1}{(2\pi)^{2N}}\int_{-\infty}^{\infty}dx_1^0\cdots dx_N^0 dx_1'^0\cdots dx_N'^0 \\ \times\exp(ip_1'^0x_1'^0+\cdots+ip_N'^0x_N'^0-ip_1^0x_1^0-\cdots-ip_N^0x_N^0) \\ \times\langle 0|T\psi(x_1')\cdots\psi(x_N')\bar{\psi}(x_N)\cdots\bar{\psi}(x_1)|0\rangle, \end{aligned} \tag{3}$$

$\psi(x)$ the electron–positron field operator in the Heisenberg picture, u_n the unperturbed atomic wave function, and $g_{nn}^{(0)}\times(E)=(E-E_n^{(0)})^{-1}$.

So as not to clutter the derivation of the formulas with minor details, we examine the case of a two-electron multiply charged ion (the general case of an N-electron ion can easily be reduced to this case). In addition, for the unperturbed wave function we take the one-determinant wave function

$$u_n=\frac{1}{\sqrt{2}}\sum_P(-1)^P\psi_{Pa}(\mathbf{x}_1)\psi_{Pb}(\mathbf{x}_2), \tag{4}$$

where P is the permutation operator. (The transition to correct wave functions is straightforward.)

To make further calculations more compact, we introduce the operator

$$I(\omega)=e^2\alpha_1^\mu\alpha_2^\nu D_{\mu\nu}(\omega), \tag{5}$$

where $\alpha^\mu\equiv\gamma^0\gamma^\mu\equiv(1,\boldsymbol{\alpha})$ are the Dirac matrices, and $D_{\mu\nu}(\omega)$ is the photon propagator. In the general covariant gauge of Ref. 15,

$$\begin{aligned} D_{\mu\nu}(\omega,\mathbf{x}-\mathbf{y})=\int\frac{d\mathbf{k}}{(2\pi)^3}e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})} \\ \times\left[\frac{-g_{\mu\nu}}{k^2-\mu^2+i0}-\frac{1-\lambda}{\lambda}\right. \\ \left.\times\frac{k_\mu k_\nu}{(k^2-\mu^2/\lambda+i0)(k^2-\mu^2+i0)}\right]\Bigg|_{k_0=\omega}, \end{aligned} \tag{6}$$

where μ is the photon mass. In the Feynman gauge ($\lambda=1$),

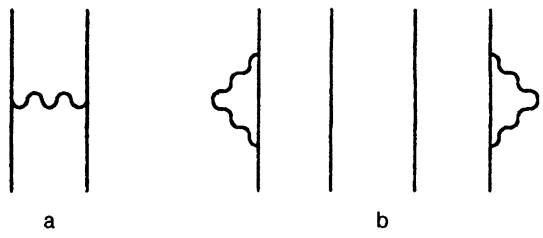

FIG. 2. The diagrams contributing to $\Delta g^{(1)}$ in Eq. (10).

$$\begin{aligned} D_{\mu\nu}(\omega,\mathbf{x}-\mathbf{y})=-g_{\mu\nu}\int\frac{d\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}(\mathbf{x}-\mathbf{y})}}{\omega^2-\mathbf{k}^2-\mu^2+i0} \\ =g_{\mu\nu}\frac{\exp[i\sqrt{\omega^2-\mu^2+i0}|\mathbf{x}-\mathbf{y}|]}{4\pi|\mathbf{x}-\mathbf{y}|}. \end{aligned} \tag{7}$$

The operator $I(\omega)$ satisfies the following symmetry property:

$$\langle ab|I(\omega)|cd\rangle=\langle ba|I(-\omega)|dc\rangle. \tag{8}$$

We also introduce the self-energy operator $\Sigma(\varepsilon)$:

$$\langle a|\Sigma(\varepsilon)|b\rangle=\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\sum_n\frac{\langle an|I(\omega)|nb\rangle}{\varepsilon-\omega-\varepsilon_n(1-i0)}. \tag{9}$$

According to (1), the second-order perturbation-theory correction to the energy is

$$\begin{aligned} \Delta E_n=\frac{1}{2\pi i}\oint_\Gamma dE\Delta E\Delta g_{nn}^{(2)}(E) \\ -\frac{1}{2\pi i}\oint_\Gamma dE\Delta E\Delta g_{nn}^{(1)}(E)\frac{1}{2\pi i}\oint_\Gamma dE\Delta g_{nn}^{(1)}(E). \end{aligned} \tag{10}$$

The diagrams contributing to $\Delta g^{(2)}$ are depicted in Fig. 1, and those contributing to $\Delta g^{(1)}$ in Fig. 2.

It is convenient to divide the contribution of the diagrams in Fig. 1a into two part, the reducible and the irreducible. By reducible we mean the part in which the energy of an intermediate state (between the self-energy loop and the electron–electron interaction) coincides with the energy of the initial state. We call the remaining part irreducible. Note that the reducible part of the diagrams in Fig. 1a must be calculated together with the second term on the right-hand side of Eq. (10).

Let us first find the contribution of the irreducible part of the diagrams in Fig. 1a. According to (2), (10), and the rules of the diagrammatic technique, we have

$$\begin{aligned} \Delta E_{\text{irred}}=\frac{1}{2\pi i}\oint_\Gamma dE\Delta E\left(\frac{i}{2\pi}\right)^2\sum_P(-1)^P\int_{-\infty}^{\infty}dp_1^0dp_1'^0 \\ \times\frac{1}{(p_1'^0-\varepsilon_{Pa}+i0)(E-p_1'^0-\varepsilon_{Pb}+i0)} \\ \times\frac{1}{(p_1^0-\varepsilon_a+i0)(E-p_1^0-\varepsilon_b+i0)} \\ \times\left[\sum_{\varepsilon_n\neq\varepsilon_a}\langle PaPb|I(p_1'^0-p_1^0)|nb\rangle\right. \end{aligned}$$

$$\frac{1}{p_1^0-\varepsilon_n(1-i0)}\langle n|\Sigma(p_1^0)|a\rangle$$

$$+\sum_{\varepsilon_n\neq\varepsilon_b}\langle PaPb|I(p_1'^0-p_1^0)|an\rangle$$

$$\times\frac{1}{E-p_1^0-\varepsilon_n(1-i0)}\langle n|\Sigma(E-p_1^0)|b\rangle$$

$$+\sum_{\varepsilon_n\neq\varepsilon_{Pa}}\langle Pa|\Sigma(p_1'^0)|n\rangle$$

$$\times\frac{1}{p_1'^0-\varepsilon_n(1-i0)}\langle nPb|I(p_1'^0-p_1^0)|ab\rangle$$

$$+\sum_{\varepsilon_n\neq\varepsilon_{Pb}}\langle Pb|\Sigma(E-p_1'^0)|n\rangle\frac{1}{E-p_1'^0-\varepsilon_n(1-i0)}$$

$$\times\langle Pan|I(p_1'^0-p_1^0)|ab\rangle\Bigg]. \tag{11}$$

Using the identity

$$\frac{1}{(p^0-\varepsilon_a+i0)(E-p^0-\varepsilon_b+i0)}$$

$$=\frac{1}{\Delta E}\left(\frac{1}{p^0-\varepsilon_a+i0}+\frac{1}{E-p^0-\varepsilon_b+i0}\right), \tag{12}$$

we can write (11) as

$$\Delta E_{\text{irred}}=\frac{1}{2\pi i}\oint_\Gamma\frac{dE}{\Delta E}\left\{\left(\frac{i}{2\pi}\right)^2\sum_P(-1)^P\int_{-\infty}^{\infty}dp_1^0dp_1'^0\right.$$

$$\times\left(\frac{1}{p_1'^0-\varepsilon_{Pa}+i0}+\frac{1}{E-p_1'^0-\varepsilon_{Pb}+i0}\right)$$

$$\times\left(\frac{1}{p_1^0-\varepsilon_a+i0}+\frac{1}{E-p_1^0-\varepsilon_b+i0}\right)$$

$$\times\Bigg[\sum_{\varepsilon_n\neq\varepsilon_a}\langle PaPb|I(p_1'^0-p_1^0)|nb\rangle$$

$$\times\frac{1}{p_1^0-\varepsilon_n(1-i0)}\langle n|\Sigma(p_1^0)|a\rangle$$

$$+\sum_{\varepsilon_n\neq\varepsilon_b}\langle PaPb|I(p_1'^0-p_1^0)|an\rangle$$

$$\times\frac{1}{E-p_1^0-\varepsilon_n(1-i0)}\langle n|\Sigma(E-p_1^0)|b\rangle$$

$$+\sum_{\varepsilon_n\neq\varepsilon_{Pa}}\langle Pa|\Sigma(p_1'^0)|n\rangle\frac{1}{p_1'^0-\varepsilon_n(1-i0)}$$

$$\times\langle nPb|I(p_1'^0-p_1^0)|ab\rangle$$

$$+\sum_{\varepsilon_n\neq\varepsilon_{Pb}}\langle Pb|\Sigma(E-p_1'^0)|n\rangle$$

$$\left.\times\frac{1}{E-p_1'^0-\varepsilon_n(1-i0)}\langle Pan|I(p_1'^0-p_1^0)|ab\rangle\Bigg]\right\}. \tag{13}$$

