Determination of the proton charge radius from the study of the hydrogen \(S\)-energy levels

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Abstract. On the basis of quasipotential method in quantum electrodynamics, the energy interval \((3S - 1S)\) in muonic hydrogen is calculated. The corrections of orders \(\alpha^3\), \(\alpha^4\), \(\alpha^5\), \(\alpha^6\) are taken into account, which are determined by relativistic effects, the effects of vacuum polarization, nuclear structure and recoil, as well as combined corrections. In the leading order proton structure effects are expressed in terms of the charge radius of the proton. In the case of two-photon exchange interaction proton structure corrections are determined by the proton electromagnetic form factors. The value of the energy interval \((3S - 1S)\) can be used for comparison with future experimental data and determining the proton charge radius with greater accuracy.

1. Introduction
The performed investigations by the CREMA collaboration in 2010-2016 \([1, 2]\) with muonic hydrogen showed that there is a significant discrepancy in the values of proton and deuteron charge radii, which were obtained from experiments with electronic and muonic atoms. In the case of other light nuclei (helium), the results are preliminary and have so far been reported only at conferences.

During 2017-2019 different new experimental results were obtained, both with electronic and muon systems, which made it possible to extract the value of the charge radius of the proton. In \([3]\), the frequency of the \((2S - 4P)\) transition in hydrogen was measured: \(\Delta \nu_{2S-4P} = 616520931626.8(2.3)\) kHz, and the extracted value \(r_p = 0.8335(95)\) fm turned out to be in agreement with the CREMA \([1]\) results.

To investigate the puzzle of the proton radius, the PRad experiment was proposed in 2011 (E12-11-1062) and was successfully carried out in 2016 at the Thomas Jefferson National Accelerator Facility with electron beams with energies of 1.1 and 2.2 GeV. In the experiment, the elastic scattering cross sections \((e-p)\) were measured at unprecedentedly low value of the square of the momentum transfer with an accuracy of one percent. The value of the charge radius of the proton was \(r_p = 0.831 \pm 0.007\) (stat) \(\pm 0.012\) (syst) fm \([4]\), which is less than the average value of \(r_p\) from previous experiments on elastic scattering \((e-p)\), but is consistent with spectroscopic results for the muonic hydrogen atom within experimental uncertainties.
A new measurement of the Lamb shift in hydrogen \((n = 2)\) was performed in \[5\]: \(\Delta E_{Ls} = 909.8717(32)\) MHz. The value of the proton charge radius, which was obtained from this experiment, \(r_p = 0.833(10)\) fm, agrees with the spectroscopic data for muonic atoms.

To solve the problem of the proton charge radius \[6, 7\] the MUSE collaboration is planning an experiment to simultaneously measure the cross sections for scattering of electrons and muons by protons \[8\]. This experiment will make it possible to determine the charge radius of the proton independently in two reactions and test lepton universality with an accuracy of an order of magnitude superior to previous scattering experiments.

It should be noted that in the recent experiment \[9\], a new measurement of the frequency of the two-photon transition \((1S - 3S)\) in hydrogen was carried out with a relative error \(9 \cdot 10^{-13}\): \(\Delta \nu_{2017}^{1S - 3S} = 2922743278671.0(4.9)\) kHz. The value of the charge radius extracted from this experimental result, \(r_p = 0.877(13)\) fm, is in good agreement with the value recommended by CODATA \[10\]. The result of the experiment \[9\] in electron hydrogen posed, in our opinion, two problems. First, it is necessary to re-analyze the theoretical calculation of the various contributions to the \((3S - 1S)\) interval in hydrogen in order to obtain the full theoretical value for the \((3S - 1S)\) transition frequency and extract the proton charge radius \[11\]. Second, it is useful to have a precise theoretical calculation of the \((3S - 1S)\) interval in muonic hydrogen as a guideline for possible future experiments with muonic hydrogen. This work is aimed at solving the second problem.

