Low energy levels in neutral muonic helium within a nonrelativistic approach

Savely G. Karshenboim,[1,2,3,*] Vladimir G. Ivanov,[3] and Vladimir I. Korobov[4]
[1]*Ludwig-Maximilians-Universität, Fakultät für Physik, 80799 München, Germany*
[2]*Max-Planck-Institut für Quantenoptik, Garching, 85748, Germany*
[3]*Pulkovo Observatory, St. Petersburg, 196140, Russia*
[4]*Joint Institute for Nuclear Research, Joliot-Curie 6, 141980 Dubna, Moscow region, Russia*

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We consider a nonrelativistic approximation for the neutral muonic helium atom, a three-body system, which consists of an electron, a muon, and a helium nucleus. We discuss the case with the muon in the ground state and study the low energy levels and the transition frequencies of the electron ($2s-1s$ and $2p-2s$). We treat neutral muonic helium both as a three-body system (with a numerical variational solution) and as a two-body system of an electron bound by a two-body compound nucleus. We compare the results of two approaches and discuss the validity and consistency of fits and of the nonrelativistic approximation.

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I. INTRODUCTION

A neutral muonic helium atom is a three-body system, consisting of an electron, a muon, and a nucleus. It is an exotic system, but within a reach. In particular, it has been successfully formed [1] and its hyperfine interval was studied [2].

With a muon at a low state, it allows the results in closed analytic form, based on the idea of a subsequent consideration of two two-body problems [3–6]. One is the problem of a two-body system of a muon and a nucleus. In its turn that system plays a role of a compound nucleus which makes a hydrogenlike atom with an electron. We remind that the compound nucleus (in the case of the muon at one of the lowest states) has a size comparable with the Compton wavelength of the electron $\lambda\!\!\!^{-}_C$, while the electron atomic cloud has a standard size of the Bohr radius a_B, which is two orders of magnitudes ($\sim\alpha^{-1}$) larger than the Compton wavelength.

The other group of the available theoretical results is from a numerical treatment which starts from a variational solution of a three-body nonrelativistic problem (see [7,8] for detail).

In this paper, we perform numerical nonrelativistic calculations for the system with the muon at the $1s$ state and the electron in the $1s$, $2s$, and $2p$ states. The calculations are performed for the infinite mass of the nucleus. To interpret the results on the energy levels in the terms of an analytic expansion, we perform several fits.

We qualitatively understand certain details of the functional dependence of the energy (in atomic units) on the mass ratio m_e/m_μ, which is the only parameter for the nonrelativistic energy levels in the case of infinitely heavy nucleus. Some coefficients of the analytic expansion are known [9]. Different fits use different portions of our understanding, which allows us to verify various hypotheses.

We discuss the numerical results, obtained on the coefficients, and improve them (in comparison with the direct numerical results) by using certain corrections due to the finite value of the actual nuclear mass.

Once we put the nuclear mass to the infinity and consider the muon in the ground state, the complete binding energy of an electronic level nl_j (expressed in atomic units) depends only on two parameters: the value of the fine structure constant α and the electron-to-muon mass ratio m_e/m_μ:

$$\begin{aligned}\mathcal{E}_{nl_j}(\alpha,m_e/m_\mu) = {}& \mathcal{E}^{(0)}_{nl_j}(m_e/m_\mu) + \alpha\,\mathcal{E}^{(1)}_{nl_j}(m_e/m_\mu) \\ & + \alpha^2\mathcal{E}^{(2)}_{nl_j}(m_e/m_\mu) \\ & + \alpha^3\mathcal{E}^{(3)}_{nl_j}(m_e/m_\mu) + \cdots . \end{aligned} \tag{1}$$

Rigorously speaking, that is not a Taylor expansion in α, but rather an indication of the order of magnitude of the contributions. The coefficients $\mathcal{E}^{(k)}_{nl_j}$, except of the first one, may include a weak α dependence such as a logarithmic one. Some relativistic and radiative corrections are discussed in [9,10]. In particular, the contributions $\mathcal{E}^{(1)}_{nl_j}$ and $\mathcal{E}^{(3)}_{nl_j}$ appear through the radiative corrections, while the $\mathcal{E}^{(2)}_{nl_j}$ term is mostly due to the relativistic effects.

The specificity of the electronic energy levels in a three-body system with a hierarchy ($m_e \ll m_\mu \ll M$) is that additionally to rather kinematic relativistic corrections for the electron, there is another way to involve the relativistic effects through the structure of the compound nucleus. The compound nucleus is compact and because of its small size the effects due to the penetration of the electron into the nucleus are of the relativistic nature. That happens in all atomic systems, including electronic and muonic two-body atoms with an ordinary nucleus. In an ordinary situation, the ratio of the nuclear radius to the characteristic electron's or muon's radius explicitly contains α indicating the presence of the relativistic effects.

*savely.karshenboim@mpq.mpg.de

In the specific case of neutral muonic helium with the muon in the ground state, the compound nucleus has a characteristic size of $\hbar/(2\alpha m_\mu c)$. Due to that the ratio of the radius of the compound nucleus to the electron's Bohr radius does not depend on α being of order of m_e/m_μ. The effects due to the penetration are relativistic ones, however, they are not "marked" with α. Because of that, the relativistic effects do contribute into $\mathcal{E}^{(0)}_{nl_j}(m_e/m_\mu)$. Analyzing our numerical results we also discuss to what extent the value of $\mathcal{E}^{(0)}_{nl_j}(m_e/m_\mu)$ agrees with the result of nonrelativistic calculations.

II. APPLICABILITY OF THE NONRELATIVISTIC APPROXIMATION

The low energy levels of the neutral muonic helium could be numerically obtained via minimization of the nonrelativistic (NR) Hamiltonian. In the case of the infinite nuclear mass ($M = \infty$), it takes the form

$$\mathcal{H}^{\rm NR} = \frac{\mathbf{p}_e^2}{2m_e} + \frac{\mathbf{p}_\mu^2}{2m_\mu} + \frac{e^2}{r_{e\mu}} - \frac{2e^2}{r_e} - \frac{2e^2}{r_\mu}, \tag{2}$$

where e is the elementary charge, while $\alpha = e^2/\hbar c$ is the fine structure constant. Here, we explicitly take into account that the nuclear charge is equal to 2.

There is a certain confusion with using words "relativistic corrections." In a narrow sense, this term is used for the corrections due v/c expansion, Breit potential, etc. In other words, they are relativistic corrections in the problem where there is no special parameter related to velocity, except of the speed of light. In more general sense, the relativistic effects are any effects where the particle is fast. The short-distance effects are the relativistic ones because they involve the high momentum and the related corrections are of the relativistic nature. The problem we consider here is the problem of relativistic effects in general context.

The results, obtained with Hamiltonian (2), require a certain interpretation. One has to check whether the calculation is restricted to nonrelativistic momenta. To understand that one may take advantage of an analytic evaluation, which has quite a limited accuracy to the date. The latter can be performed if we split Hamiltonian (2) into two parts and introduce an "unperturbed" Hamiltonian

$$\mathcal{H}^{\rm NR:unp} = \frac{\mathbf{p}_e^2}{2m_e} + \frac{\mathbf{p}_\mu^2}{2m_\mu} - \frac{e^2}{r_e} - \frac{2e^2}{r_\mu}, \tag{3}$$

which allows an exact analytic solution, and a perturbation

$$\mathcal{H}^{\rm NR:pert} = \frac{e^2}{r_{e\mu}} - \frac{e^2}{r_e}, \tag{4}$$

which, depending on the value of m_e/m_μ and on the choice of the states of interest, may allow an efficient perturbation expansion. If the expansion is possible we may interpret the numerical solution with (2) as an effective summation of the perturbation expansion for the analytic solution.

