Relativistic recoil effects on energy levels in a muonic atom: A Grotch-type calculation of the second-order vacuum-polarization contributions

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Adjusting a previously developed Grotch-type approach to a perturbative calculation of the electronic vacuum-polarization effects in muonic atoms, we find here the two-loop vacuum-polarization relativistic recoil correction of order $\alpha^2(Z\alpha)^4 m^2/M$ in light muonic atoms. The result is in perfect agreement with the one previously obtained within the Breit-type approach. We also discuss here simple approximations of the irreducible part of the two-loop vacuum-polarization dispersion density, which are applied to test our calculations and could be useful for other evaluations with an uncertainty better than 1%.

I. INTRODUCTION

High-precision tests of any advanced atomic calculations are possible only for few-body systems, and their accuracy goes down dramatically when we increase the number of particles involved. The highest accuracy has been achieved for two-body (hydrogenlike) atomic systems. To study such systems not only are binding effects and QED loops important but also recoil effects. While the nonrelativistic two-body problem is easily solved by introducing the reduced mass, the relativistic recoil effects are more complicated.

The problem of relativistic recoil effects was resolved for the pure Coulomb two-body system a long time ago. The possible solutions included the Breit equation (see, e.g., [1]) and its expansions as well as the Grotch equation [2]. For non-Coulomb systems, only the Breit-type approach has successfully been used to date.

The purpose of this paper is to develop a method suitable for a calculation of a certain class of corrections of order $\alpha^2(Z\alpha)^4 m^2/M$. The approach is applicable to medium-Z muonic and antiprotonic atoms, i.e., to the atoms whose characteristic atomic momentum $Z\alpha m$ is comparable to the electron mass m_e. In such atoms the recoil effects are more important than in ordinary (electronic) atoms. Meanwhile, the electronic vacuum-polarization (eVP) effects are also enhanced. Thus a calculation of relativistic recoil eVP corrections is important. Here we calculate such corrections to the energy levels in the second order of eVP effects, which are of order $\alpha^2(Z\alpha)^4 m^2/M$.

This paper is the third paper of the series [3,4] devoted to a general approach to calculate relativistic recoil effects and its applications. In these papers, as explained in the first paper of the series [3], we develop an approach which can be applied for a certain class of potentials (or, rather, to a certain class of corrections to the interaction between the atomic particles).

While the expressions are valid for a certain range of atoms for arbitrary states, the practical importance of the corrections depends on the value of the nuclear charge, the atomic weight of the nucleus, the mass of the orbiting particle (which is indeed different for muons and antiprotons), and the transition between what levels are studied and with what accuracy.

At this stage we are interested in deriving the method and its verification, rather than in its application to any particular transition of practical interest. Below we derive the general equations that take into account second-order eVP relativistic recoil effects. For the verification of the method we choose to calculate the corrections which are known from a calculation with an alternative (Breit-type) technique in our previous paper [5].

Generalizing the method developed by Grotch and Yennie [2] to evaluate the relativistic recoil effect in pure Coulomb systems to effects of eVP in muonic atoms, in [3,4] we derived the general expression

$$
\begin{aligned}
E = {} & m + m_R[f_{CN}(Z\alpha, Z\alpha m_R/m_e) - 1] \\
& - \frac{m_R^2}{2M}[f_{CN}(Z\alpha, Z\alpha m_R/m_e) - 1]^2 \\
& - \frac{m_R^2}{2M}\frac{\partial}{\partial \ln \kappa}[f_{CN}(Z\alpha, \kappa) - 1]^2 \bigg|_{\kappa = Z\alpha m_R/m_e} \\
& - \langle \psi_C | \left(\frac{V^2}{2M} + \frac{1}{4M}[V,[\mathbf{p}^2, W]] \right) | \psi_C \rangle,
\end{aligned}
\tag{1}
$$

which is valid for an arbitrary perturbed potential

$$
V = V_C + V_N,
$$

where V_C is the Coulomb potential and in a certain sense V_N is smaller than V_C, i.e., $V_N \sim \varepsilon V_C$, $\varepsilon \ll 1$. It is important that V_N is a kind of nonrelativistic potential in the sense that its leading nonrelativistic contribution to the energy is of order $\varepsilon(Z\alpha)^2 m$, while the first relativistic correction appears in order $\varepsilon(Z\alpha)^4 m$.

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Here, W is a specific auxiliary potential, ψ_C is the wave function of the Dirac-Coulomb problem with the reduced mass, and

$$f_{CN}(Z\alpha, Z\alpha m_R/m_e) = f_C(Z\alpha) + \Delta f_{CN}(Z\alpha, Z\alpha m_R/m_e) \quad (2)$$

is the exact dimensionless energy for the Dirac equation with the reduced mass and potential V, and we separate the corrections to it, Δf_{CN}, induced by V_N.

Expression (1) is valid for nonrecoil terms exactly in $Z\alpha$, for the nonrelativistic problem exactly in m/M, and for the leading relativistic recoil correction $(Z\alpha)^4 m^2/M$. It may be applied to an arbitrary order in ε. (In principle, it may also be applied for an ε that is not small if the appropriate wave functions and energy are found numerically.)