Allowing for the fact that the expression within the braces is analytic in energy inside the contour Γ, we can reduce the integral with respect to E to the first-order residue at $E=E_0$. By employing the relationship

$$\frac{i}{2\pi}\left(\frac{1}{x+i0}+\frac{1}{-x+i0}\right)=\delta(x) \tag{14}$$

we calculate the integral with respect to p_1^0 and $p_1'^0$ and arrive at the following expression for ΔE_{irred}:

$$\Delta E_{\text{irred}}=\sum_P(-1)^P\Bigg\{\sum_{\varepsilon_n\neq\varepsilon_a}\langle PaPb|I(\Delta)|nb\rangle$$

$$\times\frac{1}{\varepsilon_a-\varepsilon_n}\langle n|\Sigma(\varepsilon_a)|a\rangle+\sum_{\varepsilon_n\neq\varepsilon_b}\langle PaPb|I(\Delta)|an\rangle$$

$$\times\frac{1}{\varepsilon_b-\varepsilon_n}\langle n|\Sigma(\varepsilon_b)|b\rangle+\sum_{\varepsilon_n\neq\varepsilon_{Pa}}\langle Pa|\Sigma(\varepsilon_{Pa})|n\rangle$$

$$\times\frac{1}{\varepsilon_{Pa}-\varepsilon_n}\langle nPb|I(\Delta)|ab\rangle+\sum_{\varepsilon_n\neq\varepsilon_{Pb}}\langle Pb|\Sigma(\varepsilon_{Pb})|n\rangle$$

$$\times\frac{1}{\varepsilon_{Pb}-\varepsilon_n}\langle Pan|I(\Delta)|ab\rangle\Bigg\}, \tag{15}$$

where $\Delta=\varepsilon_{Pa}-\varepsilon_a$.

Let us now find the contribution of the vertex part, which is represented by the diagrams in Fig. 1b. Using the diagrammatic technique, we have

$$\Delta E_{\text{vertex}}=\frac{1}{2\pi i}\oint_\Gamma dE\Delta E\left(\frac{i}{2\pi}\right)^3$$

$$\times\sum_P(-1)^P\sum_{n_1n_2}\int_{-\infty}^{\infty}dp_1^0dp_1'^0\frac{1}{(p_1'^0-\varepsilon_{Pa}+i0)(E-p_1'^0-\varepsilon_{Pb}+i0)}\frac{1}{(p_1^0-\varepsilon_a+i0)(E-p_1^0-\varepsilon_b+i0)}$$

$$\times\Bigg[\langle n_1Pb|I(p_1'^0-p_1^0)|n_2b\rangle\left\langle Pan_2\left|\int_{-\infty}^{\infty}d\omega\frac{I(\omega)}{[p_1'^0-\omega-\varepsilon_{n_1}(1-i0)][p_1^0-\omega-\varepsilon_{n_2}(1-i0)]}\right|n_1a\right\rangle$$

$$+\langle Pan_1|I(p_1'^0-p_1^0)|an_2\rangle\left\langle Pbn_2\left|\int_{-\infty}^{\infty}d\omega\frac{I(\omega)}{[E-p_1'^0-\omega-\varepsilon_{n_1}(1-i0)][E-p_1^0-\omega-\varepsilon_{n_2}(1-i0)]}\right|n_1b\right\rangle\Bigg]. \tag{16}$$

Calculating the integrals with respect to E, p_1^0, and $p_1'^0$ in the same way as we did for ΔE_{irred}, we get

$$\Delta E_{\text{vertex}}=\sum_P (-1)^P \sum_{n_1 n_2} \frac{i}{2\pi}\left[\langle n_1 Pb|I(\Delta)|n_2 b\rangle\left\langle Pan_2\left|\int_{-\infty}^{\infty} d\omega \frac{I(\omega)}{[\varepsilon_{Pa}-\omega-\varepsilon_{n_1}(1-i0)][\varepsilon_a-\omega-\varepsilon_{n_2}(1-i0)]}\right|n_1 a\right\rangle\right.$$

$$\left.+\langle Pan_1|I(\Delta)|an_2\rangle\left\langle Pbn_2\left|\int_{-\infty}^{\infty} d\omega \frac{I(\omega)}{[\varepsilon_{Pb}-\omega-\varepsilon_{n_1}(1-i0)][\varepsilon_b-\omega-\varepsilon_{n_2}(1-i0)]}\right|n_1 b\right\rangle\right]. \tag{17}$$

The initial expression for the contribution of the reducible part of the diagrams of Fig. 1a can be written in the same way as we did for the irreducible fraction:

$$\Delta E^{(1)}_{\text{red}}=\frac{1}{2\pi i}\oint_\Gamma dE\Delta E\left(\frac{i}{2\pi}\right)^2\sum_P (-1)^P\int_{-\infty}^{\infty} dp_1^0 dp_1'^0 \frac{1}{(p_1'^0-\varepsilon_{Pa}+i0)(E-p_1'^0-\varepsilon_{Pb}+i0)}$$

$$\times\frac{\langle PaPb|I(p_1'^0-p_1^0)|ab\rangle}{(p_1^0-\varepsilon_a+i0)(E-p_1^0-\varepsilon_b+i0)}\left[\frac{1}{p_1^0-\varepsilon_a+i0}\langle a|\Sigma(p_1^0)|a\rangle+\frac{1}{E-p_1^0-\varepsilon_b+i0}\langle b|\Sigma(E-p_1^0)|b\rangle\right.$$

$$\left.+\frac{1}{p_1'^0-\varepsilon_{Pa}+i0}\langle Pa|\Sigma(p_1'^0)|Pa\rangle+\frac{1}{E-p_1'^0-\varepsilon_{Pb}+i0}\langle Pb|\Sigma(E-p_1'^0)|Pb\rangle\right]. \tag{18}$$

Let us use the first term on the right-hand side of Eq. (18), which we denote by $\Delta E^{(1)}_{\text{red}}$, as an example of how to integrate with respect to energy. Using (12) and the identity

$$\frac{1}{(p^0-\varepsilon_{Pa}+i0)^2(E-p^0-\varepsilon_{Pb}+i0)}$$

$$=\frac{1}{(\Delta E)^2}\left(\frac{1}{p^0-\varepsilon_{Pa}+i0}+\frac{1}{E-p^0-\varepsilon_{Pb}+i0}\right)$$

$$+\frac{1}{\Delta E}\frac{1}{(p^0-\varepsilon_{Pa}+i0)^2}, \tag{19}$$

we can write the expression for $\Delta E^{(1)}_{\text{red}}$ in the form

$$\Delta E^{(1)}_{\text{red}}=\frac{1}{2\pi i}\oint_\Gamma \frac{dE}{(\Delta E)^2}\left\{\left(\frac{i}{2\pi}\right)^2\sum_P (-1)^P\int_{-\infty}^{\infty} dp_1^0 dp_1'^0\right.$$

$$\times\left(\frac{1}{p_1'^0-\varepsilon_{Pa}+i0}+\frac{1}{E-p_1'^0-\varepsilon_{Pb}+i0}\right)$$

$$\times\left(\frac{1}{p_1^0-\varepsilon_a+i0}+\frac{1}{E-p_1^0-\varepsilon_b+i0}\right)$$

$$\left.\times\langle PaPb|I(p_1'^0-p_1^0)|ab\rangle\langle a|\Sigma(p_1^0)|a\rangle\right\}$$

$$+\frac{1}{2\pi i}\oint_\Gamma \frac{dE}{\Delta E}\left\{\left(\frac{i}{2\pi}\right)^2\sum_P (-1)^P\int_{-\infty}^{\infty} dp_1^0 dp_1'^0\right.$$

$$\times\left(\frac{1}{p_1'^0-\varepsilon_{Pa}+i0}+\frac{1}{E-p_1'^0-\varepsilon_{Pb}+i0}\right)$$

