Energy interval 2S-1S in muonic ions of lithium, beryllium and boron

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Abstract. Within the framework of the quasipotential method in quantum electrodynamics, the energy interval (2S − 1S) in muonic ions of lithium, beryllium and boron is calculated. Corrections of order $\alpha^3 - \alpha^6$, which are determined by relativistic effects, effects of vacuum polarization, nuclear structure and recoil, as well as combined corrections, including the above, are taken into account. Nuclear structure effects are expressed in terms of the nuclear charge radius in the case of one-photon interaction and the electromagnetic form factors of nuclei in the case of two-photon interaction. The obtained numerical values for the (2S − 1S) energy interval can be used for comparison with future experimental data and for a more accurate determination of the nuclear charge radii.

1. Introduction
At present, four complementary methods are used to obtain the charge radii of light nuclei: elastic scattering of electrons by nuclei, elastic scattering of muons by nuclei, spectroscopy of electron atoms, and high-precision laser spectroscopy in muonic atoms [1–6]. Traditionally, elastic electron scattering was the first method for determining the internal structure of nuclei. Elastic scattering of leptons by a target nucleus is described by form factors included in the theoretical expression for the scattering cross section. A proton or other light nucleus is a compound particle, and its size is determined by the charge radius $r_{nE}$. It is related to the slope of the electrical form factor of the proton (nucleus) $G_{nE}$ at $q^2 = 0$. Since $G_{nE}$ is a nonperturbative function of $q^2$, its slope must be extracted from experimental data. The most direct way to measure $r_{nE}$ is to extract the electric form factor $G_{nE}$ from the lepton-proton (nucleus) scattering and determine its slope at $q^2 = 0$. Experimental data provide detailed information about the distribution of electric charge and magnetic moment inside the nucleus. They are used to determine the absolute rms values of the nuclear charge $r_{nE}$ and magnetic $r_{nM}$ radii, usually with a percentage accuracy or slightly better. Experiments on the scattering of electrons and muons by nuclei are currently being carried out. By simultaneously determining the form factors for electron and muon scattering, these experiments will allow an accurate test of the universality of the lepton and thus contribute to the solution of the proton radius "puzzle" in the near future.
Atomic spectroscopy of hydrogen is an indirect way of determining the charge radius $r_{pE}$ of a proton (nucleus) from precision measurements of certain energy intervals. While electron scattering and spectroscopy of electron atoms have been available for a long time, muon spectroscopy became available only in 2010 thanks to the work of the CREMA collaboration. As a result of the first CREMA experiments in 2010, the value of proton charge radius $r_{pE} = 0.84184(67)$ fm was obtained, which was 10 times more accurate than all previous values from experiments with electronic systems. Moreover, this value was significantly less than the CODATA value $r_{pE} = 0.8768(69)$ fm. This difference is called the "puzzle" of the proton radius. It’s safe to say that the decade since 2010 has been the CREMA’s decade [5,8,9]. One of the future possible tasks of the CREMA is to extend the laser spectroscopy experiments with muonic systems to the elements of lithium, beryllium and others and to improve the values of charge radii and the Zemach radii of light nuclei [10,11].

In last years we calculated different energy intervals in the spectrum of muonic lithium, beryllium and boron which can be studied in experiment: the Lamb shift $(2P-2S)$ [12], hyperfine structure of S states [13], hyperfine structure of P states [14,15]. In this work we consider another basic interval $(2S-1S)$, which for many atoms (hydrogen atom, muonium) was measured with very high accuracy. One of the leading contributions to this interval is precisely determined by the charge radii of the nuclei, and, therefore, the charge radii can be extracted from the corresponding experimental data.