The analytic solution with Hamiltonian (3) allows to separate variables $\mathbf{r}_e$ and $\mathbf{r}_\mu$ and to find the wave function as a product of that for the muon one bound by the nucleus with infinite mass and charge 2 and the one for the electron bound by the infinitely heavy nucleus with charge 1. The success of the perturbative expansion obviously depends on whether

$$|r_{e\mu} - r_e| \ll r_e. \tag{5}$$

That is realized in general if the muon is located in the compact area around the nucleus which is much smaller than the area where the electron is located. The condition should be realized for *each* correction which we calculate with the perturbation series. [As we show below, the condition takes place for the neutral muonic helium for characteristic values and therefore for some leading term(s) of the perturbation series. However, it fails for higher-order terms which require the integration over singularities at low r_e.]

The neutral muonic helium atom is an example of an asymmetric three-body system. It has a heavy nucleus, either the helion h or the α particle, and two lighter orbiting particles, a muon and an electron. Their masses are not comparable: $M \gg m_\mu \gg m_e$. The asymmetric three-body system are sometimes considered as a "modified" molecular system, such as molecular ion HD^+, or a "modified" atom, such as ordinary helium atom. Based on the similarity, the nonrelativistic Hamiltonian is considered and variational numerical methods are applied.

If the particle with an "intermediate mass" is at a high state (see, e.g, the case of antiprotonic helium [11]), then it is slow (i.e., essentially slower than the electron) and one can use a kind of adiabatic approximation, similar to molecular physics. The numerical approach based on the Hamiltonian (2) is fully applicable.

In the meantime, the analytic approach should have problems because the characteristic radius of the electron (in the low state) follows its Bohr radius $a_B = \lambda\!\!\!^{-}_C/\alpha = \hbar/\alpha m_e c$, while the characteristic radius of the intermediate-mass particle (e.g., of an antiproton in antiprotonic helium [11]) *does not* follow its Bohr radius $a_{B:\overline{p}} = \lambda\!\!\!^{-}_{C:\overline{p}}/\alpha = \hbar/\alpha m_{\overline{p}} c$. The latter is of order $n^2 a_{B:\overline{p}}$, where n is the principal quantum number of that particle and in the actual cases n^2 (see, e.g, [11]) is comparable with $m_{\overline{p}}/m_e$. The condition (5) (of the applicability of the analytic approach) fails. That means that the perturbative expansion consists of comparable terms. However, with a "large" internal two-body system at high n the perturbative terms do not contain singularities at low r_e. That is why the nonrelativistic consideration based on the Hamiltonian (2) is valid.

If the intermediate-mass particle is at a low state, then it is as fast as the electron and the situation becomes tricky. Indeed, the electron *is* mostly a slow particle and can be treated nonrelativistically. The problem is, however, in the physical meaning of a solution of a three-body system. The slowness of the electron means that the most of the contribution to the energy comes from characteristic distances such as the Bohr radius. However, the details of the electron's behavior at the short distances affect the energy (which we are to minimize) as well. With the muon at the low state, the condition (5) is satisfied for the characteristic distances. We can expand the perturbation (4) in r_μ/r_e. As far as the integrations are finite (after the expansion), the values of r_e and r_μ take their characteristic values which are a_B [the (electron's) Bohr radius) and $a_{B:\mu}$ (the Bohr radius for the muon), respectively. At some moment, either because of the r_μ/r_e expansion or because of higher order in the perturbation (4), the integration becomes singular at low r_e. Roughly speaking, that means that

for singular terms $r_e \sim r_\mu \sim a_{B:\mu}$. That is not only the failure of the condition (5) for the singular corrections, but, which is more important, that is an indication that the short-distance tail of the electron's wave function is crucial for them, which is the failure of the nonrelativistic approximation and a limitation on the applicability of the nonrelativistic Hamiltonian (2).

A three-body system, such as the neutral muonic helium, has a clearly distinguished internal area $\sim a_{B:\mu}$, where the muon density is located, and a larger outer area $\sim a_B$, where the electron is located. The only real question for the solution of the nonrelativistic three-body problem, does not matter how it is solved, exactly with (2) by numerical means or analytically within a perturbation expansion with (3) and (4), is to take into account the overlap of the densities of the electron and muon. It is easy to note that $a_{B:\mu} \simeq 2/3\lambda\!\!\!^{-}_C$ and therefore in the overlapping area the electron is supposed to be a relativistic one. In a sense the dynamic condition that (i) the momentum transfer $|\mathbf{q}|$ is much smaller than $m_e c$ (which means a low velocity) while (ii) the energy transfer q_0 is much smaller than $|\mathbf{q}|$ (which means a neglection of the retardation) is broken. At least we should expect high velocities and high momentum transfer.

Returning to antiprotonic helium with "ultraslow" antiproton, we note that since the antiproton is very slow, it is localized at much larger distances from the central nucleus than $a_{B:\bar{p}}$. With the principal quantum number n we can roughly estimate it as $n^2 a_{B:\bar{p}}$, which makes it comparable with the Bohr radius of the electron a_B since in actual experiments $n \sim 30$ [11]. Penetrating the antiprotonic cloud, the electron remains a nonrelativistic one (in contrast to the case of the intermediate-mass particle in the ground state, which we consider for the muon in neutral muonic helium).

What is the leading correction to the Bohr energy levels, which are the dominant contribution in the neutral muonic helium? Normally, that may be the relativistic ones, however, in the neutral muonic helium, considered as a hydrogenlike atom with an electron and a compound nucleus, the somewhat more important effects are due to the nuclear size and nuclear structure. The largest of them is due to a single-photon exchange. Such a correction is obtained within nonrelativistic physics even in the hydrogen and muonic hydrogen (see, e.g., [13]). (In the ordinary hydrogen, the penetration into the nucleus sets the ultrarelativistic condition on the electron, while in the muonic hydrogen the muon is a relativistic one, but not ultrarelativistic.) That is because we need to use the value of the wave function in vicinity of the (compound) nucleus, but not its derivatives.

The dependence of the energy of a level on the value of m_e/m_μ is not analytic. The first few terms of the expansion around $m_e/m_\mu = 0$ are of the form

$$\mathcal{E}^{\rm NR}(nl) = \alpha^2 m_e c^2 \left\{ C_1 + C_2 \left(\frac{m_e}{m_\mu}\right)^2 + C_3 \left(\frac{m_e}{m_\mu}\right)^{5/2} + \left(\frac{m_e}{m_\mu}\right)^3 \left[C_{41} \ln\left(\frac{m_\mu}{m_e}\right) + C_{40} \right] + \cdots \right\}, \quad (6)$$

where the first term is for the Bohr levels and the second one is due to the finite size of the compound nucleus [9].