$$\times\frac{1}{(p_1^0-\varepsilon_a+i0)^2}\langle PaPb|I(p_1'^0-p_1^0)|ab\rangle$$

$$\left.\times\langle a|\Sigma(p_1^0)|a\rangle\right\}. \tag{20}$$

The two expressions within the braces are analytic in energy inside the contour Γ. Calculating the first- and second-order residues at point $E=E^{(0)}$ and taking identity (14) into account, we find that

$$\Delta E^{(1)}_{red}=\sum_P (-1)^P\frac{i}{2\pi}\int_{-\infty}^{\infty} dp_1^0\langle PaPb|I(\varepsilon_{Pa}-p_1^0)|ab\rangle$$

$$\times\langle a|\Sigma(p_1^0)|a\rangle\left[\frac{1}{(p_1^0-\varepsilon_a+i0)^2}-\frac{1}{(p_1^0-\varepsilon_a-i0)^2}\right]$$

$$+\sum_P (-1)^P\frac{i}{2\pi}\int_{-\infty}^{\infty} dp_1'^0\langle PaPb|I(p_1'^0-\varepsilon_a)|ab\rangle$$

$$\times\langle a|\Sigma(\varepsilon_a)|a\rangle\frac{-1}{(\varepsilon_{Pa}-p_1'^0+i0)^2}. \tag{21}$$

By allowing for the fact that

$$\frac{1}{(p-\varepsilon_a+i0)^2}-\frac{1}{(p-\varepsilon_a-i0)^2}$$

$$=-\frac{d}{dp}\left[\frac{1}{p-\varepsilon_a+i0}+\frac{1}{-(p-\varepsilon_a)+i0}\right]$$

$$=-\frac{2\pi}{i}\frac{d}{dp}[\delta(p-\varepsilon_a)], \tag{22}$$

and integrating by parts we obtain

$$\Delta E^{(1)}_{\text{red}}=\sum_P (-1)^P[-\langle PaPb|I'(\Delta)|ab\rangle\langle a|\Sigma(\varepsilon_a)|a\rangle$$

$$+\langle PaPb|I(\Delta)|ab\rangle\langle a|\Sigma'(\varepsilon_a)|a\rangle]$$

$$+\sum_P (-1)^P\frac{i}{2\pi}\int_{-\infty}^{\infty} dp_1'^0\frac{-1}{(\varepsilon_{Pa}-p_1'^0+i0)^2}$$

$$\times\langle PaPb|I(p_1'^0-\varepsilon_a)|ab\rangle\langle a|\Sigma(\varepsilon_a)|a\rangle, \tag{23}$$

where

$$I'(\Delta)=\left.\frac{dI(\omega)}{d\omega}\right|_{\omega=\Delta},\quad \Sigma'(\varepsilon_a)=\left.\frac{d\Sigma(\varepsilon)}{d\varepsilon}\right|_{\varepsilon=\varepsilon_a}.$$

The other terms in (18) can be calculated in a similar way:

$$\Delta E^{(2)}_{\text{"red"}}=\sum_P(-1)^P\langle PaPb|I(\Delta)|ab\rangle\langle b|\Sigma'(\varepsilon_b)|b\rangle$$
$$+\sum_P(-1)^P\frac{i}{2\pi}\int_{-\infty}^{\infty}dp_1'^0\frac{-1}{(\varepsilon_{Pa}-p_1'^0+i0)^2}$$
$$\times\langle PaPb|I(p_1'^0-\varepsilon_a)|ab\rangle\langle b|\Sigma(\varepsilon_b)|b\rangle, \quad (24)$$

$$\Delta E^{(3)}_{\text{"red"}}=\sum_P(-1)^P\{\langle PaPb|I'(\Delta)|ab\rangle\langle Pa|\Sigma(\varepsilon_{Pa})|Pa\rangle$$
$$+\langle PaPb|I(\Delta)|ab\rangle\langle Pa|\Sigma'(\varepsilon_{Pa})|Pa\rangle\}$$
$$+\sum_P(-1)^P\frac{i}{2\pi}\int_{-\infty}^{\infty}dp_1^0\frac{-1}{(\varepsilon_a-p_1^0+i0)^2}$$
$$\times\langle PaPb|I(\varepsilon_{Pa}-p_1^0)|ab\rangle\langle Pa|\Sigma(\varepsilon_{Pa})|Pa\rangle, \quad (25)$$

$$\Delta E^{(4)}_{\text{"red"}}=\sum_P(-1)^P\langle PaPb|I(\Delta)|ab\rangle\langle Pb|\Sigma'(\varepsilon_{Pb})|Pb\rangle$$
$$+\sum_P(-1)^P\frac{i}{2\pi}\int_{-\infty}^{\infty}dp_1^0\frac{-1}{(\varepsilon_a-p_1^0+i0)^2}$$
$$\times\langle PaPb|I(\varepsilon_{Pa}-p_1^0)|ab\rangle\langle Pb|\Sigma(\varepsilon_{Pb})|Pb\rangle. \quad (26)$$

Allowing for (22), we find the sum of the contributions (23)–(26):

$$\Delta E_{\text{"red"}}=\sum_P(-1)^P[2\langle PaPb|I(\Delta)|ab\rangle(\langle a|\Sigma'(\varepsilon_a)|a\rangle$$
$$+\langle b|\Sigma'(\varepsilon_b)|b\rangle)+\langle PaPb|I'(\Delta)|ab\rangle$$
$$\times(\langle a|\Sigma(\varepsilon_a)|a\rangle$$
$$+\langle b|\Sigma(\varepsilon_b)|b\rangle)]+\langle ba|I'(\Delta)|ab\rangle(\langle a|\Sigma(\varepsilon_a)|a\rangle$$
$$-\langle b|\Sigma(\varepsilon_b)|b\rangle). \quad (27)$$

As noted earlier, the contribution of the reducible part of the diagrams in Fig. 1a must be calculated together with the second term on the right-hand side of Eq. (10). We denote their sum by ΔE_{red}:

$$\Delta E_{\text{red}}=\Delta E_{\text{"red"}}-\frac{1}{2\pi i}$$
$$\times\oint_\Gamma dE\Delta E\Delta g^{(1)}_{nn}(E)\frac{1}{2\pi i}\oint_\Gamma dE\Delta g^{(1)}_{nn}(E).$$

We denote the contributions to $\Delta g^{(1)}$ of the diagrams of Figs. 2a and 2b by $\Delta g^{(1)}_a$ and $g^{(1)}_b$, respectively. Simple calculations yield

$$\frac{1}{2\pi i}\oint dE\Delta E\Delta g^{(1)}_a=\sum_P(-1)^P\langle PaPb|I(\Delta)|ab\rangle, \quad (28)$$

$$\frac{1}{2\pi i}\oint dE\Delta E\Delta g^{(1)}_b=\langle a|\Sigma(\varepsilon_a)|a\rangle+\langle b|\Sigma(\varepsilon_b)|b\rangle, \quad (29)$$

$$\frac{1}{2\pi i}\oint dE\Delta g^{(1)}_a=\sum_P(-1)^P\langle PaPb|I'(\Delta)|ab\rangle, \quad (30)$$

$$\frac{1}{2\pi i}\oint dE\Delta g^{(1)}_b=\langle a|\Sigma'(\varepsilon_a)|a\rangle+\langle b|\Sigma'(\varepsilon_b)|b\rangle. \quad (31)$$

Combining (27) and (28)–(31), we arrive at the final expression for ΔE_{red}:

$$\Delta E_{\text{red}}=\sum_P(-1)^P\langle PaPb|I(\Delta)|ab\rangle\Big[\langle a|\Sigma'(\varepsilon_a)|a\rangle$$
$$+\langle b|\Sigma'(\varepsilon_b)|b\rangle\Big]+\langle ba|I'(\Delta)|ab\rangle\Big[\langle a|\Sigma(\varepsilon_a)|a\rangle$$
$$-\langle b|\Sigma(\varepsilon_b)|b\rangle\Big]. \quad (32)$$

In the ground state ($I'(0)=0$), Eq. (32) assumes the form

$$\Delta E_{\text{red}}=\sum_P(-1)^P\langle PaPb|I(0)|ab\rangle[\langle a|\Sigma'(\varepsilon_a)|a\rangle$$
$$+\langle b|\Sigma'(\varepsilon_b)|b\rangle]. \quad (33)$$

Equations (15), (17), and (32) are formal expressions and need to be renormalized. The procedure in a stationary external field is well known.[5,16–18]. If covariant regularization is employed, the self-energy operator in (15) and (32) must be replaced by the operator $\Sigma_R(\varepsilon)$:

$$\Sigma(\varepsilon)\to\Sigma_R(\varepsilon)=\widetilde{\Sigma}(\varepsilon)-\beta\delta m-(Z_2-1)(\varepsilon-H),$$

where $H=\boldsymbol{\alpha}\mathbf{p}+\beta m+V_c(r)$ is the Dirac Hamiltonian, $\widetilde{\Sigma}(\varepsilon)$ is the self-energy operator regularized in the same way as the counterterms, and δm and Z_2 are renormalization constants. To renormalize the vertex contribution we must add to the expression (17) regularized in an appropriate manner the following counterterm:

$$\Delta E^{c.t.}_{\text{vertex}}=2(Z_1-1)\sum_P(-1)^P\langle PaPb|I(\Delta)|ab\rangle, \quad (34)$$

where Z_1 is a renormalization constant.