2. General formalism

Our approach to the precision calculation of the $(2S-1S)$ interval is based on the quasipotential method in quantum electrodynamics [16–18]. The two-particle bound state is described by the Schrödinger equation, and the leading order contribution to the particle interaction operator is determined by the Breit Hamiltonian. The main contribution to the fine structure of the spectrum of S-states of hydrogen-like atoms consisting of particles with masses $m_1$ (muon mass), $m_2$ (nuclear mass) can be represented with an accuracy of $O((Z\alpha)^6)$ ($\mu$ is the reduced mass) in the form [19]:

$$E_n = m_1 + m_2 - \frac{\mu(Z\alpha)^2}{2n^2} - \frac{\mu(Z\alpha)^4}{2n^3} \left[ 1 - \frac{3}{4n} + \frac{\mu^2}{4m_1m_2n} \right] - \frac{m_1(Z\alpha)^6}{16n^6} (2n^3 + 6n^2 - 12n + 5) = (1)$$

\[
\begin{align*}
&18689182.42 \text{ meV}, \quad (\mu_7^3 Li), \\
&33345718.84 \text{ meV}, \quad (\mu_9^3 Be), \\
&52226221.04 \text{ meV}, \quad (\mu_5^{11} B).
\end{align*}
\]

An important class of corrections to energy levels are corrections for vacuum polarization [15,18,20]. 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. One-loop vacuum polarization leads to a modification of the Coulomb potential and is determined in the coordinate representation by the following expression (the subscript $vp$ denotes here and below the electronic polarization of the vacuum, and the subscript $C$ the contribution of the Coulomb interaction):

$$V_{vp}^C(r) = \frac{\alpha}{3\pi} \int_1^{\infty} d\xi \rho(\xi) \left( -\frac{Z\alpha}{r} e^{-2m_e \xi r} \right), \quad \rho(\xi) = \frac{\sqrt{\xi^2 - 1} (2\xi^2 + 1)}{\xi^4}. \quad (2)$$
In the first order of perturbation theory, the potential \( 2 \) gives the following shifts of the energy levels \( 1S \) and \( 2S \) \((b_1 = m_e/W, W = \mu Z \alpha, Z \) is the nuclear charge):\

\[
\Delta E_{vp}(1S) = -\frac{4\mu(Z\alpha)^2 \alpha}{3\pi} \sqrt{b_1^2 - 1} \left(12\pi b_1^3 - 24b_1^2 + 9\pi b_1 - 22\right) - 6 \left(4b_1^4 + b_1^2 - 2\right) \sec^{-1}(b_1),
\]

\[
\Delta E_{vp}(2S) = -\frac{\mu(Z\alpha)^2 \alpha}{6\pi} \left(\frac{b_1(b_1(16b_1(b_1(3b_1(56b_1(\pi b_1 - 1) - 25\pi) + 68) + 6\pi) - 49) + 9\pi) - 7}{3(4b_1^2 - 1)^2}\right),
\]

\[
- i \left(3584b_1^8 - 2048b_1^6 + 300b_1^4 + 10b_1^2 - 1\right) \ln \left(\frac{-2b_1}{\sqrt{4b_1^2 - 1} - i}\right) \left(\frac{2b_1}{\sqrt{4b_1^2 - 1} - i}\right). \]

\[
\]

**Figure 1.** Effects of one-loop and two-loop vacuum polarization in 1\( \gamma \)-interaction

In the case of contributions from the fourth-order and six-order polarization operator (figures 1, 2 and 3), one can construct the interaction potential of particles and the shift of energy levels
in integral form. In the coordinate representation, the two-loop particle interaction operators take the form convenient for the subsequent calculation of the energy shift:

\[
\Delta V_{1,2\text{-loop \ vp}}(r) = -\frac{2Z\alpha}{3\pi} \left( \frac{\alpha}{\pi} \right)^2 \int_0^1 \frac{f(v)dv}{1-v^2} e^{-\frac{2m_e}{\sqrt{1-v^2}}}.
\]  

(5)

\[
V_{1,\text{vp}}(r) = \frac{\alpha^2}{9\pi^2} \int_1^\infty \rho(\xi)d\xi \int_1^\infty \rho(\eta)d\eta \left( \frac{Z\alpha}{r} \right) \frac{1}{(\xi^2-\eta^2)} \left( \xi^2 e^{-2m_e\xi r} - \eta^2 e^{-2m_e\eta r} \right).
\]  

(6)

Spectral density \( f(v) \) is written explicitly in [16]. When calculating the matrix elements (5), (6), the integration over the particle coordinates is performed analytically, and the subsequent integration over the spectral parameters is numerical. A convenient representation for the three-loop polarization operator in calculating the contributions to the energy level shifts was obtained in [21][22].