2. General formalism

We make precise calculation of the energy interval \((3S - 1S)\) on the basis of quasipotential method in quantum electrodynamics \[12 - 14\]. The two-particle bound state is described by the Schrödinger equation, and the main contribution to the particle interaction operator is determined by the amplitude of \(1\gamma\) interaction. The leading order contribution to the energy interval \((3S - 1S)\) in muonic hydrogen is determined by fine structure formula \[15\]. To extract the charge radius of a proton with high accuracy from the measurement of some spectroscopic interval, it is necessary to calculate corrections of a high order of smallness in terms of the fine structure constant and the particle mass ratio.

An important class of corrections to energy levels are corrections for vacuum polarization (VP). Although their value decreases with an increase in the number of loops in the polarization operator, it is necessary to take into account contributions up to three loops inclusive to achieve a high calculation accuracy. The electron one-loop vacuum polarization (see fig. \[1\]) leads to a modification of the Coulomb potential and gives sufficiently large value in the interval \((3S - 1S)\): \(\Delta E_{vp}(3S - 1S) = 1834.5535\) meV. The account of two-loop VP effects is done as in \[16, 17\]. Averaging corresponding potentials \(\Delta V_{\text{C}vp,vp}^C\) and \(\Delta V_{\text{2-loop}vp}^C\) from \[17\] over the Coulomb wave functions we obtain their total contribution to energy interval \((3S - 1S)\): \(\Delta E_{vp,vp}(3S - 1S) = 12.8432\) meV.

![Figure 1. Effects of one-loop and two-loop vacuum polarization in 1γ-interaction.](image-url)
Three-loop VP correction in 1\gamma interaction is determined by two sets of amplitudes with one and two fermion cycles (8 diagrams plus two diagrams)\ 17,18. General formula for the contribution of 8 diagrams with one fermion cycle has the form:

\[
\Delta E_{1\gamma}^{(1)}(3S - 1S) = \frac{64 \alpha^3}{\pi^3} \mu(Z\alpha)^2 \int_0^{\infty} \frac{s^2 \rho_1(s)}{(4 + 9s^2)^6(4 + s^2)^2} \Pi_3^{(1)} \left( \frac{s^2}{4G^2} \right),
\]

(1)

\[
\rho_1(s) = 69632 + s^2 \left( -71936 + 3s^2(239360 + 81s^2(3296 + 2688s^2 + 1053s^4)) \right),
\]

where polarization operator \( \Pi_3^{(1)} \) is written in \[17,18\]. The contribution of two diagrams with two fermion cycles can be presented as:

\[
\Delta E_{1\gamma}^{(2)}(3S - 1S) = -\frac{64 \alpha^3}{\pi^3} \mu(Z\alpha)^2 \int_0^{\infty} \frac{\rho_2(s)ds}{(4 + s^2)^2(4 + 9s^2)^6} \int_1^{\infty} \frac{\rho_2(t, s)dt}{t(t + s^2)}.
\]

(2)

\[
\rho_2(s) = s^2 \left( 3s^2(81(1053s^4 + 2688s^2 + 3296)s^2 + 239360) - 71936 \right) s^2 + 69632,
\]

where spectral density \( \rho_{2f}(s, t) \) was obtained in \[19\]. Corrections \([17]\) and \([18]\) have opposite signs and their sum is equal to 0.0246 meV.

The remaining three-loop contributions with successive loops can be calculated in the same way as the two-loop ones in fig. 1 by constructing the interaction potentials which in the coordinate representation have the form:

\[
V_{\gamma p-vp-vp}^C(r) = -\frac{Z\alpha}{r} \frac{\alpha^3}{(3\pi)^3} \int_1^{\infty} \rho(\xi)d\xi \int_1^{\infty} \rho(\eta)d\eta \int_1^{\infty} \rho(\zeta)d\zeta \times
\]

\[
\times \left[ e^{-2m_e\zeta r} \left( \frac{\zeta^4}{(\xi^2 - \zeta^2)(\eta^2 - \zeta^2)} \right) + e^{-2m_e\xi r} \left( \frac{\xi^4}{(\zeta^2 - \xi^2)(\eta^2 - \xi^2)} \right) + e^{-2m_e\eta r} \left( \frac{\eta^4}{(\xi^2 - \eta^2)(\zeta^2 - \eta^2)} \right) \right],
\]

