Low-lying electron energy levels in three-particle electron-muon ions of Li, Be, and B

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The electronic $2P$-$2S$ Lamb shift and the $2S$-$1S$ energy interval in muon-electron ions of lithium, beryllium, and boron with the muon in its ground state are calculated within the framework of perturbation theory in the fine-structure constant and the electron-muon mass ratio. The corrections of first and second orders of perturbation theory, which include the effects of vacuum polarization, nuclear structure, and recoil, are taken into account. The analytical results obtained in perturbation theory are compared with the results of calculations within the variational approach. The values obtained for the $2P$-$2S$ Lamb shift and the $2S$-$1S$ interval can be used for comparison with future experimental data and verification of quantum electrodynamics.

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I. INTRODUCTION

Muon-electron ions of lithium, beryllium, and boron (μeLi, μeBe, and μeB, respectively) are the simplest three-particle systems, consisting of a nucleus, a negatively charged muon, and an electron. The main interaction in this system is determined by the Coulomb interaction of charged particles. The masses m_e, m_μ, and M of the electron, muon, and nucleus in the exotic atom, respectively, satisfy $m_e \ll m_\mu \ll M$. As a result, the muon and the nucleus form a pseudonucleus, and in the first approximation, the muon-electron ions of lithium, beryllium, and boron can be considered as two-particle systems. Such three-particle systems are interesting in that they allow one to study simultaneously, in the energy spectrum, the corrections of small distances connected with the motion of the muon as in muonic two-particle atoms and the corrections of large distances connected with the motion of an electron as in electron atoms.

There are two ways to calculate the energy levels in three-particle muon-electron atoms and ions. The first approach, used in [1–8], is based on the perturbation theory method for the Schrödinger equation. In this case, there is an analytical solution for the three-particle wave function in the initial approximation, which allows one to take into account various corrections to energy levels from other interactions according to perturbation theory. In the other approach, Refs. [9–15] used a variational method in quantum mechanics to find the energy levels of three particles. It made it possible to obtain numerical values of the energy levels of a three-particle system with very high accuracy.

Precision muonic physics has become especially important since the first experimental results on the measurement of low-lying energy levels of muonic hydrogen were obtained by the charge radius experiments with muonic atoms (CREMA) collaboration [16]. A decade of active work of this collaboration produced interesting and unexpected results, related primarily to the determination of more accurate values of the charge radii of light nuclei (protons, deuterons, helions, and α particles). The CREMA experiments have caused a whole series of new experimental studies of the muonic systems. The physics of muonic two-particle and three-particle systems remains an urgent problem that requires appropriate theoretical studies and calculations of the observed quantities with high accuracy.

The purpose of this work is to calculate the electronic $2S$-$2P$ Lamb shift and the $2S$-$1S$ energy interval as in the framework of the first approach from [5–7] for electron-muonic ions with nuclear charges of 3, 4, and 5 and within the framework of the variational method. Note that the hyperfine structure of muonic helium was measured in [17]. New plans for precision microwave spectroscopy of the J-PARC MUSE collaboration [18] are related to the measurement of the hyperfine structure of the ground state of muonic helium with an accuracy two orders of magnitude higher than the accuracy of previous experiments. Measurement of other energy intervals, such as $2S$-$1S$ and $2S$-$2P$, in muon-electron helium or muon-electron ions of lithium, beryllium, and boron is quite feasible.

II. GENERAL FORMALISM

The Hamiltonian of the three-particle system muon-electron nucleus has the general structure [5–7]

$$H = H_0 + \Delta H + \Delta H_{\rm rec} + \Delta H_{\rm VP} + \Delta H_{\rm str}, \qquad (1)$$

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$$H_0 = -\frac{1}{2M_\mu}\nabla_\mu^2 - \frac{1}{2M_e}\nabla_e^2 - \frac{Z\alpha}{x_\mu} - \frac{(Z-1)\alpha}{x_e}, \qquad (2)$$

$$\Delta H = \frac{\alpha}{x_{\mu e}} - \frac{\alpha}{x_e},$$

$$\Delta H_{\rm rec} = -\frac{1}{M}\nabla_\mu \cdot \nabla_e,$$

where Z is the nuclear charge; $\mathbf{x}_\mu$ and $\mathbf{x}_e$ are the muon and electron radius vectors with respect to the nucleus; $x_{\mu e} = |\mathbf{x}_\mu - \mathbf{x}_e|$; $M_e = m_e M/(m_e + M)$ and $M_\mu = m_\mu M/(m_\mu + M)$ are the reduced masses of electron-nucleus and muon-nucleus subsystems, respectively; and α is the fine-structure constant. We use units $\hbar = c = 1$. The center of mass of the three particles is at rest. The Hamiltonian terms $\Delta H_{\rm VP}$, $\Delta H_{\rm str}$, and $\Delta H_{\rm rec}$ determine the vacuum polarization, nuclear structure, and recoil corrections, respectively. The form of the terms of the Hamiltonian $\Delta H_{\rm str}$ and $\Delta H_{\rm VP}$ and their contribution to the energy spectrum are discussed in Sec. III. The Hamiltonian ΔH contains part of the Coulomb interaction of particles, which is included in the perturbation operator. In the initial approximation the wave functions of the three-particle system with the muon in the ground state and the electron in the $1S$, $2S$, and $2P$ states take the form

$$\Psi_{1S}(\mathbf{x}_\mu, \mathbf{x}_e) = \frac{1}{\pi}(W_\mu W_e)^{3/2} e^{-W_\mu x_\mu} e^{-W_e x_e}, \qquad (3)$$

$$\Psi_{2S}(\mathbf{x}_\mu, \mathbf{x}_e) = \frac{1}{2\sqrt{2}\pi}(W_\mu W_e)^{3/2}\left(1 - \frac{1}{2}W_e x_e\right) e^{-W_\mu x_\mu} e^{-W_e x_e/2}, \qquad (4)$$

$$\Psi_{2P}(\mathbf{x}_\mu, \mathbf{x}_e) = \frac{1}{2\sqrt{6\pi}}(W_\mu W_e)^{3/2} W_e x_e (\boldsymbol{\varepsilon}\mathbf{n}) e^{-W_\mu x_\mu} e^{-W_e x_e/2}, \qquad (5)$$

where $W_e = (Z-1)M_e\alpha$ and $W_\mu = ZM_\mu\alpha$. The wave function of the $2P$ state is presented in tensor form and $\boldsymbol{\varepsilon}$ is the polarization vector of the state $2P$. The main contribution to the perturbation operator is determined by the term ΔH. It is known that in an electronic hydrogenlike atom the $2S$-$2P$ Lamb shift is a radiation effect of the fifth order in the fine-structure constant α and in a muonic hydrogenlike atom the Lamb shift is determined by the effect of vacuum polarization in the leading order α^3. The purely Coulomb interaction of charged particles does not give a shift between the $2S$ and $2P$ levels in two-particle atoms. In three-particle systems, the electronic Lamb shift in the leading order α^2 is determined by the purely Coulomb interaction.

In the initial approximation, the energy of the system is equal to the sum of the Coulomb energies of an electron and a muon of the order of α^2. So, for example, if both the electron and the muon are in the $1S$ state, then this energy is equal to $[-\frac{1}{2}M_e(Z-1)^2\alpha^2 - \frac{1}{2}M_\mu Z^2\alpha^2]$. In what follows, the muon energy is not of interest to us, since it will cancel out in the $2P$-$2S$ and $2S$-$1S$ intervals. In the case of the $2P$-$2S$ Lamb shift in the first order of perturbation theory, it is necessary to calculate two matrix elements of the Coulomb interaction ΔH,

$$\Delta E^{(1)}(2S) = \left\langle \Psi_{2S}\left|\left(\frac{\alpha}{x_{\mu e}} - \frac{\alpha}{x_e}\right)\right|\Psi_{2S}\right\rangle,$$
$$\Delta E^{(1)}(2P) = \left\langle \Psi_{2P}\left|\left(\frac{\alpha}{x_{\mu e}} - \frac{\alpha}{x_e}\right)\right|\Psi_{2P}\right\rangle, \qquad (6)$$

where the superscript (1) is used to denote the contribution of first-order perturbation theory. For the $2S$ electronic state the matrix element has the form

