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

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Non-relativistic second-order corrections to the wave function at 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 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 $\pi^+$ and $\pi^-$. Applications to the hyperfine structure and the Lamb shift in muonic hydrogen are also considered.

I. INTRODUCTION

A number of atomic effects and, in particular, in exotic atoms involve in the non-relativistic approximation various local operators, proportional to the $\delta$-function in coordinate space. The related contributions are proportional to the squared value of the wave function at origin $|\Psi_{NR}(0)|^2$. 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).

That is a common feature of various non-relativistic approximations and various effective non-relativistic approaches, which are based on a separation of low-energy and high-energy physics. Physics of atomic scale contributes to the non-relativistic wave functions, while the higher energies and momenta are responsible for various contact terms. That is very much similar to the operator approach in 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 non-relativistic wave function is in most problems determined by its pure Coulomb value $|\Psi_C(0)|^2$ and most of the corrections are either relativistic or have many-body origin. In contrast, in muonic and pionic atoms, there is a specific class of non-relativistic corrections, which can be still described by a non-relativistic potential. The orbiting mass $m$ in such atoms is much higher than the electron mass $m_e$ and in particular

$$m \geq m_\mu \simeq 207 m_e.$$

The characteristic momentum in such atoms $Zamc$ is higher or comparable to $m_\mu c$, and thus the electronic vacuum polarization produces a non-relativistic potential with the radius of $\sim \hbar/(m_\mu c)$, which is somewhat larger than the atomic Bohr radius $\sim \hbar/(Zamc)$.

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

Technically, in the non-relativistic case that is the reduced mass that enters the equations. It may be somewhat below the muon mass $m_\mu$. The smallest values are in systems of $\mu\mu$, $\pi\mu$ and $\pi^+\pi^-$: $m_{\mu\mu} = 0.5 m_\mu$, $m_{\pi\mu} = 0.569 \ldots m_\mu$ and $m_{\pi\pi} = 0.660 \ldots m_\mu$. 

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The related potentials depicted in Fig. 1 modify the value of the non-relativistic wave function at origin
\[ |\Psi_C(0)|^2 \rightarrow |\Psi_{NR}(0)|^2 = |\Psi_C(0)|^2 \times \left( 1 + \frac{\alpha}{\pi} c_1 + \left( \frac{\alpha}{\pi} \right)^2 c_2 + \ldots \right). \tag{1} \]

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, 2, 3, 4, 5, 6]).

FIG. 2: The first-order correction to the wave function at origin. The filled circle is for the \(\delta(r)\). The double line stands for the non-relativistic reduced Coulomb Green function.

The second-order effects (see Fig. 3) are due to subsequent iterations of the Uehling term and due to 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.

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

II. GENERAL EXPRESSION FOR THE CORRECTION TO THE WAVE FUNCTION AT ORIGIN: ORDERS \(\alpha\) AND \(\alpha^2\)

We consider a non-relativistic two-body system, which interaction
\[ V(r) = V_C(r) + V_{VP}(r) \tag{2} \]
includes the Coulomb potential and its modification by the first- and the second-order vacuum polarization (see Fig. 1).

\[ V_{VP}(r) = V_{VP}^{(1)}(r) + V_{VP}^{(1)}(r) + V_{VP}^{(2)}(r). \]

We are to find the wave function \(\Psi_V(r)\) related to a potential \(V(r)\), or rather, only its value at origin. For the latter, we can introduce an additional perturbation
\[ V_\delta(r) = A \delta(r) \]
and the obvious result of the perturbation theory, linear in \(\delta V_\delta(r)\), is
\[ \delta E_\delta = A |\Psi_{NR}(0)|^2. \]

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

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

- terms quadratic in \(V_{VP}(r)\), but including only the Uehling potential \((V_{VP}(r) \rightarrow V_{VP}^{(1)}(r))\) (see Fig. 3: and \(d\));

- terms linear in \(V_{VP}(r)\), which include the second-order vacuum polarization (both reducible and irreducible: \((V_{VP}(r) \rightarrow V_{VP}^{(1)}(r) + V_{VP}^{(2)}(r))\) (see Fig. 3: and \(b\)).