If we substitute the expression for Σ_R into Eq. (15), we see that the contribution of the second counterterm to Σ_R vanishes. This means that the irreducible part can be calculated by the method used for calculating the first-order self-energy contribution, the only difference being that instead of the diagonal matrix element we must calculate the off-diagonal matrix elements. A detailed calculation for lithium-like uranium was done in Ref. 19.

Substitution of $\Sigma_R(\varepsilon)$ into (32) and allowance for the Ward identity ($Z_1=Z_2$) show[4] that the counterterm in the vertex part is cancelled by the counterterm for the first term in the expression for the reducible part. Hence, when calculating the sum of the vertex contribution and the first term in the reducible contribution, with both regularized in the same way, the counterterms can be dropped.

Note that both (17) and (32) contain infrared divergences, which cancel when the two terms are added. In the vertex part (17) the term corresponding to $\varepsilon_{n_1}=\varepsilon_{Pa}$ and $\varepsilon_{n_2}=\varepsilon_a$ in the first term and that corresponding to $\varepsilon_{n_1}=\varepsilon_{Pb}$ and $\varepsilon_{n_2}=\varepsilon_b$ in the second term are divergent. In the reducible part (32) the term that contains an infrared divergence is the one emerging when the energy of the intermediate state, ε_n, in the operator $\Sigma'(\varepsilon)$ coincides with the energy ε_a in the first term and the energy ε_b in the second. A simple calculation of these two terms yields

$$\Delta E^{\text{``infr''}}_{\text{ver+red}}=\Delta E^{\text{``infr''}}_{\text{ver}}+\Delta E^{\text{``infr''}}_{\text{red}}=\frac{\alpha}{\pi}$$
$$\times\sum_P(-1)^P\Bigg[\sum_{\varepsilon_{n_1}=\varepsilon_a}\sum_{\varepsilon_{n_2}=\varepsilon_{Pa}}\langle n_2Pb|I(\Delta)|n_1b\rangle$$
$$\times\left\langle Pan_1\left|\left(\alpha_1^\mu\alpha_{2\mu}-\frac{1-\lambda}{2\lambda}\right)\ln r_{12}\right|n_2a\right\rangle$$
$$+\sum_{\varepsilon_{n_1}=\varepsilon_b}\sum_{\varepsilon_{n_2}=\varepsilon_{Pb}}\langle Pan_2|I(\Delta)|an_1\rangle$$
$$\times\left\langle Pbn_1\left|\left(\alpha_1^\mu\alpha_{2\mu}-\frac{1-\lambda}{2\lambda}\right)\ln r_{12}\right|n_2b\right\rangle$$
$$-\langle PaPb|I(\Delta)|ab\rangle\Bigg\{\sum_{\varepsilon_n=\varepsilon_a}\left\langle an\left|\left(\alpha_1^\mu\alpha_{2\mu}\right.\right.\right.$$
$$\left.\left.\left.-\frac{1-\lambda}{2\lambda}\right)\ln r_{12}\right|na\right\rangle+\sum_{\varepsilon_n=\varepsilon_b}\left\langle bn\left|\left(\alpha_1^\mu\alpha_{2\mu}\right.\right.\right.$$
$$\left.\left.\left.-\frac{1-\lambda}{2\lambda}\right)\ln r_{12}\right|nb\right\rangle\Bigg\}\Bigg]. \tag{35}$$

Note that in the ground state of a two-electron atom this contribution is independent of λ. Thus,

$$\Delta E_{\text{vertex}}+\Delta E_{\text{red}}=\Delta E^{\text{fin}}_{\text{ver}}+\Delta E^{\text{fin}}_{\text{red}}+\Delta E^{\text{``infr''}}_{\text{ver+red}}, \tag{36}$$

where $\Delta E^{\text{fin}}_{\text{ver}}=\Delta E_{\text{vertex}}-\Delta E^{\text{``infr''}}_{\text{ver}}$ and $\Delta E^{\text{fin}}_{\text{red}}=\Delta E_{\text{red}}-\Delta E^{\text{``infr''}}_{\text{red}}$ In the expressions for $\Delta E^{\text{fin}}_{\text{red}}$ and $\Delta E^{\text{``infr''}}_{\text{ver+red}}$ we can pass to the limit as $\mu\to 0$.

Below we restrict our discussion to the ground state ($\varepsilon_a=\varepsilon_b=\varepsilon_{1s}$) of a two- electron state and the Feynman gauge ($\lambda=1$). It has proved convenient to identify in the sum (36) the finite part of the vertex contribution, ΔE_{pole}, corresponding to $\varepsilon_{n_1}=\varepsilon_a$ and $\varepsilon_{n_2}\neq\varepsilon_a$, or $\varepsilon_{n_1}\neq\varepsilon_a$ and $\varepsilon_{n_2}=\varepsilon_a$:

$$\Delta E_{\text{vertex}}+\Delta E_{\text{red}}=\Delta E_{\text{pole}}+\Delta E_{\text{vr}}+\Delta E^{\text{``infr''}}_{\text{ver+red}}, \tag{37}$$

$$\Delta E_{\text{pole}}=2\sum_P(-1)^P\sum_{\varepsilon_{n_1}=\varepsilon_a}\sum_{\varepsilon_{n_2}\neq\varepsilon_a}\Bigg[\langle n_1Pb|I(0)|n_2b\rangle$$
$$\times\left\langle Pan_2\left|\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\right.\right.$$
$$\left.\left.\times\frac{I(\omega)}{[\varepsilon_a-\omega-\varepsilon_{n_2}(1-i0)](-\omega+i0)}\right|n_1a\right\rangle$$
$$+\langle n_2Pb|I(0)|n_1b\rangle\left\langle Pan_1\left|\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\right.\right.$$
$$\left.\left.\times\frac{I(\omega)}{[\varepsilon_a-\omega-\varepsilon_{n_2}(1-i0)](-\omega+i0)}\right|n_2a\right\rangle\Bigg]. \tag{38}$$

The integral with respect to energy can be transformed in the following manner:

$$\int_{-\infty}^{\infty}d\omega\frac{\exp(i|\omega|r_{12})}{[\varepsilon_a-\omega-\varepsilon_n(1-i0)](-\omega+i0)}$$
$$=-2i\int_0^{\infty}d\omega\frac{\exp(-\omega r_{12})}{\Delta_n^2+\omega^2}-i\pi\frac{1}{\Delta_n}, \tag{39}$$

where $\Delta_n=\varepsilon_a-\varepsilon_n$. This yields

$$\Delta E_{\text{pole}}=\frac{2}{\pi}\sum_P(-1)^P\sum_{\varepsilon_{n_1}=\varepsilon_a}\sum_{\varepsilon_{n_2}\neq\varepsilon_a}\int_0^{\infty}\frac{d\omega}{\Delta_{n_2}^2+\omega^2}$$
$$\times[\langle n_1Pb|I(0)|n_2b\rangle\langle Pan_2|I_+(i\omega)|n_1a\rangle$$
$$+\langle n_2Pb|I(0)|n_1b\rangle\langle Pan_1|I_+(i\omega)|n_2a\rangle]$$
$$+\alpha\sum_P(-1)^P\sum_{\varepsilon_{n_1}=\varepsilon_a}\sum_{\varepsilon_{n_2}\neq\varepsilon_a}\frac{1}{\Delta_{n_2}}\Bigg[\langle n_1Pb|I(0)|n_2b\rangle$$
$$\times\left\langle Pan_2\left|\frac{1-\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2}{r_{12}}\right|n_1a\right\rangle+\langle n_2Pb|I(0)|n_1b\rangle$$
$$\times\left\langle Pan_1\left|\frac{1-\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2}{r_{12}}\right|n_2a\right\rangle\Bigg], \tag{40}$$