$$\Delta E^{(1)}(2S) = \frac{(W_e W_\mu)^3}{8\pi^2}\int d\mathbf{x}_e d\mathbf{x}_\mu \left(1 - \frac{1}{2}W_e x_e\right)^2 e^{-2W_\mu x_\mu} e^{-W_e x_e}\left(\frac{\alpha}{|\mathbf{x}_\mu - \mathbf{x}_e|} - \frac{\alpha}{x_e}\right)$$
$$= \alpha W_e\left[-\frac{1}{4} + \frac{8 + a_1\{20 + a_1[12 + a_1(10 + a_1)]\}}{(2+a_1)^5}\right] = W_e\alpha\left(-\frac{1}{4}a_1^2 + \frac{5}{8}a_1^3 - \frac{63}{64}a_1^4 + O\left(a_1^5\right)\right), \qquad (7)$$

$$a_1 = \frac{W_e}{W_\mu} = \frac{(Z-1)}{Z}\frac{M_e}{M_\mu}.$$

Averaging over the orbital angular momentum projections by means of the relation

$$\frac{1}{3}\sum_\lambda \varepsilon_i^{*(\lambda)}\varepsilon_j^{(\lambda)} = \frac{1}{4\pi}\delta_{ij}, \qquad (8)$$

the matrix element for the $2P$ electronic state can be calculated analytically in the same way,

$$\Delta E^{(1)}(2P) = \frac{(W_e W_\mu)^3}{96\pi^2}\int d\mathbf{x}_e d\mathbf{x}_\mu (W_e x_e)^2 e^{-2W_\mu x_\mu} e^{-W_e x_e}\left(\frac{\alpha}{|\mathbf{x}_\mu - \mathbf{x}_e|} - \frac{\alpha}{x_e}\right)$$
$$= \alpha W_e\left[-\frac{1}{4} + \frac{\left[(2+a_1)^5 - 6a_1^4 - a_1^5\right]}{4(2+a_1)^5}\right] = W_e\alpha\left(-\frac{3}{64}a_1^4 + \frac{7}{64}a_1^5 + O\left(a_1^6\right)\right), \qquad (9)$$

and an expansion in a_1 converges well, because numerical values of a_1 for muonic ions of lithium, beryllium, and boron are small: $a_1(\mathrm{Li}) = 0.003\,276$, $a_1(\mathrm{Be}) = 0.003\,673$, and $a_1(\mathrm{B}) = 0.003\,909$. The parameter $a_1 = (Z-1)M_e/ZM_\mu$ determines the recoil effects in M_e/M_μ and acts as a small parameter used in the framework of perturbation theory for the ΔH interaction. In this approach, there are various recoil corrections, which are determined by the parameter a_1 and the

Hamiltonian $\Delta H_{\rm rec}$ (see Sec. III). We see that the recoil corrections in a_1 are smaller for the $2P$ state than for the $2S$ state. The main contribution to the electronic Lamb shift of $O(\alpha^2)$ is obtained from (7) (it is indicated by the index LO):

$$\Delta E^{(1)}_{\rm LO}(2P\text{-}2S) \approx W_e\alpha\frac{a_1^2}{4} = \frac{M_e\alpha^2}{4}\frac{(Z-1)^3M_e^2}{Z^2M_\mu^2}. \tag{10}$$

Thus, the electronic Lamb shift occurs in such three-particle systems of $O(\alpha^2)$ due to the Coulomb interaction of all particles. Note that the recoil correction $\langle\Psi|\Delta H_{\rm rec}|\Psi\rangle$ is equal to 0 for both states of the electron. The refinement of the result (10) is related to the inclusion of corrections in the higher orders of perturbation theory in α and m_e/m_μ.

In the second order of perturbation theory, the correction to energy levels is determined by the expression

$$\Delta E^{(2)} = \int \psi_{\mu0}(\mathbf{x}_\mu)\psi_{e1}(\mathbf{x}_e)\left(\frac{\alpha}{x_{\mu e}}-\frac{\alpha}{x_e}\right) \times \sum_{n,n'}\frac{\psi_{\mu n}(\mathbf{x}_\mu)\psi_{en'}(\mathbf{x}_e)\psi_{\mu n}(\mathbf{x}'_\mu)\psi_{en'}(\mathbf{x}'_e)}{E_{\mu0}+E_{e1}-E_{\mu n}-E_{en'}} \times \psi_{\mu0}(\mathbf{x}'_\mu)\psi_{e1}(\mathbf{x}'_e)\left(\frac{\alpha}{x'_{\mu e}}-\frac{\alpha}{x'_e}\right)d\mathbf{x}_\mu d\mathbf{x}'_\mu d\mathbf{x}_e d\mathbf{x}'_e, \tag{11}$$

where $\psi_{\mu0}(\mathbf{x}_\mu)$ is the muon wave function in the ground state, $\psi_{e1}(\mathbf{x}_e)$ is the electronic wave function in states $2S$ and $2P$ (or $1S$). A superscript (2) is used to denote the contribution of second-order perturbation theory. The reduced Coulomb Green's function entering (11) is determined by the sum over the excited muonic n and electronic n' states. When determining the reduced Green's function, the initial state in the sum over n and n' is excluded. Let us split the complex matrix element (11) into several simpler ones, highlighting certain states of the muon. Let the muon be in an intermediate state $n=0$. Then from (11) we get the first part of the correction

$$\Delta E^{(2)}_1 = \int \psi_{\mu0}(\mathbf{x}_\mu)\psi_{e1}(\mathbf{x}_e)\left(\frac{\alpha}{x_{\mu e}}-\frac{\alpha}{x_e}\right)\psi_{\mu0}(\mathbf{x}_\mu)\psi_{\mu0}(\mathbf{x}'_\mu) \times \sum_{n'}\frac{\psi_{en'}(\mathbf{x}_e)\psi_{en'}(\mathbf{x}'_e)}{E_{e1}-E_{en'}} \times \psi_{\mu0}(\mathbf{x}'_\mu)\psi_{e1}(\mathbf{x}'_e)\left(\frac{\alpha}{x'_{\mu e}}-\frac{\alpha}{x'_e}\right)d\mathbf{x}_\mu d\mathbf{x}'_\mu d\mathbf{x}_e d\mathbf{x}'_e, \tag{12}$$

where we use the subscript 1 to denote the contribution with $n=0$.

The reduced Coulomb Green's function of an electron for an excited state with $n=2$ has two parts. Only the part $\tilde G^e_{2S}$ gives a nonzero contribution to this matrix element, which has the form [19]

$$\tilde G^e_{2S}(r_1,r_2) = -\frac{(Z-1)\alpha M_e^2}{16\pi x_1x_2}e^{-(x_1+x_2)/2}g_{2S}(x_1,x_2),$$
$$g_{2S}(x_1,x_2) = 8x_< - 4x_<^2 + 8x_> + 12x_<x_> - 26x_<^2x_> + 2x_<^3x_> - 4x_>^2 - 26x_<x_>^2 + 23x_<^2x_>^2 - x_<^3x_>^2 + 2x_<x_>^3 - x_<^2x_>^3 + 4e^{x_<}(1-x_<)(x_>-2)x_> + 4(x_<-2)x_<(x_>-2)x_>[-2\gamma + \mathrm{Ei}(x_<) - \ln(x_<) - \ln(x_>)], \tag{13}$$

where $x_< = \min(x_1,x_2)$, $x_> = \max(x_1,x_2)$, $x_i = W_e r_i$, and γ is the Euler constant. Simple matrix elements over the muon coordinates are calculated analytically:

$$V_\mu(x_e) = \int \psi_{\mu0}(\mathbf{x}_\mu)\left(\frac{\alpha}{x_{\mu e}}-\frac{\alpha}{x_e}\right)\psi_{\mu0}(\mathbf{x}_\mu)d\mathbf{x}_\mu = -\frac{\alpha}{x_e}(1+W_\mu x_e)e^{-2W_\mu x_e}. \tag{14}$$

The remaining integration over the coordinates of the electron can also be performed analytically, giving the result

$$\Delta E^{(2)}_1(2S) = \int \psi_{e1}(\mathbf{x}_e)\left(-\frac{\alpha}{x_e}\right)(1+W_\mu x_e)e^{-2W_\mu x_e}d\mathbf{x}_e \int \psi_{e1}(\mathbf{x}'_e)\left(-\frac{\alpha}{x'_e}\right)(1+W_\mu x'_e)e^{-2W_\mu x'_e}d\mathbf{x}'_e\tilde G^e_{2S}(x_e,x'_e)$$
$$= -\frac{M_e\alpha^2}{8}\left[\frac{25}{16}a_1^3 - a_1^4\left(\frac{191}{32}+4\ln a_1\right)+O\left(a_1^5\right)\right], \tag{15}$$

where the final answer is presented with the accuracy $O(a_1^4)$ in the form of an expansion in powers of the ratio of the effective masses of particles M_e/M_μ.