(3)

\[
V_{vp-2-loop \vp}^C = -\frac{4\alpha^3(Z\alpha)}{9\pi^3r} \int_1^{\infty} \rho(\xi)d\xi \int_1^{\infty} \int_1^{\infty} \frac{f(\eta)d\eta}{\eta} \left[ e^{-2m_e\eta r} \frac{\eta^2}{\eta^2 - \xi^2} - e^{-2m_e\xi r} \frac{\xi^2}{\eta^2 - \xi^2} \right].
\]

(4)

\[
\Delta V_\gamma^C \quad \Delta V_\gamma^C \quad \Delta V_\gamma^C
\]

(3)

\[
\Delta V_\gamma^C \quad \Delta V_\gamma^C \quad \Delta V_\gamma^C
\]

(4)

\[
\Delta V_\gamma^C \quad \Delta V_\gamma^C \quad \Delta V_\gamma^C
\]

(5)

\[
\Delta V_\gamma^C \quad \Delta V_\gamma^C \quad \Delta V_\gamma^C
\]

Figure 2. Effects of one-loop and two-loop vacuum polarization in second order perturbation theory. \( \tilde{G} \) is the reduced Coulomb Green’s function.
The vacuum polarization effect changes the Breit Hamiltonian \[ \text{[20, 22]} \]. Such corrections can be called relativistic corrections taking into account the vacuum polarization. We calculate relativistic corrections with one-loop and two-loop VP effect in first and second orders of the perturbation theory (see diagrams in fig. \[ \text{2} \]) as in previous work \[ \text{[17]} \]. In second order PT we need the reduced Coulomb Green function of 1S and 3S states. If the Green’s function of the 1S state is well known and was used by us earlier in our calculations, then the Green’s function of the 3S state was obtained by us on the basis of the general expression for the Coulomb Green’s function \[ \text{[23, 24]} \] in terms of the product of Whittaker’s functions. After subtracting the pole term, the following expression is derived for the reduced Green’s function of the 3S state with two nonzero arguments:

\[
G_{3S}(r_1, r_2) = -\frac{Z\alpha\mu^2}{13122\pi r_1 r_2} e^{-\frac{1}{3}(x_1 + x_2)} g_{3S}(x_1, x_2), \tag{5}
\]

\[
g_{3S}(x_1, x_2) = 18x_<(2(x_- - 9)x_- + 27)(2(x_- - 9)x_+ + 27)x_+ \left( \text{Ei} \left( \frac{2x_-}{3} \right) - \ln(x_-) - \log \left( \frac{4x_+}{9} \right) \right) - 4x_<(2(x_- - 9)x_- + 27)x_+^2 + 2(-27e^{2x_-/3}(x_- (2x_- - 15) + 9) + x_-(36\gamma (2(x_- - 9)x_+ + 27) - 2x_-(2x_- - 135) + 891) + 1701 + 243)x_+^3 + 18(27e^{2x_-/3}(x_- (2x_- - 15) + 9) + x_-(36\gamma (2(x_- - 9)x_+ + 27) + 2x_-(2x_- - 99) + 567) - 729) - 243)x_+^4 + 27(-27e^{2x_-/3}(x_- (2x_- - 15) + 9) + x_-(2x_- - 27)x_-(2x_- - 9) - 36\gamma (2(x_- - 9)x_- + 27) - 243) + 243)x_+ + 243x_<(2(x_- - 9)x_+ + 27),
\]

where \( x_- = \min(x_1, x_2), \ x_+ = \max(x_1, x_2), \ x_i = W r_i, \) \( \gamma \) is the Euler constant.

