The Uehling correction in muonic atoms exactly in $Z\alpha$

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Abstract. The Uehling correction to the energy levels is presented in terms of the hypergeometric functions $\alpha F_1$. This presentation allows to derived various asymptotics and approximations. Further applications of this method to other atomic characteristics are also considered.

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1 Introduction

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 on muonic hydrogen $^{[1,2]}$ demand a 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 $^{[3,4]}$.

In this paper we consider contributions of the one-loop electronic vacuum polarization (the so-called Uehling potential). We intend to find such presentations of the Uehling correction, which could be successfully applied in higher-order calculations.

The first-order vacuum-polarization correction to energy levels in a hydrogen-like atom is the simplest QED correction. With a known wave function it is usually not a problem to perform a numerical computation for any desired state. However, there is a number of applications when an exact or approximate result in a closed analytic form is still preferable. Among them are the estimation of the correction for a number of levels (as a function of their quantum numbers), the calculation of a derivative of the correction for a number of levels (as a function of their energy), as well as exactly in $Z\alpha$. The relativistic results for the Uehling correction to the energy were found for the circular states in an atom with the orbiting particle of an arbitrary mass $m$ for spin 1/2 $^{[7]}$ and 0 $^{[8]}$ exactly in $Z\alpha$. For an arbitrary state of a Dirac particle in the Coulomb potential the results were obtained in $^{[9]}$.

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 and $\alpha$ is the fine structure constant.

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

\begin{align}
K_{bc}(\kappa_n) &= K_{1bc}(\kappa_n) - \frac{1}{3} K_{2bc}(\kappa_n),
\end{align}

where the dispersion density function is

\begin{align}
\rho(v) = \frac{v^2(1-v^2/3)}{1-v^2},
\end{align}

is known in a closed form in a non-relativistic approximation (see, e.g., $^{[6]}$) as well as exactly in $Z\alpha$. The relativistic results for the Uehling correction to the energy were found for the circular states in an atom with the orbiting particle of an arbitrary mass $m$ for spin 1/2 $^{[7]}$ and 0 $^{[8]}$ exactly in $Z\alpha$. For an arbitrary state of a Dirac particle in the Coulomb potential the results were obtained in $^{[9]}$.

The energy shift induced by the Uehling potential

\begin{align}
V_U(r) = -\frac{\alpha}{\pi} \frac{Z\alpha}{r} \int_0^1 dv \rho(v) \exp \left( -\frac{2m_e v^2}{\sqrt{1-v^2}} \right),
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The generalized hypergeometric function \( _3F_2 \) can be expanded as a series at low \( \kappa_n \), but not at high values of \( \kappa_n \). Even for \( \kappa_n \ll 1 \) the hypergeometric series is not always appropriate because of the increase of coefficients for \( n \gg 1 \). A real parameter of expansion for high \( n \) and low \( \kappa_n \) is \( n\kappa_n \) rather than \( \kappa_n \) (see [10]).

Due to all these problems it is hard to apply \( \kappa_n \) directly and, in fact, to find asymptotics in \([7,8]\) we used the integral presentation instead of the explicit expression:

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

Here we describe another way for the calculation of \( K_{bc} \), which is free of all the mentioned problems with large \( \kappa_n \) and \( n \) and may be applied to the higher-order perturbation theory. In principle, the non-relativistic results for the Uehling potential can be expressed in terms of certain elementary functions, which are still hard to use for asymptotics etc. The method developed here is equally efficient for non-relativistic and relativistic calculations.

2 Calculation of upper and lower limits of the basic integral \( K_{bc}(\kappa_n) \) as model calculation

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.

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

\[
K_{bc}(\kappa_n) = \kappa_n^c \int_0^1 dy f(y) y^{c - b + 1} \sqrt{1 - y} (1 + \kappa_n y)^{-c}. \tag{5}
\]

We note that the weight function

\[
f(y) = \frac{(2 + y^2)^{1/3}}{3}
\]

monotonously increases from \( f_{\text{min}} = f(0) = 2/3 \approx 0.67 \) to \( f_{\text{max}} = f(1) = \sqrt{2} \approx 1.41 \). It is also fruitful to introduce a new kind of basic integrals:

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

Because of the monotonous behavior of the weight function \([3]\) with the rest of integrand in \([5]\) being a positive factor, we arrive to the upper and lower limits of \( K_{bc}(\kappa_n) \), by substituting \( f(y) \) in \([5]\) by its minimal and maximal values, respectively:

\[
\frac{2}{3} Q_{bc}(\kappa_n) \leq K_{bc}(\kappa_n) \leq \sqrt{2} Q_{bc}(\kappa_n). \tag{8}
\]

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

\[
Q_{bc}(\kappa_n) = \kappa_n^c B(c - b + 2, 3/2)
\times \mathcal{F}_1(c, c - b + 2, c - b + 7/2; -\kappa_n). \tag{9}
\]

We remind that in contrast to \( _3F_2 \), the function \( _2F_1 \) has many well-known properties and it is much easier to deal with.

The ratio of the lower and upper limits in \([8]\) is obviously a constant \( \sqrt{2}/3 \approx 0.5 \) for any values of \( b, c \) and \( \kappa_n \). 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. We can get advantage from the knowledge of the limits, e.g., by writing an estimation

\[
K_{bc}(\kappa_n) = (1.04 \pm 0.37) Q_{bc}(\kappa_n). \tag{10}
\]

To take further advantages of the approach above we have three key problems to consider:

- an improvement in the presentation for \( Q_{bc}(\kappa_n) \), which would be easier to apply for various \( \kappa_n \);
- a derivation of estimations similar to \([8,10]\) for an arbitrary state which involves a number of \( K_{bc} \) integrals with different values of \( b \) and \( c \);
- an improvement in the accuracy of the estimation \([10]\).

Below we proceed with all three problems and consider in addition further applications of the approach.

3 Improved presentations for the basic integral \( Q_{bc}(\kappa_n) \)

3.1 Low-\(\kappa_n\) adjusted presentation

The presentation \([8]\) for \( Q_{bc}(\kappa_n) \) allows to derive easily a series at low \( \kappa_n \). Meanwhile, its applicability is rather limited since the coefficients \( b \) and \( c \) may be quite large in the case of \( n \gg 1 \) (see \([10]\) for detail). As a first issue, we improve a presentation for \( Q_{bc}(\kappa_n) \) at low and medium \( \kappa_n \). 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 \([11]\)), but not for \( _3F_2 \). In particular, applying Eq. (e.5) from \([11]\) we find

\[
Q_{bc}(\kappa_n) = \left( \frac{\kappa_n}{1 + \kappa_n} \right)^c B(c - b + 2, 3/2)
\times _2F_1 \left( c, 3/2, c - b + 7/2; \frac{\kappa_n}{1 + \kappa_n} \right). \tag{11}
\]

Apparently, the advantage of this presentation is that the argument of the hypergeometric function is always below unity (since \( \kappa_n \) is positive). We note the appearance of pre-factor \( (\kappa_n/(1 + \kappa_n))^c \) in \([11]\), 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 \( \kappa_n \) (see Sect. 6.3 in \([10]\); cf. Eq. (13) in this paper).

For an arbitrary state we discuss the problem in Sect. 4 and here we present examples for the non-relativistic case with the circular states \((l = n - 1)\) only, for which the whole correction to the energy is determined by a single
The series in (9) is finite only for a limited range of \( \kappa_n \) for the 1s state: (a) – the exact function \( Q_{bc}(\kappa_1) \), (b) – the first five terms of expansion of \( 2F_1 \) in (9), (c) – the same for (11), (d) – the same for (13).

Indeed, the speed of the convergency of the series in (9) and (11) is also quite different and in particular at low \( \kappa_n \), the convergency is much faster for high \( n \) for \( 2F_1 \) in (11) than in (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. 1 and 2 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. 7). As explained in [11][13], the actual parameter of the naive low-\( \kappa_n \) expansion, based on (9), is \( n\kappa_n \) and at \( n\kappa_n \to 1 \) the error of the related five-term approximation becomes very high. In contrast to that, the presentation (11) allows an improved low-\( \kappa_n \) 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. 3 and 4. One can note that the 5-term approximations are quite successful in a broad area. E.g., as seen in Figs. 11[14] the improved low-\( \kappa_n \) expansion is accurate up to \( \kappa_n \sim 1 \).

\[ 2F_1(\alpha, \alpha', \beta; z) = \frac{\Gamma(\beta)}{\Gamma(\alpha)\Gamma(\alpha')} \sum_{k=0}^{\infty} \frac{\Gamma(\alpha + k)\Gamma(\alpha' + k)}{\Gamma(\beta + k)} \frac{z^k}{k!} \]

is different in terms of \( \kappa_n \) for different presentations. While the series in (9) is finite only for a limited range of low \( \kappa_n \), the series in the presentations (11) is convergent for \( 0 < \kappa_n < \infty \).