Note, the dependence on m_e/m_μ is not analytic. We expect the continuity for small positive values of m_e/m_μ and rely only on it, while small negative values are not allowed. That is rather a standard assumption in atomic physics of simple atoms. Even in a simpler case of a two-body atom, which has two small parameters, the Coulomb strength $Z\alpha$ and orbiting-particle-to-nucleus mass ratio m/M, we have no analyticity around their zero values but only the continuity for small positive values [12]. The analyticity at zero would mean that zero is a regular point and a switch from small positive values, at which the atom exists, to a small negative value of either parameter, at which the atom does not exist, is smooth and continuous.

The negative value of m_e/m_μ could be achieved by considering a negative value of m_μ, at which the neutral muonic helium as a system of bound states does not exist. The analyticity at $m_e/m_\mu = 0$ is impossible. Since the behavior at small positive values of m_e/m_μ is nonanalytic, we expect that the dependence is more complicated than just a Taylor series. The most simple case is appearance of terms with semi-integer exponentials and logarithms. Such terms *do* appear in theory of the hyperfine structure of the neutral atomic helium. The semi-integer exponentials appear in [5], while a logarithmic term is found in [6]. The leading contributions to (6) have been found previously. They relate to terms with C_1 and C_2 [9]. They do not contain any nonanalytic terms. Once we suggest that such terms may appear as early as possible, we arrive at the expansion suggested above. We cannot prove it mathematically as a kind of theorem, but we have a naive estimation which confirms a possibility of such contributions at so early stage. Which is more important, a consistency and stability of the fits performed below confirm that, as a base of the fit, this expansion is reasonable.

The next-to-leading finite-nuclear-structure term is due to the two-photon exchange, which involves the polarizability of the compound nucleus and its higher-order finite-size effects. The latter is presented by the so-called Friar term, which is similar to the leading finite-size term to the hyperfine splitting (the so-called Zemach term). The details on these two terms can be found, e.g., in [13]. The Friar term is of the form

$$\begin{aligned} \Delta E_{\rm Friar}(ns) &= -\frac{2(Z\alpha)^5 m_r^4}{\pi n^3} \int_0^\infty \frac{dq}{q^4} \\ &\quad \times \{[G_E(q^2)]^2 - 1 - 2G'_E(0)\, q^2\} \\ &= -\frac{(Z\alpha)^5 m^4}{3n^3} \langle r^3 \rangle_{(2)}, \end{aligned} \quad (7)$$

where Z is the nuclear charge, G_E is the electric charge form factor, q is the momentum transfer, and in the nonrecoil limit

$$\langle r^n \rangle_{(2)} \equiv \int d^3r\, d^3r'\, \rho_E(\mathbf{r}) \rho_E(\mathbf{r}') |\mathbf{r} - \mathbf{r}'|^n \quad (8)$$

is the nth Zemach momentum with $\rho_E(\mathbf{r})$ being the density of the electric charge density distribution. In this relativistic formula, we use the relativistic units in which $\hbar = c = 1$. The third Zemach momentum is also referred to as the Friar momentum.

The specifics of this term is that once we consider the nucleus as a nonrelativistic one $R_N \ll \lambda\!\!\!^{-}_{C:N}$ (which is the case for ordinary hydrogen, muonic hydrogen, and neutral muonic helium as a two-body atom with a compound nucleus), the

retardation can be neglected and we arrive at (7), which is related to the external-field approximation. The two-photon contributions in (7) have a nonrelativistic shape of the integrand, while the area of integration is ultrarelativistic for hydrogen and relativistic (but not ultrarelativistic) for muonic hydrogen and neutral muonic helium. That happens because of a "poor" γ-matrix structure. Already three-photon exchange is described with more complicated expressions and involves terms which do not have relativistic shape because of a more rich γ-matrix structure. Such terms cannot be treated perturbatively within a nonrelativistic approach because the characteristic loop momenta are relativistic. A similar situation is the nuclear polarizability correction, which in neutral muonic helium is larger than the elastic two-photon contributions.

Some time ago the hyperfine interval in neutral muonic helium was intensively discussed (see, e.g., [3–6]). The one of the important corrections there is due to two-photon exchange. Its elastic finite-size part has a form similar to that in (7) and contains a certain Zemach momentum. Again, once we assume that the nucleus is a nonrelativistic one, we arrive at an integral with a nonrelativistic shape of the integrand, but with the area of integration which is a relativistic one. That is the well-known Zemach contribution (see, e.g., [13])

$$\begin{aligned}\Delta E_{\rm Zemach}(ns) &= -\frac{8(Z\alpha)\,m\,E_F}{\pi n^3}\int_0^\infty \frac{dq}{q^2}\\ &\quad\times\left[\frac{2G_E(q^2)G_M(q^2)}{g_N}-1\right]\\ &= -\frac{2(Z\alpha)\,m\,E_F}{n^3}\,\langle r\rangle_{(2:EM)}, \qquad (9)\end{aligned}$$

where G_M is the magnetic form factor of the compound nucleus, and the involved Zemach momentum is found with a convolution of the densities of the electric charge and magnetic moment. The Fermi energy E_F is the standard leading nonrelativistic contribution to the hyperfine interval, and g_N is the nuclear g factor.

In the neutral muonic helium atom, $Z\alpha m R_N \sim m_e/m_\mu$ and therefore the Friar term [which is a (part of the) spin-independent two-photon correction] is of the same order in $Z\alpha$ as the leading nonrelativistic (Bohr) term, but of a different order in m_e/m_μ. The Zemach term [which is a (part of the) spin-dependent two-photon correction] is of the same order in $Z\alpha$ as the Fermi energy E_F, which is the leading nonrelativistic spin-dependent term, but it is of a different order in m_e/m_μ.

In the ordinary and muonic hydrogen atoms the situation is very similar in the terms of the integrands and numerical values of the parameters, however the two-photon-exchange contributions (Friar's and Zemach's) are of order $(Z\alpha)^5$ (in contrast to neutral muonic helium), while the leading nonrelativistic contributions due to the finite size and hyperfine interaction are both of order $(Z\alpha)^4$ (as well as in the case of neutral muonic helium).

Therefore, those two-photon-exchange contributions have the integrands of the nonrelativistic shape but with a fully relativistic integration area. Nevertheless, in the muonic helium they are of the same order in the terms $Z\alpha$ as the nonrelativistic terms. The two-photon-exchange contributions are included into a theory based on Hamiltonian (2), and does not matter whether it is done exactly or perturbatively. Such a theory cannot produce terms of higher order in $Z\alpha$ (without an additional relativistic perturbation $\Delta\mathcal{H}_{\rm rel}$), but can produce contributions of different order in m_e/m_μ. The results with Hamiltonian (2) in atomic units are not even sensitive to the value of $Z\alpha$. (The relativistic corrections with $\Delta\mathcal{H}_{\rm rel}$ are.) A confusion can come from the fact that in both ordinary and muonic (two-body) atoms the parameter $Z\alpha m R_N$ explicitly involves $Z\alpha$ and therefore it is clearly recognized as a kind of relativistic effect. On the contrary, in the neutral muonic helium atom, interpreted as a two-body electronic atom with a compound nucleus, the parameter does not involve $Z\alpha$ since $Z\alpha m R_N \propto m_e/m_\mu$, and it does not look like a relativistic effect. (Technically, the difference is because in ordinary and muonic atoms, the theory includes one more independent parameter R_N. Its value in atomic units is equal to the ratio R_N/a_B and it is therefore α dependent.)