In [4] we describe a method to calculate the recoil correction to the energy of order $\alpha/\pi (Z\alpha)^4 m^2/M$, and here we aim to obtain the recoil correction of the next order in α. For that we consider a potential of the form

$$V_N = V_U + V_{11} + V_2, \quad (3)$$

where

$$V_U = -Z\alpha \int_0^1 dv\, \rho_1(v) \frac{e^{-\lambda r}}{r}$$

is the Uehling potential,

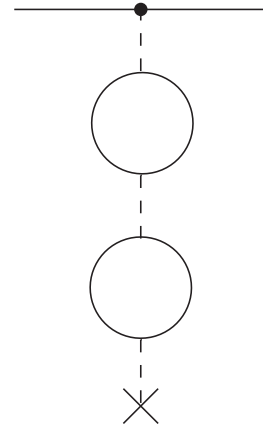$$V_{11} = -Z\alpha \int_0^1 dv\, \rho_{11}(v) \frac{e^{-\lambda r}}{r}$$

FIG. 1. Diagram of the reducible part of the Källen-Sabry potential V_{11}.

corresponds to the reducible two-loop eVP potential (see Fig. 1), and

$$V_2 = -Z\alpha \int_0^1 dv\, \rho_2(v) \frac{e^{-\lambda r}}{r}$$

is for its irreducible part (see Fig. 2). The dispersion parameter is

$$\lambda^2 = \frac{4m_e^2}{1 - v^2},$$

and the eVP dispersion density functions are defined as [6–9]

$$\rho_1(v) = \left(\frac{\alpha}{\pi}\right) \frac{v^2(1 - v^2/3)}{1 - v^2}, \quad (4)$$

$$\rho_{11}(v) = -\frac{1}{9}\left(\frac{\alpha}{\pi}\right)^2 \frac{v^2(1 - v^2/3)}{1 - v^2}\left\{16 - 6v^2 + 3v(3 - v^2)\ln\left(\frac{1 - v}{1 + v}\right)\right\}, \quad (5)$$

$$\rho_2(v) = \frac{2}{3}\left(\frac{\alpha}{\pi}\right)^2 \frac{v}{1 - v^2}\left((3 - v^2)(1 + v^2)\left\{\mathrm{Li}_2\left(-\frac{1 - v}{1 + v}\right) + 2\mathrm{Li}_2\left(\frac{1 - v}{1 + v}\right) + \ln\left(\frac{1 + v}{1 - v}\right)\left[\frac{3}{2}\ln\left(\frac{1 + v}{2}\right) - \ln(v)\right]\right\}\right.$$

$$\left. + \left[\frac{11}{16}(3 - v^2)(1 + v^2) + \frac{1}{4}v^4\right]\ln\left(\frac{1 + v}{1 - v}\right) + \frac{3}{2}v(3 - v^2)\ln\left(\frac{1 - v^2}{4}\right) - 2v(3 - v^2)\ln(v) + \frac{3}{8}v(5 - 3v^2)\right), \quad (6)$$

where $\mathrm{Li}_2(z)$ is the Euler dilogarithm [10].

It is important that Eq. (1) includes only the first derivative with respect to κ. That is because a shift in the effective mass is at most $O((Z\alpha)^2(m/M)m)$ and terms quadratic in the shift are at most of the order $\varepsilon(Z\alpha)^6(m/M)^2 m$. To evaluate the derivative we apply the identity

$$\frac{\partial[f_{CN}(Z\alpha, \kappa) - 1]^2}{\partial \ln \kappa} = -\frac{\partial[f_{CN}(Z\alpha, Z\alpha m_R/m_e) - 1]^2}{\partial \ln m_e},$$

which allows us to avoid differentiating the α^2 term in $f_{CN}(Z\alpha, Z\alpha m_R/m_e)$, found by means of numerical computation, and instead allows to calculate numerically an integral which contains a derivative of the potential over the parameter m_e.

The result for the Dirac equation with the reduced mass and the potential defined in Eq. (3) can be, in principle, obtained

by many means. Recently, such a result for low-lying states in light muonic atoms was found by applying a nonrelativistic perturbation theory in [5].
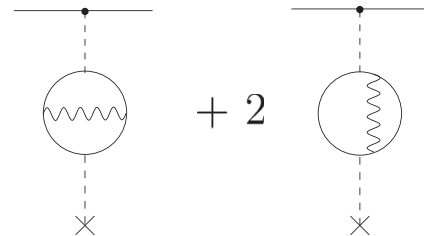

FIG. 2. Diagrams of the irreducible part of the Källen-Sabry potential V_2.

II. eVP RELATIVISTIC RECOIL CORRECTIONS TO THE SECOND ORDER OF α

Let us expand Eq. (2) in terms of ε:

$$f_{CN}(Z\alpha, Z\alpha m_R/m_e) = f_C(Z\alpha) + f_N(Z\alpha, Z\alpha m_R/m_e) + f_{NN}(Z\alpha, Z\alpha m_R/m_e), \quad (7)$$

where f_N is linear in ε and f_{NN} is quadratic.