Similarly, we can consider another contribution when the muon is in excited intermediate states $n\neq0$. This contribution can be represented as

$$\Delta E^{(2)}_2(2S) = \int \psi_{\mu0}(\mathbf{x}_\mu)\psi_{e1}(\mathbf{x}_e)\frac{\alpha}{|\mathbf{x}_\mu-\mathbf{x}_e|}d\mathbf{x}_\mu d\mathbf{x}_e\sum_{n\neq0}\psi_{\mu n}(\mathbf{x}_\mu)\psi_{\mu n}(\mathbf{x}'_\mu)G^e(\mathbf{x}_e,\mathbf{x}'_e,z)\frac{\alpha}{|\mathbf{x}'_\mu-\mathbf{x}'_e|}\psi_{\mu0}(\mathbf{x}'_\mu)\psi_{e1}(\mathbf{x}'_e)d\mathbf{x}'_\mu d\mathbf{x}'_e, \tag{16}$$

where we use the subscript 2 to denote the contribution with $n\neq0$.

The Coulomb Green's function of the electron standing here depends on the parameter $z = E_{\mu0}-E_{\mu n}+E_{e1}$. In the leading order with respect to the particle mass ratio, we approximate $G^e(\mathbf{x}_e,\mathbf{x}'_e,z)$ in the form of the Green's function of a free electron [1,2]:

$$G^e(\mathbf{x}_e,\mathbf{x}'_e,z) = -\frac{M_e}{2\pi}\frac{1}{|\mathbf{x}_e-\mathbf{x}'_e|}e^{-b|\mathbf{x}_e-\mathbf{x}'_e|}, \quad b=\sqrt{2M_e(E_{\mu0}-E_{\mu n}+E_{e1})}. \tag{17}$$

As discussed in [1,2], the terms that we neglect in this case in the energy spectrum have, in comparison with the ones left, the smallness factor $O((M_e/M_\mu)^{1/2})$.

Then the second part of the correction in the second order of the perturbation theory takes the form

$$\Delta E_2^{(2)}(2S) = -\frac{M_e\alpha^2}{2\pi}\int \psi_{\mu 0}(\mathbf{x}_\mu)\psi_{e1}(\mathbf{x}_e)\frac{1}{|\mathbf{x}_\mu-\mathbf{x}_e|}d\mathbf{x}_\mu d\mathbf{x}_e\sum_{n\neq 0}\psi_{\mu n}(\mathbf{x}_\mu)\psi_{\mu n}(\mathbf{x}'_\mu)$$
$$\times\frac{1}{|\mathbf{x}_e-\mathbf{x}'_e|}e^{-b|\mathbf{x}_e-\mathbf{x}'_e|}\frac{1}{|\mathbf{x}'_e-\mathbf{x}'_\mu|}\psi_{\mu 0}(\mathbf{x}'_\mu)\psi_{e1}(\mathbf{x}'_e)d\mathbf{x}'_\mu d\mathbf{x}'_e. \tag{18}$$

Replacing the value of the electronic wave function $\psi_{e1}(\mathbf{x}'_e)$ with its value at zero, we first perform integration over $\mathbf{x}'_e$,

$$\begin{aligned} I &= \int d\mathbf{x}'_e\psi_{e1}(\mathbf{x}'_e)\frac{1}{|\mathbf{x}_e-\mathbf{x}'_e||\mathbf{x}'_e-\mathbf{x}'_\mu|}e^{b|\mathbf{x}_e-\mathbf{x}'_e|}\\ &= \frac{4\pi}{b^2}\psi_{e1}(0)\frac{1}{|\mathbf{x}_e-\mathbf{x}'_\mu|}\left(1-e^{-b|\mathbf{x}_e-\mathbf{x}'_\mu|}\right)\\ &= 4\pi\psi_{e1}(0)\left[\frac{1}{b}-\frac{1}{2}|\mathbf{x}_e-\mathbf{x}'_\mu|+\frac{b}{6}|\mathbf{x}_e-\mathbf{x}'_\mu|^2+\cdots\right], \end{aligned} \tag{19}$$

where we also expanded the function in (19) in $b|\mathbf{x}_e-\mathbf{x}'_\mu|$. The corrections that we neglect using the approximation in (19) are of order M_e/M_μ. The term $1/b$ in square brackets vanishes due to the orthogonality of the muon wave functions. Leaving the leading term in square brackets proportional to $|\mathbf{x}_e-\mathbf{x}'_\mu|$, we will use the completeness relation in calculating the integrals over the coordinates of the particles:

$$\sum_{n\neq 0}\psi_{\mu n}(\mathbf{x}_3)\psi^*_{\mu n}(\mathbf{x}_2) = \delta(\mathbf{x}_3-\mathbf{x}_2)-\psi_{\mu 0}(\mathbf{x}_3)\psi^*_{\mu 0}(\mathbf{x}_2). \tag{20}$$

Direct calculation of integrals with functions from the right-hand side (18) gives the following results corresponding to two terms in (20) after expansion in a_1:

$$\Delta E_{21}^{(2)}(2S) = -16M_e\alpha^2, \quad \Delta E_{22}^{(2)}(2S) = M_e\alpha^2\left[16+\frac{105}{128}a_1^3-\frac{481}{512}a_1^4+O(a_1^5)\right]. \tag{21}$$

We denote these contributions by the subscripts 21 and 22.

Let us now calculate the second-order correction of perturbation theory for the $2P$ state. Let us first choose a muon in an intermediate state with $n=0$. Such a contribution will be determined by the integral

$$\Delta E_1^{(2)}(2P) = \int\psi_{e1}(\mathbf{x}_e)\left(-\frac{\alpha}{x_e}\right)(1+W_\mu x_e)e^{-2W_\mu x_e}d\mathbf{x}_e\int\psi_{e1}(\mathbf{x}'_e)\left(-\frac{\alpha}{x'_e}\right)(1+W_\mu x'_e)e^{-2W_\mu x'_e}d\mathbf{x}'_e\tilde{G}^e_{2P}(x_e,x'_e). \tag{22}$$

The reduced Coulomb Green's function of the electron for the excited state $2P$ has the form

$$\begin{aligned} \tilde{G}(2P) &= -\frac{Z\alpha\mu^2}{36x_1^2x_2^2}e^{-(x_1+x_2)/2}\frac{3}{4\pi}\frac{\mathbf{x}_1\mathbf{x}_2}{x_1x_2}g_{2P}(x_1,x_2),\\ g_{2P}(x_1,x_2) &= 24x_<^3+36x_<^3x_>+36x_<^3x_>^2+24x_>^3+36x_<x_>^3+36x_<^2x_>^3+49x_<^3x_>^3-3x_<^4x_>^3-12e^{x_<}(2+x_<+x_<^2)x_>^3-3x_<^3x_>^4\\ &\quad+12x_<^3x_>^3[-2C+\mathrm{Ei}(x_<)-\ln(x_<)-\ln(x_>)]. \end{aligned} \tag{23}$$

As in the case of the $2S$ state, all coordinate integrals can be calculated analytically. Expanding the final result in powers of $a_1=W_e/W_\mu$ with precision $O(a_1^6)$, we get

$$\Delta E^{(2)}(2P) = -M_e\alpha^2\left[\frac{7}{2048}a_1^5-\frac{9}{8192}a_1^6+O\left(a_1^7\right)\right]. \tag{24}$$

As it follows from the expansions (9) and (24), the order of the correction in a_1 for the $2P$ electronic state increases in comparison with the $2S$ electronic state and its magnitude decreases significantly. Let us study the second contribution for the $2P$ state connected with muonic excitations, which initially can be written in the form

$$\Delta E_2^{(2)}(2P) = -\frac{M_e\alpha^2}{8\pi^2}\int\psi_{\mu 0}(\mathbf{x}_\mu)\psi_{e2P}(\mathbf{x}_e)\frac{d\mathbf{x}_e}{|\mathbf{x}_\mu-\mathbf{x}_e|}d\mathbf{x}_\mu\sum_{n\neq 0}\psi_{\mu n}(\mathbf{x}_\mu)\psi_{\mu n}(\mathbf{x}'_\mu)\frac{d\mathbf{x}'_e}{|\mathbf{x}'_\mu-\mathbf{x}'_e|}$$
$$\times e^{-b|\mathbf{x}_e-\mathbf{x}'_e|}\frac{1}{|\mathbf{x}_e-\mathbf{x}'_e|}\psi_{\mu 0}(\mathbf{x}'_\mu)\psi_{e2P}(\mathbf{x}'_e). \tag{25}$$