where

$$I_+(\omega)=\alpha\frac{\alpha_\mu\alpha^\mu}{r_{12}}\exp(i\omega r_{12}).$$

The expression for ΔE_{vr} can be written in terms of the Green's function as follows:

$$\Delta E_{vr}=2\alpha^2\sum_P(-1)^P\frac{i}{2\pi}\int_{-\infty}^{\infty}d\omega\int d\mathbf{x}d\mathbf{y}d\mathbf{z}$$
$$\times\frac{\exp(i|\omega||\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|}\Bigg[\psi^\dagger_{Pa}(\mathbf{x})\alpha_\nu\int d\mathbf{z}_1$$
$$\times\frac{\psi^\dagger_{Pb}(\mathbf{z}_1)\alpha_\mu\psi_b(\mathbf{z}_1)}{|\mathbf{z}-\mathbf{z}_1|}\tilde{G}(\varepsilon_a-\omega,\mathbf{x},\mathbf{z})\alpha^\mu$$
$$\times\tilde{G}(\varepsilon_a-\omega,\mathbf{z},\mathbf{y})\alpha^\nu\psi_a(\mathbf{y})-\left\langle PaPb\left|\frac{1-\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2}{r_{12}}\right|ab\right\rangle$$
$$\times\psi^\dagger_a(\mathbf{x})\alpha_\nu\tilde{G}(\varepsilon_a-\omega,\mathbf{x},\mathbf{z})\tilde{G}(\varepsilon_a-\omega,\mathbf{z},\mathbf{y})\alpha^\nu\psi_a(\mathbf{y})\Bigg], \tag{41}$$

where

$$\tilde{G}(\varepsilon,\mathbf{x},\mathbf{y})=G(\varepsilon,\mathbf{x},\mathbf{y})-\sum_{\varepsilon_n=\varepsilon_a}\frac{\psi_n(\mathbf{x})\psi_n^\dagger(\mathbf{y})}{\varepsilon-\varepsilon_a+i0}, \tag{42}$$

with $G(\varepsilon,\mathbf{x},\mathbf{z})$ the Coulomb Green's function of the Dirac equation, and $\psi_a(\mathbf{x})$ and $\psi_b(\mathbf{x})$ are the $1s$-state wave func-

tions with $+\frac{1}{2}$ and $-\frac{1}{2}$ projections of angular momentum. In going over from (17) and (33) to (41) we joined the coinciding integrations in the reducible and vertex contributions and allowed for the fact that

$$\frac{\partial G(\varepsilon,\mathbf{x},\mathbf{y})}{\partial\varepsilon}=-\int d\mathbf{z}G(\varepsilon,\mathbf{x},\mathbf{z})G(\varepsilon,\mathbf{z},\mathbf{y}).$$

Bearing in mind the forthcoming numerical calculations, we rotate the contour of integration with respect to ω in (41) in the complex ω plane so that it coincides with the imaginary axis. Since in the process of contour deformation the contour crosses no singularities of the integrand, we get

$$\begin{aligned}\Delta E_{vr}=&-\frac{2\alpha^2}{\pi}\sum_P(-1)^P\int_0^\infty d\omega\int d\mathbf{x}d\mathbf{y}d\mathbf{z}\frac{e^{-\omega|\mathbf{x}-\mathbf{y}|}}{|\mathbf{x}-\mathbf{y}|}\\&\times\Bigg[\psi^\dagger_{Pa}(\mathbf{x})\alpha_\nu\int d\mathbf{z}_1\frac{\psi^\dagger_{Pb}(\mathbf{z}_1)\alpha_\mu\psi_b(\mathbf{z}_1)}{|\mathbf{z}-\mathbf{z}_1|}\\&\times\mathrm{Re}\{\tilde G(\varepsilon_a-i\omega,\mathbf{x},\mathbf{z})\alpha^\mu\tilde G(\varepsilon_a-i\omega,\mathbf{z},\mathbf{y})\}\\&\times\alpha^\nu\psi_a(\mathbf{y})-\left\langle PaPb\left|\frac{1-\boldsymbol{\alpha}_1\boldsymbol{\alpha}_2}{r_{12}}\right|ab\right\rangle\psi^\dagger_a(\mathbf{x})\alpha_\nu\\&\times\mathrm{Re}\{\tilde G(\varepsilon_a-i\omega,\mathbf{x},\mathbf{z})\tilde G(\varepsilon_a-i\omega,\mathbf{z},\mathbf{y})\}\alpha^\nu\psi_a(\mathbf{y})\Bigg].\end{aligned}\tag{43}$$

3. NUMERICAL CALCULATIONS

3.1. The irreducible contribution

It is convenient to write the irreducible contribution of the diagrams of Fig. 1a as

$$\Delta E_{\mathrm{irred}}=2[\langle\xi|\Sigma_R(\varepsilon_a)|a\rangle+\langle a|\Sigma_R(\varepsilon_a)|\xi\rangle],\tag{44}$$

where

$$|\xi\rangle=\sum_{\varepsilon_n\neq\varepsilon_a}\frac{|n\rangle[\langle nb|I(0)|ab\rangle-\langle nb|I(0)|ba\rangle]}{\varepsilon_a-\varepsilon_n}.\tag{45}$$

The numerical calculation of $\Delta E_{\mathrm{irred}}$, just as that of all other contributions, is performed for a point nucleus. The function $|\xi\rangle$ was calculated by the method of B-splines for the Dirac equation.[20] Zero boundary conditions and the grid $r_i=\rho^4\gamma/Z$, where $\gamma=\sqrt{1-(\alpha Z)^2}$, were used in the calculations.[21,22] To calculate the off-diagonal matrix elements of the selfenergy operator in (44) we used a generalization of the numerical renormalization method based on an expansion of the mass operator[23] in partial waves.[24–26] According to this method, the divergent integrals for the unrenormalized contribution and the mass renormalization counterterm are replaced by divergent series of finite partial contributions. Term-by-term integration yields a series that converges to the correct value of self-energy in the first order. According to our analysis, to generalize the expression for the mass counterterm in Refs. 24–26 to the off-diagonal matrix elements considered here, the mass operator must be taken in the form

$$\begin{aligned}M=&\frac{\alpha}{\pi}\sum_{l=0}^\infty(2l+1)\\&\times\int_0^\infty dk\,k\sum_{p_1\kappa_1m_1a_1}\sum_{p_2\kappa_2m_2a_2}\sum_{p_3\kappa_3m_3a_3}|p_1\kappa_1m_1a_1\rangle\\&\times\langle p_1\kappa_1m_1a_1|\alpha_\mu j_l(kr_1)C^l(1)|p_2\kappa_2m_2a_2\rangle\\&\times\frac{1}{2}\left\{\frac{1}{\varepsilon_{p_2}-\varepsilon_{p_1}+a_2k}+\frac{1}{\varepsilon_{p_2}-\varepsilon_{p_3}+a_2k}\right\}\\&\times\langle p_2\kappa_2m_2a_2|\alpha^\mu j_l(kr_2)C^l(2)|p_3\kappa_3m_3a_3\rangle\langle p_3\kappa_3m_3a_3|,\end{aligned}\tag{46}$$

where, as in Ref. 26, the quantum numbers p_i, κ_i, m_i, and a_i characterize the spherical waves of a free Dirac equation, with p_i the radial momentum,

$$\kappa_i=(-1)^{j_i+l_i+1/2}(j_i+l_i+\tfrac{1}{2}),$$

j_i and l_i the electron's total and orbital angular momenta, m_i the projection of the total angular momentum, and $a_i=\mathrm{sgn}(\varepsilon_{p_i})$, $\varepsilon_{p_i}=a_i\sqrt{p_i^2+m^2}$, j_l are spherical Bessel functions,

$$C^l_m=\sqrt{\frac{4\pi}{2l+1}}Y^l_m,$$

and Y^l_m are spherical harmonics. It is assumed that a scalar product is taken between spherical tensors. Summation with respect to p_i means integration over the continuum of radial momenta. The integrals of three Bessel functions in (46) were calculated recursively by an algorithm discussed in Ref. 27. To shorten the computation time, the overlap integrals $\langle a|p_i\kappa_im_ia_i\rangle$ and $\langle\xi|p_i\kappa_i,m_ia_i\rangle$ were first calculated on a fixed grid in p and were then interpolated with allowance for their behavior at infinity. While one can easily obtain an analytic expression for the overlap integral $\langle a|p_i\kappa_im_ia_i\rangle$, calculating the integral $\langle\xi|p_i\kappa_im_ia_i\rangle$ requires a numerical procedure that may require some enhancement at large values of p. For fixed momenta k and p_2, integration with respect to p_1 and p_3 is done only on the interval $(|k-p_2|,k+p_2)$. In calculating the integrals one must bear in mind that because of the energy denominator the integrand has singularities, which lie outside the integration range but for large momenta are close to the limits of that range. The behavior of the integrand was accounted for by using a grid tending to the limits of integration in a power-like manner. All calculations of integrals in the present work were done by Gaussian quadrature formulas. Since integrations with respect to p_1 and p_3 are independent, both integrals were calculated simultaneously. The entire range of integration with respect to p_2 was divided into two parts, $(0,k)$ and (k,∞), since the derivative of the integrand has a discontinuity at the point $p_2=k$. Integration was then done by replacing the infinitely large interval with a finite interval by an appropriate change of variables.