\( K_{bc} \) integral [7][10] with \( b = 2 \) and \( c = 2n \). In this particular case, we note another advantage of presentation (11).
3.2 High-κn adjusted presentation

In contrast to the presentation [3] for $K_{bc}$ with $3F_2$, the presentations [11] for $Q_{bc}$ with $2F_1$ are easy to adjust for the high-κn case.

To derive a presentation efficient at high κn, we apply to (11) the transformation (e,7) from [11] and find

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

$$\times 2F_1 \left( c, 3/2, b - 1; \frac{1}{1 + \kappa_n} \right) \left. + (1 + \kappa_n)^{b-2}B(-2 + b, c - b + 2) \times 2F_1 \left( c - b + 2, 7/2 - b, 3 - b; \frac{1}{1 + \kappa_n} \right) \right] .$$

(12)

We note that for the case of integer b, which actually takes place for any state, the expression contains a singularity and should be properly regularized. In a general case we apply the substitute $b \rightarrow b + \epsilon$ in (11), which is obviously valid, next apply the transformation (e,7) from [11] and then consider a limit of $\epsilon \rightarrow 0$ in (12). That delivers us a finite well-determined result. Eventually, the result for $b = 2$ reads

$$Q_{2c}(\kappa_n) = \left( \frac{\kappa_n}{1 + \kappa_n} \right)^c \times \left[ \partial_{\epsilon} 2F_1 \left( c - \epsilon, 3/2 - \epsilon, 1 - 2\epsilon, \frac{1}{1 + \kappa_n} \right) \right.$$

$$\left. + \left[ \ln(1 + \kappa_n) - \psi(3/2) - \psi(c) + 2\psi(1) \right] \times 2F_1 \left( c, 3/2, 1; \frac{1}{1 + \kappa_n} \right) \right] ,$$

(13)

where $\psi(x)$ is the logarithmic derivative of Euler’s gamma function. A comparison of approximation of this presentation by a partial sum of the hypergeometric series is summarized in Figs. 1 and 2. The results for general value of $b$ is presented in App. A.

Obviouisly the high-κn asymptotics (cf. [7]) should contain ln κn, 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. 3 and 4). We see that $c = 2n$ and other parameters of $2F_1$ are of the order of unity, therefore for high κn the expansion is effectively done in $n/\kappa_n$ (cf. [10]).

As long as we deal with [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 App. A for more detail).

4 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 non-relativistic result for an arbitrary nl state is of the form [10]

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

(14)

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

(15)

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 [9]

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

(16)

or a presentation with derivatives of $K_{bc}$ [10]

$$F_{nl}(\kappa_n) = \frac{(n + l)!}{n_r!(2n - 1)!} \sum_{i=0}^{n_r - 1} \frac{1}{(2l + i + 1)!} K_{2l+2i+2}(\kappa_n) .$$
\[
\times \left( \frac{1}{\kappa_n} \right)^{2(n_r-i)} \left( \frac{n_r^2}{(n_r-i)!} \right)^2 \left( 2 \frac{\partial}{\partial \kappa_n} \right)^{2(n_r-i)}
\times \kappa_n^{2(l+i+1)} \left( \frac{\partial}{\partial \kappa_n} \right)^{2(l+i)} \frac{F_{10}(\kappa_n)}{\kappa_n^2}, \tag{17}
\]

which expresses the correction for an arbitrary non-relativistic state in terms of the result for the 1s state, which is well known (see two previous equations at \([6]\)). One more presentation for \(F_{nl}(\kappa_n)\) can be found in \([12]\).