After the variable shifts $\mathbf{x}_e \to \mathbf{x}_e + \mathbf{x}_\mu$ and $\mathbf{x}'_e \to \mathbf{x}'_e + \mathbf{x}'_\mu$ we can neglect $\mathbf{x}_\mu$ and $\mathbf{x}'_\mu$ in electronic wave functions and present the leading-order contribution in the mass ratio M_e/M_μ in (25) as follows:

$$\Delta E_2^{(2)}(2P) = -\frac{M_e\alpha^2}{192\pi^2}W_e^5\int\frac{d\mathbf{x}_e}{x_e}\frac{d\mathbf{x}'_e}{x'_e}e^{-W_e x_e/2}e^{-W_e x'_e/2}e^{-b|\mathbf{x}_e-\mathbf{x}'_e|}\frac{1}{|\mathbf{x}_e-\mathbf{x}'_e|}$$
$$\times\sum_{n\neq 0}\psi_{\mu n}(\mathbf{x}_\mu)\mathbf{x}_\mu\psi_{\mu 0}(\mathbf{x}_\mu)\psi_{\mu n}(\mathbf{x}'_\mu)\mathbf{x}'_\mu\psi_{\mu 0}(\mathbf{x}'_\mu). \tag{26}$$

Then all integrals over the electronic coordinates can be calculated analytically, giving the result

$$\Delta E_2^{(2)}(2P) = -\frac{M_e\alpha^2(Z-1)}{36Z}\frac{W_e^3}{W_\mu^3}(S^d+S^c) = \begin{cases} {}^7_3\mathrm{Li}\mu e, & -0.014\ \mathrm{GHz} \\ {}^9_4\mathrm{Be}\mu e, & -0.023\ \mathrm{GHz} \\ {}^{11}_5\mathrm{B}\mu e, & -0.029\ \mathrm{GHz}, \end{cases}$$
$$S^d = \sum_{n=2}^{\infty}\frac{n^2}{n^2-1}|\langle\psi_{\mu 0}|W_\mu\mathbf{x}_\mu|\psi_{\mu n}\rangle|^2 = \sum_{n=2}^{\infty}\frac{2^8n^9(n-1)^{2n-6}}{(n+1)^{2n+6}} = 2.747\,443\ldots, \tag{27}$$
$$S^c = \int_0^\infty kdk\frac{2^8}{(1-e^{-2\pi/k})}\frac{1}{(k^2+1)^6}\left|\left(\frac{1+ik}{1-ik}\right)^{i/k}\right|^2 = 0.627\,556\ldots.$$

The results obtained show that the expansion parameter, which works in the framework of perturbation theory in ΔH [Eq. (2)], is the particle mass ratio $M_e/M_\mu \approx m_e/m_\mu$.

Let us conclude this section by calculating the interaction correction ΔH in the second order of perturbation theory for the electronic state $1S$:

$$\Delta E^{(2)}(1S) = \int\psi_{\mu 0}(\mathbf{x}_\mu)\psi_{e0}(\mathbf{x}_e)\left(\frac{\alpha}{x_{\mu e}}-\frac{\alpha}{x_e}\right)\sum_{n,n'}\frac{\psi_{\mu n}(\mathbf{x}_\mu)\psi_{en'}(\mathbf{x}_e)\psi_{\mu n}(\mathbf{x}'_\mu)\psi_{en'}(\mathbf{x}'_e)}{E_{\mu 0}+E_{e0}-E_{\mu n}-E_{en'}}$$
$$\times\psi_{\mu 0}(\mathbf{x}'_\mu)\psi_{e0}(\mathbf{x}'_e)\left(\frac{\alpha}{x'_{\mu e}}-\frac{\alpha}{x'_e}\right)d\mathbf{x}_\mu d\mathbf{x}'_\mu d\mathbf{x}_e d\mathbf{x}'_e. \tag{28}$$

Let us first extract, as before, the contribution of the muon in the ground state $n = 0$:

$$\Delta E_1^{(2)}(1S) = \int\psi_{\mu 0}(\mathbf{x}_\mu)\psi_{e0}(\mathbf{x}_e)\left(\frac{\alpha}{x_{\mu e}}-\frac{\alpha}{x_e}\right)\psi_{\mu 0}(\mathbf{x}_\mu)\psi_{\mu 0}(\mathbf{x}'_\mu)\sum_{n'}\frac{\psi_{en'}(\mathbf{x}_e)\psi_{en'}(\mathbf{x}'_e)}{E_{e0}-E_{en'}}$$
$$\times\psi_{\mu 0}(\mathbf{x}'_\mu)\psi_{e0}(\mathbf{x}'_e)\left(\frac{\alpha}{x'_{\mu e}}-\frac{\alpha}{x'_e}\right)d\mathbf{x}_\mu d\mathbf{x}'_\mu d\mathbf{x}_e d\mathbf{x}'_e. \tag{29}$$

The reduced Coulomb Green's function of the electron for the ground state $\tilde{G}^e_{1S}$ has the form

$$\tilde{G}^e_{1S}(r_1,r_2) = -\frac{(Z-1)\alpha M_e^2}{\pi}e^{-(x_1+x_2)}g_{1S}(x_1,x_2), \tag{30}$$

$$g_{1S}(x_1,x_2) = \frac{1}{2x_>}-\ln 2x_> - \ln 2x_< + \mathrm{Ei}(2x_<) + \frac{7}{2} - 2\gamma - (x_1+x_2) + \frac{1}{2x_<}(1-e^{2x_<}).$$

As in the case of (16), all integrals are calculated analytically and the result of the calculation is

$$\Delta E_1^{(2)}(1S) = -M_e\alpha^2\left[\frac{25}{16}a_1^3 + a_1^4\left(\frac{1}{32}-4\ln 2-4\ln a_1\right) + a_1^5\left(-\frac{565}{32}+20\ln 2+20\ln a_1\right)+O\left(a_1^6\right)\right], \tag{31}$$

which we presented in the form of an expansion in terms of a_1. Since the expansion starts from the third power of a_1, this contribution to the $2S$-$1S$ interval is numerically small compared to the contribution of the leading order.

When calculating the contribution of muonic intermediate states with $n \neq 0$, we replace the Green's function of the electron by the free Green's function (17) and use the relation completeness, as in (20). Then the second part of the correction will be determined by the expression

$$\Delta E_2^{(2)}(1S) = M_e\alpha^2\psi_{e0}(0)\int\psi_{\mu 0}(\mathbf{x}_2)\psi_{e0}(\mathbf{x}_1)\frac{|\mathbf{x}_1-\mathbf{y}_2|}{|\mathbf{x}_1-\mathbf{x}_2|}d\mathbf{x}_1 d\mathbf{x}_2\psi_{\mu 0}(\mathbf{y}_2)d\mathbf{y}_2[\delta(\mathbf{x}_2-\mathbf{y}_2)-\psi_{\mu 0}(\mathbf{x}_2)\psi^*_{\mu 0}(\mathbf{y}_2)]. \tag{32}$$

The δ-function term contributes $\Delta E^{(2)}_{21}(1S) = 8M_e\alpha^2$ and the second part in the completeness condition reduces to the integral

$$\Delta E^{(2)}_{22}(1S) = -2M_e\alpha^2 a_1^3 \int_0^\infty dx\, e^{-4x(1+a_1/4)}(-1-x+e^{2x})(-2-x+2e^{2x}(1+x^2)]$$
$$= -2M_e\alpha^2\left[4 + 2a_1^2 - \frac{105}{32}a_1^3 + O\big(a_1^4\big)\right]. \tag{33}$$

As a result, the second part of the correction in the second order of the perturbation theory for the $1S$ state takes the form

$$\Delta E^{(2)}_{2}(1S) = \Delta E^{(2)}_{21}(1S) + \Delta E^{(2)}_{22}(1S) = -2M_e\alpha^2\left[2a_1^2 - \frac{105}{32}a_1^3 + O\big(a_1^4\big)\right]. \tag{34}$$