The calculation of the terms in the partial-wave expansion of the matrix element of the unrenormalized self-energy operator (9) is done by employing the relativistic Coulomb Green's function. For convenience of calculation we rotated

TABLE I. The first-order self-energy contribution for the $1s$-state expressed in terms of the function $F(\alpha Z)$ (here $E_{SE}=(\alpha/\pi)(\alpha Z)^4 F(\alpha Z)mc^2$).

Z	Present work	Mohr's data[30]
20	3.2464(5)	3.2462556(1)
30	2.5521(5)	2.5520151(1)
40	2.1354(5)	2.1352284(1)
50	1.8646(5)	1.8642743(2)
60	1.6839(5)	1.6838358(3)
70	1.5673(5)	1.5674075(4)
80	1.5027(5)	1.5027775(4)
92	1.4908(5)	1.4909160(3)
100	1.5302(5)	1.5301997(4)
110	1.6600(5)	1.660063(1)

the contour of integration with respect to ω in the complex ω plane so that the contour coincided with the imaginary axis. As a result the oscillatory behavior of the integrand was replaced by exponential decay. The calculation of the relativistic Coulomb Green's function was done by employing Whittaker functions, with the calculation algorithms taken from Ref. 28. By using the algorithm discussed in Ref. 29 in the range of variation of $|\kappa|$ of interest ($|\kappa| \in (1,22)$), we avoided applying quadrupole accuracy in calculating the Whittaker function $W_{\alpha\beta}(x)$, which considerably reduced the calculation time in comparison to the scheme suggested in Ref. 28. Radial integration was done by an approach similar to the one suggested by Mohr.[28] In each partial wave, integration with respect to energy was done for the difference of the unrenormalized contribution and the counterterm by replacing the infinitely large interval with a finite interval via an appropriate change of variables.

As a result, after term-by-term subtraction of two divergent series, one for the unrenormalized contribution and the other for the counterterm, we arrive at a convergent alternating series in powers of $|\kappa|$. Applying the lowest-order Euler transformation to this series, as done in Ref. 26, improves its convergence. In practice the calculation was done up to $|\kappa|=22$. Table I compares the results of first-order calculations of the self-energy with the most exact data of Ref. 30. The numerical values for the irreducible contribution defined by Eqs. (44) and (45) are listed in the second column of Table II.

3.2. The pole term

After integration with respect to the angular variables the expression (40) for ΔE_{pole} assumes the form

$$\Delta E_{\rm pole}=\alpha^2\sum_{\kappa_n=-1,2}\sum_{L=0,1}(-1)^{L+1}\begin{Bmatrix}1/2 & 1/2 & L\\ 1/2 & j_n & L\end{Bmatrix}\times\sum_{\varepsilon_n\neq\varepsilon_a}\frac{[R_L(0,anaa)]^2}{\varepsilon_a-\varepsilon_n}$$

$$+\frac{2\alpha^2}{\pi}\sum_{\kappa_n=-1,2}\int_0^\infty d\omega\sum_{L_2=0,1}\sum_{\varepsilon_n\neq\varepsilon_a}\frac{R_{L_2}(\omega,anaa)}{\Delta_n^2+\omega^2}\times\left[\sum_{L_1=0,1}(-1)^{L_1+1}\begin{Bmatrix}1/2 & 1/2 & L_1\\ 1/2 & j_n & L_2\end{Bmatrix}\right.$$

$$\left.\times R_{L_1}(0,anaa)\right]. \tag{47}$$

Here we have introduced the following notation:

$$R_0(\omega,anaa)=2\delta_{\kappa_n,-1}\int_0^\infty dr_1\int_0^\infty dr_2 r_1^2 r_2^2\tilde{g}_0(\omega,r_1,r_2)\times W_{aa}(r_1)W_{na}(r_2),$$

$$R_1(\omega,anaa)=(-1)^{j_n+1/2}\sqrt{2(2j_n+1)}(\kappa_n-1)\int_0^\infty dr_1\times\int_0^\infty dr_2 r_1^2 r_2^2\tilde{g}_1(\omega,r_1,r_2)V_{aa}(r_1)V_{na}(r_2),$$

$$\tilde{g}_L(\omega,r_1,r_2)=\frac{1}{\sqrt{r_1 r_2}}I_{L+1/2}(\omega r_<)K_{L+1/2}(\omega r_>),$$

$r_<=\min(r_1,r_2)$, $r_>=\max(r_1,r_2)$; $I_n(r)$ and $K_n(r)$ are modified Bessel functions, and

$$W_{ab}(r)=g_a(r)g_b(r)+f_a(r)f_b(r),$$

$$V_{ab}(r)=g_a(r)f_b(r)+f_a(r)g_b(r),$$

where $g(r)$ and $f(r)$ are, respectively, the large and small radial components of the Dirac wave function:

$$\psi_{n\kappa m}(\mathbf{r})=\begin{pmatrix} g_{nk}(r)\Omega_{\kappa m}(\mathbf{n})\\ if_{n\kappa}(r)\Omega_{-\kappa m}(\mathbf{n})\end{pmatrix}.$$

The calculation of the pole term, as well as the wave function $|\xi\rangle$ in the irreducible contribution, was done by the method of B-splines for the Dirac equation. In the final calculations we used 55 splines of the 10th order on the interval $(0,r_{\max})$. The radius $r_{\max}$ of the box bounding the system was chosen large enough that a further increase had no effect on the final result. In our case the value $r_{\max}=0.3$ a.u. for $Z=80$ proved sufficient. For specific calculations we replaced the B-spline representation of the wave functions with a representation in which the wave functions are a single polynomial in each interval (r_i,r_{i+1}). The results of calculations of $\Delta E_{\rm pole}$ are listed in the third column of Table II.

3.3. The contribution ΔE_{vr}

After integration with respect to the angular variables the expression (43) for ΔE_{vr} assumes the form

$$\Delta E_{vr}=-\frac{2\alpha^2}{\pi}\sum_\kappa\int_0^\infty d\omega\int_0^\infty dy\int_0^1 dr\int_0^\infty dz S_\kappa(\omega,r,y,z), \tag{48}$$

$$S_\kappa(\omega,r,y,z)=\frac{(2\alpha Z)^{-3}}{\Gamma^2(2\gamma+1)}r^{\gamma+1}y^{2\gamma+3}z^2\times\exp\left[-\frac{(r+1)y}{2}\right]T_\kappa(\omega,r,y,z), \tag{49}$$

$$T_\kappa(\omega,r,y,z)=[R_1(z)-R_0]\left[|\kappa|\tilde{g}_l\{\mathbf{D}_\kappa\}^{\rm I}\right.$$

TABLE II. Contribution of the diagrams of screened self-energy for the ground state of helium-like ions ($\Delta E_{\rm irred}$, $\Delta E_{\rm pole}$, $\Delta E_{\rm vr}$, and $\Delta E^{\rm ``infr''}_{\rm red+red}$ are defined in Eqs. (15), (40), (42), and (35), respectively; ΔE is the total contribution, ΔE_{LO} is the contribution, determined via Eq. (59), of the diagrams of the screened self-energy in the lowest order in αZ). The atomic system of units is used.