The effect of vacuum polarization leads to a change not only in the Coulomb potential, but also in other terms in the Breit Hamiltonian, which will contribute to the energy spectrum of order \( \alpha(Z\alpha)^4 \). This order of contribution suggests that the numerical values of the corrections can be significant. The modification of the Breit potential due to the one-loop vacuum polarization is determined in the case of S-states by the following terms (the subscript "B" denotes the Breit potential) [23][24]:

\[
\Delta V_{1,\text{vp}}(r) = \frac{\alpha}{3\pi} \int_1^\infty \rho(\xi)d\xi \sum_{i=1}^{3} \Delta V_{i,\text{vp}}(r),
\]  

(7)

\[
\Delta V_{1,\text{vp}} = \frac{Z\alpha}{8} \left( \frac{1}{m_1^2} + \frac{1}{m_2^2} \right) \left[ 4\pi \delta(r) - \frac{4m_2^2\xi^2}{r} e^{-2m_e\xi r} \right],
\]  

(8)

\[
\Delta V_{2,\text{vp}} = -\frac{Z\alpha m_2^2\xi^2}{m_1m_2r} e^{-2m_e\xi r}(1 - m_e\xi r),
\]  

(9)

\[
\Delta V_{3,\text{vp}} = -\frac{Z\alpha}{2m_1m_2p_i} e^{-2m_e\xi r} \left[ \delta_{ij} + \frac{r_ir_j}{r^2} \left( 1 + 2m_e\xi r \right) \right] p_j.
\]  

(10)

The largest numerical contribution (more than 80%) comes from the term \( \Delta V_{1,\text{vp}} \), whose matrix elements are calculated analytically for 1S and 2S states:

\[
\Delta E_{1,\text{vp}}(1S) = \frac{\alpha(Z\alpha)^4\mu^3}{18\pi} \left( \frac{1}{m_1^2} + \frac{1}{m_2^2} \right) \left( 1 + 6b_1^2 - 3b_3^3 \pi \right) + \frac{1}{\sqrt{1 - b_1^2}} \left( 6 - 3b_1^2 + 6b_1^4 \right) \ln \frac{1 + \sqrt{1 - b_1^2}}{b_1}.
\]  

(11)

\[
\Delta E_{1,\text{vp}}(2S) = \frac{\alpha(Z\alpha)^4\mu^3}{288\pi} \left( \frac{1}{m_1^2} + \frac{1}{m_2^2} \right) \left[ \frac{2}{9} \left( 8b_1 \left( 48b_1^3 - 3\pi \left( 1 - 4b_1^2 \right)^2 - 22b_1 \right) - 29 \right) b_1^2 + 11 \right.
\]  

\[
- \left. \frac{12 \left( 256b_1^8 - 160b_1^6 + 66b_1^4 + 10b_1^2 + 1 \right) \ln \left( \frac{2b_1}{\sqrt{1 - 4b_1^2}} \right) \right] \right] .
\]  

(12)

In order to increase the accuracy of the calculation we also take into account the contribution of relativistic corrections with effects of one-loop, two-loop and three-loop vacuum polarization in second order perturbation theory (PT) as in [18]. The Wichman-Kroll and light-by-light contributions are calculated using the interaction potentials from [19][25].
Another group of corrections which should be taken into account is related with the nuclear structure. Expanding the charge form factor of the nucleus at small momentum transfers, we find that in the leading order the effect of the structure of the nucleus is determined in the energy spectrum by the following correction proportional to the square of the charge radius $r^2_N$ [19] (see figure 4 (a)) (the $\text{str}$ subscript denotes here and below a correction for the nuclear structure):

$$\Delta E_{\text{str}}(2S - 1S) = -\frac{7\mu^3(Z\alpha)^4}{12} < r^2_N > = \begin{cases} -3868.1341 r^2_{^7Li} \text{ meV,} & (\mu_3^3 Li), \\ -12355.5147 r^2_{^9Be} \text{ meV,} & (\mu_3^9 Be), \\ -30369.8008 r^2_{^5B} \text{ meV,} & (\mu_3^5 B), \end{cases}$$

where we have extracted the coefficient at $r^2_N$, and the value of the charge radius itself is taken in fm. For the subsequent numerical evaluation of the contributions (13), we used the values of the charge radii of the nuclei from [26].