Since the integrands keep the nonrelativistic shape, the exact (in the term of photon exchanges) solution of the numerical variational nonrelativistic problem gives a correct result for the two-photon-exchange contribution. The problem of the applicability of the three-body numerical solutions appears with three-photon exchanges. Below, we perform a numerical evaluation with Hamiltonian (2) with the different values of m_e/m_μ and fit the results in order to recover the coefficients of the expansion in m_e/m_μ in (1). As far as we deal with the one-photon and two-photon exchanges, we expect that the solution of the nonrelativistic problem with (2) agrees with $\mathcal{E}^{(0)}$, the leading term of α expansion in (1). While for the three-photon-exchange contributions we expect that the numerical nonrelativistic solution delivers us only a part of result. We identify the physical origin of the terms of the expansion (1) and assign an additional uncertainty to the contributions which are related to multiphoton exchanges.

Concluding this section, we note that there are two parameters in two-body atoms which describe relativistic effects. One is $Z\alpha$, while the other is mR_N. The inverse value of the second parameter $(1/mR_N)$ shows what should be momentum-to-mass ratio (which is the velocity in the nonrelativistic limit) for the orbiting particle penetrating into the nucleus. This parameter is essentially above unity for ordinary hydrogenic atoms, and it is comparable with the unity in two-body muonic atoms. In the neutral muonic helium (with the muon in its ground state), understood as a two-body atom with a compound nucleus, it is about unity as well. The parameter m_e/m_μ appears in a sense as a combination of two parameters for relativistic expansion, $Z\alpha$ and $Z\alpha m_\mu/m_e$. The higher-order (in m_e/m_μ) contributions to the energy are in part of the relativistic origin. In contrast to ordinary atoms, where the nuclear-finite-size effects are small and the relativistic effects are well recognized in the final expressions as a result of $Z\alpha$ expansion, in the neutral muonic helium the relativistic corrections (for the electron) may be of the same order in $Z\alpha$ as the leading term, as it is seen in the case of the Friar and Zemach contributions.

Examining the expression of the energy in form (6), we note that the contributions with coefficients C_1 and C_2 are purely nonrelativistic. The contributions with C_3 and C_{41} come in part from the integration of the nonrelativistic expressions over the relativistic momentum area, which in this particular case is consistent with the numerical variational consideration, as

explained above. In contrast to that, the C_{40} and C_5 contributions also come in part from the relativistic area of the integration over nonrelativistic expressions, but those expressions may be incomplete. Until this question is clarified, we should consider those two terms of the expansion (6) as only partial contributions to the *complete* expression for the energy $\mathcal{E}^{(0)}$.

III. VARIATIONAL NUMERICAL CALCULATIONS

Our strategy is to perform numerical calculations with a nonrelativistic Hamiltonian and to interpret the results, using a low-m_e/m_μ expansion. Since we intend to rely on the expansion, we have chosen to set the nuclear mass M to infinity in order to avoid an expansion in two small parameters. For the numerical evaluation we apply the atomic units, and Hamiltonian (2) takes the form

$$\mathcal{H}^{\rm NR} = \frac{\mathbf{p}_1^2}{2} + \frac{\mathbf{p}_2^2}{2}\frac{m_e}{m_\mu} + \frac{1}{r_{12}} - \frac{2}{r_1} - \frac{2}{r_2}, \tag{10}$$

where we use the following notation: $\mathbf{r}_1$ and $\mathbf{p}_1$ stand for the radius vector and momentum of the electron, $\mathbf{r}_2$ and $\mathbf{p}_2$ are for the muon, while $\mathbf{r}_{12}$ is the difference of the two mentioned radius vectors. Afterwards, we are to partially restore the finite nuclear mass by taking advantage of a perturbative approach with considering the electron and compound nucleus as a two-body system [9].

In our numerical calculations of $\mathcal{E}^{\rm NR}$ we use the variational method based on exponential expansion with randomly generated parameters [14,15]. The wave function is taken in the form

$$\Psi_L(l_1,l_2) = \sum_{k=1}^{N}\{U_k \mathrm{Re}[e^{-\alpha_k r_1-\beta_k r_2-\gamma_k r_{12}}] + W_k \mathrm{Im}[e^{-\alpha_k r_1-\beta_k r_2-\gamma_k r_{12}}]\}\mathcal{Y}_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2), \tag{11}$$

where $\mathcal{Y}_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2)$ are the solid bipolar harmonics as defined in Ref. [16]:

$$\mathcal{Y}_{LM}^{l_1,l_2}(\mathbf{r}_1,\mathbf{r}_2) = r_1^{l_1} r_2^{l_2}\left\{Y_{l_1}\otimes Y_{l_2}\right\}_{LM},$$

L is the total orbital angular momentum of a state and N is the number of the basis-set functions. Complex parameters α_k, β_k, and γ_k are generated in a quasirandom manner:

$$\alpha_k = \left[\left\lfloor \tfrac{1}{2}k(k+1)\sqrt{p_\alpha}\right\rfloor(A_2 - A_1) + A_1\right] + i\left[\left\lfloor \tfrac{1}{2}k(k+1)\sqrt{q_\alpha}\right\rfloor(A_2' - A_1') + A_1'\right], \tag{12}$$

TABLE I. The binding energy of the electron for the states $1s$, $2s$, and $2p$ in the neutral muonic helium atom with the muon in the ground state as follows from Hamiltonian (10) as function of the muon mass. The numerical data are variational solutions of the stationary Schrödinger problem calculated for variational basis of 2000 and 2500 functions, correspondingly. The results are presented in atomic units; for the muon mass we apply a parameter $x = m_e/m_\mu = 2^n/206.768\,2826$.

n	$1s$ (2000)	$1s$ (2500)
−4	−0.500 000 047 199 227 225 321	−0.500 000 047 199 227 225 331
−3	−0.500 000 191 033 578 786 047	−0.500 000 191 033 578 786 062
−2	−0.500 000 775 880 845 228 706	−0.500 000 775 880 845 228 717
−1	−0.500 003 163 466 276 532 681	−0.500 003 163 466 276 532 687
0	−0.500 012 946 805 678 863 497	−0.500 012 946 805 678 863 510
1	−0.500 053 122 904 815 614 566	−0.500 053 122 904 815 615 242
2	−0.500 217 876 896 591 416 291	−0.500 217 876 896 591 465 248
3	−0.500 888 144 061 291 219 534	−0.500 888 144 061 293 438 269
4	−0.503 568 095 182 590 249 853	−0.503 568 095 182 675 564 693
n	$2s$ (2000)	$2s$ (2500)
−4	−0.125 000 005 899 652 947 057	−0.125 000 005 899 652 947 058
−3	−0.125 000 023 877 234 369 411	−0.125 000 023 877 234 369 413
−2	−0.125 000 096 969 819 874 234	−0.125 000 096 969 819 874 238
−1	−0.125 000 395 315 118 616 248	−0.125 000 395 315 118 616 271
0	−0.125 001 617 443 163 665 292	−0.125 001 617 443 163 665 573
1	−0.125 006 633 402 083 161 331	−0.125 006 633 402 083 165 702
2	−0.125 027 180 466 047 089 480	−0.125 027 180 466 047 181 806
3	−0.125 110 576 444 206 900 294	−0.125 110 576 444 210 373 858
4	−0.125 442 046 467 181 785 896	−0.125 442 046 467 367 399 492
n	$2p$ (2000)	$2p$ (2500)
−4	−0.125 000 000 000 157 601 972 240	−0.125 000 000 000 157 601 972 240
−3	−0.125 000 000 001 248 075 857 305	−0.125 000 000 001 248 075 857 310
−2	−0.125 000 000 009 848 331 444 529	−0.125 000 000 009 848 331 444 646
−1	−0.125 000 000 077 354 540 592 515	−0.125 000 000 077 354 540 593 944
0	−0.125 000 000 604 139 162 379 714	−0.125 000 000 604 139 162 448 957
1	−0.125 000 004 687 050 097 369 309	−0.125 000 004 687 050 099 840 290
2	−0.125 000 036 106 709 083 244 451	−0.125 000 036 106 709 376 329 842
3	−0.125 000 276 366 319 547 065 399	−0.125 000 276 366 335 073 308 025
4	−0.125 002 105 596 572 398 961 282	−0.125 002 105 596 723 266 258 334