Validity of estimations presented in Sect. 2 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 non-relativistic case is of the form

\[
\Delta E = -\frac{\alpha(Z\alpha)}{\pi} \int d^3r \int_0^1 dv \rho(v)
\times P(r) \frac{1}{r} \exp \left( -\frac{2Z\alpha e_r r}{\sqrt{1-v^2}} \right), \tag{18}
\]

Here \(v\) is the spectral parameter for the Schwinger presentation \([13]\) of the vacuum polarization, \(\rho(v)\) is the spectral function, which in the one-loop case is defined in \([2]\), 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 non-relativistic case reads

\[P_{\text{NR}}(r) = |\Psi(r)|^2,\]

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

\[P_{\text{rel}}(r) = |f(r)|^2 + |g(r)|^2,\]

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

All evaluations in Sect. 2 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 \([14]\). 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 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 \([15]\) and \([19]\)). Concerning \([17]\), we remind that it is deduced from a presentation without derivatives by using certain recurrent relations \([14]\) (see also \([7]\)). Meanwhile, the relations are maintained by the shape of \([14]\) for any spectral function \(\rho(v)\) and thus allow any substitution for \(f(y)\).

In the presentation \([16]\) \(b = 2\) for all integrals and \(c\) can take various values, while in the case of \([15]\) the situation is opposite: \(c = 2n\) and \(b\) varies. The consideration above and in particular the high-\(\kappa_n\) expansion in Sect. 3.2 is derived only for \(b = 2\). Applying this approach to sum \([16]\), one can arrive to more complicated identities (see App. A for more detail).

5 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 \([5]\) (in particular, replacing it by a constant) we succeeded to simplify the integral and present the result in substantially simpler terms than in \([3]\).

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

\[f(y) = \sum_{k=0}^{\infty} c_k y^k, \tag{19}\]

\[f(y) = \sum_{k=0}^{\infty} c_k^* (1-y)^k. \tag{20}\]

The finite series of this kind can already be used as an approximation (see, e.g., Fig. 5), but direct approximations lead to even simpler and more accurate presentations for the energy shift (see Sect. [5] 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 App. A.

Before considering any particular expansion or approximation based on \([19]\) and \([20]\), we note that the weight function \(f(y)\) is positive as well as the integrand, as discussed in Sect. 4.

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

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

to the exact value as

\[\Delta E = -N(\overline{\tau}) \int_0^1 dy f(y) R(y) = N(\overline{\tau}) \Delta E, \tag{21}\]

where \(\overline{\tau}\) is a certain unknown intermediate value \(0 < \overline{\tau} < 1\). 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: \([N(y)-1] \leq \delta\). So, the relative uncertainty of the approximation is at least below \(\delta\). That is valid for arbitrary \(R(y)\) and in particular for the energy shift for an arbitrary state in a muonic atom.
Fig. 5. Top: plots of $f(y)$ [5] (bold line), its partial sums with first the first three terms for series [19] and [20] (thin lines) and the linear approximation (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).

| $k$ | $c_k$ | $c'_k$ |
|-----|-------|--------|
| 0   | 2/3   | $\sqrt{2}$ |
| 1   | 1/3   | $-\frac{1}{\sqrt{2}}$ |
| 2   | 1/4   | $\frac{1}{2}\sqrt{2}$ |
| 3   | 5/24  | $\frac{64\sqrt{2}}{7}$ |
| 4   | -13/192| $\frac{64\sqrt{2}}{7}$ |
| 5   | 5/128 | $\frac{64\sqrt{2}}{7}$ |
| $k \to \infty$ | $(-1)^{k+1}e^{\gamma/2} \left( \frac{1}{2} + \frac{1}{2k} \right)$ | $\frac{1}{2}$ |

Table 1. Coefficients of the Taylor series for $f(y)$ expansions [19] and [20].

5.1 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 [19] and [20], which are summarized in Table 1.

Applying the series [19] to the integral [15] leads to an infinite sum

$$K_{bc}(\kappa_n) = \sum_{k=0}^{\infty} c_k Q_{b-k,c}(\kappa_n), \quad (22)$$

Table 2. Coefficients of various approximations of $f(y)$ in [21]. The approximations are denoted as $f_i(y)$.

| $f_i$ | $f_0$ | $f_1$ | $f_2$ | $f_3$ |
|------|-------|-------|-------|-------|
| $d_0$ | 0     | -0.47733 | -0.418767 | -0.41490 |
| $d_1$ | 0     | 0     | -0.135733 | -0.15737 |
| $d_2$ | 0     | 0     | 0     | 0.02412 |
| $\delta$ | 13% | 0.7% | 0.03% | 0.0063% |

where one can use for $Q_{b-k,c}$ an appropriate presentation (see, e.g., [9, 11, 13] etc.).