Z	$\Delta E_{\rm irred}$	$\Delta E_{\rm pole}$	$\Delta E_{\rm vr}$	$\Delta E^{\rm ``infr''}_{\rm ver+red}$	ΔE	ΔE_{LO}
20	−0.00971(5)	−0.00883	0.01332(10)	−0.00000	−0.0052(1)	−0.00379
30	−0.01991(5)	−0.01285	0.01866(4)	−0.00004	−0.01414(9)	−0.00706
40	−0.03524(5)	−0.01688	0.02316(2)	−0.00015	−0.02911(7)	−0.00711
50	−0.05736(5)	−0.02112	0.02687(2)	−0.00047	−0.05209(7)	
60	−0.08886(5)	−0.02585	0.02972(2)	−0.00119	−0.08618(7)	
70	−0.13377(5)	−0.03144	0.03159(2)	−0.00262	−0.13625(7)	
80	−0.19882(5)	−0.03843	0.03228(2)	−0.00523	−0.21020(7)	
90	−0.29595(5)	−0.04767	0.03146(2)	−0.00971	−0.32187(7)	
92	−0.32095(5)	−0.04990	0.03108(2)	−0.01091	−0.35068(7)	
100	−0.44880(8)	−0.06063	0.02863(2)	−0.01707	−0.49787(10)	
110	−0.7129(2)	−0.08024	0.02275(2)	−0.02891	−0.7993(2)	

$$
-\sum_{JL}\left(J+\frac{1}{2}\right)\tilde{g}_L\{\mathbf{D}_\kappa\}^{\rm II}_{\kappa\kappa,JL}\Bigg]+R_2(z)
$$

$$
\times\sum_{\kappa'}\frac{(-1)^{\kappa'}\alpha Z(\kappa+\kappa')}{\sqrt{6}}C_1(-\kappa,\kappa')
$$

$$
\times\Bigg[\delta_{l,l'}(-1)^{j-j'+l}2\sqrt{|\kappa\kappa'|}
$$

$$
\times\begin{Bmatrix}1/2 & 1/2 & 1\\ j' & j & l\end{Bmatrix}\tilde{g}_l\{\mathbf{P}_{\kappa\kappa'}\}^{\rm I}
$$

$$
-\sum_J(-1)^J(2J+1)\begin{Bmatrix}1/2 & 1/2 & 1\\ j' & j & J\end{Bmatrix}
$$

$$
\times\sum_L\tilde{g}_L\{\mathbf{P}_{\kappa\kappa'}\}^{\rm II}_{\kappa\kappa',JL}\Bigg], \qquad (50)
$$

where the angular momenta j,l, and j',l' correspond to the quantum numbers κ and κ', respectively, and

$$
\{\mathbf{A}\}^{\rm I}\equiv(1+\gamma)A^{11}-\alpha ZA^{12}-\alpha ZA^{21}+(1-\gamma)A^{22},
$$

$$
\begin{aligned}
\{\mathbf{A}\}^{\rm II}_{\kappa\kappa',JL}\equiv&(1-\gamma)A^{11}S_{JL}(1,\kappa)S_{JL}(1,\kappa')\\
&+\alpha ZA^{12}S_{JL}(1,\kappa)S_{JL}(-1,-\kappa')\\
&+\alpha ZA^{21}S_{JL}(-1,-\kappa)S_{JL}(1,\kappa')\\
&+(1+\gamma)A^{22}S_{JL}(-1,-\kappa)S_{JL}(-1,-\kappa'),
\end{aligned}
$$

$$
\begin{aligned}
D^{11}_\kappa=&\tilde{G}^{11}_\kappa(\omega,ru,z)\tilde{G}^{11}_\kappa(\omega,z,u)\\
&+\tilde{G}^{12}_\kappa(\omega,ru,z)\tilde{G}^{21}_\kappa(\omega,z,u),\\
D^{12}_\kappa=&\tilde{G}^{11}_\kappa(\omega,ru,z)\tilde{G}^{12}_\kappa(\omega,z,u)\\
&+\tilde{G}^{12}_\kappa(\omega,ru,z)\tilde{G}^{22}_\kappa(\omega,z,u),\\
D^{21}_\kappa=&\tilde{G}^{21}_\kappa(\omega,ru,z)\tilde{G}^{11}_\kappa(\omega,z,u)\\
&+\tilde{G}^{22}_\kappa(\omega,ru,z)\tilde{G}^{21}_\kappa(\omega,z,u),\\
D^{22}_\kappa=&\tilde{G}^{21}_\kappa(\omega,ru,z)\tilde{G}^{12}_\kappa(\omega,z,u)\\
&+\tilde{G}^{22}_\kappa(\omega,ru,z)\tilde{G}^{22}_\kappa(\omega,z,u),
\end{aligned}
$$

$$
\begin{aligned}
P^{ij}_{\kappa\kappa'}=&\tfrac{1}{2}(\tilde{P}^{ij}_{\kappa\kappa'}+\tilde{P}^{ji}_{\kappa'\kappa}),\\
\tilde{P}^{11}_{\kappa\kappa'}=&\tilde{G}^{11}_\kappa(\omega,ru,z)\tilde{G}^{21}_{\kappa'}(\omega,z,u)\\
&+\tilde{G}^{12}_\kappa(\omega,ru,z)\tilde{G}^{11}_{\kappa'}(\omega,z,u),\\
\tilde{P}^{12}_{\kappa\kappa'}=&\tilde{G}^{11}_\kappa(\omega,ru,z)\tilde{G}^{22}_{\kappa'}(\omega,z,u)\\
&+\tilde{G}^{12}_\kappa(\omega,ru,z)\tilde{G}^{12}_{\kappa'}(\omega,z,u),\\
\tilde{P}^{21}_{\kappa\kappa'}=&\tilde{G}^{21}_\kappa(\omega,ru,z)\tilde{G}^{21}_{\kappa'}(\omega,z,u)\\
&+\tilde{G}^{22}_\kappa(\omega,ru,z)\tilde{G}^{11}_{\kappa'}(\omega,z,u),\\
\tilde{P}^{22}_{\kappa\kappa'}=&\tilde{G}^{21}_\kappa(\omega,ru,z)\tilde{G}^{22}_{\kappa'}(\omega,z,u)\\
&+\tilde{G}^{22}_\kappa(\omega,ru,z)\tilde{G}^{12}_{\kappa'}(\omega,z,u).
\end{aligned}
$$

Here the functions $\tilde{G}^{ij}_\kappa(\omega,x,y)$ are the radial components of $\tilde{G}(\omega,\mathbf{x},\mathbf{y})$ defined by Eq. (42), $u=y/2\alpha Z$, $\gamma=\sqrt{1-(\alpha Z)^2}$,

$$
\tilde{g}_L\equiv\tilde{g}_L(\omega,r,u)=\frac{1}{u\sqrt{r}}I_{L+1/2}(\omega ru)K_{L+1/2}(\omega u)
$$

($I_L(x)$ and $K_L(x)$ are modified Bessel functions), and

$$
\begin{aligned}
R_1(z)=&\frac{(2\alpha Z)^{2\gamma+1}}{z}\Bigg[\int_0^z dx x^{2\gamma}e^{-2\alpha Zx}\\
&+z\int_z^\infty dx x^{2\gamma-1}e^{-2\alpha Zx}\Bigg],\\
R_2(z)=&\frac{(2\alpha Z)^{2\gamma+1}}{z^2}\Bigg[\int_0^z dx x^{2\gamma+1}e^{-2\alpha Zx}\\
&+z^3\int_z^\infty dx x^{2\gamma-2}e^{-2\alpha Zx}\Bigg],
\end{aligned}
$$

$$
R_0=\frac{1}{\alpha}\Gamma(2\gamma+1)\Delta E^{(1)},
$$

where $\Delta E^{(1)}$ is the one-photon correction to the energy of the ground state of a two-electron ion. A simple analytic calculation of this correction yields[31]

$$\Delta E^{(1)}=\Delta E^{(1)}_{\text{Coul}}+\Delta E^{(1)}_{Br}, \tag{51}$$

$$\Delta E^{(1)}_{\text{Coul}}=\frac{\alpha^2 Z}{\gamma}mc^2\left[1-\frac{\Gamma(2\gamma+1/2)}{\sqrt{\pi}\Gamma(2\gamma+1)}\right], \tag{52}$$

$$\Delta E^{(1)}_{Br}=\frac{4}{3}\frac{\alpha^4 Z^3}{\gamma(2\gamma-1)}\left[\gamma+\frac{1}{2}-\frac{(6\gamma+1)\Gamma(2\gamma+1/2)}{2\sqrt{\pi}\Gamma(2\gamma+1)}\right]. \tag{53}$$

The angular coefficients $S_{JL}(\kappa_a,\kappa_b)$ are nonzero only at $L=J-1$, J, $J+1$ and have the following form:

$$S_{JJ+1}(\kappa_a,\kappa_b)=\sqrt{\frac{J+1}{2J+1}}\left(1+\frac{\kappa_a+\kappa_b}{J+1}\right)C_J(-\kappa_b,\kappa_a),$$

$$S_{JJ}(\kappa_a,\kappa_b)=\frac{\kappa_a-\kappa_b}{\sqrt{J(J+1)}}C_J(\kappa_b,\kappa_a),$$

$$S_{JJ-1}(\kappa_a,\kappa_b)=\sqrt{\frac{J}{2J+1}}\left(-1+\frac{\kappa_a+\kappa_b}{J}\right)\times C_J(-\kappa_b,\kappa_a),$$

$$C_J(\kappa_b,\kappa_a)=(-1)^{j_b+1/2}\sqrt{(2j_a+1)(2j_b+1)}\times\begin{pmatrix} j_a & J & j_b \\ 1/2 & 0 & -1/2\end{pmatrix}\Pi(l_a,l_b,J),$$

where Π stands for the even triangle rule.