III. VACUUM POLARIZATION, NUCLEAR STRUCTURE, AND RECOIL CORRECTIONS

The electron vacuum polarization correction $\Delta V_{\rm VP}$ in (1) has three contributions, one for each pair of charged particles. They are determined by the expressions

$$\Delta V^{eN}_{\rm VP}(x_e) = \frac{\alpha}{3\pi}\int_1^\infty \rho(\xi)\Big(-\frac{Z\alpha}{x_e}\Big)e^{-2m_e\xi x_e}d\xi, \quad \rho(\xi) = \frac{\sqrt{\xi^2-1}(2\xi^2+1)}{\xi^4}, \tag{35}$$

$$\Delta V^{\mu N}_{\rm VP}(x_\mu) = \frac{\alpha}{3\pi}\int_1^\infty \rho(\xi)\Big(-\frac{Z\alpha}{x_\mu}\Big)e^{-2m_e\xi x_\mu}d\xi, \tag{36}$$

$$\Delta V^{e\mu}_{\rm VP}(|\mathbf{x}_e-\mathbf{x}_\mu|) = \frac{\alpha}{3\pi}\int_1^\infty \rho(\xi)\frac{\alpha}{x_{e\mu}}e^{-2m_e\xi x_{e\mu}}d\xi. \tag{37}$$

When studying the energy levels of light two-particle muonic atoms, it was found that the contribution of the electron vacuum polarization is the main one both for the $2P$-$2S$ Lamb shift and for the $2S$-$1S$ interval [20,21]. Therefore, we will take into account the correction for vacuum polarization to the Coulomb potential (36). For any electronic states $1S$, $2S$, and $2P$, this correction in the energy spectrum is the same; therefore, for the $2P$-$2S$ and $2S$-$1S$ intervals, the contribution is zero. In the second order of perturbation theory, the vacuum polarization contribution (36) is determined by the integral expression

$$\Delta E^{(2)\mu N}_{\rm VP} = \frac{2\alpha}{3\pi}\int \psi_{\mu 0}(\mathbf{x}_\mu)\psi_{e1}(\mathbf{x}_e)\Big(-\frac{Z\alpha}{x_\mu}\Big)\sum_{n,n'}\frac{\psi_{\mu n}(\mathbf{x}_\mu)\psi_{en'}(\mathbf{x}_e)\psi_{\mu n}(\mathbf{x}'_\mu)\psi_{en'}(\mathbf{x}'_e)}{E_{\mu 0}+E_{e1}-E_{\mu n}-E_{en'}}$$
$$\times\,\rho(\xi)e^{-2m_e\xi x_\mu}d\xi\,\psi_{\mu 0}(\mathbf{x}'_\mu)\psi_{e1}(\mathbf{x}'_e)\Big(\frac{\alpha}{x'_{\mu e}}-\frac{\alpha}{x'_e}\Big)d\mathbf{x}_\mu d\mathbf{x}'_\mu d\mathbf{x}_e d\mathbf{x}'_e. \tag{38}$$

Taking into account the orthogonality of the electronic wave functions in the initial and intermediate states, it is necessary to set $n' = nL$ ($1S$, $2S$, and $2P$). Then the difference in the contribution of the muon-nuclear polarization of the vacuum will be connected with the remaining integral over the coordinates of the electron in this matrix element. For the states $1S$, $2S$, and $2P$ these integrals have the form

$$J_1 = \int \big|\psi^e_{1S}(\mathbf{x}'_e)\big|^2\Big(\frac{\alpha}{x'_{\mu e}}-\frac{\alpha}{x'_e}\Big) = 2\alpha W_e\frac{e^{-W_e x'_\mu}}{W_e x'_\mu}\big[-W_e x'_\mu\cosh(W_e x'_\mu)+\sinh(W_e x'_\mu)\big], \tag{39}$$

$$J_2 = \int \big|\psi^e_{2S}(\mathbf{x}'_e)\big|^2\Big(\frac{\alpha}{x'_{\mu e}}-\frac{\alpha}{x'_e}\Big) = \frac{\alpha W_e}{4}\frac{1}{2W_e x'_\mu}(8-2W_e x'_\mu+e^{-W_e x'_\mu}\{-8-W_e x'_\mu[6+W_e x'_\mu(2+W_e x'_\mu)]\}), \tag{40}$$

$$J_3 = \int \big|\psi^e_{2P}(\mathbf{x}'_e)\big|^2\Big(\frac{\alpha}{x'_{\mu e}}-\frac{\alpha}{x'_e}\Big) = \frac{\alpha W_e}{48}\frac{1}{W_e x'_\mu}[-12W_e x'_\mu - 36W_e x'_\mu e^{-W_e x'_\mu}$$
$$+48(1-e^{-W_e x'_\mu})-12(W_e x'_\mu)^2 e^{-W_e x'_\mu}-2(W_e x'_\mu)^3 e^{-W_e x'_\mu}]. \tag{41}$$

Given the explicit expressions for J_i, it is possible to perform analytical integration over the particle coordinates in (38). Expanding in the parameter a_1 and integrating over the remaining spectral parameter ξ, we obtain the contribution in the form

$$\Delta E^{(2)\mu N}_{\rm VP}(1S) = \frac{64\alpha^2 W_\mu}{3\pi}\int\rho(\xi)d\xi\int_0^\infty x_\mu dx_\mu\int_0^\infty x'_\mu dx'_\mu g_{1S}(x_\mu,x'_\mu)e^{-2x_\mu(1+a_2\xi)}e^{-2x'_\mu(1+a_1/2)}[-a_1x'_\mu\cosh(a_1x'_\mu)+\sinh(a_1x'_\mu)]$$
$$= \frac{\alpha^2 W_\mu a_1^3}{432\pi\big(1-a_2^2\big)^{9/2}}\Bigg\{-8\big(1-a_2^2\big)^{3/2}\big(-152+978a_2^2-2763a_2^4+2924a_2^6-1032a_2^8-516\pi a_2^3+1548\pi a_2^5$$
$$-1548\pi a_2^7+516\pi a_2^9\big)+24\big(48-216a_2^2+948a_2^4-2285a_2^6+2709a_2^8-1548a_2^{10}+344a_2^{12}\big)\ln\frac{a_2}{1-\sqrt{1-a_2^2}}\Bigg\}, \tag{42}$$

$$\Delta E^{(2)\mu N}_{\rm VP}(2S) = \frac{\alpha^2 W_\mu a_1^3}{3456\pi\left(1-a_2^2\right)^4}\left\{-\left[1216+a_2^2\left(-9040+a_2\left(29\,928a_2-45\,496a_2^3+31\,648a_2^5-8256a_2^7+4128\left(1-a_2^2\right)\pi\right)\right)\right]\right.$$
$$\left.+24\sqrt{1-a_2^2}\left(-48+168a_2^2-780a_2^4+1505a_2^6-1204a_2^8+344a_2^{10}\right)\ln\frac{a_2}{1+\sqrt{1-a_2^2}}\right\}, \tag{43}$$

$$\Delta E^{(2)\mu N}_{\rm VP}(2P) = \frac{\alpha^2 W_\mu a_1^5}{230\,400\pi\left(1-a_2^2\right)^{11/2}}\left\{\sqrt{1-a_2^2}\left(32\,804-290\,020a_2^2+1\,252\,145a_2^4-2\,539\,811a_2^6\right.\right.$$
$$+2\,636\,152a_2^8-1\,368\,800a_2^{10}+283\,200a_2^{12}+141\,600\pi a_2^3-708\,000\pi a_2^5+14\,116\,000\pi a_2^7-1\,416\,000\pi a_2^9$$
$$+708\,000\pi a_2^{11}-141\,600\pi a_2^{13}\big)+15\big(-1920+10\,560a_2^2-59\,010a_2^4+174\,877a_2^6-273\,565a_2^8$$
$$\left.\left.+233\,640a_2^{10}-103\,840a_2^{12}+18\,880a_2^{14}\right)\ln\frac{a_2}{1-\sqrt{1-a_2^2}}\right\}, \tag{44}$$

where the parameter $a_2 = m_e/W_\mu$. We have presented here only the first terms of the expansions in the parameter a_1, which give the numerical values of the contributions with high accuracy.