A similar evaluation of [20] leads to the result

$$K_{bc}(\kappa_n) = \left( \frac{\kappa_n}{1 + \kappa_n} \right)^c \sum_{k=0}^{\infty} c_k B \left( c - b + 2, k + \frac{3}{2} \right) \times F_1 \left( c, \frac{3}{2} + k, -b + \frac{7}{2} + k; \frac{\kappa_n}{1 + \kappa_n} \right). \quad (23)$$

A presentation similar to [19] and [13] 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 [19] are regularly sign-alternating (except of few first terms), coefficients in [20] 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 App. B). To conservatively estimate the remainder of the series, we do the estimation prior the estimation of accuracy of a partial sum of either series (see Fig. 5). The results of various approximations are summarized in Table 2.

5.2 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

$$f(y) \simeq \tilde{f}(y) = f(0) \cdot (1 - y) + f(1) \cdot y + y(1 - y) \cdot (d_0 + d_1 y + d_2 y^2 + \ldots) \quad (24)$$

and to tune the coefficients $d_k$ to minimize the value

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

For instance, a very rough linear approximation

$$\tilde{f}(y) = f_0(y) = f(0) \cdot (1 - y) + f(1) \cdot y \quad (25)$$

is already compatible with the partial three-term sums for either series considered above (see Fig. 5). The results of various approximations are summarized in Table 2.

Including one more coefficient we improve the accuracy substantially. Apparently, we can continue and reach
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 \([22]\) and \([23]\), is quite straightforward. Some other need more consideration to estimate the fractional uncertainty. That concerns, in particular, the approximation \([26]\). When the complete \(y\) integrand does not change sign, we can apply an estimation from Table 2 otherwise we consider our approach as a ‘good’ approximation, the uncertainty of which is to be revisited in each particular case.

6.1 Relativistic Uehling correction for a Dirac particle

The relativistic expression for the energy shift of the \(nlj\) state in a hydrogen-like atom with a Dirac particle (the electron, muon or antiproton) reads as \([9]\)

\[
\Delta E_{nlj} = \frac{\alpha}{\pi} \frac{(Z\alpha)^2}{n^2} F_{nlj}(\kappa_n),
\]

\[
F_{nlj}(\kappa_n) = \frac{n'^2 \eta^2}{(Z\alpha)^2} \frac{\Gamma(2\zeta + n'_j + 1)n'_j!}{\nu} \\
\times \sum_{i,k=0}^{n'_j} \frac{(-1)^{i+k}}{i!(n'_j - i)!k!(n'_j - k)!} \times \frac{\Gamma(2\zeta + i + k)}{\Gamma(2\zeta + i + 1)\Gamma(2\zeta + k + 1)} \\
\times \left\{ m \left( \frac{Z\alpha}{\eta} - \nu \right)^2 + (n'_j - i)(n'_j - k) \right\} \\
- E_{nlj} \left( \frac{Z\alpha}{\eta} - \nu \right) (2n'_j - i - k) \\
\times K_{2,i+k+2\zeta}(\kappa_n),
\]

where

\[
\nu = (-1)^{l+i+1/2}(j + 1/2), \\
\zeta = \sqrt{\nu^2 - (Z\alpha)^2}, \\
\eta = \sqrt{1 - E_{nlj}/m^2}, \\
n'_j = n - |m|, \\
\kappa_n = n \eta k_n/(Z\alpha)
\]

and

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

is the exact relativistic energy of the state for the Dirac-Coulomb problem. The non-relativistic limit of the relativistic expression above is given by \([16]\) \([9]\).

The efficiency of our approach in the relativistic case is illustrated for the 3d5/2 state in Figs. 7 and 8.