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

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 literature (see, e.g., [1, 2, 3, 4, 5, 6]), while the results for \(c_2\) are found in this work. The accuracy of the presented results is determined by rounding of the numerical results.

| Atom | \(m_r/m_e\) | \(1s\) | \(2s\) |
|------|-------------|-------|-------|
|      | \(c_1\) | \(c_2\) | \(c_1\) | \(c_2\) |
| \(\pi^-\pi^+\) | 136.566 | 1.35025 | 5.4378 | 1.13440 | 4.3723 |
| \(\mu H\) | 185.841 | 1.73115 | 7.2558 | 1.40425 | 5.5552 |
| \(\mu D\) | 195.742 | 1.80116 | 7.6038 | 1.45230 | 5.7730 |
| \(\pi H\) | 237.764 | 2.07748 | 9.0209 | 1.63850 | 6.6402 |
| \(\pi D\) | 254.215 | 2.17742 | 9.5504 | 1.70477 | 6.9584 |

More details of the calculation of the \(c_2\) coefficient can be found in Table II, where we present separately all contributions for the \(1s\) state. The result for the Fig. 3 contribution is split into two terms. That 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])

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

(3)

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

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

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

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

TABLE II: Contributions to the value of $c_2(1s)$ for different diagrams in Fig. 3 The result for the Fig. 3 and $d$ contributions is split into two parts (cf. (2)).

| Atom | $c_2^{(a)}(1s)$ | $c_2^{(b)}(1s)$ | $c_2^{(c)}(1s)$ | $c_2^{(d)}(1s)$ | $c_2(1s)$ |
|------|----------------|----------------|----------------|----------------|-----------|
| $\pi^-$ | 1.3336 | 3.1031 | 0.6502 − 0.0719 | 0.4558 − 0.0330 | 5.4378 |
| $\mu H$ | 1.8551 | 3.7967 | 1.0755 − 0.1525 | 0.7492 − 0.0682 | 7.2558 |
| $\mu D$ | 1.9509 | 3.9166 | 1.1655 − 0.1719 | 0.8110 − 0.0765 | 7.6038 |
| $\pi H$ | 2.3937 | 4.3693 | 1.5575 − 0.2635 | 1.0790 − 0.1150 | 9.0209 |
| $\pi D$ | 2.5608 | 4.5253 | 1.7137 − 0.3032 | 1.1853 − 0.1315 | 9.5501 |

To calculate the complete $\alpha^2$ corrections to any quantity one indeed has to take into account relativistic corrections and corrections to the operators, which are not universal. Let us briefly discuss possible applications.

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

(i) For the pionium a part of the $\alpha^2$ corrections is known [8] and progress in experiment [10] requires improvement of theory and calculation of remaining $\alpha^2$ 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 $\alpha^2$ 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 will deliver accurate results, one can consider a specific difference [8]

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

(5)

and for this difference the calculation of the $\alpha^2$ terms are relevant. The contribution induced by the correction to the wave function is only a part of the complete result (cf. Fig. 4) for the VP contributions, which is (see [13] for detail).

$$\Delta E^{\text{VP}}(1s) = \left( 2.61419 \frac{\alpha}{\pi} + 12.54584 \left( \frac{\alpha}{\pi} \right)^2 \right) \Delta E^{(0)}_{\text{hfs}}(1s) ,$$  

(6)

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

(7)

where

$$\Delta E^{(0)}_{\text{hfs}}(ns) = \frac{8}{3} (1 + a_\mu) \frac{\alpha(Z\alpha)^3 n^2}{m} \frac{\mu}{m_p} \left( \frac{m_n}{m} \right)^3 ,$$  

(8)

$\mu_N$ is the nuclear magneton, $\mu$ stands for the proton magnetic moment, and $m_r$ is the reduced mass.

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

Performing a calculation of third terms depicted in Fig. 3 and Fig. 4 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. 5: The $\alpha^3 m$ correction to the Lamb shift in muonic hydrogen: the only contribution of the third order of non-relativistic perturbation theory (see [14]).

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 a particular interest because of the PSI experiment [12]. We have also calculated the same quantity and found

$$\Delta E^{(\text{Fig. 5})}_{2p-2s} (\text{this work}) = \left[ -7.3861 \cdot 10^{-6} + 0.3511 \cdot 10^{-6} \right]$$
\[-(0.0025412+0.0013661) \frac{\alpha^5}{\pi^3} m_e c^2 = 0.0011681 \frac{\alpha^5}{\pi^3} m_e c^2 \]

(9)

where the first parenthesis is for the \(2p\) contribution, while the second is for the \(2s\) one; each parenthesis consists of a main term and a subtraction term as introduced in [3].

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

\[
\Delta E_{2p-2s}^{\text{Fig. 5}} \text{(Ref. [14])} = 0.002535(1) \frac{\alpha^5}{\pi^3} m_e c^2 .
\]

(10)

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

Concluding, we calculated non-relativistic corrections in the relative order \(\alpha^2\) to the wave function at origin in muonic and exotic atoms for the \(1s\) and \(2s\) states, presented a result on the non-relativistic \(\alpha^2\) correction to the hyperfine structure in muonic hydrogen for the same states and corrected the result [14] on the \(\alpha^2 m_e c^2\) contribution to Lamb shift in muonic hydrogen. Details of our calculations of the second-order vacuum polarization effects for the wave function at 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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