where $\lfloor x \rfloor$ designates the fractional part of x, p_α and q_α are some prime numbers, and $[A_1, A_2]$ and $[A_1', A_2']$ are real variational intervals, which need to be optimized. Parameters β_k and γ_k are obtained in a similar way. For more details, see [17].

Hamiltonian (10) has only one parameter, namely, m_e/m_μ. We perform our numerical calculations for an equidistant (in logarithmic scale) set of hypothetical values of $x = m_e/m_\mu$ with the actual value in the middle point of the set. To keep the numerical stability of calculations at large value of N, an octuple precision (64 decimal digits) has been used. Results of these calculations versus size of the basis set for the states of interest are presented in Table I. The results are given for three lowest states: $nl = 1s$, $2s$, and $2p$.

Variational parameters were optimized manually for the basis set with the actual value of m_e/m_μ. For scaled values of x, the variational parameter related to variable r_2 was scaled proportionally to keep the set of parameters close to optimal values. Basis sets with $N = 2000$ and 2500 functions were used. As it is seen from Table I, the worst case of $n = 4$ provides 12 significant digits for the nonrelativistic energy. For the actual value of $x = m_e/m_\mu$, a number of significant digits increases to about 18 digits, which should be more than sufficient for reliable analysis of the fits.

IV. FITTING THE VARIATIONAL RESULTS WITH THEORETICALLY INSPIRED FITS

To interpret the numerical results for $\mathcal{E}^{\rm NR}$ in terms of $\mathcal{E}^{(0)}(m_e/m_\mu)$ properly, we have to split the total numerical results in the terms of expansion at low m_e/m_μ. Once we present the energy in such a form, we could discuss whether the individual (nonrelativistic) contributions are correctly found within the nonrelativistic approximation, and corrections in which orders in m_e/m_μ may be required.

To find the coefficients, we consider five different fits of a similar shape [cf. (6)]. Their difference is in a different number of terms and in different suggestions we use for the fit parameters.

A very important issue is the uncertainty of the data points. The computational uncertainty, found from the difference between the values obtained with the 2000 and 2500 functions, is not appropriate for fitting. The fits (introduced with a realistic shape and a reasonable number of terms) have huge values of χ^2 (of orders of magnitudes above the number of degrees of freedom), while fitting the data with such uncertainty as it is (i.e., with the computational uncertainty only). That is because the data points are extremely accurate and a "true" approximation with a comparable uncertainty should have a very large number of terms. Indeed, we may set a large number of parameters, and in such a case we can improve the value of χ^2, but that would be just a fit, i.e., a function which has no physical sense, but well consistent with the data. If we intend to find a function, for which parameters would have a physical meaning, we need to use another strategy.

Prior to discussion of the details of the fit, we have to mention that the fits are basically an expansion around $m_e/m_\mu = 0$ [cf. (6)]. If we would know correct coefficients of such an expansion, then the approximated function with the true coefficients should deviate from the data within the uncertainty of the approximation which is determined by the first missing terms. In our fits, we "manually" introduce an uncertainty which is proportional to the biggest missing term. That makes the fits more stable once we add additional terms, etc. That is *not* a rigorously correct procedure because that uncertainty is proportional to the error, but not (approximately) equal to it (since we have no accurate way to estimate the coefficient for the biggest missing term). If it would be the only problem of scaling the uncertainty, it should make a bad value of χ^2, but a good central value. However, in combination with the numerical uncertainty, estimated as the difference between the values obtained with the 2000 and 2500 functions, the choice of the (unknown) proportionality coefficient affects the central value as well. The other problem is that the shift related to the first missing term is a systematic one. We recognize all those difficulties and comment the values of χ^2 of various fits as well as evolution of the coefficients from fit to fit.

The fits are described below.

(i) Fit A is a fit

$$\mathcal{E}^{\rm NR}(nl) = C_1 + C_2\left(\frac{m_e}{m_\mu}\right)^2 + C_3\left(\frac{m_e}{m_\mu}\right)^{5/2} + \left(\frac{m_e}{m_\mu}\right)^3\left[C_{41}\ln\left(\frac{m_\mu}{m_e}\right) + C_{40}\right]. \quad (13)$$

The additional uncertainty (to the computational one) is assigned for each data point as $(m_e/m_\mu)^{7/2}/n^3$ and treated as a random one. The fit is a "free" fit and we do not set any constraints on its parameters.

(ii) Fit B has the same shape as fit A, however, we take the advantage of two known leading coefficients [9], namely,

$$C_1(nl) = -\frac{1}{2n^2}, \quad C_2(nl) = -\frac{\delta_{l0}}{2n^3}. \quad (14)$$

The uncertainty is treated the same way as for fit A.

(iii) Fit C is a somewhat more advanced fit than the previous ones:

$$\mathcal{E}^{\rm NR}(nl) = C_1 + C_2\left(\frac{m_e}{m_\mu}\right)^2 + C_3\left(\frac{m_e}{m_\mu}\right)^{5/2} + \left(\frac{m_e}{m_\mu}\right)^3\left[C_{41}\ln\left(\frac{m_\mu}{m_e}\right) + C_{40}\right] + C_5\left(\frac{m_e}{m_\mu}\right)^{7/2}, \quad (15)$$

with constraints (14). It has one more term comparing with the previous fits and the additional random uncertainty to each data point is now assigned as $(m_e/m_\mu)^4/n^3$.

The fits A–C are performed for each of three states, $1s$, $2s$, and $2p$ independently.

(iv) Fit D is based on fit B, however, we set a constraint

$$C_3(nl) = C_3(1s)\,\frac{\delta_{l0}}{n^3}, \; C_{41}(nl) = C_{41}(1s)\,\frac{\delta_{l0}}{n^3}, \quad (16)$$

which means two additionally known coefficients for $2p$ and relations between the values of two pairs of the coefficients for the $1s$ and $2s$ states.

The fitting for $1s$ and $2s$ is not performed independently anymore, but as a single procedure.