It is convenient to consider different parts of the perturbing potential independently, setting appropriate ε in different cases.

A. The first-order contribution of V_{11} and V_2

To take into account the contributions of V_{11} and V_2, we can set $\varepsilon = (\alpha/\pi)^2$ and take the first order of the perturbation theory (in ε), which has been already studied in Ref. [4][1],

$$E_{Nq}^{(1)} = m_R f_{Nq} + \Delta E_q^{(1)}, \quad (8)$$

where the index q corresponds to either V_{11} or V_2,

$$\Delta E_q^{(1)} = -\frac{m_R^2}{M}(f_C - 1)f_{Nq} - \frac{m_R^2}{M}(f_C - 1)\frac{\partial}{\partial \ln \kappa} f_{Nq}$$
$$- \langle \psi_C | \left(\frac{V_q V_C}{M} + \frac{1}{4M}[V_C,[\mathbf{p}^2, W_q]] \right.$$
$$+ \left. \frac{1}{4M}[V_q,[\mathbf{p}^2, W_C]] \right) | \psi_C \rangle, \quad (9)$$

$| \psi_C \rangle$ is the Coulomb wave function, and it is sufficient to consider it in the nonrelativistic (NR) approximation (cf. [4]). The related auxiliary potential takes the form [cf. Eq. (10) of [4]]

$$W_q(\mathbf{k}) = 8\pi(Z\alpha) \int_0^1 dv \frac{\rho_q(v)}{(\mathbf{k}^2 + \lambda^2)^2},$$
$$W_q(r) = (Z\alpha) \int_0^1 dv \, \rho_q(v) \frac{e^{-\lambda r}}{\lambda}. \quad (10)$$

Proceeding in the same way as in [4] [cf. Eq. (32) there], we obtain for these contributions (cf. [11,12])

$$\Delta E_{Nq}^{(NR)} = \frac{(Z\alpha)^4}{n^3} \frac{m_R^2}{M} \sum_{i,k=0}^{n-l-1} B_{ik}^{(NR)}$$
$$\times \left[-\frac{1}{2n} K_{2,2l+i+k+2}^{(q)}(\kappa_n) \right.$$
$$- \frac{2l+i+k+2}{2n\kappa_n} K_{3,2l+i+k+3}^{(q)}(\kappa_n)$$
$$+ \left. \frac{1}{\kappa_n} K_{3,2l+i+k+2}^{(q)}(\kappa_n) \right], \quad (11)$$

where

$$B_{ik}^{(NR)} = \frac{(-1)^{i+k}(n-l-1)!}{i!(n-l-i-1)!k!(n-l-k-1)!}$$
$$\times \frac{(n+l)!(2l+i+k+1)!}{(2l+i+1)!(2l+k+1)!} \quad (12)$$

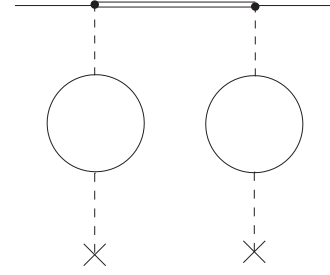[1]To simplify notation we drop the arguments in terms of Eq. (1).

FIG. 3. The second-order Uehling contributions to the energy.

and functions

$$K_{bc}^{(q)}(\kappa) = \int_0^1 dv \frac{\rho_q(v)}{(1-v^2)^{b/2-1}} \left(\frac{\kappa\sqrt{1-v^2}}{1+\kappa\sqrt{1-v^2}} \right)^c \quad (13)$$

differ from the base integrals $K_{bc}(\kappa)$ [11,12], introduced earlier and expressed in terms of spectral functions.

For the low-lying states of interest ($n = 1,2$) in light muonic atoms the results are

$$\Delta E_q^{(NR)}(1s) = (Z\alpha)^4 \frac{m_R^2}{M}$$
$$\times \frac{1}{\kappa} \left[-\frac{\kappa}{2} K_{22}^{(q)}(\kappa) + K_{32}^{(q)}(\kappa) - K_{33}^{(q)}(\kappa) \right],$$

$$\Delta E_q^{(NR)}(2s) = (Z\alpha)^4 \frac{m_R^2}{32M}$$
$$\times \left\{ -K_{24}^{(q)}(\kappa_2) + \frac{4}{\kappa_2} \left[K_{34}^{(q)}(\kappa_2) - K_{35}^{(q)}(\kappa_2) \right] \right.$$
$$+ \left. \frac{2}{\kappa_2^3} \left[\kappa_2 K_{44}^{(q)}(\kappa_2) + 4K_{54}^{(q)}(\kappa_2) - 4K_{55}^{(q)}(\kappa_2) \right] \right\},$$

$$\Delta E_q^{(NR)}(2p) = (Z\alpha)^4 \frac{m_R^2}{M} \frac{1}{\kappa_2} \left[-\frac{\kappa_2}{2} K_{2,4}^{(q)}(\kappa_2) \right.$$
$$+ \left. 2K_{3,4}^{(q)}(\kappa_2) - 2K_{3,5}^{(q)}(\kappa_2) \right]. \quad (14)$$

The required integrals $K_{bc}^{(11)}$ and $K_{bc}^{(2)}$ should be calculated numerically. The numerical results are considered in Sec. III.