Let us consider the calculation of other corrections for vacuum polarization, which are determined by the potentials (35) and (37) and appear already in the first order of perturbation theory. In the electron-nucleus interaction, the correction for vacuum polarization for S states is determined by the expression

$$\Delta E^{(1)eN}_{\rm VP}(nS) = -\frac{4\alpha(Z\alpha)m_e}{15\pi}\left(\frac{W_e}{m_e}\right)^3. \tag{45}$$

To estimate the value of the $2S$-$1S$ energy interval, this correction is not very significant, since it has values of tens of gigahertz. It is more important for the total value of the $2P$-$2S$ Lamb shift. In the case of the $2P$ state, the correction for vacuum polarization has the form

$$\Delta E^{(1)eN}_{\rm VP}(2P) = -\frac{\alpha(Z\alpha)m_e}{560\pi}\left(\frac{W_e}{m_e}\right)^5 \tag{46}$$

and is very small. Therefore, the value of this correction to the $2P$-$2S$ shift is determined by (45):

$$\Delta E^{(1)eN}_{\rm VP}(2P-2S) = \begin{cases} {}^7_3{\rm Li}\mu e, & 0.650\ {\rm GHz} \\ {}^9_4{\rm Be}\mu e, & 2.929\ {\rm GHz} \\ {}^{10}_5{\rm B}\mu e, & 8.680\ {\rm GHz}. \end{cases} \tag{47}$$

The correction of the muon-electron vacuum polarization [the potential (37)] is also important for the $2P$-$2S$ shift. Taking into account the expansion terms a_1^2 and a_1^3, it takes the form

$$\Delta E^{(1)e\mu}_{\rm VP}(2P\text{-}2S) = -\frac{\alpha^2 W_e}{3\pi}a_1^2\left\{\frac{2}{5a_2^2}+\frac{a_1}{480a_2^4\sqrt{4-a_2^2}}\left[\sqrt{4-a_2^2}\left(-620a_2^4-120a_2^6-150\pi a_2-270\pi a_2^3+135\pi a_2^5+30\pi a_2^7\right)\right.\right.$$
$$\left.\left.+30a_2^4\left(-40+5a_2^2+2a_2^4\right)\ln\frac{2-\sqrt{4-a_2^2}}{a_2}\right]\right\} = \begin{cases} {}^7_3{\rm Li}\mu e, & -0.212\ {\rm GHz} \\ {}^9_4{\rm Be}\mu e, & -0.711\ {\rm GHz} \\ {}^{11}_5{\rm B}\mu e, & -1.670\ {\rm GHz}. \end{cases} \tag{48}$$

Another correction in the energy spectrum that improves the accuracy of the results is the correction for the structure of the nucleus. In two-particle muonic atoms, the correction for the structure of the nucleus is significant, since the muon is closer to the nucleus than the electron. The interaction potentials of a muon and a nucleus and of an electron and a nucleus, necessary for calculating the correction, are determined by the formulas

$$\Delta V^{\mu N}_{\rm str}(\mathbf{x}_\mu) = \frac{2}{3}\pi(Z\alpha)r_N^2\delta(\mathbf{x}_\mu),$$
$$\Delta V^{eN}_{\rm str}(\mathbf{x}_e) = \frac{2}{3}\pi(Z\alpha)r_N^2\delta(\mathbf{x}_e), \tag{49}$$

respectively, where r_N is the nuclear charge radius. The potential $\Delta V^{\mu N}_{\rm str}(\mathbf{x}_\mu)$ does not contribute to the $2S$-$1S$ and $2P$-$2S$ shifts in the first order of perturbation theory, since it depends only on the muon coordinate. The $\Delta V^{\mu N}_{\rm str}(\mathbf{x}_\mu)$ contribution in the second order of perturbation theory is expressed in terms of the reduced Coulomb Green's function of the muon $1S$ state with one zero argument, which has the form

$$\tilde G^\mu_{1S}(\mathbf{r}) = \frac{Z\alpha M_\mu^2}{4\pi}\frac{e^{-x}}{x}g_{1S}(x),$$
$$g_{1S}(x) = \left[4x(\ln 2x + C) + 4x^2 - 10x - 2\right]. \tag{50}$$

The different kind of correction for the electronic states $1S$, $2S$, and $2P$ is determined by the same functions J_i [Eqs. (39)–(41)] as for vacuum polarization. The initial integral expression for this correction is presented as

$$\Delta E^{(2)\mu N}_{\rm str}(nL) = \frac{4}{3}(Z\alpha) r_N^2 W_\mu^3 \int \tilde{G}^{\mu}_{1S}(\mathbf{x}_\mu) J_i(\mathbf{x}_\mu) e^{-W_\mu x_\mu} d\mathbf{x}_\mu. \quad (51)$$

For all electronic states, coordinate integration is performed analytically and the results can be presented as

$$\Delta E^{(2)\mu N}_{\rm str}(1S) = \frac{8}{3}\alpha(Z\alpha) r_N^2 W_\mu^2 M_\mu a_1^3 \left[-\frac{11}{6} + \frac{155}{24} a_1 + O\big(a_1^2\big)\right], \quad (52)$$

$$\Delta E^{(2),\mu N}_{\rm str}(2S) = \frac{1}{3}\alpha(Z\alpha) r_N^2 W_\mu^2 M_\mu a_1^3 \left[-\frac{11}{6} + \frac{155}{24} a_1 + O\big(a_1^2\big)\right], \quad (53)$$

$$\Delta E^{(2)\mu N}_{\rm str}(2P) = -\frac{1}{2880}\alpha(Z\alpha) r_N^2 W_\mu^2 M_\mu a_1^5 \big[591 - 1659 a_1 + O\big(a_1^2\big)\big]. \quad (54)$$

The high degree of a_1 in (54) for the $2P$ state makes this correction in the Lamb shift negligible. The second potential from (49) gives a known contribution already in the first order of perturbation theory:

$$\Delta E^{(1),eN}_{\rm str}(nS) = \frac{2}{3n^3}(Z\alpha)^4 r_N^2 M_e^3 \delta_{l0}. \quad (55)$$

The numerical values of the corrections (53) and (55) are important to refine the results on the Lamb shift, since they are tenths of a gigahertz.

The nuclear recoil contribution is determined by the Hamiltonian $\Delta H_{\rm rec}$. In the first-order perturbation theory the recoil correction is equal to zero due to the vanishing of the integral over the angular variables. For the same reason, the state of the muon with $n = 0$ in the second order of perturbation theory does not contribute. The muon contribution with $n \neq 0$ can be written in the second-order perturbation theory as

$$\Delta E^{(2)}_{\rm rec}(2S) = -\frac{M_e W_\mu^2 W_e^2}{8\pi m_N^2} \int \psi_{\mu 0}(\mathbf{x}_\mu) \frac{\partial}{\partial x'_e} \psi_{e2S}(\mathbf{x}_e) \frac{\mathbf{x}_\mu \mathbf{x}_e}{x_\mu x_e} d\mathbf{x}_\mu d\mathbf{x}_e \sum_{n\neq 0} \psi_{\mu n}(\mathbf{x}_\mu) \psi^*_{\mu n}(\mathbf{x}'_\mu) \frac{e^{-b|\mathbf{x}_e - \mathbf{x}'_e|}}{|\mathbf{x}_e - \mathbf{x}'_e|} \frac{\mathbf{x}'_\mu \mathbf{x}'_e}{x'_\mu x'_e} \psi_{\mu 0}(\mathbf{x}'_\mu) \frac{\partial}{\partial x'_e} \psi_{e2S}(\mathbf{x}'_e) d\mathbf{x}'_\mu d\mathbf{x}'_e. \quad (56)$$

In this expression, the integral symmetric tensor in the coordinates of the electron can be distinguished

$$J^{ij} = \int d\mathbf{x}_e d\mathbf{x}'_e \frac{x_e{}^i x'_e{}^j}{x_e x'_e} \frac{e^{-b|\mathbf{x}_e - \mathbf{x}'_e|}}{|\mathbf{x}_e - \mathbf{x}'_e|} \frac{\partial}{\partial x'_e} \psi_{e2S}(\mathbf{x}_e) \frac{\partial}{\partial x'_e} \psi_{e2S}(\mathbf{x}'_e) = \delta^{ij} A, \quad (57)$$

where the value of the integral is found after convolution with the tensor δ^{ij}:

$$A = \frac{\pi}{3W_e^2}(4b_1^2 - 13b_1^4), \quad b_1^2 = \frac{M_e}{M_\mu}\frac{(Z-1)^2}{Z^2}\frac{n^2}{n^2-1}. \quad (58)$$