We calculated the function $\tilde{G}_\kappa(\varepsilon,x,y)$ in (50) by subtracting

$$\sum_{\varepsilon_n=\varepsilon_a}\frac{\psi_n(\mathbf{x})\psi_n^\dagger(\mathbf{y})}{\varepsilon-\varepsilon_n+i0}$$

from the Green's function $G_\kappa(\varepsilon,x,y)$ at $\kappa=-1$. Certain numerical cancellations emerge in the process, and these may be considerable for low energies. This requires that the Green's function be calculated to high accuracy.

To reduce the computation time, we calculated the functions $R_1(z)$ and $R_2(z)$ beforehand on a fixed grid, and then in the computation process found specific values by interpolation with allowance for the behavior at infinity. Next, for each value of ω and $|\kappa|$ we also used a fixed grid in the radial variable to calculate the four Whittaker functions needed for finding the Green's function, and then by interpolation could calculate these functions at any point. Here we allowed for the asymptotic behavior of the Whittaker functions for $r\to 0$ and $r\to\infty$. Numerical integration was performed via Gauss–Legendre quadratures. First integration with respect to z was done. Here the integrand has discontinuities at the points where the radial arguments of the Green's functions coincide. The entire interval was partitioned into three intervals: $(0,ru)$, (ru,u), and (u,∞). Within each interval integration was done separately by an appropriate change of variables. Then integration with respect to the variables r and y was carried out. The correctness of integration with respect to z, r, and y was verified via the identity

$$\int d\mathbf{x}\,d\mathbf{y}\,d\mathbf{z}\;\psi_a^\dagger(\mathbf{x})G_{-1}(\varepsilon,\mathbf{x},\mathbf{z})G_{-1}(\varepsilon,\mathbf{z},\mathbf{y})\psi_a(\mathbf{y})=\frac{1}{(\varepsilon-\varepsilon_a)^2}.$$

The last step was integration with respect to energy.

As a result of these calculations we obtained an alternating convergent series in powers of the parameter $|\kappa|$. For large values of Z (here Z is the charge of the nucleus) the terms in the series decrease as $1/|\kappa|^3$, and the convergence gradually weakens as Z decreases. Summation was done up to the value $|\kappa|=12$. The remainder of the series was estimated on the assumption that the terms in the series decrease according to the following law:

$$\frac{1}{|\kappa|^3}\left(A+\frac{B}{|\kappa|}+\cdots\right).$$

The results of calculations of ΔE_{vr} are listed in the fourth column in Table II.

3.4. The "infrared" term $\Delta^{\text{"infr"}}_{\text{vert+red}}$

After calculating the angular integrals and performing the necessary transformations for the ground state, we arrive at the following expression for (35):

$$\Delta E^{\text{"infr"}}_{\text{ver+red}}=\frac{16}{9}\frac{\alpha}{\pi}\Delta E^{(1)}_{Br}\int_0^\infty dr_1\int_0^\infty dr_2 r_1^2 r_2^2 a_1(r_1,r_2)\times V_{aa}(r_1)V_{aa}(r_2). \tag{54}$$

Here $V_{aa}(r)=2g_a(r)f_a(r)$, with $g_a(r)$ and $f_a(r)$ the large and small radial components of the wave functions of the $1s$-state, respectively;

$$a_1(r_1,r_2)=\frac{3}{2}\int_{-1}^{1}d\xi\,\ln\sqrt{r_1^2+r_2^2-2r_1r_2\xi}\;P_1(\xi),$$

with $P_1(\xi)=\xi$ the first-order Legendre polynomial; and $\Delta E^{(1)}_{Br}$ is the correction to the ground-state energy due to the exchange of a single Breit photon and specified by Eq. (53). The integrals in (54) were calculated analytically. The result is

$$\Delta E^{\text{"infr"}}_{\text{ver+red}}=\frac{4\alpha}{3\pi}(\alpha Z)^2\Delta E^{(1)}_{Br}\frac{\Gamma(4\gamma+2)}{\Gamma^2(2\gamma+1)}(I_1-I_2), \tag{55}$$

where

$$I_1=\frac{\sqrt{\pi}\,\Gamma(2\gamma-1)}{2^{4\gamma-2}8\Gamma(2\gamma+1/2)}\times\left[-2+C+2\ln 2+\psi\left(2\gamma+\frac{1}{2}\right)\right], \tag{56}$$

$$I_2=\frac{{}_2F_1(4\gamma+2,2\gamma,2\gamma+1,-1)}{2\gamma}+\frac{{}_2F_1(4\gamma+2,2\gamma+2,2\gamma+3,-1)}{2(\gamma+1)}, \tag{57}$$

TABLE III. Verifying calculations of the correction caused by the interaction with an additional external field $\Delta V=-\alpha/r$ in the first-order self-energy diagram. (The results are compared with dE_{SE}/dZ.) The atomic system of units is employed.

Z	ΔE_{irred}	ΔE_{pole}	ΔE_{vr}	ΔE	dE_{SE}/dZ
20	0.02003	0.01320	−0.02219	0.01104	0.01102
30	0.03969	0.01837	−0.02917	0.02888	0.02885
40	0.06795	0.02274	−0.03359	0.05710	0.05713
50	0.10722	0.02645	−0.03537	0.09830	0.09832
60	0.16148	0.02973	−0.03458	0.15662	0.15663
70	0.23749	0.03292	−0.03095	0.23946	0.23946
80	0.34748	0.03666	−0.02386	0.36027	0.36027
92	0.55983	0.04364	−0.00891	0.59456	0.59456
100	0.79500	0.05193	−0.00727	0.85420	0.85426
110	1.3307	0.07241	−0.04120	1.4443	1.44427

where C is Euler's constant, and $\psi(x)$ is the logarithmic derivative of the gamma function. In the lowest order in αZ this expression has the simple form

$$(\Delta E^{\text{"infr"}}_{\text{ver+red}})_{\text{LO}}=-\frac{2}{9\pi}\alpha^2(\alpha Z)^5 mc^2. \tag{58}$$

The values of the "infrared" term are listed in the fifth column of Table II.

The values of the total contribution of the diagrams of screened self-energy are listed in the sixth column of Table II.

4. DISCUSSION

We have calculated the contribution of the diagrams of screened self-energy for the ground state of helium-like ions. For U^{90+} it amounts to -9.54 eV.

To check the results of numerical calculations we computed the correction to the first-order self-energy diagram produced by an external field $\Delta V=-\alpha/r$. In this case the total contribution of all terms, ΔE_{irred}, ΔE_{red}, and ΔE_{vertex} ($\Delta E^{\text{"infr"}}_{\text{ver+red}}=0$), must be equal to dE_{SE}/dZ, where E_{SE} is the first-order self-energy contribution. In Table III the results of our calculations are compared with the values of dE_{SE}/dZ found by interpolation of the most precise values of E_{SE} from Ref. 30.

Let us compare the results of our calculations with those done in the lowest order in αZ. Using the results of Refs. 32–34, we found that the contribution of the diagrams of screened self-energy in the lowest order in αZ amounted to

$$\Delta E_{LO}=\alpha^5 Z^3 mc^2(1.346\ln Z-5.251). \tag{59}$$

The values of ΔE_{LO} are listed in the last column of Table II. For detailed comparison we wrote ΔE for small values of Z as

$$\Delta E=\alpha^5 Z^3 mc^2(C_1\ln Z+C_2+C_3\alpha Z) \tag{60}$$

and found the coefficients C_1 and C_2 from our numerical values of ΔE at $Z=20$, 25, and 30. The result was $C_1=1.36$ and $C_2=-5.32$.

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