B. The second-order contribution of V_U

To deal with the second-order contributions of V_U (see, e.g., Fig. 3) we should address terms in (1) which are second order in $\varepsilon = \alpha/\pi$.

For the case of general V_N, selecting terms of the corresponding order ε^2 in Eq. (1), we arrive at

$$E_N^{(2)} = m_R f_{NN} + \Delta E_N^{(2a)} + \Delta E_N^{(2b)}, \quad (15)$$

where

$$\Delta E_N^{(2a)} = -\frac{m_R^2}{M} \left((f_C - 1)f_{NN} + \frac{(f_N)^2}{2} \right)$$
$$- \frac{m_R^2}{M} \left((f_C - 1)\frac{\partial}{\partial \ln \kappa} f_{NN} + f_N \frac{\partial}{\partial \ln \kappa} f_N \right). \quad (16)$$

Note that in the last expression we need only the leading nonrelativistic contribution to various f, and in particular, it

TABLE I. The α^2 eVP relativistic recoil corrections to energies of the muonic hydrogen in units of $(\alpha/\pi)^2(Z\alpha)^4 m_R^2/M$. See Eq. (20) for notation.

	$1s$	$2s$	$2p$
$\Delta E_{11}^{(1)}$	0.505	0.0721	0.000133
$\Delta E_2^{(1)}$	0.139	0.0576	0.002879
$\Delta E_U^{(2a)}$	−0.154	−0.0024	−0.000060
$\Delta E_U^{(2b)}$	0.678	0.0685	0.000367
$\Delta E^{(\text{rec}-\text{VP2})}$	1.168	0.1958	0.003319

is sufficient to write

$$f_{NN} = \frac{\langle \psi_C | V_N G_C' V_N | \psi_C \rangle}{m_R}, \quad (17)$$

where G_C' is the reduced Coulomb wave function for the corresponding state.

The second term in (15), $\Delta E^{(2b)}$, corresponds to the W contribution of the matrix element in (1), which in the second order of ε provides us with

$$\Delta E_N^{(2b)} = -\langle \psi_C | \left(\frac{V_N^2}{2M} + \frac{1}{4M}[V_N,[\mathbf{p}^2,W_N]] \right) |\psi_C\rangle$$
$$- 2\langle \psi_C | \left(\frac{V_C V_N}{M} + \frac{1}{4M}[V_N,[\mathbf{p}^2,W_C]] \right.$$
$$+ \left. \frac{1}{4M}[V_C,[\mathbf{p}^2,W_N]] \right) |\psi_N\rangle, \quad (18)$$

where

$$|\psi_N\rangle = G_C' V_N |\psi_C\rangle \quad (19)$$

is the correction to the wave function induced by V_N.

To calculate the correction to the second order in the Uehling potential we set $V_N = V_U$ in general expressions (16)–(19).

Equation (15) presents the complete result for the relativistic terms of order $\alpha^2(Z\alpha)^4 m$ and $\alpha^2(Z\alpha)^4 m^2/M$ in terms of the sum of the Dirac term with the reduced mass $m_R f_{NN}$ and the recoil corrections $\Delta E_U^{(2a)}$ and $\Delta E_U^{(2b)}$. Since the expressions for the corrections deal with nonrelativistic wave functions and Green's functions, the result for the eVP relativistic recoil correction depends on orbital momentum l and does not depend on total muon angular momentum j, which means that there is no corrections to the fine splitting in this order behind the result of the Dirac equation with the reduced mass.

III. RESULTS

The expressions presented above allow us to calculate the recoil correction to the energy of order $(\alpha/\pi)^2(Z\alpha)^4 m_R^2/M$. The contributions to the correction for the lowest states of the muonic hydrogen

$$\Delta E^{(\text{rec}-\text{VP2})} = \Delta E_{11}^{(1)} + \Delta E_2^{(1)} + \Delta E_U^{(2a)} + \Delta E_U^{(2b)} \quad (20)$$

are listed for muonic hydrogen in Table I.

The first-order Källen-Sabry potential contributions are calculated numerically in a rather straightforward way. To control the calculation of the irreducible part we have also

TABLE II. The α^2 relativistic recoil eVP corrections to energies of the light muonic hydrogenlike atoms in units of $(\alpha/\pi)^2(Z\alpha)^4 m_R^2/M$.

	$1s$	$2s$	$2p$
H	1.168	0.1958	0.003319
D	1.192	0.2016	0.003551
^{3}He$^+$	1.445	0.2867	0.006866
^{4}He$^+$	1.447	0.2878	0.006900

used various approximate representations for the dispersion function. They are discussed in Appendix A.

