Uehling correction in muonic atoms to all orders of $Z\alpha$

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The Uehling correction to the energy levels is presented in terms of the hypergeometric functions ${}_2F_1$. This presentation allows to derive various asymptotics and approximations. Further applications of this method to other atomic characteristics are also considered.

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I. INTRODUCTION

Theory of muonic atoms has a few specific features which are different from the case of conventional atoms. Two of them are importance of the vacuum-polarization corrections and nuclear structure effects. Both are determined by the fact that the characteristic radius of an atomic orbit in muonic atoms is shorter than in related electronic atoms by a factor of $m_\mu/m_e \sim 207$. While the vacuum polarization can be calculated analytically, nuclear-size effects require a numerical evaluation. For this reason vacuum-polarization effects are often computed numerically for the case of a distributed nuclear charge rather than analytically for a pointlike nucleus.

Still, there is a certain domain where a pointlike approximation for a nucleus is appropriate. It is related to the case of $l \neq 0$ and is better for higher l. Since the muonic wave function vanishes in vicinity of the nucleus, the nuclear-size effects are suppressed for such states and can be successfully considered perturbatively, which eventually allows one to develop for higher l states a more accurate theory than for s states. Precision studies of higher l states are of interest in particular for determination of the mass of negative muon (the $3d_{5/2}$-$2p_{3/2}$ transition in muonic ^{24}Mg and ^{28}Si was used in [1] to determine m_μ/m_e). Similar experiments have been also performed in pionic atoms to determine the pion mass. One of the problems in such measurements is a calibration of the x-ray standards and in fact it is the ratio m_π/m_μ that has been measured. In [2] the $5f$-$4g$ transition in pionic nitrogen and the $6h$-$5f$ one in pionic neon were compared with $5f$-$4g$ transitions in muonic oxygen. A successful determination of the pion mass, in its turn, allows to use spectra of pionic atoms as x-ray standards [3], where the $6h$-$5f$ transition in pionic neon is used as the reference line.

Another case when the nuclear-size effects can be successfully treated as a perturbation is that of low Z, e.g., muonic hydrogen. One more application of analytic treatment is due to the g factor of a bound muon, which may be expressed via its binding energy [4], but the relation between the energy and the g factor includes derivatives. Besides, an exact or approximate result in a closed analytic form is preferable to make various preliminary estimations, e.g., for the contribution of a large number of levels (as a function of their quantum numbers) and/or for relativistic and recoil corrections etc.

Still, the analytic calculation of the first-order vacuum-polarization correction to energy levels in a hydrogenlike atom with pointlike nuclei, exact or approximate, is not an issue of any practical importance because there is no problem to perform a related numerical calculation for any desired state. While that is correct for the leading order contribution, it is not obvious for the second- and the third-order terms. The latter can be calculated with help of the Sturmian expansion and in this case the matrix elements to be calculated are very similar to the first-order calculations. We study such corrections and apply the technique developed here for our calculations of higher-order vacuum-polarization effects [5–7].

Vacuum-polarization effects play an important role in quantum electrodynamics of bound states, especially in the case of muonic and exotic atoms. They are responsible for the dominant QED correction to the Coulomb energy levels. Recent and planned activities in muonic hydrogen [8,9] demand precision theory, which in particular involves higher-order vacuum-polarization contributions. For instance, for muonic hydrogen such contributions at the second and the third order were found in [10,11].

Having in mind this close analogy in the calculation of the radial integrals for the leading vacuum-polarization term and the higher-order corrections, we consider in this paper some effective approaches for approximate analytic calculations of the leading contribution. We intend to find such presentations of the leading correction, which could be successfully applied in higher-order calculations.

The one-loop electronic vacuum-polarization energy shift is induced by the so-called Uehling potential

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$$V_U(r) = -\frac{\alpha}{\pi}\frac{Z\alpha}{r}\int_0^1 dv\,\rho(v)\exp\left(-\frac{2m_e r}{\sqrt{1-v^2}}\right), \qquad (1)$$

where the dispersion density function is

$$\rho(v) = \frac{v^2(1-v^2/3)}{1-v^2}, \qquad (2)$$

and this energy

$$\Delta E = \int d^3r |\Psi(\mathbf{r})|^2 V_U(r),$$

where $\Psi(\mathbf{r})$ is the related wave function, is known in a closed form in a nonrelativistic approximation (see, e.g., [12]) as well as exactly in $Z\alpha$. The relativistic results for the Uehling energy correction were found for the circular states in an atom with the orbiting particle of an arbitrary mass m for spin 1/2 [13] and 0 [14] exactly in $Z\alpha$. For an arbitrary state of a Dirac particle in the Coulomb potential the results were obtained in [15].

Here and throughout the paper the relativistic units in which $\hbar = c = 1$ are applied; m_e is the electron mass, Z is the nuclear charge, α is the fine structure constant and n is the principle quantum number.

The analytic results expressed in terms of the basic integral $K_{bc}(\kappa_n)$ are cumbersome:

$$K_{bc}(\kappa_n) = K_{1bc}(\kappa_n) - \frac{1}{3}K_{2bc}(\kappa_n),$$

$$\begin{aligned} K_{abc}(\kappa_n) = {} & \frac{1}{2}\kappa_n^c B\left(a+\frac{1}{2}, 1-\frac{b}{2}+\frac{c}{2}\right) \\ & \times {}_3F_2\left(\frac{c}{2}, \frac{c}{2}+\frac{1}{2}, 1-\frac{b}{2}+\frac{c}{2}; \frac{1}{2}, a+\frac{3}{2}-\frac{b}{2}+\frac{c}{2}; \kappa_n^2\right) \\ & - \frac{c}{2}\kappa_n^{c+1} B\left(a+\frac{1}{2}, \frac{3}{2}-\frac{b}{2}+\frac{c}{2}\right) \\ & \times {}_3F_2\left(\frac{c}{2}+1, \frac{c}{2}+\frac{1}{2}, \frac{3}{2}-\frac{b}{2}+\frac{c}{2}; \frac{3}{2}, a+2\right. \\ & \left. -\frac{b}{2}+\frac{c}{2}; \kappa_n^2\right), \end{aligned} \qquad (3)$$

where ${}_3F_2$ is the generalized hypergeometric function, $B(x,y)$ is the beta function and

$$\kappa_n = Z\alpha m/(nm_e).$$

The generalized hypergeometric function ${}_3F_2$ can be expanded as a series at low κ_n, but not at high values of κ_n. Even for $\kappa_n \ll 1$ the hypergeometric series is not always appropriate because of the increase of coefficients for $n \gg 1$.

In previous papers [15,16] we discussed "natural parameters" and "fast convergence" of various expansions for the Uehling energy shift as a function of κ_n at high and low κ_n. In particular, comparing values of a few first terms of the expansion we found that real expansion parameters for high n and low κ_n are $n\kappa_n$ rather than κ_n.

To be accurate, we should clearly distinguish between a formal convergence of a series for a generalized hypergeometrical function ${}_mF_n(\alpha_1,\ldots,\alpha_m;\beta_1,\ldots,\beta_n;z)$ and a possibility to approximate it by very few first terms.

The convergence for ${}_3F_2$ and ${}_2F_1$ is determined by the condition $|z|<1$ and does not depend on parameters α_i and β_i (except for a special case of negative integer values of one of α and β: we remind that in the case of a negative integer α_i the series becomes polynomial, while for the integer β_i value it is infinite).

Meanwhile the possibility for a successful few-term approximation strongly depends on the values of parameters. In particular, if some of them are large (e.g., $\alpha_1 \sim N \gg 1$ and all other α and β are ~ 1), then the first N terms will be numerically enhanced and for a successful approximation by a few first terms the condition $N \cdot z \ll 1$ should be held, which is a stronger requirement than that of the convergence of the series.

While performing some higher-order perturbative calculations of the asymptotic behavior or of contributions in a sum over intermediate states, we should be interested in a successful few-term approximation rather than in a formal convergence of the series. For that we have to try to rearrange the series to avoid appearance of coefficients with large and/or fast increasing values in the beginning of the hypergeometric series.

