Second-order corrections to the wave function at the origin in muonic hydrogen and pionium

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Nonrelativistic second-order corrections to the wave function at the origin in muonic and exotic atoms are considered. The corrections are due to the electronic vacuum polarization. Such corrections are of interest due to various effective approaches, which take into account QED and hadronic effects. The wave function at the origin plays a key role in the calculation of the pionium lifetime, various finite nuclear size effects, and the hyperfine splitting. The results are obtained for the 1s and 2s states in pionic and muonic hydrogen and deuterium and in pionium, a bound system of π^+ and π^- . Applications to the hyperfine structure and the Lamb shift in muonic hydrogen are also considered.

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I. INTRODUCTION

A number of atomic effects, particularly in exotic atoms, in the nonrelativistic approximation involve various local operators, which are proportional to the δ function in coordinate space. The related contributions are proportional to the squared value of the wave function at the origin $|\Psi_{\text{NR}}(0)|^2$. Two examples of such operators are the operator of interaction of the muon spin and the nuclear spin in a muonic atom (that is responsible for the hyperfine structure) and the $\pi^+\pi^-\pi^0\pi^0$ vertex operator (that is responsible for the lifetime of the pionium atom).

These are common features of various nonrelativistic approximations and various effective nonrelativistic approaches, which are based on a separation of low-energy and high-energy physics. Atomic scale physics contributes to the nonrelativistic wave functions, while the higher energies and momenta are responsible for various contact terms. This is very similar to the operator approach in the theory of strong interactions.

Meanwhile, there is an important difference between "conventional" atoms and various exotic atoms in the calculation of $|\Psi_{NR}(0)|^2$. In conventional (electronic) atoms the nonrelativistic wave function is, in most cases, determined by its pure Coulomb value $|\Psi_C(0)|^2$ and most of the corrections are either relativistic or have a manybody origin. In contrast, in muonic and pionic atoms, there is a specific class of nonrelativistic corrections, which can still be described by a nonrelativistic potential. The orbiting mass *m* in such atoms is much higher than the electron mass m_e and, in particular,¹

$$m \geq m_{\mu} \simeq 207 m_{e}$$
.

The characteristic momentum in such atoms $Z\alpha mc$ is higher or comparable to m_ec , and thus the electronic vacuum polarization produces a nonrelativistic potential with a radius of $\sim \hbar/(m_ec)$, which is somewhat larger than the atomic Bohr radius $\sim \hbar/(Z\alpha mc)$.

The related potentials depicted in Fig. 1 modify the value of the nonrelativistic wave function at the origin,

$$|\Psi_{C}(0)|^{2} \rightarrow |\Psi_{\rm NR}(0)|^{2} = |\Psi_{C}(0)|^{2} \left(1 + \frac{\alpha}{\pi}c_{1} + \left(\frac{\alpha}{\pi}\right)^{2}c_{2} + \ldots\right).$$
(1)

The related diagrams are presented in Fig. 2. The coefficient c_1 for the one-loop corrections is due to the Uehling potential and was evaluated for a number of problems (see, e.g., [1–6]).

The second-order effects (see Fig. 3) are due to subsequent iterations of the Uehling term and to the Källen-Sabry potential, and here we present a calculation of c_2 for the 1s and 2s states in muonic and pionic hydrogen and deuterium, and for the pionium atom.

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¹Technically, in the nonrelativistic case the reduced mass enters the equations. It may be somewhat below the muon mass m_{μ} . The smallest values are in systems of $\bar{\mu}\mu$, $\pi\mu$, and $\pi^+\pi^-$: $m_{\mu\mu} = 0.5m_{\mu}$, $m_{\pi\mu} \simeq 0.569m_{\mu}$, and $m_{\pi\pi} = 0.660m_{\mu}$.



FIG. 1. Vacuum polarization corrections to the electrostatic Coulomb potential $(V_{\rm VP})$: the Uehling potential $(V_{\rm VP}^{(1)})$, and the reducible two-loop $(V_{\rm VP}^{(1\cdot1)})$ and irreducible two-loop $(V_{\rm VP}^{(2)})$ potentials (the Källen-Sabry potential).



FIG. 2. The first-order correction to the wave function at the origin. The filled circle is for $\delta(\mathbf{r})$. The double line stands for the nonrelativistic reduced Coulomb Green function.



FIG. 3. The second-order vacuum polarization correction to the wave function at the origin.