The corrections of the second order in the Uehling potential were computed using two different representations of the reduced nonrelativistic Coulomb Green's functions, which are summarized in Appendix B. The results produced with two representations are consistent.

The calculations were also performed for various isotopes of muonic hydrogen and helium ions. The results are presented in Table II.

It is interesting to compare results obtained with the Grotch-type calculations in this paper with the Breit-type calculation we performed previously [5].

A comparison of the Grotch-type results with the complete Breit-type ones is summarized in Table III. The Breit-type results are exact in m/M, while the Grotch-type recoil correction includes only a term linear in m/M. As explained in [4,5] (see also [13]), one can rearrange the Breit Hamiltonian and separate the linear recoil and higher-order terms. As stated in [5], the linear recoil terms in the Breit-type approach are consistent with the results obtained here; in fact they agree within an uncertainty of numerical integration, and therefore all digits in the results given for the Grotch-type evaluation in Table III are valid.

As one can see from Table III, the higher-order terms in m/M are important for the complete recoil results. For the s states in muonic hydrogen they are about 10% of the linear term. [Here in Table III the Darwin-Foldy-type terms are included for all atoms. If, following [14,15], we exclude them,

TABLE III. The α^2 relativistic recoil eVP corrections to energies of light muonic hydrogenlike atoms in units of μeV. The eVP2 results of the Grotch-type evaluation of this paper are given in roman type. The complete results of the Breit-type calculations [5] are presented in italics. Note that the complete Breit-type recoil results [5] of order $\alpha^2(Z\alpha)^4 m$ are exact in m/M, while the Grotch-type recoil contributions include only terms linear in m_R/M.

Atom	$1s$	$2s$	$2p_{1/2}$	$2p_{3/2}$
H	0.172	0.0288	0.000488	0.000488
	0.155	*0.0259*	*0.000737*	*0.000289*
D	0.0973	0.0165	0.000290	0.000290
	0.0921	*0.0156*	*0.000370*	*0.000227*
^{3}He$^+$	1.31	0.259	0.00621	0.00621
	1.26	*0.250*	*0.00810*	*0.00492*
^{4}He$^+$	1.00	0.200	0.00478	0.00478
	0.97	*0.194*	*0.00590*	*0.00403*

the results are shifted and become 0.0635 μeV (1s), 0.0126 μeV (2s) for muonic deuterium and 0.75 μeV (1s), 0.172 μeV (2s) for muonic helium-4]. For the p states the $(m/M)^2$ contribution is even larger in fractional units; however, the total recoil contribution for the $2p$ state is small in comparison with the related $2s$ contribution and can be neglected for the $2p - 2s$ difference while calculating the Lamb shift. A similar situation actually also takes place for the one-loop eVP contribution [4,13].

The Breit-type calculations [5] delivered all the contributions within a nonrelativistic perturbation theory (NRPT) with various relativistic perturbations of the Coulomb potential.

Within the Breit-equation approach, the recoil and nonrecoil terms of the Breit Hamiltonian are treated in the same way (see, e.g., [1]). As a result, the technique applied in [5] to obtain the relativistic nonrecoil term (i.e., the relativistic correction to the one-particle equation with the reduced mass) was the same as for the recoil term. Actually, within the NRPT approach there is no need for a separation between the recoil and nonrecoil terms.

Here, the recoil correction is obtained in a quite different way. Thus, we conclude that our NRPT calculation of both the nonrecoil and recoil relativistic contributions [5] is correct.

To conclude, the results of this paper include the development of a method to calculate the second-order eVP relativistic recoil correction for an arbitrary state in an arbitrary hydrogenlike muonic atom. That is a purely theoretical result. As for an application to practically important transitions,

we have calculated the relativistic recoil correction of order $\alpha^2(Z\alpha)^4 m^2/M$ for the Lamb shift in muonic hydrogen. It is small by itself. As we explain above, such a calculation serves as a confirmation of our eVP results previously obtained by means of NRPT [5]. Because of the way relativistic recoil and nonrecoil contributions were treated there, the result of this paper confirms the whole relativistic eVP contribution of [5] and, in particular, its relativistic nonrecoil correction of order $\alpha^2(Z\alpha)^4 m$. That correction, in contrast to the recoil term, is somewhat smaller than, but still compatible with, the uncertainty of actual experiments (see [5] for details).