It is hard to apply (3) directly and, in fact, to find asymptotics in [13,14] we used the integral presentation instead of the explicit expression,

$$K_{bc}(\kappa_n) = \int_0^1 dv \frac{\rho(v)}{(1-v^2)^{b/2-1}}\left(\frac{\kappa_n\sqrt{1-v^2}}{1+\kappa_n\sqrt{1-v^2}}\right)^c. \qquad (4)$$

To proceed with analytic calculations, we have to find some alternative. Here we describe another way of the calculation of K_{bc}, which is free of all mentioned problems with large κ_n and n and may be applied to the higher-order perturbation theory both for the nonrelativistic and relativistic[1] case. In principle, the nonrelativistic results for the Uehling potential can be expressed in terms of certain elementary functions, which are still difficult to use for asymptotics and even to "generate" lengthy expressions for high excited states. The method developed here is equally efficient for nonrelativistic and relativistic calculations.

Our goal is to achieve as accurate results as necessary and in principle we demonstrate that the method allows that. However, improvement of the accuracy is always a result of increasing the number of approximating terms at various stages. Here we present a number of explicit results with an uncertainty of a few parts in 10^4 and 10^5.

However, to explain our approach, we simplify the problem and derive at first the upper and lower limits for $K_{bc}(\kappa_n)$ instead of its calculation. They allow to arrive at the approximation with an uncertainty of about 35%.

It is a crucial element of our approach, that our approximation is not for the radial integral, which is specific for

[1]In the case of a spin-1/2 particle, for which the relativistic effects are described by the Dirac equation

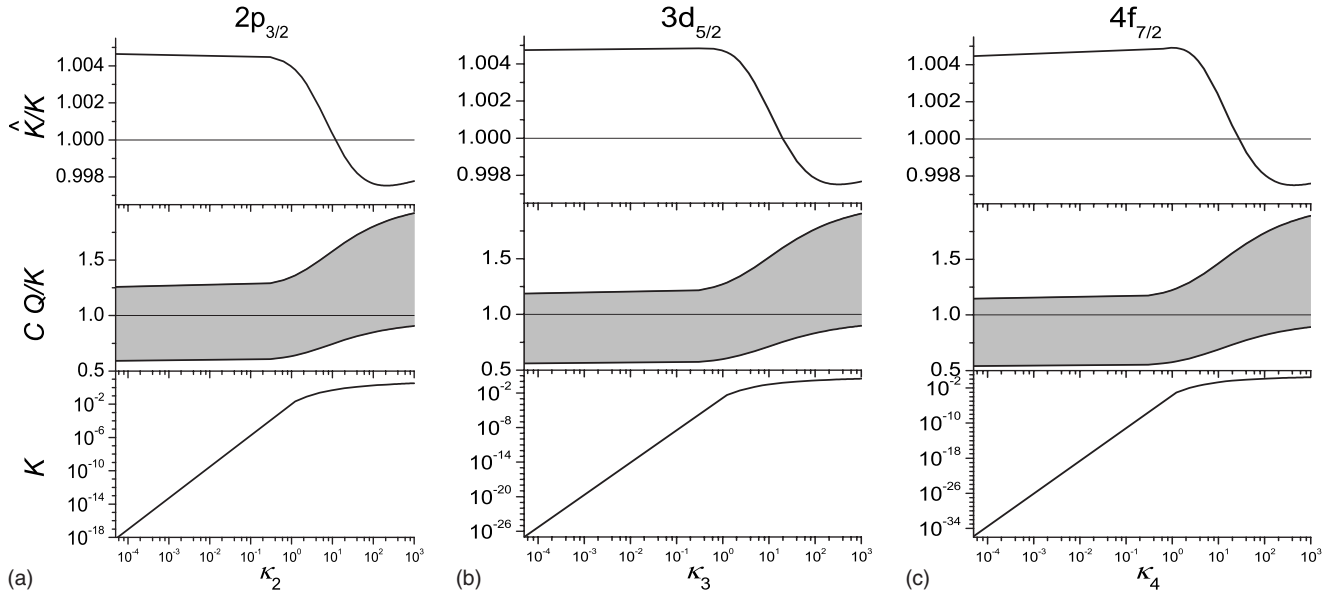

FIG. 1. Comparison of $K_{bc}(\kappa_n)$ (lower panels) with its upper and lower estimations (middle panels) CQ_{bc}, with $C_{\rm up}=\sqrt{2}$ and $C_{\rm lo}=2/3$ [Eq. (8)], and the approximation $\hat{K}_{bc}(\kappa_n)$ [Eq. (11)] (upper panels) for the case of circular states $2p_{3/2}$, $3d_{5/2}$ and $4f_{7/2}$, for which energies are expressed via a single integral $K_{2,2\xi}(\kappa_n)$ [Eq. (12)].

each wave function, but for the dispersion function (2) of the Uehling potential, which is universal.

First, we change the variable in the integral presentation (4), introducing $y=\sqrt{1-v^2}$, and for the basic integral arrive to an equivalent form

$$K_{bc}(\kappa_n)=\kappa_n^c\int_0^1 dyf(y)y^{c-b+1}(1-y)^{1/2}(1+\kappa_n y)^{-c}. \quad (5)$$

We note that the weight function

$$f(y)=\frac{(2+y^2)\sqrt{1+y}}{3} \quad (6)$$

monotonously increases from $f_{\rm min}=f(0)=2/3\simeq 0.67$ to $f_{\rm max}=f(1)=\sqrt{2}\simeq 1.41$. It is also fruitful to introduce a new type of basic integrals,

$$Q_{bc}(\kappa_n)=\kappa_n^c\int_0^1 dyy^{c-b+1}(1-y)^{1/2}[1-(-\kappa_n y)]^{-c}. \quad (7)$$

Because of the monotonous behavior of the weight function (6) and positivity of the rest of the integrand in Eq. (5), we arrive to the upper and lower limits of $K_{bc}(\kappa_n)$ by substituting $f(y)$ in Eq. (5) by its minimal and maximal values, respectively,

$$\frac{2}{3}Q_{bc}(\kappa_n)\le K_{bc}(\kappa_n)\le\sqrt{2}Q_{bc}(\kappa_n). \quad (8)$$

Furthermore, taking advantage of the simplification of the integral, we arrive in Eq. (7) to the generic integral presentation of the hypergeometric function and find

$$Q_{bc}(\kappa_n)=\kappa_n^c B(c-b+2,3/2)\times {}_2F_1(c,c-b+2,c-b+7/2;-\kappa_n). \quad (9)$$

We remind that in contrast to ${}_3F_2$, the function ${}_2F_1$ has many well-known properties and is much easier to deal with.

The ratio of the lower and upper limits in Eq. (8) is obviously a constant $\sqrt{2}/3\approx 0.5$ for any values of b,c and κ_n. That is not a trivial issue by itself, because in the wide range from $\kappa_n\ll 1$ to $\kappa_n\gg 1$ the integral $K_{bc}(\kappa_n)$ is changing by many orders of magnitude (see Fig. 1). We can get advantage from the knowledge of the limits, e.g., by writing an estimation

$$K_{bc}(\kappa_n)=(1.04\pm 0.37)Q_{bc}(\kappa_n). \quad (10)$$

In Fig. 1 the upper and lower limits [Eq. (8)] are compared with the exact value for relativistic $2p_{3/2}$, $3d_{5/2}$, and $4f_{7/2}$ states.

Indeed, the accuracy of the approximation above is not enough for any real calculations, neither it can be directly applied for the evaluation of asymptotic behavior at low and high κ. To take real advantages of the approach above we have three key problems to consider.

(i) As we mentioned, the accuracy of the estimation (10) is not appropriate and we are to improve it. As it is demonstrated in Sec. IV, an arbitrary accuracy can be reached. In particular, the approximation of K_{bc} by

$$\hat{K}_{bc}(\kappa_n)=0.66667Q_{bc}(\kappa_n)+0.270214Q_{b-1,c}(\kappa_n)+0.477333Q_{b-2,c}(\kappa_n) \quad (11)$$

has an uncertainty below 0.7% for an arbitrary state. The quoted figure is not a standard deviation but a conservative estimation of the uncertainty and for any K_{bc},

$$|K_{bc} - \hat{K}_{bc}| \leq 0.7\%.$$

The quality of the approximation for the lowest circular ($l=n-1$, $j=l+1/2$) states is shown in Fig. 1. If we introduce one or two additional Q_{bc} terms, the uncertainty will be below than 0.03% or 0.003%, respectively.