II. GENERAL EXPRESSION FOR THE CORRECTION TO THE WAVE FUNCTION AT THE ORIGIN: ORDERS α AND α^2

We consider a nonrelativistic two-body system, with the interaction

$$V(r) = V_C(r) + V_{VP}(r),$$
 (2)

which includes the Coulomb potential and its modification by the first- and the second-order vacuum polarization (see Fig. 1),

$$V_{\rm VP}(r) = V_{\rm VP}^{(1)}(r) + V_{\rm VP}^{(1\cdot1)}(r) + V_{\rm VP}^{(2)}(r).$$

We find that the wave function $\Psi_V(r)$ is related to a potential V(r), or rather, only its value at the origin. For the latter, we can introduce an additional perturbation,

$$V_{\delta}(r) = A\delta(\mathbf{r}),$$

and the obvious result of the perturbation theory, which is linear in $\delta V_{\delta}(r)$, is

$$\delta E_{\delta} = A |\Psi_{\rm NR}(0)|^2.$$

This means that instead of finding the wave function, we can calculate the perturbation theory expansion for energy with the perturbation $V_{\rm VP}(r) + V_{\delta}(r)$, taking terms linear in *A* and of a proper order in α .

So, to find the coefficient c_1 it is enough to consider linear terms in $V_{\rm VP}(r)$, and for the latter to apply the Uehling term only. To find c_2 we have to evaluate two kinds of contributions, which are

- (i) terms quadratic in V_{VP}(r), but including only the Uehling potential [V_{VP}(r) → V⁽¹⁾_{VP}(r)] [see Figs. 3(c) and 3(d)];
- (ii) terms linear in $V_{\rm VP}(r)$, which include the secondorder vacuum polarization, both reducible and irreducible: $V_{\rm VP}(r) \rightarrow V_{\rm VP}^{(1\cdot1)}(r) + V_{\rm VP}^{(2)}(r)$ [see Figs. 3(a) and 3(b)].

The results of the calculation of the coefficients c_1 and c_2 are collected in Table I.

More details of the calculation of the c_2 coefficient can be found in Table II, where we present separately all contributions for the 1*s* state. The result for the contribution in Fig. 3(d) is split into two terms. This reflects the fact that, in general, a contribution in the third order of a perturbative theory is determined by the expression (see, e.g., [7,8])

$$\Delta E^{(3)}(ns) = \langle \Psi_{ns} | \delta V \tilde{G}[\delta V - \Delta E^{(1)}_{ns}] \tilde{G} \delta V | \Psi_{ns} \rangle, \quad (3)$$

where $\Delta E_{ns}^{(1)} = \langle \Psi_{ns} | \delta V | \Psi_{ns} \rangle$, δV is a sum of all perturbations under consideration, and Ψ_{ns} and \tilde{G} are the wave function and the reduced Green function, respectively, of the unperturbed problem (i.e., of the nonrelativistic Coulomb problem in our case).

A calculation of the subtraction term in (3), which is of the form

$$\Delta E^{\rm sub}(ns) = -\Delta E_{ns}^{(1)} \times \langle \Psi_{ns} | \delta V \tilde{G}^2 \delta V | \Psi_{ns} \rangle, \quad (4)$$

is different from that of the main term in (3), and in fact, for the wave function it is even somewhat more complicated.

To calculate the complete α^2 corrections to any quantity, one indeed has to take into account relativistic corrections

TABLE I. The results of the calculation of the coefficients c_1 and c_2 in various atoms for the 1s and 2s states. The c_1 coefficient was discussed in the literature (see, e.g., [1–6]), while the results for c_2 are found in this work. The accuracy of the presented results is determined by rounding the numerical results.

Atom	m_r/m_e	1s		2s	
		c_1	c_2	c_1	c_2
$\pi^-\pi^+$	136.566	1.350 25	5.4378	1.134 40	4.3723
μH	185.841	1.731 15	7.2558	1.404 25	5.5552
μD	195.742	1.801 16	7.6038	1.452 30	5.7730
πH	237.764	2.077 48	9.0209	1.638 50	6.6402
<i>πD</i>	254.215	2.177 42	9.5504	1.70477	6.9584

TABLE II. Contributions to the value of $c_2(1s)$ for different diagrams in Fig. 3. The results for the contributions in Figs. 3(c) and 3(d) are split into two parts [cf. (3)].

Atom	$c_2^{(a)}(1s)$	$c_2^{(b)}(1s)$	$c_2^{(c)}(1s)$	$c_2^{(d)}(1s)$	$c_2(1s)$
$\overline{\pi^{-}\pi^{+}}$	1.3336	3.1031	0.6502 - 0.0719	0.4558 - 0.0330	5.4378
μH	1.8551	3.7967	1.0755 - 0.1525	0.7492 - 0.0682	7.2558
μD	1.9590	3.9166	1.1655 - 0.1719	0.8110 - 0.0765	7.6038
πH	2.3937	4.3693	1.5575 - 0.2635	1.0790 - 0.1150	9.0209
πD	2.5608	4.5253	1.7137 - 0.3032	1.1853 - 0.1315	9.5504

and corrections to the operators, which are not universal. Let us briefly discuss possible applications.