A similar calculation for the $2P$ state gives a factor $4b_1^2 - \frac{7}{3}b_1^4$ in the corresponding integral for the $2P$ state. In the difference, the first terms cancel out and the final result has the form

$$\Delta E^{(2)}_{\rm rec}(2P\text{-}2S) = -\frac{16}{9}\frac{M_e \alpha^2 M_e^2 (Z-1)^4}{Z^2 m_N^2} \int d\mathbf{x}_\mu \int d\mathbf{x}'_\mu \sum_{n\neq 0} \psi^*_{\mu 0}(\mathbf{x}_\mu) \frac{\mathbf{x}_\mu}{x_\mu} \psi_{\mu n}(\mathbf{x}_\mu) \psi^*_{\mu 0}(\mathbf{x}'_\mu) \frac{\mathbf{x}'_\mu}{x'_\mu} \psi_{\mu n}(\mathbf{x}'_\mu) \frac{n^4}{(n^2-1)^2}. \quad (59)$$

The square of the radial integral for the $1S \to nP$ transition has the form

$$\big(I^{nP}_{1S}\big)^2 = \frac{4}{n(n^2-1)}\left[1 - \frac{(5n^2-1)}{(n^2-1)}\frac{(n-1)^n}{(n+1)^n}\right]^2, \quad I^{nP}_{1S} = \int_0^\infty R_{10}(r) R_{n1}(r) r\, dr. \quad (60)$$

Then the contributions of discrete and continuous spectra in (59) are determined by the expressions

$$C^d = \sum_{n=2}^{\infty} \frac{4n^3}{(n^2-1)^3}\left[1 - (5n^2-1)\frac{(n-1)^{n-1}}{(n+1)^{n+1}}\right] = 0.474\,899\ldots, \quad (61)$$

$$C^c = \int_0^\infty \frac{4k\,dk}{(k^2+1)^3(1-e^{-2\pi/k})}\left[1 - \frac{(5+k^2)}{(1+k^2)}\left(\frac{1+ik}{1-ik}\right)^{i/k}\right]^2 = 0.129\,105\ldots. \quad (62)$$

As a result, the total value of the correction (59) in the Lamb shift is

$$\Delta E^{(2)}_{\rm rec}(2P\text{-}2S) = -\frac{16}{27}\frac{M_e \alpha^2 M_e^2 (Z-1)^4}{Z^2 m_N^2}(C^d + C^c) = \begin{cases} {}^7_3{\rm Li}\mu e, & -0.026\ {\rm GHz} \\ {}^9_4{\rm Be}\mu e, & -0.044\ {\rm GHz} \\ {}^{11}_5{\rm B}\mu e, & -0.060\ {\rm GHz}. \end{cases} \quad (63)$$

TABLE I. Electronic $2S$-$1S$ energy interval in gigahertz.

Contribution	$(\mu e\,{}^{7}_{3}\mathrm{Li})$	$(\mu e\,{}^{9}_{4}\mathrm{Be})$	$(\mu e\,{}^{11}_{5}\mathrm{B})$
Eq. (65)	$9.868\,999\times10^{6}$	$22.205\,543\times10^{6}$	$39.476\,833\times10^{6}$
vacuum polarization correction	2.140	13.418	45.433
nuclear structure correction	−0.188	−0.527	−1.286
relativistic correction	481.832	2439.636	7711.943
QED correction	−95.367	−420.460	−1189.068
summary	9.8690×10^{6}	22.2055×10^{6}	39.4768×10^{6}

IV. NUMERICAL RESULTS

The total analytical contribution of the perturbation operators ΔH and $\Delta H_{\rm rec}$ obtained in the first and second orders of perturbation theory to the $2P$-$2S$ Lamb shift is

$$\Delta E(2P\text{-}2S)=M_e\alpha^2\Big[\frac{Z-1}{4}a_1^2-\frac{5Z}{8}a_1^3-\frac{Z-1}{36Z}a_1^3(S^d+S^c)-\frac{16}{27}\frac{M_e^2(Z-1)^4}{Z^2m_N^2}(C^d+C^c)+\Big(\frac{15Z}{16}-\frac{381}{512}\Big)a_1^4-\frac{1}{2}a_1^4\ln a_1\Big]. \tag{64}$$

Similarly, the $2S$-$1S$ energy interval obtained taking into account the recoil effects according to the perturbation theory with the Hamiltonian ΔH is

$$\Delta E(2S\text{-}1S)=M_e\alpha^2\Big[\frac{(Z-1)^2}{2}+\tfrac{7}{4}(Z-1)a_1^2+\Big(5-\frac{25}{8}Z\Big)a_1^3+\Big(\frac{513}{64}Z-\frac{4203}{512}\Big)a_1^4+\tfrac{1}{2}a_1^4\ln a_1\Big]. \tag{65}$$

Using the values of the fundamental parameters of the theory, one can obtain from the formulas (64) and (65) numerical estimates of the electronic Lamb shift and the $2S$-$1S$ interval for muonic lithium (${}^{7}_{3}$Li), beryllium (${}^{9}_{4}$Be), and boron (${}^{11}_{5}$B) ions, which are presented in Tables I and II. The calculation of the $2S$-$1S$ and $2P$-$2S$ energy intervals is also performed by us within the framework of the variational method formulated in [14,15] with very high accuracy (see Sec. V). Our analytical results coincide with numerical calculations of $2S$-$1S$ in the variational approach with an accuracy of 0.0001 GHz. In the case of the Lamb shift, the difference between the results from Table II (see row 1) from the variational calculations turns out to be more significant. Here are the results of the variational method with an accuracy of 0.001 GHz:

$$\begin{aligned}\Delta E_{\rm Li}(2P\text{-}2S)7&=36.568\ \text{GHz},\\ \Delta E_{\rm Be}(2P\text{-}2S)&=68.015\ \text{GHz},\\ \Delta E_{\rm B}(2P\text{-}2S)&=101.947\ \text{GHz}.\end{aligned} \tag{66}$$

This difference between (66) and the results in line 1 of Table II is due to the approximation that we use in analytical calculations in the second order of perturbation theory. Expanding in the parameter b [Eq. (19)], we take into account the leading-order correction in M_e/M_μ and therefore neglect the contributions of $O(\sqrt{M_e/M_\mu})$ with respect to the contribution considered.

TABLE II. Electronic $2P$-$2S$ Lamb shift in gigahertz.

Contribution	$(\mu e\,{}^{7}_{3}\mathrm{Li})$	$(\mu e\,{}^{9}_{4}\mathrm{Be})$	$(\mu e\,{}^{11}_{5}\mathrm{B})$
Eq. (64)	34.837	65.684	99.214
vacuum polarization correction	0.306	1.916	6.491
nuclear structure correction	−0.027	−0.075	−0.184
relativistic correction	0	0	0
QED correction	−14.257	−63.273	−180.004
summary	20.859	4.252	−74.483

The corrections for the nuclear structure and vacuum polarization calculated in Sec. III are included in Tables I and II in separate rows. They are important for refining the $2P$-$2S$ Lamb shift. There are two more important corrections that must be taken into account when obtaining the total numerical value of the energy interval: the relativistic correction and the QED correction, which is the main one for obtaining the Lamb shift in the hydrogen atom. An analytical expression is known for it, which we represent in the form without vacuum polarization correction [22]:

$$\Delta E_{\rm QED}(nS)=\frac{\alpha[(Z-1)\alpha]^4}{\pi n^3}\frac{M_e^3}{m_e^2}\Big[\frac{4}{3}\ln\frac{m_e}{M_e(Z-1)^2\alpha^2}-\frac{4}{3}\ln k_0(nS)+\frac{10}{9}\Big], \tag{67}$$

$$\Delta E_{\rm QED}(2P)=\frac{\alpha[(Z-1)\alpha]^4}{8\pi}\frac{M_e^3}{m_e^2}\Big[-\frac{4}{3}\ln k_0(2P)-\frac{m_e}{6M_e}\Big]. \tag{68}$$

Relativistic corrections of $O(\alpha^4)$ and $O(\alpha^6)$ connected with the motion of the electron are also known in analytical form [22]. They can be important only for the $2S$-$1S$ interval. As we noted at the beginning of this work, the electronic Lamb shift in muon-electron ions of lithium, beryllium, and boron appears already in $O(\alpha^2)$ [Eq. (64)], but the main term is also proportional to a_1^2. Thus, Eq. (64) contains two small expansion parameters. Although the QED corrections (67) and (68) have a high order of smallness in α, they also depend on the nuclear charge Z, which leads to an increase in this correction when passing to ions with large Z. As a result, with

TABLE III. Various contributions to the $\Delta E(2S\text{-}1S)$ and $\Delta E(2P_{1/2}\text{-}2S)$ energy intervals in the $(\mu e\,{}^7_3\mathrm{Li})$ ion (in gigahertz) in the variational method.