(ii) It is possible to write an exact inequality for K_{bc} with any bc and a result for the Uehling correction to the energy of any state in hydrogenlike atoms can be presented in terms of K_{bc} (see, e.g., [15,16]). In particular, for a circular state this correction is

$$\Delta E_{n,n-1,n-1/2} = -\frac{\alpha}{\pi}\frac{(Z\alpha)^2 m}{n\zeta} K_{2,2\zeta}(\kappa_n), \tag{12}$$

where $\zeta=\sqrt{n^2-(Z\alpha)^2}$. However, for other states the result includes more K_{bc} terms with different values of b,c and it is not necessary for a result for an arbitrary state to be presented as a sum with positive coefficients. To control accuracy it is important to prove an inequality similar to Eq. (8) for the case of a correction which involves a number of different K_{bc} integrals with different values of b and c. That is considered in Sec. III for both nonrelativistic and relativistic (for a Dirac particle) cases and the exact inequality can be derived for an arbitrary state. That allows to derive a conservative uncertainty for the approximate calculation of the leading Uehling contribution to the energy which depends neither on a state nor on parameters of the atom.

(iii) Even in the simplest approximation (10), the expression (7) for high n involves ${}_2F_1$ with large parameters [cf. Eqs. (12) and (9)], which creates a problem to approximate ${}_2F_1$ by a few terms in case of both low and high κ_n. We have to transform Eq. (7) to a form better suited for the ${}_2F_1$ approximation by a few first terms. That is done in Sec. II, where a presentation improved for low-κ expansion involving ${}_2F_1[\alpha,\alpha';\beta;\kappa_n/(1+\kappa_n)]$ and that adjusted for a high-κ case dealing with ${}_2F_1(\alpha,\alpha';\beta;1/(1+\kappa_n)$, are presented. In both cases α, α', β are about unity for any atomic state. It is particularly important to mention that the high-κ asymptotics contains the logarithmic terms because of the logarithmic correction to the effective electric charge at high momentum transfer. It is helpful that we managed to present the K_{bc} integrals in the form

$$K_{bc}(\kappa) = A_{bc}(\kappa) + B_{bc}(\kappa)\ln(\kappa),$$

where the A and B coefficient functions do not involve logarithmic terms at high κ.

The results in Sec. II are for nonrelativistic calculations and the problem for the K_{bc} integrals, typical of the case of a Dirac particle, are covered in other.

In addition, further applications of the approach are described in Sec. V. They include a consideration of the g factor of a bound muon, pionic atoms (while most of relativistic calculations in the paper are for a Dirac particle, such as muon or electron, i.e., for spin 1/2, the pion has spin 0) and the Uehling correction to the wave function for the ground state in a nonrelativistic approximation.

II. IMPROVED PRESENTATIONS FOR THE BASIC INTEGRAL $Q_{bc}(\kappa_n)$

A. Low-κ_n adjusted presentation

The presentation (9) for $Q_{bc}(\kappa_n)$ allows to derive easily a series at low κ_n. Meanwhile, its applicability is rather limited since the coefficients b and c may be quite large in the case of $n \gg 1$ (see [16] for detail). As a first issue, we improve a presentation for $Q_{bc}(\kappa_n)$ at low and medium κ_n. We achieve that by applying a proper transformation of the hypergeometric function, many of which are well known for ${}_2F_1$ (see, e.g., Appendix in [17]), but not for ${}_3F_2$. In particular, applying Eq. (e,5) from [17], we find

$$Q_{bc}(\kappa_n) = \left(\frac{\kappa_n}{1+\kappa_n}\right)^c B(c-b+2,3/2) \times {}_2F_1\left(c,3/2,c-b+7/2;\frac{\kappa_n}{1+\kappa_n}\right). \tag{13}$$

Apparently, the advantage of this presentation is that the argument of the hypergeometric function is always below unity (since κ_n is positive). We note the appearance of prefactor $[\kappa_n/(1+\kappa_n)]^c$ in Eq. (13), which carries most of the changes in the value of $K_{bc}(\kappa_n)$, while the remaining factor is a slow-changing smooth function of κ_n [see Sec. 6.3 in [16]; cf. Eq. (15) in this paper].

For an arbitrary state we discuss the problem in Sec. III, and here we present examples for the nonrelativistic case with the circular states ($l=n-1$) only, for which the whole correction to the energy is determined by a single K_{bc} integral [13,16] with $b=2$ and $c=2n$. In this particular case, we note another advantage of presentation (13). The convergency of the hypergeometric series

$${}_2F_1(\alpha,\alpha',\beta;z) = \frac{\Gamma(\beta)}{\Gamma(\alpha)\Gamma(\alpha')}\sum_{k=0}^{\infty}\frac{\Gamma(\alpha+k)\Gamma(\alpha'+k)}{\Gamma(\beta+k)}\frac{z^k}{k!}$$

is different in terms of κ_n for different presentations. While the series in Eq. (9) is finite only for a limited range[2] of low κ_n, the series in the presentations (13) is convergent for $0<\kappa_n<\infty$.

Indeed, the speed of convergency of the series in Eqs. (9) and (13) is also quite different and in particular at low κ_n the convergency is much faster for high n for ${}_2F_1$ in Eq. (13) than in Eq. (9). That is because in the former case for high n the parameters are: $\alpha\sim\beta\sim 2n$ and $\alpha'\sim 3/2$, while in the latter presentation: $\alpha\sim\alpha'\sim\beta\sim 2n$.

The results for $Q_{bc}(\kappa_n)$ related to the ground state and to a circular state at $n=10$ are presented in Figs. 2 and 3, respectively. To check how fast the convergency is we consider only the first five terms of the hypergeometric series for each presentation of ${}_2F_1$.

The behavior of the five-term approximation in (9) is very notable (cf. also Fig. 8). As explained in [16,18], the actual parameter of the naive low-κ_n expansion, based on Eq. (9), is $n\kappa_n$ and at $n\kappa_n\to 1$ the error of the related five-term approxi-

[2]E.g., for $c\gg 1$ and $b=2$ the series is convergent for $c\kappa_n/2<1$ [16].

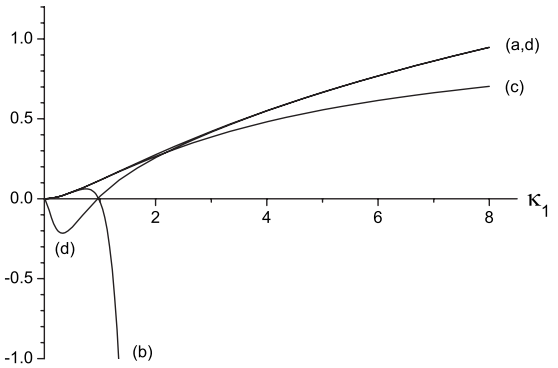

FIG. 2. Comparison of the convergence of the hypergeometric function in relations (9), (13), and (15) for the 1*s* state: (a)—the exact function $Q_{bc}(\kappa_1)$, (b)—the first five terms of expansion of ${}_2F_1$ in Eq. (9), (c)—the same for Eq. (13), (d)—the same for Eq. (15).

mation becomes very high. In contrast to that, the presentation (13) allows an improved low-κ_n approximation which is successful at least up to $\kappa_n \sim 1$.

We can also check how many terms of the hypergeometric series we need to reach a proper level of accuracy. The results are collected in Figs. 4 and 5. One can note that the five-term approximations are quite successful in a broad area. E.g., as seen in Figs. 2–5, the improved low-κ_n expansion is accurate up to $\kappa_n \simeq 1$.

