Properties and hyperfine structure of helium-muonic atoms

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Basic geometrical and dynamical properties of the $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ helium-muonic atoms are determined from high-precision, variational calculations. Only the bound ground states with $L=0$ are discussed. The estimated hyperfine splitting between $^{1/2}S$ and $^{3/2}S$ states in the $^3He^{2+}\mu^-e^-$ atom is $\Delta\nu=4166.389$ MHz. The analogous result for the hyperfine splitting between ^0S and ^1S states in the $^4He^{2+}\mu^-e^-$ atom is $\Delta\nu=4464.555$ MHz. Both obtained figures agree very well with the known experimental values. The evaluated hyperfine splitting for the $^6Li^{3+}\mu^-e^-$ ion is ≈ 29311.4 MHz and for the $^7Li^{3+}\mu^-e^-$ ion is ≈ 36790.8 MHz.

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In this paper we report the results of high-precision calculations of various geometrical and dynamical properties for the bound ground $S(L=0)$ states in helium-muonic atoms. The main goal of this study is to evaluate very accurately the hyperfine splitting between $^{1/2}S$ and $^{3/2}S$ states in the $^3He^{2+}\mu^-e^-$ atom and analogous difference between ^0S and ^1S states in the $^4He^{2+}\mu^-e^-$ atom. These values can be measured experimentally with good accuracy. In fact, the maximal error of such measurements does not exceed a few kHz. In contrast with this, the best theoretical estimations had significantly poorer accuracy (≈ 1 MHz) (see, e.g., [1–4] and references therein). In the present study, we determine the hyperfine splitting with the maximal error which is less than 5 kHz. This means that both nucleus-electron and muonic-electron δ functions must be calculated with maximal error $\approx 1\times 10^{-7}$ a.u. As it follows from the atomic three-body calculations, the cusp between two negative particles (i.e., electrons) can be determined quite accurately when the total error in the total energy is less than 1×10^{-12} a.u.. Since the total ground-state energy of the $He^{2+}\mu^-$ ion is ≈ -400 a.u., this gives the maximal possible error in the total bound-state energy $\approx 1\times 10^{-15}$ for each of the helium-muonic atoms.

Hyperfine splitting in helium-muonic atoms was studied in a number of papers almost 20 years ago [5–10]. Those works were stimulated by experiments with helium-muonic atoms performed a few years earlier (see references in Refs. [6] and [9]). All theoretical studies at that time were based on the two-shell model which describes approximately the structure and properties of the helium-muonic atoms. The two-shell model for the helium-muonic atoms means that their actual structure is represented (with very good accuracy) as one-electron motion in the field of the quasinucleus which is a singly-charged hydrogenlike ion $He^{2+}\mu^-$. The muon mass is ≈ 206.77 times larger than the electron mass, therefore, the muon shell radius is $\approx (m_\mu/m_e)(Z/e)\approx 413$ times smaller than the appropriate electron shell radius.

By using the two-shell model one may derive some analytical expressions for the expectation values of two-particle Dirac δ functions and other properties in such systems. However, some of these analytical expressions include infinite sums and depend upon three different dimensionless parameters (the three mass ratios), thus restricting the final accuracy of earlier studies. Likewise, expectation values for the Dirac δ functions could not be evaluated easily. The first highly accurate numerical calculations of the two-particle δ functions were performed in Chen's papers [1–3], where the Hylleraas variational expansion of the trial wave function was used throughout. In our earlier study of the helium-muonic atoms [4] (see also Ref. [11]) we applied an exponential variational expansion producing the ground-state energies much better than the values derived in previous calculations. Moreover, we have determined not only δ functions, but also all three two-particle cusps. By using the agreement between computed and predicted cusp values, one can easily evaluate the reliability of the δ function expectation values used in calculations. Unfortunately, in [4] such good agreement was observed only for the muon-nucleus cusp.

Furthermore, our method used in Ref. [4] obviously could not provide the relative accuracy even comparable with 1×10^{-15}. However, recently we have developed a very effective two-stage strategy [12] to construct high-precision variational wave functions. This strategy can be used to determine the bound state energies in few-body systems, in principle, with an arbitrarily high accuracy. In the present study this strategy is applied to the high-precision calculation of the bound states in the helium-muonic atoms. A detailed description of the two-stage strategy for the helium-muonic atoms can be found below. Finally, the hyperfine splitting for the helium-muonic atoms has been determined with the maximal error of a few kHz. Such improved theoretical values coincide very well with the known experimental data (for both helium-muonic atoms). In particular, the coincidence of our presently computed and known experimental results is significantly better than observed previously. This indicates that the ignored relativistic corrections are much smaller than it was predicted in earlier papers.