Our approach for the approximation consists of two parts: firstly, we approximate a combination of \(K_{bc}\) by a

### 6 Further applications

Above we have developed a method for calculation of the non-relativistic Uehling correction to the energy. Below we
presentation with $2F_1$. The simplest of such presentations (cf. (25)) is

$$K_{bc}(\kappa_n) = f(0) Q_{bc}(\kappa_n) + [f(1) - f(0)] Q_{b-1,c}(\kappa_n).$$

(29)

Secondly, we approximate the latter by few first terms of the related $2F_1$, which may have different arguments in different presentations and thus is well adjusted for expansion in a certain region of $\kappa_n$. 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 Sect. 6.4 all non-relativistic results for uncertainty due to the approximation at the first stage (see, e.g., Table 2) are valid for the Dirac relativistic consideration.

To study the efficiency at the second step we rely on (20) as an example. The functions $Q_{bc}(\kappa_n)$ are typical functions used in the approximations in Table 2 and we approximate $Q_{bc}$ related to $3d_{5/2}$, by first five terms in (9), (11) and (13). The results are summarized in Figs. 7 and 8 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. 7 and 8 we remind that the effects contribute to the prefactors in (28), to the index $c = i + k + 2\zeta$ of the $K_{bc}(\kappa_n)$ integral and to its argument $\kappa_n$. The figures present only approximations of $K_{bc}$ at a given argument $\kappa_n$, i.e. only a part of relativistic effects.

6.2 Corrections to the bound $g$ factor

As found in [58], 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:

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

(30)

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.

6.3 Relativistic Uehling correction for a Klein-Gordon particle

Recently, a perturbative series of the Klein-Gordon bound particle was discussed [15] and the Uehling correction was found for circular states [59]. It was shown that the Uehling correction is still expressed in terms of $K_{bc}(\kappa_n)$, where

$$\kappa_n = \kappa_n \left(1 + \frac{2n - 2l - 1}{2n^2(2l + 1)}(Z\alpha)^2 + \ldots\right).$$

(31)

6.4 Non-relativistic corrections to the wave function at origin $\Psi(0)$

An accurate value of the non-relativistic 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 [10], for the pionium lifetime [16] etc.

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

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

(32)

where $G'_{ns}(r', r)$ is the non-relativistic reduced Coulomb Green function. The values of $G'_{ns}(0, r)$ are known in a simple form (see, e.g., [17]) and in particular

$$G'_{1s}(0, r) = \frac{m e^{-Z\text{am}}}{2\pi r} \left\{2Z\text{amr}[\ln(2Z\text{amr}) - \psi(1)] + 2(Z\text{amr})^2 - 5Z\text{amr} - 1\right\}.$$  

(33)
instance, we can apply the simplest approximations for \( \kappa \) to ones obtained above for the energy corrections. For we use for its evaluation relations based on (21), similar to relativistic case for Dirac and Klein-Gordon particles. For we use for its evaluation relations based on (21), similar to relativistic case for Dirac and Klein-Gordon particles.

\[
\frac{\delta \Psi_{f_1}(0)}{\Psi_{f_1}(0)} = \frac{\alpha}{\pi} \kappa_1 \int_0^1 dy \frac{f(y)}{\sqrt{1-y(1+\kappa_1 y)^{-3}}} \times \left[ (2+\kappa_1 y)(1+3\kappa_1 y) + 2\kappa_1 y \ln \frac{1+\kappa_1 y}{\kappa_1 y} \right] = \frac{\alpha}{\pi} \left\{ \kappa_1^2 K_{43}(\kappa_1) + \frac{7}{2} \kappa_1 K_{33}(\kappa_1) + \frac{3}{2} \kappa_1^2 K_{23}(\kappa_1) - \frac{\partial}{\partial \epsilon} K_{2,2+\epsilon}(\kappa_1) \right\}_{\epsilon=0}.
\]

Since the sign of the integrand in (34) does not change\(^2\), we use it for its evaluation relations based on (21), similar 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 2 (see Fig. 9).

### 7 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 non-relativistic consideration as well as in the relativistic case for Dirac and Klein-Gordon particles.

\(^2\) We have found that it also takes place for the 2s state.

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 in principle not a problem for numerical calculations. Our concern is rather the higher order corrections and we expect our results can be applied there.