APPENDIX A: APPROXIMATION FOR THE IRREDUCIBLE PART OF THE KÄLLEN-SABRY DISPERSION FUNCTION WITH AN UNCERTAINTY BETTER THAN 1%

The exact expression for the irreducible part of the dispersion weight function of the Källen-Sabry potential [6–8],

$$\rho_2(v) = \frac{2}{3}\left(\frac{\alpha}{\pi}\right)^2 \frac{v}{1-v^2}\left((3-v^2)(1+v^2)\left\{\mathrm{Li}_2\left(-\frac{1-v}{1+v}\right) + 2\mathrm{Li}_2\left(\frac{1-v}{1+v}\right) + \ln\left(\frac{1+v}{1-v}\right)\left[\frac{3}{2}\ln\left(\frac{1+v}{2}\right) - \ln(v)\right]\right\}\right.$$
$$\left. + \left[\frac{11}{16}(3-v^2)(1+v^2) + \frac{1}{4}v^4\right]\ln\left(\frac{1+v}{1-v}\right) + \frac{3}{2}v(3-v^2)\ln\left(\frac{1-v^2}{4}\right) - 2v(3-v^2)\ln(v) + \frac{3}{8}v(5-3v^2)\right), \quad \text{(A1)}$$

is somewhat complicated. It does not allow us exact analytic evaluations in muonic atoms. Meanwhile, an approximate representation by Schwinger [6],

$$\rho_2^{(s)}(v) = \left(\frac{\alpha}{\pi}\right)^2 \frac{v^2\left(1-\frac{v^2}{3}\right)}{1-v^2}\left\{\frac{\pi^2}{2v} - \frac{3+v}{4}\left(\frac{\pi^2}{2} - \frac{3}{4}\right)\right\}, \quad \text{(A2)}$$

is a well-known successful approximation. It allows us to find contributions of the irreducible two-loop vacuum polarization to various values with a high accuracy. Since it reproduces the correct behavior of the dispersion density at $v \simeq 0$ (i.e., for $s \simeq s_{\text{threshold}}$) and $v \simeq 1$ (i.e., for $s \to \infty$), it may be considered as an extrapolation formula. Because of that, it is useful not only to approximately find various numeric contributions but also to approximate certain asymptotics.

Here, we present a few more extrapolations which in certain respects are more accurate than Schwinger's [6]. They are

$$\rho_2^{(1)}(v) = \left(\frac{\alpha}{\pi}\right)^2 \frac{v}{1-v^2}$$
$$\times \left\{\frac{1}{2}v^2 + (1-v^2)\left(\frac{\pi^2}{2} - 2.62\,v\right)\right\}, \quad \text{(A3)}$$

$$\rho_2^{(2)}(v) = \left(\frac{\alpha}{\pi}\right)^2 \frac{v}{1-v^2}\left\{\left[\frac{1}{2} + 0.288(1-v^2)\right]v^2\right.$$
$$\left. + (1-v^3)\left(\frac{\pi^2}{2} - 3.695\,v\right)\right\}, \quad \text{(A4)}$$

$$\rho_2^{(3)}(v) = \left(\frac{\alpha}{\pi}\right)^2 \frac{v}{1-v^2}\left\{\left[\frac{1}{2} + 1.08(1-v^2)\right]v^2\right.$$
$$\left. + (1-v^3)\left(\frac{\pi^2}{2} - 3.97\,v - 0.28\,v^3\right)\right\}. \quad \text{(A5)}$$

The quality of these approximations can be discussed in the following way. We note that the density function is always positive. If we are to calculate a matrix element which does not change sign, such as an average of the irreducible part of the Källen-Sabry potential over a certain state, then the fractional error cannot exceed the maximal fractional error of the approximation of $\rho_2(v)$ in (A1) by an approximate function. In general, if there are not specific cancelations, the fractional error determines the fractional uncertainty of any integrals.
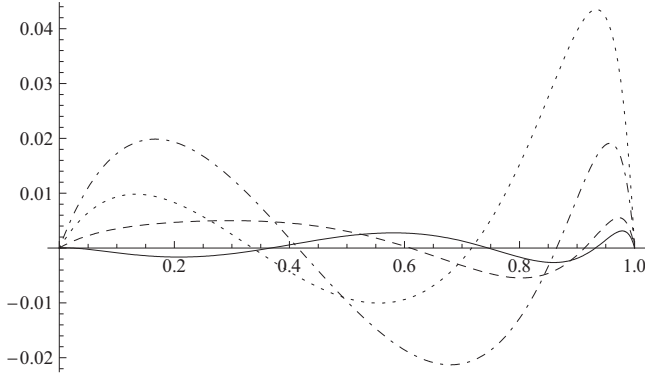
FIG. 4. Fractional deviation $\delta^{\text{approx}}(v)$ of the approximations from the exact dispersion density $\rho_2(v)$. The dotted line presents a deviation for the original Schwinger extrapolation $\rho_2^{(s)}$, the dot-dashed line is for $\rho_2^{(1)}$, the dashed is for $\rho_2^{(2)}$, and the fractional deviation for $\rho_2^{(3)}$ is plotted as a solid line.

Such an error

$$\delta^{\text{approx}}(v) = \frac{\rho_2^{\text{approx}}(v) - \rho_2(v)}{\rho_2(v)}$$

is plotted for the considered approximations in Fig. 4 along with the Schwinger approximation. The maximal values δ^{max} of the fractional deviation are collected in Table IV.