TABLE II. The fit coefficients for the $1s$ state and the properties of the fits. Fits A–C are performed for the $1s$ state separately and their χ^2 and χ^2/d.o.f. are found only for the $1s$ data and fits. In the case of fits D and E, the fits are performed on the set of the $1s$ and $2s$ data. The value of χ^2 shows a deviation of the $1s$ data from the fits, while the value of χ^2/d.o.f. is given for the combined $1s$ and $2s$ data since the number of degrees of freedom are defined only for the combined data.

Fit	C_1	C_2	C_3	C_{41}	C_{40}	C_5	χ^2	χ^2/d.o.f.
A	−0.500 000 000 00(1)	−0.4999(7)	−1.05(5)	0.5(2)	1.2(6)		6×10^{-3}	2×10^{-3}
B	−1/2	−1/2	−1.049(3)	0.53(5)	1.2(2)		1×10^{-2}	3×10^{-3}
C	−1/2	−1/2	−1.0494(4)	0.53(1)	1.19(8)	0.1(3)	0.7	0.17
D	−1/2	−1/2	−1.049(2)	0.53(3)	1.2(2)		$2.4 \cdot 10^{-2}$	3×10^{-3}
E	−1/2	−1/2	−1.0495(3)	0.534(8)	1.17(6)	0.2(2)	0.9	0.14

(v) Fit E is a modification of fit C with an additional constraint (16) (the same the constraint introduced for fit D).

In principle, all the fits should be consistent. The results of the fits are summarized in Tables II, III, and IV. The fits for the $1s$ energy are also compared in Fig. 1.

V. ACCURACY AND CONSISTENCY OF THE FITS

Let us discuss the results of the fitting procedure and compare the results of the different fits. The fits A, B, and D deal with the same additional random error of the data points. They have very low value of χ^2. As we see from the fits C and E, the coefficient C_5 is either very small or equal to zero. In the meantime, for the estimation of the uncertainty for A, B, and D we should set $C_5 = \pm 1/n^3$ (since we have no *a priori* reason to do otherwise). In other words (as we learned from more advanced fits), the uncertainty of the fits A, B, and D is an overestimation of the error.

Next, we see for the fits A, B, and D that the value of χ^2 increases as well as the value of χ^2/d.o.f. (while going from A to D through B). That is because the fits have the same number of parameters, but the fit A does not have constraints on them. Next, we introduce constraints (14) on fit B, and additional constraints (16) on fit C, reducing the number of free parameters. Introducing the constraints we make the fits less flexible and make them worse as fits. Nevertheless, the constraints improve the fits as approximations, i.e., they improve the determination of the coefficients.

The fits C and E have a different additional random uncertainty comparing with A, B, and D. Since the total effective uncertainty of the data points is different, a comparison of the value of χ^2 of, e.g., the fits A and C, does not make sense. The values of χ^2 for the fits C and E are more reasonable than the very small values for the fits A, B, and D, which indicates that the random uncertainty is more reasonably estimated.

From experimental perspectives, we are interested in the $2s - 1s$ and $2p - 2s$ intervals. A comparison of direct results and the results obtained using the fit coefficients (but ignoring their correlations) is presented in Tables V and VI.

We note that the direct calculations at $m_e/m_\mu \simeq 1/207$ from Table I are more accurate than the fits, but the results of the fits are consistent with them. The accuracy of the fits is determined not by the computational uncertainty, but by the errors of the fit.

We have two comments on that. They both are related to the fact that the fit is a truncated version of a certain true function for the expansion around $m_e/m_\mu = 0$. For the sake of simplicity, we refer to any expansion around zero as to an extended Taylor expansion and to any fit which has the same shape as a truncated extended Taylor expansion as to extended polynomials.

The coefficients of an extended Taylor expansion are defined as certain derivatives or limit values at zero. For example,

$$C_3 = \left[\frac{E(x) - C_1 - C_2 x^2}{x^{5/2}}\right]_{x=0},$$
$$C_4 = \left[x\frac{\partial}{\partial x}\frac{E(x) - C_1 - C_2 x^2 - C_3 x^{5/2}}{x^3}\right]_{x=0}, \quad (17)$$

which is a certain generalization of the presentation of the standard Taylor series in the terms of the derivatives at zero. Here, $x = m_e/m_\mu$ and $E(x)$ is the true function for the energy we are to restore with the fits.

Therefore, the determination of the coefficients of an extended Taylor series requires extrapolations because $x = 0$ is slightly outside of the edge of the data interval. Such extrapolated values are always more uncertain than the data themselves.

The extended Taylor series has two important differences from the extended polynomials.

TABLE III. The fit coefficients for the $2s$ state and the properties of the fits. Concerning values of χ^2 and χ^2/d.o.f. (see the caption to Table II).

Fit	C_1	C_2	C_3	C_{41}	C_{40}	C_5	χ^2	χ^2/d.o.f.
A	−0.125 000 000 000(2)	−0.06250(8)	−0.131(7)	0.07(3)	0.15(7)		3×10^{-3}	9×10^{-4}
B	−1/8	−1/16	−0.1312(4)	0.066(6)	0.16(3)		5×10^{-3}	1×10^{-3}
C	−1/8	−1/16	−0.131 20(5)	0.067(1)	0.15(1)	0.02(4)	0.4	0.11
D	−1/8	−1/16	−0.1312(3)	0.066(4)	0.16(2)		$1.6 \cdot 10^{-2}$	3×10^{-3}
E	−1/8	−1/16	−0.131 19(3)	0.067(1)	0.156(7)	0.00(3)	0.7	0.14

TABLE IV. The fit coefficients for the $2p$ state and the properties of the fits.

Fit	C_1	C_2	C_3	C_{41}	C_{40}	C_5	χ^2	χ^2/d.o.f.
A	−0.125 000 000 000(2)	−0.000 00(8)	0.000(7)	0.00(3)	0.00(7)		1×10^{-6}	3×10^{-7}
B	−1/8	0	0.0000(4)	0.000(6)	0.00(3)		4×10^{-5}	9×10^{-6}
C	−1/8	0	0.000 00(5)	0.000(1)	0.00(1)	0.00(4)	4×10^{-4}	1×10^{-4}
D	−1/8	0	0	0	−0.006(2)		8×10^{-3}	1×10^{-3}
E	−1/8	0	0	0	−0.006(1)	0.007(5)	3×10^{-2}	4×10^{-3}

(i) All the fits are optimized to the area where the data are present. Therefore, in the case of our consideration the result for the actual value of m_e/m_μ from the fit function should be in a very good agreement with the data and it is. The actual deviation of the fit from the data for this actual value is rather smaller than the uncertainty found with ignoring the correlations between the coefficients. (The correlations are often the negative ones since a change in one coefficient may be compensated by a change in another.) The fit coefficients by themselves are the most uncertain part of the fit because they require an extrapolation and a differentiation. We partly overcome the problem "punishing" the data points by introducing the uncertainty increasing with m_e/m_μ. Such an uncertainty should optimize the fit for the low edge of the data, rather than for the center of the data interval.

(ii) The residuals of the data in respect to a fit are randomly distributed, while the true function should rather systematically deviate from the data. The "model," i.e., the way we treat the "additional" uncertainty suggests a random distribution. To probe the correlations, we used the different fits, introducing the correlations between the results for different states, such as $1s$ and $2s$. To check the importance of the correlation of the errors of the approximation between data for different m_e/m_μ, we introduced an additional term in fits C (comparing with B) and E (comparing with D). Introducing an additional term into the fit function and reducing the random uncertainty is a way to model the correlation between the deviations of the data from the approximation for different m_e/m_μ.