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### Appendix

#### A Transformation of \( 2F_1 \) adjusted for the \( 1/\kappa_n \) expansion

The transformation (12) contains singular terms and in the text of the paper we consider only the case of \( b = 2 \) (see (13)). For integer \( b \neq 2 \) we apply the identity

\[
2F_1(\alpha, \alpha', \beta, z) = \sum_{k=0}^{N-1} \frac{\Gamma(\alpha + k)\Gamma(\alpha' + k)\Gamma(\beta)\Gamma(\beta) \, z^k}{\Gamma(\alpha)\Gamma(\alpha')\Gamma(\beta + k) \, k!}
\]

\[
+ \frac{\Gamma(\alpha + N)\Gamma(\alpha' + N)\Gamma(\beta)\Gamma(\beta) \, z^N}{\Gamma(\alpha)\Gamma(\alpha')\Gamma(\beta + N) \, N!}
\]

\[
\times _3F_2(\alpha + N, \alpha' + N, 1; \beta + N, N + 1; z).
\]

to separate the pole of the function for negative integer \( b \) (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 \( \kappa_n \). The result for integer \( b > 2 \) is

\[
Q_{bc}(\kappa_n) = \left( \frac{\kappa_n}{1 + \kappa_n} \right)^c \frac{1}{\Gamma(7/2 - b)} \left\{ (-1)^b \sqrt{\pi} \frac{1}{2(b - 2)!} \right. \\
+ \left. \left[ 2F_1 \left(c, 3/2, -1 + b, \frac{1}{1 + \kappa_n} \right) \times \left[ \frac{\ln(1 + \kappa_n) - \psi(3/2) - \psi(b - 1) + \psi(1)}{2} \right] + \frac{\partial}{\partial \epsilon} 3F_2 \left( c - \epsilon, 3/2 - \epsilon, 1; \left. b - 1 - \epsilon, 1 - \epsilon; \frac{1}{1 + \kappa_n} \right| \epsilon = 0 \right) \right] \right. \\
+ \left. \frac{(1 + \kappa_n)^{b-2}}{\Gamma(c)} \sum_{k=0}^{b-3} \Gamma(2 - b + c + k) \Gamma\left( \frac{7}{2} - b + 2 \right) \times \frac{(b - k - 3)!}{k!} \left( -\frac{1}{1 + \kappa_n} \right)^k \right\}.
\]

(35)
while for the case of integer $b < 2$ we obtain

$$Q_{bc}(\kappa_n) = \left(\frac{\kappa_n}{1 + \kappa_n}\right)^c \frac{1}{\Gamma(c)} \left\{ (-1)^b (1 + \kappa_n)^{b-2} \Gamma(c + 2 - b) \right\} 
\times \left[ 2 F_1 \left( c + 2 - b, 7/2 - b, 3 - b, \frac{1}{1 + \kappa_n} \right) \right.
\times \left[ \ln(1 + \kappa_n) + \psi(1) - \psi(7/2 - b) \right.
\left. - \psi(c - b + 2) + \psi(3 - b) \right]
+ \frac{\partial}{\partial \epsilon} \left[ \ln(1 + \kappa_n) + \psi(1) - \psi(7/2 - b) \right]
\left. - \psi(c - b + 2) + \psi(3 - b) \right]
\times \frac{\Gamma(7/2 - b)}{\Gamma(3/2 + k)}
\times \frac{(1 - b - k)!}{k!} \left( \frac{1}{1 + \kappa_n} \right)^k \right\}. \quad (36)$$

At $b = 2$ the summation in (35) and (36) vanishes $(\sum_{k=0}^{b-3} = \sum_{k=0}^{b-2} \equiv 0)$ and both results coincide with (19).

**B Estimation of uncertainty of series for $f(y)$ and related results for the energy shifts**

Accordingly to (21) 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 $\left| c_{k+1} \right| < \left| c_k \right|$, $c_k \cdot c_{k+1} < 0$, $k \geq 3$. Therefore the fractional uncertainty of the sum is less than $c_{N}/f(1)$. E.g., for the first five terms of (22) the relative error for $K_{bc}$ is below 10%, and for the first 14 terms it is below 1%.

**B.1 Finite $y$-series (19) and its uncertainty**

To estimate uncertainty of the presentation of $f(y)$ by the sum of the first $N$ terms of (22), we note that the coefficients of (19) satisfy the conditions

$$|c_{k+1}| < |c_k|, \quad c_k \cdot c_{k+1} < 0, \quad k \geq 3. \quad (37)$$

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