Contribution	$\Delta E(2S\text{-}1S)$	$\Delta E(2P_{1/2}\text{-}2S)$
E_{NR}	9 869 022.575	36.568
ΔE_{BP}	482.067	116.833
$\Delta E_{\mathrm{fs}}(2P_{1/2})$		−117.019
$\Delta E_{\mu N}$	−0.649	−0.056
ΔE_{VP}	3.038	0.434
ΔE_{QED}	−95.367	−14.257
$\Delta E_{\mathrm{HO\text{-}QED}}$	−1.56(2)	−0.221(2)
E_{tot}	9 869 410.10(2)	22.160(2)

an increase in Z, the effect of compensation for two corrections is observed. If for the lithium ion the value of the $2P$-$2S$ shift is positive, then for the boron ion it becomes negative and for the beryllium ion the QED correction and (64) are almost completely canceled. The obtained total values of the $2P$-$2S$ and $2S$-$1S$ energy intervals in Tables I and II can serve as a reference point for comparison with future experimental data. They are presented with an accuracy of three digits after the decimal point according to the obtained analytical formulas. Nevertheless, the calculation accuracy is not so high, since a number of approximations are used in the work to calculate the recoil effects M_e/M_μ. We can estimate the contribution of some of the unaccounted for terms to the $2P$-$2S$ Lamb shift connected with this expansion to 0.5 GHz. We have estimated the uncalculated terms using the main factors α and M_e/M_μ determining the order of the contribution, as well as the obtained numerical results. It is possible that the exact calculation of the corresponding coefficients will lead to the coincidence of the complete variational results and the results of analytical perturbation theory.

V. EXPLICIT THREE-BODY FORMALISM

The obtained results can be improved using the variational method in the three-body problem. Numerically, the nonrelativistic Schrödinger solution may be obtained via a variational approach with almost arbitrary precision [23]. The variational approach also allows us to calculate different corrections by the perturbation theory. Let us focus on the calculation of relativistic corrections which are equal to zero in a two-body approximation. Relativistic corrections are determined by the Breit-Pauli Hamiltonian [24,25]

$$H_{\mathrm{BP}} = -\frac{p_e^4}{8m^3} + \frac{1}{8m^2}4\pi[Z\delta(\mathbf{x}_e) - \delta(\mathbf{x}_{\mu e})] + \frac{Z}{2}\frac{p_e^i}{m_e}\left(\frac{\delta^{ij}}{r_1} + \frac{r_1^i r_1^j}{r_1^3}\right)\frac{P_N^j}{M} - \frac{1}{2}\frac{p_e^i}{m_e}\left(\frac{\delta^{ij}}{x_{\mu e}} + \frac{x_{\mu e}^i x_{\mu e}^j}{x_{\mu e}^3}\right)\frac{p_\mu^j}{m_\mu}, \tag{69}$$

where $\mathbf{P}_N = -(\mathbf{p}_\mu + \mathbf{p}_e)$ and $\mathbf{x}_{\mu e} = \mathbf{x}_e - \mathbf{x}_\mu$. For the $2P$ state we have as well the fine-structure contribution to the Hamiltonian

$$\Delta H_{\mathrm{fs}} = b_{\mathrm{fs}}(\mathbf{s}_e \cdot \mathbf{L}), \tag{70}$$

where $\mathbf{L}$ is an operator of the total orbital momentum of the three-body system and b_{fs} is expressed in terms of the reduced matrix elements of the three-body operators as [23,25]

$$b_{\mathrm{fs}} = (2\,\mathrm{Ry})\frac{\alpha^2}{\sqrt{L(L+1)(2L+1)}}\left\{\frac{Z(1+2a_e)}{2m_e^2}\left\langle L\left\|\frac{\mathbf{x}_e\times\mathbf{p}_e}{x_e^3}\right\|L\right\rangle + \frac{Z(1+a_e)}{Mm_e}\left\langle L\left\|\frac{\mathbf{x}_e\times\mathbf{P}_N}{x_e^3}\right\|L\right\rangle\right.$$
$$\left. -\frac{1+2a_e}{2m_e^2}\left\langle L\left\|\frac{\mathbf{x}_{\mu e}\times\mathbf{p}_e}{x_{\mu e}^3}\right\|L\right\rangle - \frac{1+a_e}{m_\mu m_e}\left\langle L\left\|\frac{\mathbf{x}_{\mu e}\times\mathbf{p}_\mu}{x_{\mu e}^3}\right\|L\right\rangle\right\},$$

where Ry is the Rydberg constant and a_e is the electron anomalous magnetic moment. The results of numerical computation of relativistic and other corrections for the $\mu e\,{}^7_3\mathrm{Li}$ ion are summarized in Table III.

The largest contribution to the leading-order QED (one-loop) corrections is the vacuum polarization (36) due to the small subsystem (μN). For the case of the $\mu e\,{}^7_3\mathrm{Li}$ ion $\Delta E_{\mathrm{VP}}^{\mu N} = -14\,814\,915$ GHz. Still, the total contribution of this leading vacuum polarization correction to the $2S$-$1S$ energy interval is smaller than 1 GHz, since the wave function of the small subsystem differs too little between the states under consideration.

The other QED contributions can be calculated using a simplified two-body approximation with a pseudonucleus μN by means of the formulas (35) and (37) for the vacuum polarization and Eqs. (67) and (68) for the one-loop self-energy. Higher-order QED contributions are also important and have to be included. The following one- and two-loop corrections [26] have been taken into consideration,

$$\Delta E_{\text{1-loop}}(nS) = \frac{\alpha(Z^*\alpha)^5}{\pi n^3}\left\{4\pi\left(\frac{139}{128} - \frac{1}{2}\ln 2 + \tfrac{5}{192}\right)\right.$$
$$+ (Z^*\alpha)[-\ln^2(Z^*\alpha)^{-2}$$
$$\left. + A_{61}(nS)\ln(Z^*\alpha)^{-2}]\right\} + \cdots,$$
$$\Delta E_{\text{1-loop}}(2P_{1/2}) = \frac{\alpha(Z^*\alpha)^6}{\pi n^3}\left[\frac{103}{180}\right]\ln(Z^*\alpha)^{-2},$$
$$\Delta E_{\text{2-loop}}(nS) = \frac{\alpha^2(Z^*\alpha)^4}{\pi^2 n^3}[0.538\,941], \tag{71}$$

where $Z^* = Z - 1$ is the charge of a pseudonucleus and the state-dependent coefficient $A_{61}(nS)$ is taken as in [26] [Eq. (2.5) therein]. For the purposes of our study, the accuracy that is determined by the formula (71) is sufficient. Numerical

TABLE IV. The $\Delta E(2S\text{-}1S)$ and $\Delta E(2P_{1/2}\text{-}2S)$ energy intervals for muonic He, Li, Be, and B ions (in gigahertz) in the variational method.

Muonic ion	$\Delta E(2S\text{-}1S)$	$\Delta E(2P_{1/2}\text{-}2S)$
$(\mu e\,^4_2\mathrm{He})$	2 467 150.79(1)	9.665(1)
$(\mu e\,^7_3\mathrm{Li})$	9 869 410.10(2)	22.160(2)
$(\mu e\,^9_4\mathrm{Be})$	22 207 596.32(8)	4.022(8)
$(\mu e\,^{11}_5\mathrm{B})$	39 483 388.3(4)	−82.03(4)

calculations of higher-order corrections were performed in Ref. [27].

The final results of calculations in the three-body formalism are presented in Table IV. The uncertainties indicated stem from two sources: the uncalculated higher-order contributions and the imperfectness of the pointlike model for the pseudonucleus.

VI. CONCLUSION

In this work we investigated the energy levels in a muon-electron-nucleus three-particle system. We calculated the electronic $2S$-$1S$ energy interval and electronic $2P$-$2S$ Lamb shift in electron-muon ions of lithium, beryllium, and boron using the analytic perturbation theory method and the variational approach. The results of the calculation in analytic perturbation theory were presented in Tables I and II. The results of the calculation on the basis of the variational method were presented in Tables III and IV. The results obtained by different methods are in agreement, taking into account the theoretical errors. We investigated the dependence of the electronic $2P$-$2S$ Lamb shift on the nuclear charge Z. An interesting effect of $2P$ and $2S$ level reorientation was discovered when passing from a beryllium ion to a boron ion. The extension of studies of the energy levels of electron-muonic helium in [18] to three-particle systems with other nuclei could facilitate the experimental study of this issue.

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