Among the amplitudes in fig. \[ \text{2} \] the largest contribution of order \( \alpha^2(Z\alpha)^2 \) is given by the amplitude (c), which contains two Coulomb potentials corrected for vacuum polarization. The integration over coordinates is carried out analytically, and over spectral parameters numerically. Since, after integration over coordinates, the result has a cumbersome form, we present here the initial integral expression for this correction and its numerical values in the interval \( (3S - 1S) \):

\[
\Delta E_{sop}^{vp, vp}(1S) = -\frac{16\mu^2(Z\alpha)^2}{9\pi^2} \int_1^\infty \rho(\xi) d\xi \int_1^\infty \rho(\eta) d\eta \times \tag{6}
\]

\[
\int_0^\infty x_1 e^{-x_1(1-2m_\xi)} dx_1 \int_0^\infty x_2 e^{-x_2(1-2m_\eta)} g_{1S}(x_1, x_2) dx_2,
\]

\[
\Delta E_{sop}^{vp, vp}(3S) = -\frac{8\mu^2(Z\alpha)^2}{1594323\pi^2} \int_1^\infty \rho(\xi) d\xi \int_1^\infty \rho(\eta) d\eta \times \tag{7}
\]

\[
\int_0^\infty \left( 1 - \frac{x_1}{3} + \frac{x_1^2}{27} \right) e^{-x_1(2/3 - 2m_\xi)} dx_1 \int_0^\infty \left( 1 - \frac{2x_2}{3} + \frac{x_2^2}{27} \right) e^{-x_2(2/3 - 2m_\eta)} g_{1S}(x_1, x_2) dx_2,
\]

\[
\Delta E_{sop}^{vp, vp}(3S - 1S) = 1.9955 \text{ meV}.
\]

Nuclear structure corrections play a special role in the energy spectrum. In the leading order they are determined by the following expression proportional to the square of the charge radius \( r_p^2 \) \[ \text{[15]} \] (the \( str \) subscript denotes here and below a correction for the nuclear structure):

\[
\Delta E_{str}(3S - 1S) = -\frac{52\mu^2(Z\alpha)^4}{81} r_p^2 = -40.039631 \ r_p^2 = -28.3105 \text{ meV}, \tag{9}
\]
where we have extracted the coefficient at $r_p^2$, and the value of the charge radius itself is taken in fm. For a numerical estimate of the contributions [1], the value of the proton charge radius from [1] was used. The next most important correction for muonic hydrogen is the correction for the structure of the nucleus of order $(Z\alpha)^5$ of two-photon exchange amplitudes, which is expressed in terms of the Dirac $F_1$ and Pauli $F_2$ form factors of the proton. Neglecting the relative momenta of particles in the initial and final states, one can represent this contribution to the shift of $S$ levels in the integral form:

$$
\Delta E^{2\gamma}_{str}(nS) = -\frac{\mu^3(Z\alpha)^5}{\pi n^3} \delta \int_0^\infty \frac{d\xi}{k} V_{2\gamma}(k) = 0.18 \text{ meV},
$$

$$
V_{2\gamma}(k) = \frac{2(F_1^2 - 1)}{m_1 m_2} + \frac{8 m_1 [F_2(0) + 4 m_Z^2 F_1(0)]}{m_2 (m_1 + m_2) k} +
\begin{align*}
&\frac{k^2}{2 m_1^2 m_2^2} [2(F_1^2 - 1)(m_1^2 + m_2^2) + 4 F_1 F_2 m_1^2 + 3 F_2^2 m_1^2] + \frac{\sqrt{k^2 + 4 m_1^2}}{2 m_1^2 m_2 (m_1^2 - m_2^2) k} \times \\
&\left\{ k^2 [2(F_1^2 - 1)m_1^2 + 4 F_1 F_2 m_1^2 + 3 F_2^2 m_1^2] - 8 m_1^2 F_1 F_2 + \frac{16 m_1^2 m_2^2 (F_1^2 - 1)}{k^2} \right\} - \\
&- \frac{\sqrt{k^2 + 4 m_2^2 m_1}}{2 m_2^2 (m_1^2 - m_2^2) k} \left\{ k^2 [2(F_1^2 - 1) + 4 F_1 F_2 + 3 F_2^2] - 8 m_2^2 F_1 F_2 + \frac{16 m_2^2 (F_1^2 - 1)}{k^2} \right\},
\end{align*}
$$

In the numerical integration in (10), we use the parametrization of the proton form factors from [25]. The error in calculating this contribution is estimated at 1%, therefore the result is given with an accuracy of two digits after the decimal point. The magnitude of this correction in muonic hydrogen increases significantly in comparison with electron hydrogen. The contribution of two-photon amplitudes in the case of a point nucleus is also taken into account in the form known from the calculation with hydrogen atom [15].