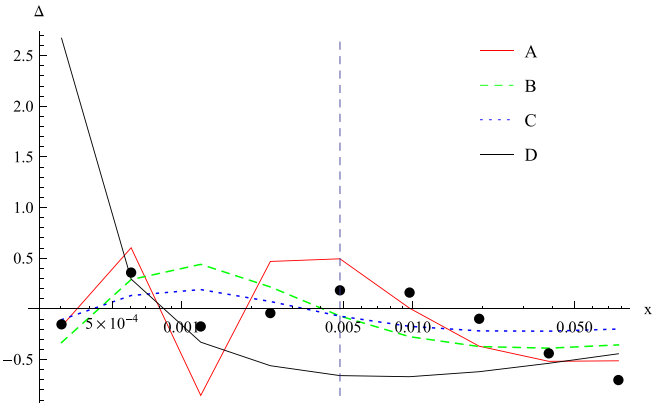

FIG. 1. The differences $\Delta = \frac{f(x)-f_E(x)}{x^4}$, where $x = m_e/m_\mu$, and f corresponds to fits A, B, C, and D and to the direct calculation (black closed circles) for the $1s$ state; $f_E(x)$ stands for the results of fit E. The value of x^4 is the uncertainty introduced for fits C and E. (The uncertainty for fits A, B, and D being $x^{7/2}$ is somewhat larger.) The vertical dashed line is for the actual value of m_e/m_μ.

We have already considered in Sec. II the applicability of nonrelativistic Hamiltonian (2) and the expansion (6) to find $\mathcal{E}^{(0)}_{nl_j}(m_e/m_\mu)$. The contributions with C_1, C_2, C_3, and C_{41} have a clear nonrelativistic origin being related to nonrelativistic integrands of the perturbation approach. The area of the integration does not affect the interpretation. The contributions with C_{40} and C_5 in (6) correspond to relativistic integrations over integrands which are not reduced to those with a pure nonrelativistic shape. That means that we have obtained only partial results for the related terms of the expansion of $\mathcal{E}^{(0)}_{nl_j}(m_e/m_\mu)$ in m_e/m_μ.

VI. RESTORING A FINITE VALUE OF THE NUCLEAR MASS

Once we study the three-body neutral muonic helium atom as a hierarchy system of an electron bound by a compound two-body nucleus, it is clear that all the terms should contain corrections in m_e/M and m_μ/M, which cannot be covered by the introducing the reduced mass. As for the first two terms of the expansion in (6), the correction can be done by a substitution [9]

$$C_1 \to C_1\left(\frac{M+m_\mu}{m_e+m_\mu+M}\right) \simeq C_1\left(1-\frac{m_e}{M+m_\mu}+\frac{2m_e^2}{M^2}\right), \tag{18}$$

$$C_2\left(\frac{m_e}{m_\mu}\right)^2 \to C_2\left(\frac{m_e}{m_\mu}\right)^2 \times\left(1-\frac{2m_\mu^2}{M^2}\right)\left(\frac{M+m_\mu}{m_e+m_\mu+M}\right)^3 \simeq C_2\left(\frac{m_e}{m_\mu}\right)^2\left(1-\frac{2m_\mu^2}{M^2}-\frac{3m_e}{M+m_\mu}\right). \tag{19}$$

TABLE V. The $2s-1s$ interval in atomic units (with the infinite nuclear mass and the actual value of m_e/m_μ) from numerical calculations with Hamiltonian (10). The results are given in atomic units.

Method	$2s-1s$ interval
Direct	0.375 011 329 362 515 1979(3)
Fit A	0.375 011 3(2)
Fit B	0.375 011 33(4)
Fit C	0.375 011 33(1)
Fit D	0.375 011 33(3)
Fit E	0.375 011 329(8)

TABLE VI. The $2p-2s$ interval in atomic units (with the infinite nuclear mass and the actual value of m_e/m_μ) from numerical calculations with Hamiltonian (10). The results are given in atomic units.

Method	$2p-2s$ interval
Direct	0.000 001 616 839 024 5031(3)
Fit A	0.000 001 62(3)
Fit B	0.000 001 617(7)
Fit C	0.000 001 617(2)
Fit D	0.000 001 617(3)
Fit E	0.000 001 617(1)

(Note that the results are in atomic units, in which $m_e = 1$, but the reduced mass of the electron

$$\frac{m_e(M+m_\mu)}{m_e+m_\mu+M}$$

is not equal to the unity.)

A comparison with available numerical results obtained for neutral ^{3}He and ^{4}He [8] are presented in Tables VII and VIII. We clearly see a difference between our results and those from [8]. It should be attributed to incomplete restoration of m_μ/M and m_e/M corrections. We have restored the recoil corrections in (18) and (19) to two leading terms. Accidentally, the linear m_μ/M correction to the C_2 term vanishes and the first nonzero correction is suppressed, being proportional to $(m_\mu/M)^2$.

The C_2 term might have an m_μ/M correction, but it cancels out. The C_3 term may also have such a correction and there is no reason to expect its cancellation. Until the issue is clarified by direct perturbative calculation, we consider the value of

$$\frac{5}{2}\,C_3\left(\frac{m_e}{m_\mu}\right)^{5/2}\frac{m_\mu}{M}$$

as an additional uncertainty to be included into the eventual result. The factor of $\frac{5}{2}$ appears naturally if we substitute m_μ for m_r in (6). Such a substitution with the use of the reduced mass of the muon has a correct sign and covers the most of the correction.

The problem of higher order m_e/M and m_μ/M terms could be also resolved by fitting a set of data with different values of m_μ and M. Anyway, the uncertainty due to the applicability of the nonrelativistic calculations (see below) is comparable with the contribution above and we leave it as it is.

TABLE VII. The $2s-1s$ interval for ^{3}He (with the actual value for nuclear mass). The results of the fits are given with the corrections in Eqs. (18) and (19) introduced. The results are given in atomic units.

Ref.	$2s-1s$ interval in ^{3}He
[8] (direct)	0.374 945 745 405 113 94
Fit A	0.374 945 5(2)
Fit B	0.374 945 55(4)
Fit C	0.374 945 55(1)
Fit D	0.374 945 55(3)
Fit E	0.374 945 548(8)

TABLE VIII. The $2s-1s$ interval for ^{4}He (with the actual value for nuclear mass). The results of the fits are given with the corrections in Eqs. (18) and (19) introduced. The results are given in atomic units.

Ref.	$2s-1s$ interval in ^{4}He
[8] (direct)	0.374 961 469 887 0687
Fit A	0.374 961 3(2)
Fit B	0.374 961 32(4)
Fit C	0.374 961 32(1)
Fit D	0.374 961 32(3)
Fit E	0.374 961 323(8)

VII. CONCLUSIONS

Now, we can write the final results for the $2s-1s$ and $2p-2s$ energy intervals, based on the fit E, as

$$\begin{aligned}
\mathcal{E}^{(0)}(^3\mathrm{He}, 2s-1s) &= 0.374\,9455(2)\ \text{a.u.},\\
\mathcal{E}^{(0)}(^4\mathrm{He}, 2s-1s) &= 0.374\,9613(2)\ \text{a.u.},\\
\mathcal{E}^{(0)}(^3\mathrm{He}, 2p_{1/2}-2s) &= 1.62(3)\ \times 10^{-6}\ \text{a.u.},\\
\mathcal{E}^{(0)}(^4\mathrm{He}, 2p_{1/2}-2s) &= 1.62(2)\ \times 10^{-6}\ \text{a.u.}
\end{aligned} \tag{20}$$

The individual contributions to the central values and their uncertainties are summarized in Table IX for the muonic ^{3}He and in Table X for muonic ^{4}He. The values correspond to the physical masses of the electron, muon, and the nuclei. The hyperfine effects are neglected and the results correspond to the values averaged over the spin of the compound nucleus.