Contributions of the 5th order in $\alpha$ also give the amplitudes of particle interaction, which contain both the effects of the nuclear structure and vacuum polarization (see figure 4). The particle interaction operator in coordinate representation, corresponding to the diagram in figure 4 (b) has the form:

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

Using the expression (14), you can perform analytical integration over all variables when calculating the matrix elements. For 1S and 2S states, the energy level shifts are equal:

$$\Delta E_{\text{str}}^{1S} = \frac{2\alpha(Z\alpha)^4 r^2_N \mu^3}{27\pi \sqrt{1 - b_1^2}} \left[ (6b_1^4 - 3b_1^2 + 6) \ln \left( \frac{1 - b_1^2 + 1}{b_1} \right) + \sqrt{1 - b_1^2}(-3\pi b_3^3 + 6b_1^2 + 1) \right],$$

$$\Delta E_{\text{str}}^{2S} = \frac{\alpha(Z\alpha)^4 r^2_N \mu^3}{216\pi (4b_1^2 - 1)^{5/2}} \left\{ \sqrt{4b_1^2 - 1} \left[ 2(8b_1 \left( 48b_3^3 - 3\pi (1 - 4b_1^2)^2 - 22b_1 \right) - 29) b_1^2 + 11 \right] + 12i(256b_1^8 - 160b_1^6 + 66b_1^4 - 10b_1^2 + 1) \ln \left( \frac{-2ib_1 (4b_1^2 - 1)^{1/2}}{(4b_1^2 - i\sqrt{4b_1^2 - 1} - 1)} \right) \right\}. $$

We calculate also the contribution to the energy spectrum of the same order $\alpha(Z\alpha)^4$ which is determined by the same effects in the second order of the perturbation theory (see figure 4 (c)). More complicated correction on the nuclear structure and two-loop vacuum polarization are calculated in a similar way (see figure 5 for the correction in second order perturbation theory).
Figure 5. Nuclear structure and two-loop vacuum polarization effects in the second order PT.

So far, we have considered corrections of various orders in the \((2S - 1S)\) interval, which are specific for each muonic atom. But there is also another set of contributions that are known analytically and were obtained in the study of the fine structure of the spectrum of the hydrogen atom \[19\]. Using analytical results from Tables 5-10 \[19\] we make numerical estimation of these corrections for muonic ions of Li, Be and B and include them in total results.

3. Conclusion
Total theoretical results for the energy interval \((2S - 1S)\) in muonic ions of lithium, beryllium and boron have the form: \[\Delta E(\mu Li) = 18721.85385 \text{ eV}, \Delta E(\mu Be) = 33393.43067 \text{ eV}, \Delta E(\mu B) = 52283.31345 \text{ eV}.\] The accuracy of the results obtained is not as high as written. It refers only to pure QED effects, and the corrections for the nuclear structure are known to within hundredths of an eV. If we do not fix the numerical values of the corrections to the nucleus structure, then the complete results can be presented as:

\[
\Delta E^{\text{tot}}(2S - 1S) = \begin{cases} 
18744.95385 - 3.868134141 \ r^2_{Li} \text{ eV}, & (\mu^7_{Li}), \\
33471.83067 - 12.355514666 \ r^2_{Be} \text{ eV}, & (\mu^9_{Be}), \\
52459.12345 - 30.369800775 \ r^2_{B} \text{ eV}, & (\mu^1_{B}).
\end{cases}
\] (17)

Thus, a precision measurement of the \((2S - 1S)\) transition frequency can give new, more accurate values of the charge radii of light nuclei. So, for example, measuring the \((2S - 1S)\) shift in muonic ions with a relative error of 1-2 ppm will reduce the error in determining the nucleus charge radius to 0.001 fm.

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