We note that the accuracy of polynomial approximations for the expression in the large parentheses in Eq. (A1) is limited. It is clear that the behavior close to $v = 0$ and $v = 1$ should include logarithmic factors $\ln(v)$ and $\ln(1 - v)$, respectively. Those cannot be approximated with polynomials. However, approximations of $\rho_2(v)$ with uncertainty below 1% are possible.

The application of the approximate formulas to the calculation of the relativistic and relativistic recoil corrections is summarized in Tables V and VI. The fractional errors do not exceed the values of δ^{max} collected in Table IV.

The application of the approximations could be useful not only for tests but also for approximate analytic expressions (cf. [11,12,16,17]).

APPENDIX B: REPRESENTATION OF THE REDUCED NONRELATIVISTIC COULOMB GREEN'S FUNCTION IN COORDINATE SPACE

The nonrelativistic Coulomb Green's function

$$G_E(\mathbf{r}, \mathbf{r}') = \sum \frac{|\lambda\rangle\langle\lambda|}{E - E_\lambda}$$

TABLE IV. The maximal values δ^{max} of the fractional deviation $\delta^{\text{approx}}(v)$ for various approximations.

Approximation	δ^{max}
$\rho_2^{(s)}(v)$	4%
$\rho_2^{(1)}(v)$	2%
$\rho_2^{(2)}(v)$	0.55%
$\rho_2^{(3)}(v)$	0.3%

TABLE V. The relativistic contribution to the energies for the irreducible part of the Källen-Sabry potential in muonic hydrogen. Units are $(\alpha/\pi)^2(Z\alpha)^4 m_R$. The numerical results are for the solution of the Dirac equation with the reduced mass.

$\rho_2(v)$	$1s_{1/2}$	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$
Exact $\rho_2(v)$	-0.5856	-0.1026	-0.03110	-0.003754
$\rho_2^{(s)}(v)$	-0.5909	-0.1035	-0.03124	-0.003763
$\rho_2^{(1)}(v)$	-0.5844	-0.1024	-0.03100	-0.003754
$\rho_2^{(2)}(v)$	-0.5861	-0.1027	-0.03114	-0.003759
$\rho_2^{(3)}(v)$	-0.5859	-0.1027	-0.03112	-0.003756

and its reduced form

$$G'_{E,nlm}(\mathbf{r}, \mathbf{r}') = \sum{}' \frac{|\lambda\rangle\langle\lambda|}{E - E_\lambda},$$

where one has to sum over all intermediate states λ for G_E and over all but the reference state nlm for the reduced one, have a number of useful representations.

It is helpful to separate the radial and angular parts for the partial contributions in the full Green's function

$$G_E(\mathbf{r}, \mathbf{r}') = \sum_{lm} G_{E,nl}(r,r')\, Y_{lm}^\star(\Omega) Y_{lm}(\Omega')$$

$$= \frac{2l+1}{4\pi}\, G_{E,nl}(r,r')\, P_l(\cos\theta), \quad \text{(B1)}$$

where $Y_{lm}(\Omega)$ are spherical harmonics, m is the projection of orbital momentum, Ω is the angular variable, $P_l(\cos\theta)$ is the Legendre polynomial, and θ is the angle between $\mathbf{r}$ and $\mathbf{r}'$. A similar separation can be also done for the reduced Green's functions.

In our calculations we deal with matrix elements as

$$\langle nlm|A G'_{E_{nlm},nlm} B|nlm\rangle,$$

where A and B are for central potentials. In such a case the only partial contribution surviving in the sum over lm in (B1) is $G_{E,nlm}$. The result for the matrix element does not depend on m. For further consideration we denote it as $G_{E,nl}$. For the reduced Green's function with $E = E_{nl}$, we denote the surviving term in the partial sum as G'_{nl}.

In our paper we apply two representations, which are described below.

TABLE VI. The relativistic recoil contribution to the energies $\Delta E_2^{(1)}$ for the irreducible part of the Källen-Sabry potential in muonic hydrogen in units of $(\alpha/\pi)^2(Z\alpha)^4 m_R^2/M$.

$\rho_2(v)$	$1s$	$2s$	$2p$
Exact $\rho_2(v)$	0.1390	0.05762	0.002879
$\rho_2^{(s)}(v)$	0.1425	0.05837	0.002895
$\rho_2^{(1)}(v)$	0.1401	0.05765	0.002868
$\rho_2^{(2)}(v)$	0.1392	0.05767	0.002881
$\rho_2^{(3)}(v)$	0.1391	0.05765	0.002880

1. The Hostler presentation

One of the efficient representations of the nonrelativistic Coulomb Green's function was derived by Hostler [18],

$$G_{E,nl}(\mathbf{r},\mathbf{r}') = \frac{4Z\alpha\, m_r^2}{\nu\, z_> z_<} \frac{\Gamma(1+l-\nu)}{\Gamma(2l+2)}$$
$$\times W_{\nu,l+1/2}(z_>)M_{\nu,l+1/2}(z_<), \qquad (B2)$$

where

$$\nu = \frac{Z\alpha\, m_r}{\sqrt{-2m_r E}}, \qquad (B3)$$

$$z_> = \frac{2Z\alpha\, m_r}{\nu} \max(r,r'), \qquad (B4)$$

$$z_< = \frac{2Z\alpha\, m_r}{\nu} \min(r,r'), \qquad (B5)$$

$\Gamma(x)$ is the Gamma function, and $M_{\mu\nu}(x)$ and $W_{\mu\nu}(x)$ are the Whittaker functions [19].