B. High-κ_n adjusted presentation

In contrast to the presentation (3) for K_{bc} with ${}_3F_2$, the presentations (13) for Q_{bc} with ${}_2F_1$ are easy to adjust for the high-κ_n case. To derive a presentation efficient at high κ_n, we apply to Eq. (13) the transformation (e,7) from [17] and find

$$Q_{bc}(\kappa_n) = \left(\frac{\kappa_n}{1+\kappa_n}\right)^c \Bigg[B(2-b,3/2) \times {}_2F_1\left(c,3/2,b-1;\frac{1}{1+\kappa_n}\right) + (1+\kappa_n)^{b-2} B(-2+b,c-b+2) \times {}_2F_1\left(c-b+2,7/2-b,3-b;\frac{1}{1+\kappa_n}\right)\Bigg]. \tag{14}$$

We note that for the case of integer b, which actually takes place for any state in the nonrelativistic approximation, the expression contains a singularity and should be properly regularized. In a general case we apply the substitute $b \to b+\epsilon$ in Eq. (13), which is obviously valid, next apply the transformation (e,7) from [17] and then consider a limit of $\epsilon \to 0$ in Eq. (14). That delivers us a finite well-determined result. Eventually, the result for $b=2$ reads

$$Q_{2c}(\kappa_n) = \left(\frac{\kappa_n}{1+\kappa_n}\right)^c \Bigg\{ \frac{\partial}{\partial\epsilon} {}_2F_1\left(c-\epsilon,\frac{3}{2}-\epsilon,1-2\epsilon,\frac{1}{1+\kappa_n}\right)\Bigg|_{\epsilon=0} + [\ln(1+\kappa_n) - \psi(3/2) - \psi(c) + 2\psi(1)] \times {}_2F_1\left(c,\frac{3}{2},1,\frac{1}{1+\kappa_n}\right)\Bigg\}, \tag{15}$$

where $\psi(x)$ is the logarithmic derivative of Euler's gamma function. A comparison of approximation of this presentation[3] by a partial sum of the hypergeometric series is summarized in Figs. 2 and 3. The results for general value of b are presented in Appendix A.

Obviously the high-κ_n asymptotics (cf. [13]) should contain $\ln \kappa_n$, which follows from well-known asymptotics of the vacuum polarization. The derived presentation allows to separate the logarithmic contribution explicitly.

With appearing of the ${}_2F_1$ function of the argument $1/(1+\kappa_n)$ one can consider the approximation of ${}_2F_1$ by a few first terms of the hypergeometric series (see Figs. 4 and 5). We see that $c=2n$ and other parameters of ${}_2F_1$ are of the order of unity, therefore for high κ_n the expansion is effectively done in n/κ_n (cf. [16]).

As long as we deal with Eqs. (8) and (10), we can present the result for any state with combinations of $Q_{2c}(\kappa_n)$. However, improvements of estimation (10), which we consider below, involve various cases of ${}_2F_1$ and the transformation becomes more complicated (see Appendix A for more detail).

III. ESTIMATIONS FOR CORRECTIONS TO THE ENERGY SHIFTS

The estimations above are achieved for the basic integral $K_{bc}(\kappa_n)$, while the results for any state except circular ones contain a set of such integrals. In particular, the nonrelativistic result for an arbitrary nl state is of the form [16]

$$\Delta E_{nl} = \frac{\alpha}{\pi}\frac{(Z\alpha)^2 m}{n^2} F_{nl}(\kappa_n), \tag{16}$$

$$F_{nl}(\kappa_n) = -\frac{(n+l)!}{n_r!}\sum_{i=0}^{n_r}\frac{1}{i!\,(2l+i+1)!} \times \left(\frac{n_r!}{(n_r-i)!}\right)^2 \frac{K_{2(n_r-i+1),2n}(\kappa_n)}{\kappa_n^{2(n_r-i)}}, \tag{17}$$

where $n_r = n-l-1$.

This expression is a sum of terms with the same sign and we can apply to each K_{bc} separately the approach based on our approximation for $f(y)$. Before doing that, we like to mention that the approach can be also applied to various other representation, such as a sign-alternating series [15]

$$F_{nl}(\kappa_n) = -\sum_{i=0}^{n_r}\sum_{k=0}^{n_r}\frac{(-1)^{i+k} n_r!\,(n+l)!}{i!\,(n_r-i)!\,k!\,(n_r-k)!} \times \frac{(2l+i+k+1)!}{(2l+i+1)!\,(2l+k+1)!} K_{2,2l+i+k+2}(\kappa_n) \tag{18}$$

or a presentation with derivatives of K_{bc} [16]

[3] Referring through the paper to five-term expansion of an expression with ${}_2F_1$ we mean approximation of each hypergeometric function in the expression by five first terms. The expression by itself may contain few ${}_2F_1$ terms.

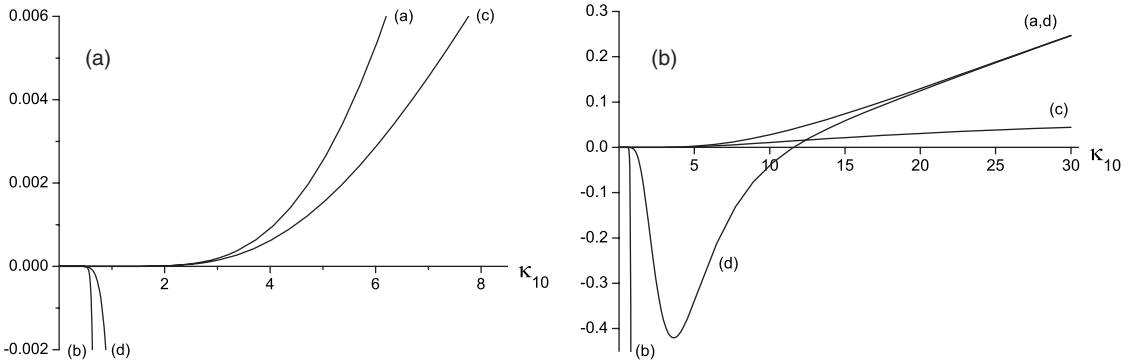

FIG. 3. Comparison of the convergence of the hypergeometric function in relations (9), (13), and (15) for the circular state with $n=10$: (a)—the exact function $Q_{bc}(\kappa_{10})$, (b)—the first five terms of expansion of ${}_2F_1$ in Eq. (9), (c)—the same for Eq. (13), (d)—the same for Eq. (15).

$$F_{nl}(\kappa_n) = \frac{(n+l)!}{n_r!\,(2n-1)!}\sum_{i=0}^{n-l-1}\frac{1}{(2l+i+1)!\,i!}\times\left(\frac{1}{\kappa_n}\right)^{2(n_r-i)} \times\left(\frac{n_r!}{(n_r-i)!}\right)^2\left(\kappa_n^2\frac{\partial}{\partial\kappa_n}\right)^{2(n_r-i)}\times\kappa_n^{2(l+i+1)} \times\left(\frac{\partial}{\partial\kappa_n}\right)^{2(l+i)}\frac{F_{10}(\kappa_n)}{\kappa_n^2}, \tag{19}$$

which expresses the correction for an arbitrary nonrelativistic state in terms of the well known result [12] for the $1s$ state

$$F_{10}(\kappa) = -K_{22}(\kappa).$$

One more presentation for $F_{nl}(\kappa_n)$ can be found in [19].

Validity of estimations presented in Sec. I and similar can be easily proved not through any explicit analytic presentations of F_{nl}, but via related original expressions for the energy shift before any integrations are taken.

Such an expression in both relativistic (Dirac's) and nonrelativistic case is of the form

$$\Delta E = -\frac{\alpha(Z\alpha)}{\pi}\int d^3r\int_0^1 dv\,\rho(v)\times P(r)\frac{1}{r}\exp\left(-\frac{2m_e r}{\sqrt{1-v^2}}\right). \tag{20}$$

Here v is the spectral parameter for the Schwinger presentation [20] of the vacuum polarization, $\rho(v)$ is the spectral function, which in the one-loop case is defined in Eq. (2), while $P(r)$ is a positive weight function which describes the density of the distribution of the electric charge of the atomic bound particle. The latter in the nonrelativistic case reads

$$P_{\mathrm{NR}}(r) = |\Psi(\mathbf{r})|^2,$$

where $\Psi(\mathbf{r})$ is the Schrödinger wave function of the related atomic state, while in the relativistic case it is defined as

$$P_{\mathrm{Rel}}(r) = |f(r)|^2 + |g(r)|^2,$$

where $f(r)$ and $g(r)$ are the radial parts of the upper and lower components of the Dirac wave function.

All evaluations in Sec. I (cf. Sec. II and V A) are based on a certain manipulation with $\rho(v)$ and on the fact that the v integrand is positive. The same can be seen in Eq. (20). That means that for any state we can replace $f(y)$ [which is a result of a certain transformation of $\rho(v)$] by its minimum and maximum and in this way we arrive at the upper and lower limits for the whole F_{nl}. To derive such limits we may apply any presentation for F_{nl} listed above, by substitute K_{bc} in the right-hand side for its upper and lower limit.