The nonrelativistic Hamiltonian H of the helium-muonic atoms takes the following general form:

$$H=-\frac{\hbar^2}{2}\left[\frac{1}{m_e}\nabla_e^2+\frac{1}{m_\mu}\nabla_\mu^2+\frac{1}{m_N}\nabla_N^2\right]+\frac{e^2}{r_{e\mu}}-2\frac{e^2}{r_{eN}}-2\frac{e^2}{r_{\mu N}}, \tag{1}$$

where the notation μ designates the negatively charged

TABLE I. The convergence for the total energies in atomic units for the ground state in the helium-muonic atoms.

N^a	$^3He^{2+}\mu^-e^-$	$^4He^{2+}\mu^-e^-$	$^\infty He^{2+}\mu^-e^-$
200	−399.042336832862230	−402.637263035135090	−414.036536946808025
300	−399.042336832862295	−402.637263035135158	−414.036536946808084
400	−399.042336832862342	−402.637263035135222	−414.036536946808125
500	−399.042336832862371	−402.637263035135262	−414.036536946808156
550	−399.042336832862384	−402.637263035135275	−414.036536946808169
600	−399.042336832862399	−402.637263035135289	−414.036536946808176
700	−399.042336832862417	−402.637263035135314	−414.036536946808198

[a]These results correspond to the short-term (i.e., booster) wave function $\Psi_1(N_0=200)$.

muon μ^-, while N stands for the helium nucleus ^{3}He, ^{4}He, or $^\infty$He. In atomic units $\hbar=1$, $e^2=1$, and $m_e=1$ it is written in the form

$$H=-\frac{1}{2}\left[\nabla_e^2+\frac{1}{m_\mu}\nabla_\mu^2+\frac{1}{m_N}\nabla_N^2\right]+\frac{1}{r_{e\mu}}-\frac{2}{r_{eN}}-\frac{2}{r_{\mu N}}, \tag{2}$$

where the both m_μ and m_N masses are expressed in atomic units (i.e., in the electron mass). In the present study, no assumptions are made that some parts of this Hamiltonian are negligible in comparison to others. Note also, that (1) our present calculations are completely nonadiabatic, and Eq. (2) they have been performed in atomic units ($\hbar=1, m_e=1$, and $e=1$). In these units the following values for the particle masses [13]

$$m_\mu=206.768262, \quad M_{^\infty He^{2+}}=\infty,$$

$$M_{^3He^{2+}}=5495.8852, \quad M_{^4He^{2+}}=7294.2996,$$

were used in calculations.

Our present consideration is restricted to the case of the bound ground S states ($L=0$) in the helium-muonic atoms. In the case of S states the trial wave function $\psi_{L=0}$ in the relative coordinates r_{32}, r_{31}, and r_{21} takes the form

$$\psi_{L=0}(r_{32},r_{31},r_{21})=\sum_{i=1}^{N} C_i\exp(-\alpha_i r_{32}-\beta_i r_{31}-\gamma_i r_{21}), \tag{3}$$

where N is the number of terms in the variational expansion. The subscript 1 denotes the electron, the subscript 2 designates muon μ^-, while subscript 3 stands for the helium nucleus. This means $r_{32}=r_{23}=r_{\mu N}=|\vec{r}_\mu-\vec{r}_N|$, $r_{31}=r_{13}=r_{eN}=|\vec{r}_e-\vec{r}_N|$, and $r_{21}=r_{12}=r_{e\mu}=|\vec{r}_e-\vec{r}_\mu|$, respectively. The linear parameters C_i are determined by the solution of the variational (eigenvalue) problem. The principal question is the choice of the nonlinear parameters $\alpha_i, \beta_i, \gamma_i$, where $i=1,2,\ldots,N$. The regular [14] or quasirandom choices of these parameters obviously cannot provide a final accuracy sufficient for the helium-muonic atoms (see above and our results from [4]). Presently, to improve the final accuracy drastically we shall apply our two-stage procedure proposed in [12].

In this approach the trial wave function Ψ is represented by the sum of the very well-optimized, short-term (or booster) function Ψ_1 and roughly optimized (or even nonoptimized), long-term function Ψ_2. If the total number of terms equals N, then we may write $\Psi(N)=\Psi_1(N_0)+\Psi_2(N-N_0)$, where $N_0 \ll N$ (but also $N_0 \gg 1$). For the exponential variational expansion, each of the basis functions contains three nonlinear parameters. Therefore, the short-term $\Psi_1(N_0)$ function includes $3N_0$ nonlinear parameters, while the second $\Psi_2(N-N_0)$ function contains $3(N-N_0)$ such parameters. Correspondingly, the first stage of the procedure is to well optimize only the $3N_0$ nonlinear parameters, which is significantly smaller than the total number of these parameters ($3N$) in the trial wave function Ψ. In the second stage the total number of nonlinear parameters grows extensively, but they can be chosen by approximate optimization or even without optimization, e.g., in a regular [14] or quasirandom manner (see, e.g., [4] and references therein).