Contributions of the 5th order in $\alpha$ are given by the amplitudes of particle interactions, which contain both the effects of the nuclear structure and vacuum polarization. Corresponding particle interaction operator in the coordinate representation has the form:

$$
\Delta V_{str}^{\alpha}(r) = \frac{2}{3} \pi Z \alpha^2 \frac{\alpha^2}{r^3} \int_1^\infty \rho(\xi) d\xi \left[ \delta(r) - \frac{m_e^2 \xi^2}{\pi r} e^{-2 m_e \xi r} \right].
$$

Using the expression (11), you can perform analytical integration over all variables when calculating the matrix elements. For 1$S$ and 3$S$ states, the energy level shifts are equal:

$$
\Delta E_{str}^{\alpha}(1S) = \frac{2 \alpha (Z\alpha)^4 r_p^2 \mu^3}{27 \pi \sqrt{1 - b_1^2}} \left[ (6 b_1^2 - 3 b_1^2 + 6) \ln \left( \frac{\sqrt{1 - b_1^2} + 1}{b_1} \right) \right.
+ \left. \sqrt{1 - b_1^2} \left( -3 \pi b_1^3 + 6 b_1^2 + 1 \right) \right],
$$

$$
\Delta E_{str}^{\alpha}(3S) = \frac{\alpha (Z\alpha)^4 r_p^2 \mu^3}{1458 \pi (1 - 9 b_1^2)^{9/2}} \left[ \sqrt{1 - 9 b_1^2} \times \left[ 32 + 9 b_1^2 \right] - 116 + 9 b_1 (3b_1 (19 + 
+ 6 b_1 (-5 - 414 b_1^2 + 972 b_1^4)) - 4 (1 - 9 b_1^2)^3) \right] + 3 \left( 8 + 81 b_1^2 (-4 + 9 b_1^2 (10 + 
+ b_1^2 (-89 + 162 b_1^2 (5 - 18 b_1^2 + 36 b_1^4)))) \right) \ln \frac{3b_1}{1 - \sqrt{1 - 9 b_1^2}} \right].
$$
Similar corrections are calculated also in second order PT. We have considered numerous corrections of various orders in the \((3S - 1S)\) interval, which are specific for muonic hydrogen using our approach as in \([17]\). Other contributions that are known analytically for hydrogen atom were used for numerical estimation in muonic hydrogen (see Tables 5–10 \([15]\)).

3. Conclusion

The interest in the transitions between the \(S\)-energy levels in the hydrogen atom is due to the fact that the study of such transitions opens up yet another possibility of refining the value of the charge radius of the proton. In this work, we continue our studies \([13, 14, 17, 22]\) of low-lying energy levels of muonic hydrogen, which have been intensively investigated in recent years experimentally and theoretically. The \((3S - 1S)\) transition was chosen as the energy interval for precise calculations, the measurement accuracy of which in the case of electron hydrogen is very high \([9]\). Various potentially important interactions in muonic hydrogen were analyzed and their contribution to the structure of \(S\) states was calculated within the quasipotential method in quantum electrodynamics.

Total theoretical result for the energy interval \((3S - 1S)\) in muonic hydrogen has the form

\[
\Delta E(\mu p) = 2249398.5478 \text{ meV.}
\]

Theoretical error in the calculation of the interval \((3S - 1S)\) connected with the calculation of the QED corrections is, according to our estimates, about 0.005 meV. If we do not fix the numerical value of the leading order nuclear structure correction, then the full result can be presented as:

\[
\Delta E^{\text{tot}}(3S - 1S) = 2249426.8578 - 40.039631 \ r_p^2 \ \text{meV. \ \ (14)}
\]

Thus, a precision measurement of the frequency of the \((3S - 1S)\) transition in muonic hydrogen can give a new, more exact value of the proton’s charge radius. So, for example, measuring the \((3S' - 1S)\) shift in muonic hydrogen with a relative error \((1 \div 3) \ ppb\) will reduce the error in determining the proton charge radius to 0.0001 fm.

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