That would not be clear from the point of view of the presentations above by themselves, which include positive and negative contributions as well as derivatives. However, substituting $f(y)$ by $f(0)$ [or $f(1)$], we should arrive at such a limitation. That is obvious, as seen from the consideration above for any presentation without derivatives [such as Eqs. (17) and (18)]. Concerning Eq. (19), we remind that it is deduced from a presentation without derivatives by using certain recurrent relations [16] (see also [13]). Meanwhile, the relations are maintained by the shape of Eq. (4) for any

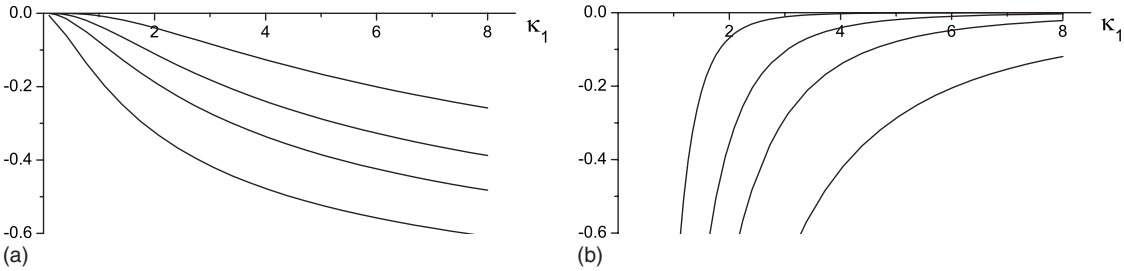

FIG. 4. Relative errors for the hypergeometric function expansions in relations (13) (top) and (15) (bottom) as compared with the exact value for different number of nontrivial terms in the expansion (from bottom to up: 1,2,3,5 terms). The results are for the $1s$ state.

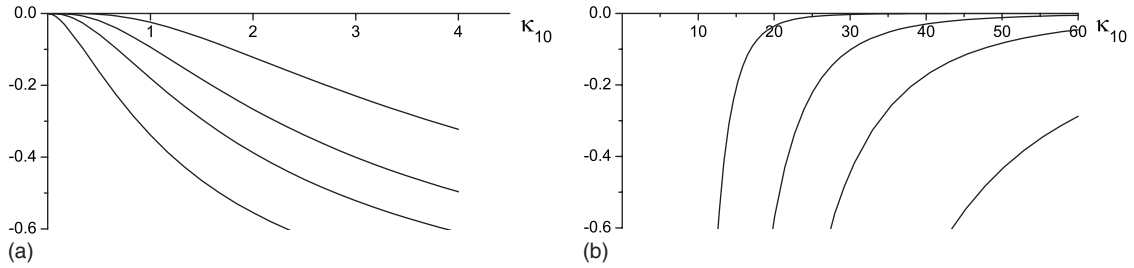

FIG. 5. Relative errors for the hypergeometric function expansions in relations (13) (top) and (15) (bottom) as compared with the exact value for different number of nontrivial terms in the expansion (from bottom to up: 1,2,3,5 terms). The results are for the circular state with $n=10$.

spectral function $\rho(v)$ and thus allow any substitution for arbitrary weight function $f(y)$, which does not alternate its sign.

In the presentation (18) $b=2$ for all integrals and c can take various values, while in the case of Eq. (17) the situation is opposite: $c=2n$ and b varies. The consideration above and in particular the high-κ_n expansion in Sec. II B is derived only for $b=2$. Applying this approach to sum (18), one can arrive to more complicated identities (see Appendix A for more detail).

IV. PRESENTATION OF THE WEIGHT FUNCTION $f(y)$ AS INFINITE SERIES EXACTLY AND ITS DIRECT APPROXIMATION BY POLYNOMIALS

Above we found that simplifying the function $f(y)$ in Eq. (5) (in particular, replacing it by a constant) we succeeded to simplify the integral and present the result in substantially simpler terms than in Eq. (3).

In this section we consider a presentation of $f(y)$ by infinite series in terms of either form

$$f(y)=\sum_{k=0}^{\infty} c_k y^k, \tag{21}$$

$$f(y)=\sum_{k=0}^{\infty} c'_k (1-y)^k. \tag{22}$$

The finite series of this kind can already be used as an approximation (see, e.g., Fig. 6), but direct approximations lead to even simpler and more accurate presentations for the energy shift (see Sec. IV B below).

Here we consider series and approximations for the basic integral $K_{bc}(\kappa_n)$, leaving discussions of uncertainties of partial sums of series for Appendix B.

Before considering any particular expansion or approximation based on Eqs. (21) and (22), we note that the weight function $f(y)$ is positive as well as the integrand, as discussed in Sec. III.

In particular, we start from

$$\Delta E=-\int_0^1 dy f(y)R(y),$$

where $R(y)$ is a certain positive function. Considering the approximation of $f(y)$ by $\tilde{f}(y)$ and introducing the correction factor

$$\tilde{f}(y)=N(y)f(y),$$

we relate the approximation of the energy shift

$$\widetilde{\Delta E}=-\int_0^1 dy \tilde{f}(y)R(y)$$

to the exact value as

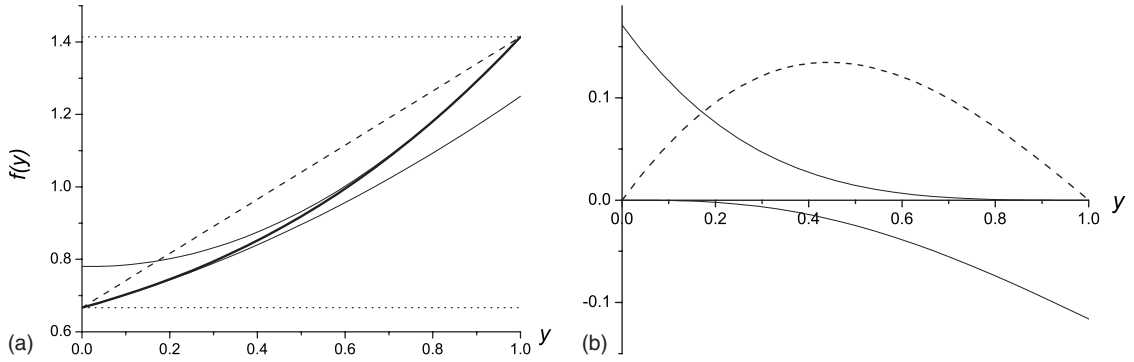

FIG. 6. Top: plots of $f(y)$ [Eq. (5)] (bold line), its partial sums with first the first three terms for series (21) and (22) (thin lines) and the linear approximation (27) (dashes). The maximal and minimal values of $f(y)$ are denoted by the dotted lines. Bottom: the relative errors of the three-term partial sum (thin lines) and the linear approximation (dashes).

TABLE I. Coefficients of the Taylor series for $f(y)$ expansions (21) and (22).

k	c_k	c'_k
0	$\frac{2}{3}$	$\sqrt{2}$
1	$\frac{1}{3}$	$-\frac{11}{6\sqrt{2}}$
2	$\frac{1}{4}$	$\frac{15}{16\sqrt{2}}$
3	$\frac{5}{24}$	$-\frac{9}{64\sqrt{2}}$
4	$-\frac{13}{192}$	$-\frac{47}{3072\sqrt{2}}$
5	$\frac{5}{128}$	$-\frac{15}{4096\sqrt{2}}$
$k\to\infty$	$(-1)^{k+1}e^{7/2}\frac{1}{2\sqrt{\pi}}\frac{1}{k^2}$	$-e^{7/2}\frac{1}{\sqrt{2\pi}}\frac{1}{2^k k^2}$
k	$\frac{(-1)^{k+1}(2k^2-6k+5)}{4\sqrt{\pi}}\times\frac{\Gamma(k-5/2)}{k!}$	$-\frac{(4k^2-8k+15)}{2^{k+2}\sqrt{2\pi}}\times\frac{\Gamma(k-5/2)}{k!}$

$$\widetilde{\Delta E} = -N(\bar{y})\int_0^1 dy f(y)R(y) = N(\bar{y})\Delta E, \tag{23}$$

where $\bar{y}$ is a certain unknown intermediate value $0<\bar{y}<1$. To make a successful approximation it is enough to approximate the function $f(y)$ in such a way that it does not exceed a certain margin: $|N(y)-1|\le\delta$. So, the relative uncertainty of the approximation is at least below δ. That is valid for arbitrary $R(y)$ and in particular for the energy shift for an arbitrary state in a muonic atom.