Let us consider two systems, namely, pionium and muonic hydrogen.

- (i) For the pionium, some of the α^2 corrections are known [9], and progress in experiment [10] requires improvement of theory and the calculation of the remaining α^2 terms, which are, in particular, presented in this paper.
- (ii) Another application of interest is due to the hyperfine splitting in muonic hydrogen. In this case the complete result includes various nuclear-structure dependent effects, and the α^2 corrections are rather irrelevant for comparison with expected experimental data, both for the 1s [11] and the 2s [12] hyperfine intervals. However, if both experiments deliver accurate results, one can consider a specific difference [5],

$$\Delta E_{21} = 8 \times E_{\rm hfs}(2s) - E_{\rm hfs}(1s), \tag{5}$$

and for this difference the calculation of the α^2 terms is relevant. The contribution induced by the correction to the wave function is only part of the complete result (cf. Fig. 4) for the vacuum polarization contributions, which is (see [13] for details)

$$\Delta E^{\rm VP}(1s) = \left(2.614\,19\frac{\alpha}{\pi} + 12.545\,84\left(\frac{\alpha}{\pi}\right)^2\right) \\ \times \Delta E^{(0)}_{\rm hfs}(1s), \tag{6}$$

$$\Delta E^{\rm VP}(2s) = \left(2.31451\frac{\alpha}{\pi} + 10.65790\left(\frac{\alpha}{\pi}\right)^2\right) \times \Delta E^{(0)}_{\rm hfs}(2s),\tag{7}$$

where

$$\Delta E_{\rm hfs}^{(0)}(ns) = \frac{8}{3}(1+a_{\mu})\frac{\alpha(Z\alpha)^3mc^2}{n^3}\frac{m}{m_p}\frac{\mu}{\mu_N}\left(\frac{m_{\rm r}}{m}\right)^3.$$
(8)

 μ_N is the nuclear magneton, μ stands for the proton magnetic moment, and m_r is the reduced mass.

Performing a calculation of third-order terms depicted in Figs. 3(d) and 4(g) as a test, we also calculated a contribution to the Lamb shift (see Fig. 5), which was previously calculated for muonic hydrogen in [14].



FIG. 4. The second-order vacuum polarization corrections to the hyperfine splitting in muonic hydrogen. The wavy line stands for the hyperfine interaction.



FIG. 5. The $\alpha^5 m$ correction to the Lamb shift in muonic hydrogen: the only third-order contribution of nonrelativistic perturbation theory [see (3)].

The result [14] was for the correction to the Lamb shift (i.e. for a splitting of the 2s and 2p states). This value is of particular interest because of the Paul Scherrer Institute experiment [12]. We have also calculated the same quantity and have found

$$\Delta E_{2p-2s}^{(\text{Fig. 5})}(\text{this work})$$

$$= [(-7.3861 \times 10^{-6} + 0.3511 \times 10^{-6}) - (-0.0025412 + 0.0013661)] \frac{\alpha^5}{\pi^3} m_r c^2$$

$$= 0.0011681 \frac{\alpha^5}{\pi^3} m_r c^2,$$

where the terms in the first set of brackets are for the 2p contribution, while the terms in the second set of brackets are for the 2s one; each set of brackets consists of a main term and a subtraction term as introduced in (3).

Our result disagrees with the result published in [14],

$$\Delta E_{2p-2s}^{(\text{Fig. 5})}(\text{Ref. [14]}) = 0.002\,535(1)\frac{\alpha^5}{\pi^3}m_rc^2.$$
(10)

After this work was finished, we contacted the authors of [14]. As a result of our communications, it has been agreed that our results for the main terms for both states (2s and 2p) confirm calculations in [14], while the subtraction term was missing there. After correcting for subtraction, their result agrees with ours (see [15] for details).

In conclusion, we calculated nonrelativistic corrections in the relative order α^2 to the wave function at the origin in muonic and exotic atoms for the 1s and 2s states, presented a result for the nonrelativistic α^2 correction to the hyperfine structure in muonic hydrogen for the same states, and corrected the result [14] for the $\alpha^5 m_{\mu}c^2$ contribution to the Lamb shift in muonic hydrogen. Details of our calculations of the second-order vacuum polarization effects for the wave function at the origin in various atoms, and the hyperfine splitting and the Lamb shift in muonic hydrogen are in preparation and will be published elsewhere.

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