The required radial parts of the reduced Coulomb Green's functions of the states of interest are [20–22]

$$G'_{1s}(r,r') = 4Z\alpha\, m_r^2 \exp\left(-\frac{z_>+z_<}{2}\right)$$
$$\times \left\{ \frac{1}{z_>} + \frac{1}{z_<} + \frac{7}{2} - \frac{z_>+z_<}{2} + \mathrm{Ei}(z_<) - 2C \right.$$
$$\left. - \ln(z_> z_<) - \frac{e^{z_<}}{z_<} \right\}, \qquad (B6)$$

$$G'_{2s}(r,r') = Z\alpha\, m_r^2 \frac{\exp\left(-\frac{z_>+z_<}{2}\right)}{4z_> z_<}\{8z_< - 4z_<^2 + 8z_>$$
$$+ 12z_> z_< - 26z_> z_<^2 + 2z_> z_<^3 - 4z_>^2$$
$$- 26z_>^2 z_< + 23z_>^2 z_<^2 - z_>^2 z_<^3 + 2z_>^3 z_<$$
$$- z_>^3 z_<^2 + 4(z_> - 2)z_>(1 - z_<)e^{z_<}$$
$$+ 4(z_> - 2)z_>(z_< - 2)z_<$$
$$\times [-2C + \mathrm{Ei}(z_<) - \ln(z_> z_<)]\}, \qquad (B7)$$

$$G'_{2p}(r,r') = Z\alpha\, m_r^2 \frac{\exp\left(-\frac{z_>+z_<}{2}\right)}{36(z_> z_<)^2}\{24z_<^3 + 36z_> z_<^3$$
$$+ 36z_>^2 z_<^3 + 24z_>^3 + 36z_>^3 z_< + 36z_>^3 z_<^2$$
$$+ 49z_>^3 z_<^3 - 3z_>^3 z_<^4 - 3z_>^4 z_<^3$$
$$- 12z_>^3(2 + z_< + z_<^2)e^{z_<} + 12z_>^3 z_<^3$$
$$\times [-2C + \mathrm{Ei}(z_<) - \ln(z_> z_<)]\}, \qquad (B8)$$

where $C = 0.577\,216\ldots$ is the Euler constant and

$$\mathrm{Ei}(x) = \int_{-\infty}^{x} \frac{e^t}{t} dt$$

is the exponential integral.

2. The Sturmian representation

The Sturmian presentation of the nonrelativistic Coulomb Green's function is a presentation in terms of a basis set which consists of solutions of the related Sturm-Liouville problem.

The basis functions satisfy the equation

$$\mathbf{p}^2 \Phi_{klm}(\nu;\ \mathbf{r}) = 2m_r\left(\frac{k}{\nu}\frac{Z\alpha}{r} + E\right)\Phi_{klm}(\nu;\ \mathbf{r}), \qquad (B9)$$

where

$$\nu = \sqrt{-\frac{(Z\alpha)^2 m}{2E}}.$$

They can be presented in the form

$$\Phi_{klm}(\nu;\ \mathbf{r}) = R_{kl}(\nu; r)Y_{lm}(\Omega),$$

where

$$R_{kl}(\nu;\ r) = \left(\frac{k}{\nu}\right)^{3/2} R_{kl}\left(\frac{k}{\nu} r\right)$$

and $R_{kl}(r)$ stands for the radial part of the standard wave function of the nonrelativistic Coulomb problem (see, e.g., [23]).

The radial part of the Coulomb Green's function is of the form [24]

$$G_{El}(r;r') = \frac{\nu^2}{(Z\alpha)^2 m} \sum_{k=l+1}^{\infty} \frac{k}{k-\nu} R_{kl}(\nu;\ r)R_{kl}(\nu;\ r'). \qquad (B10)$$

The required radial part of the reduced Coulomb Green's function (at $E = E_n$) is of the form [24]

$$G'_{nl}(r,r') = \frac{n^2}{(Z\alpha)^2 m_r}\left\{ \sum_{\substack{k=l+1 \\ k\neq n}}^{\infty} \frac{k}{k-n} R_{kl}(n;r)R_{kl}(n;r') \right.$$
$$+ \frac{3}{2} R_{nl}(n;r)R_{nl}(n;r') + r R'_{nl}(n;r)R_{nl}(n;r')$$
$$\left. + r' R'_{nl}(n;r')R_{nl}(n;r) \right\}, \qquad (B11)$$

where

$$R'_{nl}(n;r) = \frac{\partial}{\partial r} R_{nl}(n;r).$$

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