A. Presentation of $f(y)$ by an infinite series and the results for the integral $K_{bc}(\kappa_n)$

Presenting $f(y)$ as a Taylor series, one can find the coefficients of either series (21) and (22), which are summarized in Table I.

Applying the series (21) to the integral (5) leads to an infinite sum

$$K_{bc}(\kappa_n) = \sum_{k=0}^{\infty} c_k Q_{b-k,c}(\kappa_n), \tag{24}$$

where one can use for $Q_{b-k,c}$ an appropriate presentation [see, e.g., Eqs. (9), (13), and (15) etc.].

A similar evaluation of Eq. (22) leads to the result

$$K_{bc}(\kappa_n) = \left(\frac{\kappa_n}{1+\kappa_n}\right)^c \sum_{k=0}^{\infty} c'_k B\left(c-b+2, k+\frac{3}{2}\right) \times {}_2F_1\left(c, \frac{3}{2}+k, c-b+\frac{7}{2}+k; \frac{\kappa_n}{1+\kappa_n}\right). \tag{25}$$

A presentation similar to Eqs. (9) and (15) can be also derived.

An important property of the both series for $f(y)$ is that the coefficients are quite regular. Their absolute values decrease with k. While the coefficients in Eq. (21) are regularly sign-alternating (except of few first terms), coefficients in Eq. (22) are all negative (except of a few first terms). Such a regular structure allows a simple conservative estimation of accuracy of a partial sum of either series (see Appendix B). To conservatively estimate the remainder of the series for the correction to the energy for a particular state, we do the estimation prior the y integration, dealing only with a certain expansion of function $f(y)$, which is indeed universal for any state.

TABLE II. Coefficients of various approximations of $f(y)$ in Eq. (26). The approximations are denoted as $f_i(y)$.

	f_0	f_1	f_2	f_3
d_0	0	−0.477333	−0.418767	−0.41490
d_1	0	0	−0.135733	−0.15737
d_2	0	0	0	0.02412
δ	13%	0.7%	0.03%	0.003%

B. Polynomial approximations

The series above allow in principle to reach any accuracy. However, one very seldom needs the accuracy substantially better than 0.01%, and it may be more fruitful not to expand the function, but to approximate it.

To obtain an approximation for $K_{bc}(\kappa_n)$ we need to approximate successfully $f(y)$, e.g., in a form

$$f(y) \simeq \tilde{f}(y) = f(0)(1-y) + f(1)y + y(1-y)(d_0 + d_1 y + d_2 y^2 + \cdots) \tag{26}$$

and to tune the coefficients d_k to minimize the value [cf. Eq. (23)]

$$\delta = \max_{0\le y\le 1} |N(y)-1|.$$

For instance, a very rough linear approximation

$$\tilde{f}(y) = f_0(y) = f(0)(1-y) + f(1)y \tag{27}$$

is already compatible with the partial three-term sums for either series considered above (see Fig. 6). The results of various approximations are summarized in Table II.

Including one more coefficient, we improve the accuracy substantially. Apparently, we can continue and reach any required accuracy. We already know that a successful polynomial approximation is possible because of the existence of series Eqs. (21) and (22), meanwhile here we use a more direct strategy to minimize the uncertainty of an approximation with a fixed number of terms.

Applying to Eq. (5) the approximation

$$\tilde{f}(y) = \sum_{k=0}^{N} \tilde{d}_k y^k,$$

where

$$\tilde{d}_0 = f(0), \quad \tilde{d}_1 = f(1) - f(0) + d_0,$$
$$\tilde{d}_k = d_{k-1} - d_{k-2} \quad \text{for } k \ge 2,$$

we obtain the corresponding approximation for K_{bc}

$$\tilde{K}_{bc}(\kappa_n) = \sum_{k=0}^{N} \tilde{d}_k Q_{b-k,c}(\kappa_n). \tag{28}$$

We expect our estimation of accuracy to be rather conservative. A fractional error of the approximation $\tilde{f}(y)$ is plotted in Fig. 7 for the nonrelativistic basic integral K_{2c}, which, we

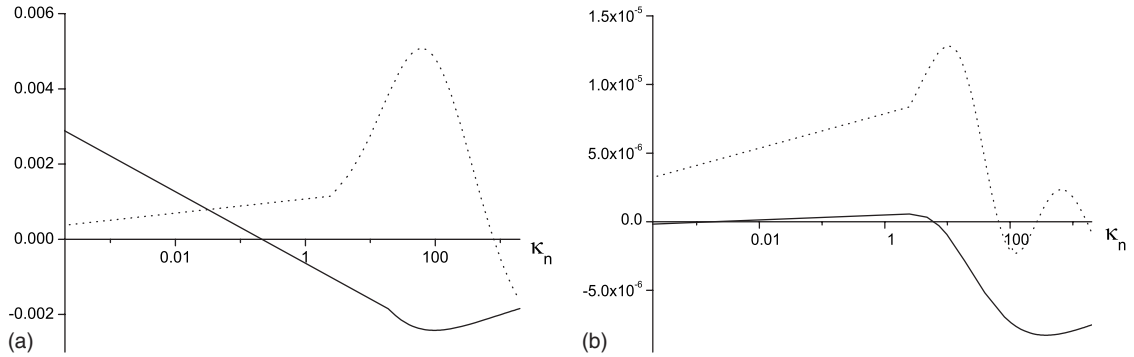

FIG. 7. Top: the relative error of the approximative functions $K_{2,2n}(\kappa_n)$, corresponding to function $\tilde{f}(y)=f_1(y)$, for $n=1$ (solid line) and $n=100$ (dots). Bottom: the same for function $\tilde{f}(y)=f_3(y)$.

remind, completely determines the energy shift for the circular state with $n=c/2$.

V. FURTHER APPLICATIONS

Above we have developed a method for calculation of the Uehling correction to the energy. The examples were related to the nonrelativistic case and, in particular, we implied that some coefficients were integer, which is not the case for relativistic calculations, which may be performed in a similar matter (see below).

Below we discuss possible further applications. Prior to the discussion we have to note that the application of some results, such as a presentation by the infinite series (24) and (25), is quite straightforward. Some other need more consideration to estimate the fractional uncertainty. That concerns, in particular, the approximation (28). When the complete y integrand does not change sign, we can apply an estimation from Table II, otherwise we consider our approach as a "good" approximation, the uncertainty of which is to be revisited in each particular case.

A. Relativistic Uehling correction for a Dirac particle

The relativistic expression for the energy shift of the nl_j state in a hydrogenlike atom with a Dirac particle (the electron, muon or antiproton) reads as [15]

$$\Delta E_{nlj} = \frac{\alpha}{\pi}\frac{(Z\alpha)^2}{n^2} F_{nlj}(\tilde{\kappa}_n), \tag{29}$$

$$\begin{aligned} F_{nlj}(\tilde{\kappa}_n) = & -\frac{n^2\eta^2}{(Z\alpha)^2}\frac{\Gamma(2\zeta+n_r'+1)n_r'!}{\frac{Z\alpha}{\eta}-\nu} \\ & \times \sum_{i,k=0}^{n_r'} \frac{(-1)^{i+k}}{i\,!\,(n_r'-i)\,!\,k\,!\,(n_r'-k)!} \\ & \times \frac{\Gamma(2\zeta+i+k)}{\Gamma(2\zeta+i+1)\Gamma(2\zeta+k+1)} \times \left\{ m\left[\left(\frac{Z\alpha}{\eta}-\nu\right)^2 \right.\right. \\ & \left.\left. + (n_r'-i)(n_r'-k)\right] - E_{nlj}\left(\frac{Z\alpha}{\eta}-\nu\right)(2n_r'-i-k)\right\} \\ & \times K_{2,i+k+2\zeta}(\tilde{\kappa}_n), \end{aligned} \tag{30}$$

where

$$\nu = (-1)^{j+l+1/2}(j+1/2),$$

$$\zeta = \sqrt{\nu^2-(Z\alpha)^2},$$

$$\eta = \sqrt{1-(E_{nlj}/m)^2},$$

$$n_r' = n - |\nu|,$$

$$\tilde{\kappa}_n = n\,\eta\kappa_n/(Z\alpha)$$

and

$$E_{nlj} = m\left[1+\frac{(Z\alpha)^2}{(\zeta+n_r')^2}\right]^{-1/2}$$

is the exact relativistic energy of the state for the Dirac-Coulomb problem. The nonrelativistic limit of the relativistic expression above is given by Eq. (18) [15].