We remind that the eventual uncertainty consists of three contributions already mentioned in the text.

(u1) The uncertainty of the fit E presents the uncertainty of the fitting procedure. It contains the uncertainties due to those of the coefficients (which are already included into individual

TABLE IX. The individual contributions to $2s-1s$ and $2p_{1/2}-2s$ intervals in the neutral muonic ^{3}He (in a.u.). The terms #i are for a contribution with the coefficient C_i according to fit E. The contributions to the uncertainty ("u1," etc.) and the higher-order (in α) terms are explained in the text.

Term	$2s-1s$	$2p_{1/2}-2s$
#1	0.375	0
(18)	$-6.574\,73\times10^{-5}$	0
#2	$1.023\,32\times10^{-5}$	$1.461\,88\times10^{-6}$
(19)	$-3.433\,52\times10^{-8}$	$-4.905\,03\times10^{-9}$
#3	$1.4938(4)\times10^{-6}$	$2.134\,0(5)\times10^{-7}$
#41	$-2.82(5)\times10^{-7}$	$-4.02(6)\times10^{-8}$
#40	$-1.14(6)\times10^{-7}$	$-1.82(8)\times10^{-8}$
#5	$-2(2)\times10^{-9}$	$0(2)\times10^{-10}$
u1	$\pm8.3\times10^{-9}$	$\pm1.0\times10^{-9}$
u2	$\pm1.4\times10^{-7}$	$\pm2.0\times10^{-8}$
u3	$\pm1.1\times10^{-7}$	$\pm1.8\times10^{-8}$
Total $\mathcal{E}^{(0)}$	0.374 9455(2)	$1.62(3)\times10^{-6}$
$\alpha\,\mathcal{E}^{(1)}$	-3.0×10^{-8}	-4.3×10^{-9}
$\alpha^2\mathcal{E}^{(2)}$	4.58×10^{-6}	0
$\alpha^3\mathcal{E}^{(3)}$	-1.08×10^{-6}	-1.60×10^{-7}
Total $\mathcal{E}$	0.374 9490(2)	$1.46(3)\times10^{-6}$

TABLE X. The individual contributions to $2s-1s$ and $2p_{1/2}-2s$ intervals in the neutral muonic ^{4}He (in a.u.). The notation used is the same as in Table IX.

Term	$2s-1s$	$2p_{1/2}-2s$
#1	0.375	0
(18)	$-4.998\,62\times10^{-5}$	0
#2	$1.023\,32\times10^{-5}$	$1.461\,88\times10^{-6}$
(19)	$-2.053\,03\times10^{-8}$	$-2.932\,90\times10^{-9}$
#3	$1.4938(4)\times10^{-6}$	$2.1340(5)\times10^{-7}$
#41	$-2.82(5)\times10^{-7}$	$-4.02(6)\times10^{-8}$
#40	$-1.14(6)\times10^{-7}$	$-1.82(8)\times10^{-8}$
#5	$-2(2)\times10^{-9}$	$0(2)\times10^{-10}$
u1	$\pm8.3\times10^{-9}$	$\pm1.0\times10^{-9}$
u2	$\pm1.1\times10^{-7}$	$\pm1.5\times10^{-8}$
u3	$\pm1.1\times10^{-7}$	$\pm1.8\times10^{-8}$
Total $\mathcal{E}^{(0)}$	0.374 9613(2)	$1.62(2)\times10^{-6}$
$\alpha\,\mathcal{E}^{(1)}$	-3.0×10^{-8}	-4.2×10^{-9}
$\alpha^2\mathcal{E}^{(2)}$	4.58×10^{-6}	0
$\alpha^3\mathcal{E}^{(3)}$	-1.08×10^{-6}	-1.60×10^{-7}
Total $\mathcal{E}$	0.374 9648(2)	$1.46(2)\times10^{-6}$

contributions in Tables IX and X) and an additional systematic uncertainty of the fit as the whole defined as $(m_e/m_\mu)^4/n^3$. The latter is denoted as u1.

(u2) The uncertainty due to the recoil corrections (i.e., the corrections in m_e/M and m_μ/M) are estimated with a dominant missing correction as $2.5\,C_3\,(m_e/m_\mu)^{5/2}(m_\mu/M)$.

(u3) The uncertainty due to the applicability of the nonrelativistic Hamiltonian (10) to calculation of $\mathcal{E}^{(0)}$ is estimated as $C_{40}(m_e/m_\mu)^3$.

It is important that the uncertainty items u2 and u3 are essentially larger than the uncertainty due to the fitting procedure. The uncertainty of the fitting procedure (both item u1 and the uncertainty due to those of coefficients C_i) is a rough estimation because any extended Taylor series with true coefficients should have a systematic deviation from the data. We imitate the deviations with a statistical error. As long as these types of errors do not dominate, such estimations are acceptable.

Additionally, there are also higher-order corrections in α [see (1)]. They are also summarized in Table IX for the neutral muonic ^{3}He atom and in Table X for the muonic ^{4}He. Note that the α term is a result of the Uehling correction to the radius of the compound nucleus [10] and the leading term scales as $\alpha\times(m_e/m_\mu)^2$ which makes it small. The α^2 term is mostly due to the standard relativistic corrections and the α^3 term is for the leading QED corrections to the Lamb shift in standard hydrogenlike atoms (see [9] for detail). Taking all the individual contributions into account, we arrive at the results

$$\begin{aligned}
\mathcal{E}(^3\mathrm{He},2s-1s) &= 0.374\,9490(2)\ \text{a.u.},\\
\mathcal{E}(^4\mathrm{He},2s-1s) &= 0.374\,9648(2)\ \text{a.u.},\\
\mathcal{E}(^3\mathrm{He},2p_{1/2}-2s) &= 1.46(3)\times10^{-6}\ \text{a.u.},\\
\mathcal{E}(^4\mathrm{He},2p_{1/2}-2s) &= 1.46(2)\times10^{-6}\ \text{a.u.}
\end{aligned}\tag{21}$$

or

$$\begin{aligned}
h\nu(^3\mathrm{He},2s-1s) &= 2.467\,046(1)\times10^9\ \text{MHz},\\
h\nu(^4\mathrm{He},2s-1s) &= 2.467\,150(1)\times10^9\ \text{MHz},\\
h\nu(^3\mathrm{He},2p_{1/2}-2s) &= 9.6(2)\times10^2\ \text{MHz},\\
h\nu(^4\mathrm{He},2p_{1/2}-2s) &= 9.6(2)\times10^2\ \text{MHz}.
\end{aligned}\tag{22}$$

That is the main theoretical prediction of the paper.

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