The efficiency of our approach in the relativistic case is illustrated for the $3d_{5/2}$ state in Figs. 8 and 9. Our approach for the approximation consists of two parts: first, we approximate a base integral K_{bc} by a combination of Q_{bc} integrals, which may be expressed in terms of ${}_2F_1$. The simplest of such approximations [cf. Eq. (27)] is

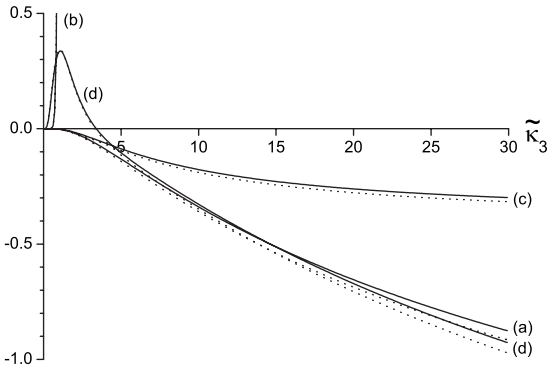

FIG. 8. Comparison of different approximations of Eq. (31) for $3d_{5/2}$ state: (a)—the relation (31), (b)—the first five terms of expansion for Eq. (9), (c)—the same for Eq. (13), (d)—the same for Eq. (15). Solid lines correspond to $Z=1$, dotted lines to $Z=92$.

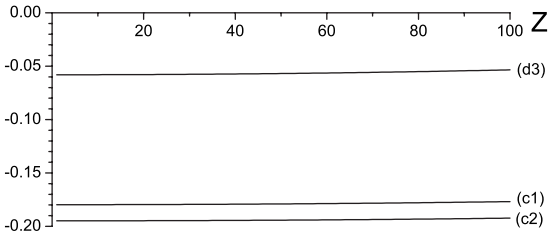

FIG. 9. Relative errors of different approximations of Eq. (31) for $3d_{5/2}$ state. (c1)—the first five terms of expansion for Eq. (13) and $\tilde{\kappa}_3=0.3$, (c2)—the same for $\tilde{\kappa}_3=0.9$, (d3)—the same for Eq. (15) and $\tilde{\kappa}_3=8$. The relative errors of the other approximations (a, b, c at $\tilde{\kappa}_3=0.3,0.9,8$, which are not shown, are above 40%).

$$\tilde{K}_{bc}(\tilde{\kappa}_n)=f(0)Q_{bc}(\tilde{\kappa}_n)+[f(1)-f(0)]Q_{b-1,c}(\tilde{\kappa}_n). \quad (31)$$

Various more complicated (and more accurate) approximations are discussed above.

Second, we approximate the latter by few first terms of the related ${}_2F_1$, which may have different arguments in different presentations and may be specifically adjusted for expansion in a certain region of κ_n. At both stages we can apply approximations of the same kind, varying the number of approximation terms. That improves accuracy, but does not change situation in general, because we do not change the character of the expressions.

As we have already proved in Sec III, all nonrelativistic results for uncertainty due to the approximation at the first stage (see, e.g., Table II) are valid for the Dirac relativistic consideration. To study the efficiency at the second step we rely on Eq. (31) as an example and consider properties of $\tilde{K}_{bc}(\kappa)$ as function of κ. The functions $Q_{bc}(\kappa_n)$ are typical functions used in the approximations in Table II and we approximate Q_{bc}, related to $3d_{5/2}$, by first five terms in Eqs. (9), (13), and (15). The results are summarized in Figs. 8 and 9 and confirm that the efficiency of the approach does not depend on whether we proceed relativistically or not. Concerning the value of the relativistic effects in Figs. 8 and 9, we remind that the effects contribute to the prefactors in Eq. (30), to the index $c=i+k+2\zeta$ of the $K_{bc}(\tilde{\kappa}_n)$ integral and to its argument $\tilde{\kappa}_n$. The figures present only approximations of K_{bc} at a given argument $\tilde{\kappa}_n$, i.e., only a part of relativistic effects.

B. Corrections to the bound g factor

As found in [4], to obtain the correction to the bound g factor in the case of an arbitrary potential for a Dirac or Schrödinger particle it is enough to know analytically the energy E at the related level of parametrical accuracy,

$$g_{\rm bound}(nl_j)=-\frac{\nu}{2j(j+1)}\left[1-2\nu\frac{\partial E_{nlj}}{\partial m}\right]. \quad (32)$$

Differentiating the function, for which we can numerically control the accuracy of approximation, we cannot be sure that the numerical accuracy of the derivative is good enough. However, we expect that the better is the approximation of the energy the better is the result for the g factor.

C. Relativistic Uehling correction for a Klein-Gordon particle

Recently, a perturbative series of the Klein-Gordon bound particle was discussed [21] and the Uehling correction was found for circular states [14]. It was shown that the Uehling correction is still expressed in terms of $K_{bc}(\tilde{\kappa}'_n)$, where

$$\tilde{\kappa}'_n=\kappa_n\left(1+\frac{2n-2l-1}{2n^2(2l+1)}(Z\alpha)^2+\cdots\right). \quad (33)$$

D. Nonrelativistic corrections to the wave function at origin $\Psi(0)$

An accurate value of the nonrelativistic wave function at origin, $\Psi(0)$, was discussed in muonic and exotic atoms for a number of occasions. Its value is important for the finite-nuclear-size corrections in muonic and pionic atoms, for the hyperfine structure in muonic atoms [22], for the pionium lifetime [19,22] etc.

The correction to the wave functions of the ns state $\Psi_{ns}(0)$ induced by the Uehling potential is of the form

$$\delta\Psi_{ns}(0)=\int G'_{ns}(0,r)V_U(r)\Psi_{ns}(r)d^3r, \quad (34)$$

where $G'_{ns}(r',r)$ is the nonrelativistic reduced Coulomb Green's function. The values of $G'_{ns}(0,r)$ are known in a simple form (see, e.g., [23]) and in particular

$$G'_{1s}(0,r)=\frac{m}{2\pi}\frac{e^{-Z\alpha mr}}{r}\{2Z\alpha mr[\ln(2Z\alpha mr)-\psi(1)] +2(Z\alpha mr)^2-5Z\alpha mr-1\}. \quad (35)$$

For the $1s$ wave function we obtain (cf. [22])

$$\frac{\delta\Psi_{1s}(0)}{\Psi_{1s}(0)}=\frac{\alpha}{\pi}\frac{\kappa_1}{2}\int_0^1 dyf(y)\sqrt{1-y}(1+\kappa_1 y)^{-3} \times\left[(2+\kappa_1 y)(1+3\kappa_1 y_1)+2\kappa_1 y\ln\frac{1+\kappa_1 y}{\kappa_1 y}\right] =\frac{\alpha}{\pi}\left\{\frac{1}{\kappa_1^2}\left[K_{43}(\kappa_1)+\frac{7}{2}\kappa_1 K_{33}(\kappa_1)+\frac{3}{2}\kappa_1^2 K_{23}(\kappa_1)\right] -\frac{\partial}{\partial\epsilon}K_{2,2+\epsilon}(\kappa_1)\Big|_{\epsilon=0}\right\}. \quad (36)$$

Since the sign of the integrand in Eq. (36) does not change[4], we use for its evaluation relations based on Eq. (23), similar

[4]We have found that it also takes place for the $2s$ state.

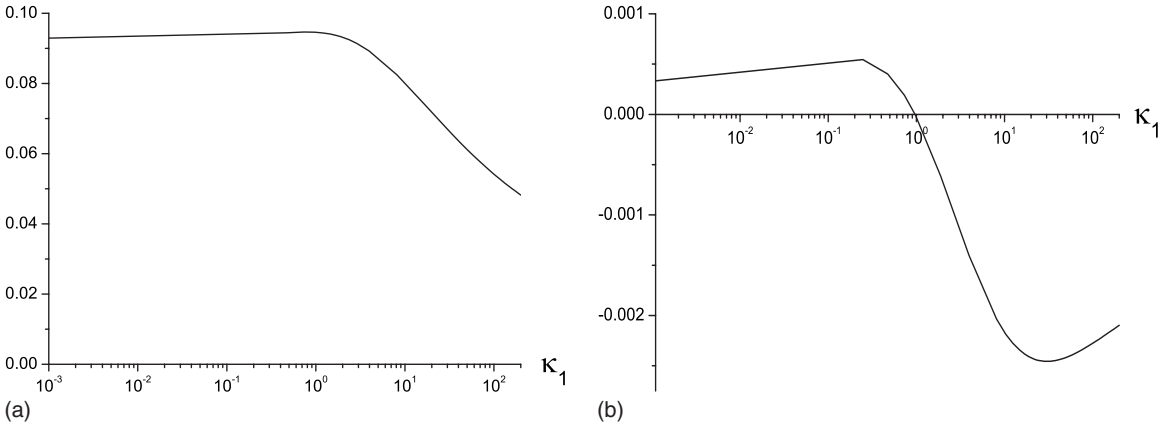

FIG. 10. The relative error of $\delta\Psi_{1s}(0)/\Psi_{1s}(0)$ approximation as a function of κ_1 for $f=f_0$ (top) and $f=f_1$ (bottom) from Table II.

to ones obtained above for the energy corrections. For instance, we can apply the simplest approximations for $f(y)$ and apply conservative estimation of the uncertainty as presented in Table II (see Fig. 10).

VI. SUMMARY

Above we have developed a method which allows to study the Uehling correction to the energy levels and some other atomic characteristics. The method can be efficiently applied to the nonrelativistic consideration as well as in the relativistic case for Dirac and Klein-Gordon particles.

The results are presented in terms well defined at any arguments and using the well-known hypergeometric function ${}_2F_1$. The approach allows to derive various approximations and find useful asymptotics. The free one-loop vacuum polarization is by itself not a problem for numerical calculations. Our concern is rather higher-order corrections and we expect our results to be applied there.

Our method is for a semianalytic calculation of radial and dispersion integrals of generic form

$$\int dr r^k e^{-\omega r} U(r)$$

where

$$U(r) = \int dv F(v) \exp\left(-\frac{2mr}{\sqrt{1-v^2}}\right).$$

Such integrals are not exceptional, which are used only for the one-loop vacuum-polarization contributions. They are rather characteristic of many-loop evaluations with a pointlike nucleus. They appear in certain methods and that allows to simplify the computational procedure.

Recently, we have performed calculations of higher-order vacuum-polarization effects for the Lamb shift [6,7], hyperfine structure [5,7] and wave function at origin [7] in muonic and exotic atoms applying the Sturmian expression for the muon reduced Green's function in the Coulomb field. The intermediate radial integrations appeared in this way are similar to those considered here and approximate calculations and applications of high-κ asymptotics happens to be helpful.

ACKNOWLEDGMENTS

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APPENDIX A: TRANSFORMATION OF ${}_2F_1$ ADJUSTED FOR THE $1/\kappa_n$ EXPANSION

The transformation (14) contains singular terms and in the text of the paper we consider only the case of $b=2$ [see Eq. (15)]. For integer $b\neq 2$ we apply the identity

$$\begin{aligned}{}_2F_1(\alpha,\alpha',\beta,z) = &\sum_{k=0}^{N-1} \frac{\Gamma(\alpha+k)\Gamma(\alpha'+k)\Gamma(\beta)}{\Gamma(\alpha)\Gamma(\alpha')\Gamma(\beta+k)}\frac{z^k}{k!} \\ &+ \frac{\Gamma(\alpha+N)\Gamma(\alpha'+N)\Gamma(\beta)}{\Gamma(\alpha)\Gamma(\alpha')\Gamma(\beta+N)}\frac{z^N}{N!} \\ &\times {}_3F_2(\alpha+N,\alpha'+N,1;\beta+N,N+1;z).\end{aligned}$$

to separate the pole of the function for negative integer β (we choose for that $N=-\beta+1$). That makes the result for $Q_{bc}(\kappa_n)$ more complicated, however, with $z=1/(1+\kappa_n)$ one can easily derive a related expansion for high κ_n. The result for integer $b>2$ is

$$Q_{bc}(\kappa_n)=\left(\frac{\kappa_n}{1+\kappa_n}\right)^c\frac{1}{\Gamma(7/2-b)}\left\{\frac{(-1)^b\sqrt{\pi}}{2(b-2)!}\left[{}_2F_1\left(c,3/2,-1+b,\frac{1}{1+\kappa_n}\right)[\ln(1+\kappa_n)-\psi(3/2)-\psi(c)+\psi(b-1)+\psi(1)]\right.\right.$$
$$\left.+\frac{\partial}{\partial\epsilon}{}_3F_2\left(c-\epsilon,3/2-\epsilon,1;b-1-\epsilon,1-\epsilon;\frac{1}{1+\kappa_n}\right)\right|_{\epsilon=0}\Bigg]+\frac{(1+\kappa_n)^{b-2}}{\Gamma(c)}\sum_{k=0}^{b-3}\Gamma(2-b+c+k)\Gamma\left(\frac{7}{2}-b+2\right)$$
$$\left.\times\frac{(b-k-3)!}{k!}\left(-\frac{1}{1+\kappa_n}\right)^k\right\}, \tag{A1}$$

while for the case of integer $b<2$ we obtain

$$Q_{bc}(\kappa_n)=\left(\frac{\kappa_n}{1+\kappa_n}\right)^c\frac{1}{\Gamma(c)}\left\{\frac{(-1)^b(1+\kappa_n)^{b-2}\Gamma(c+2-b)}{(2-b)!}\left[{}_2F_1\left(c+2-b,7/2-b,3-b,\frac{1}{1+\kappa_n}\right)\right.\right.$$
$$\times[\ln(1+\kappa_n)+\psi(1)-\psi(7/2-b)-\psi(c-b+2)+\psi(3-b)]$$
$$\left.+\frac{\partial}{\partial\epsilon}{}_3F_2\left(c+2-b-\epsilon,7/2-b-\epsilon,1;3-b-\epsilon,1-\epsilon;\frac{1}{1+\kappa_n}\right)\right|_{\epsilon=0}\Bigg]+\sum_{k=0}^{1-b}\frac{(-1)^k\Gamma(c+k)\Gamma(3/2+k)}{\Gamma(7/2-b)}$$
$$\left.\times\frac{(1-b-k)!}{k!}\left(\frac{1}{1+\kappa_n}\right)^k\right\}. \tag{A2}$$

At $b=2$ the summation in Eqs. (A1) and (A2) vanishes ($\Sigma_{k=0}^{b-3}=\Sigma_{k=0}^{1-b}\equiv 0$) and both results coincide with Eq. (15).

APPENDIX B: ESTIMATION OF UNCERTAINTY OF SERIES FOR $f(y)$ AND RELATED RESULTS FOR THE ENERGY SHIFTS

Accordingly to Eq. (23) and the related discussion, to estimate the uncertainty of approximation of either a particular base integral or the correction to the energy for a certain level, it is enough to find accuracy of the approximation of $f(y)$. Here we consider its approximation by a partial finite sum of series (21) and (22).

1. Finite y-series (21) and its uncertainty

To estimate uncertainty of the presentation of $f(y)$ by the sum of the first N terms of Eq. (24), we note that the coefficients of Eq. (21) satisfy the conditions

$$|c_{k+1}|<|c_k|,$$

$$c_k\cdot c_{k+1}<0,\quad k\geq 3. \tag{B1}$$

Therefore the fractional uncertainty of the sum is less than $c_N/f(1)$. E.g., for the first five terms of Eq. (24) the relative error for K_{bc} is below 10%, and for the 14 terms it is below 1%.

2. Finite $(1-y)$-series (22) and its uncertainty

To estimate uncertainty due to partial summation in Eq. (25), we note that

$$f'_N(0)=\sum_{k=N}^{\infty}c'_k \tag{B2}$$

and $c'_k<0$ for $k\geq 3$. That allows to estimate easily a sum of coefficients $s'_N=\Sigma_{k=N}^{\infty}c'_k$ which enter the remaining series. The difference between the infinite series for the base integral and the N-term partial sum has a fractional value which does not exceed $s'_N/f(1)$. E.g., the error of approximation of K_{bc} by the first three terms of Eq. (25) is below 20%, and by the first five terms the error is below 1%.

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