For the considered helium-muonic atoms the number of basis functions in the booster functions has been chosen equal 200, i.e., $N_0=200$. The 600 nonlinear parameters in the booster function have been optimized carefully for each of the three helium-muonic atoms considered, i.e. for the $^3He^{2+}\mu^-e^-$, $^4He^{2+}\mu^-e^-$, and $^\infty He^{2+}\mu^-e^-$ atoms. Finally, the variational energies obtained with such booster functions (200 basis functions in each) are significantly better than energies determined for these systems in [4] with 400 nonoptimized basis functions. The final accuracy with 700 basis functions is sufficient to stabilize at least 15 significant figures, i.e., to reach the relative accuracy 1×10^{-15} for the total energy. This gives 1×10^{-12} a.u. for the helium-muonic atoms.

The variational energies obtained in calculations are presented in Table I. The numerical values for some of the properties (i.e., expectation values) can be found in Table II. In both Tables I and II only atomic units are used: $m_e=1$, $e=1$, and $\hbar=1$. As follows from Table I, the accuracy achieved for the total energies E by using the two-stage approach is significantly higher than that obtained in the previous works. Note that, in principle, such accuracy can also be increased drastically by performing better optimization for the short-term Ψ_1 function. The physical meaning for all of the expectation values in Table II is quite clear from the notations used (for more detail, see [12]). Now, we want to

TABLE II. The expectation values in atomic units ($m_e=1,\hbar=1,e=1$) of some properties for the ground S states ($L=0$) of the $^i\mathrm{He}^{2+}\mu^-e^-$ atoms (where $i=3,\ 4$, and ∞).

System	$^3\mathrm{He}^{2+}\mu^-e^-$	$^4\mathrm{He}^{2+}\mu^-e^-$	$^\infty\mathrm{He}^{2+}\mu^-e^-$
Particles	3 2 1	3 2 1	3 2 1
$\langle r_{21}^{-2}\rangle$	1.99913907599	1.99931125680	1.99985633100
$\langle r_{31}^{-2}\rangle$	1.99969855311	1.99986366763	2.00038742025
$\langle r_{32}^{-2}\rangle$	317672.089970	323428.825393	342024.895809
$\langle r_{21}^{-1}\rangle$	0.9998492589984	0.9998912308494	1.000024296854
$\langle r_{31}^{-1}\rangle$	0.9998638509791	0.9999057441944	1.000038566251
$\langle r_{32}^{-1}\rangle$	398.5423976114	402.1373029064	413.5365105290
$\langle (r_{31}r_{32})^{-1}\rangle$	398.4877927370	402.0990589015	413.5521314933
$\langle (r_{32}r_{21})^{-1}\rangle$	398.4849137616	402.0961688833	413.5492072979
$\langle (r_{31}r_{21})^{-1}\rangle$	1.992047926597	1.992280422629	1.993010072434
$\langle (r_{32}r_{31}r_{21})^{-1}\rangle$	794.90908505	802.16418121	825.17752181
$\langle r_{21}\rangle$	1.500229562409	1.500166624663	1.499967090001
$\langle r_{31}\rangle$	1.500223659552	1.500160720184	1.499961186483
$\langle r_{32}\rangle$	$3.763715066031\times10^{-3}$	$3.730069344784\times10^{-3}$	$3.627249315637\times10^{-3}$
$\langle r_{21}^2\rangle$	3.000925384153	3.000673562997	2.999875258280
$\langle r_{31}^2\rangle$	3.000907793135	3.000655963785	2.999857652388
$\langle r_{32}^2\rangle$	$0.188874018542\times10^{-4}$	$0.1855122346652\times10^{-4}$	$0.1754258380434\times10^{-4}$
$\langle r_{21}^3\rangle$	7.503489911979	7.502545354839	7.499551220113
$\langle r_{31}^3\rangle$	7.503437239738	7.502492656457	7.499498497710
$\langle r_{32}^3\rangle$	$0.118478003453\times10^{-6}$	$0.1153289216446\times10^{-6}$	$0.1060522129237\times10^{-6}$
$\langle r_{21}^4\rangle$	22.51402052822	22.51024148604	22.49826332561
$\langle r_{31}^4\rangle$	22.51384507503	22.51006594791	22.49808771573
$\langle r_{32}^4\rangle$	$0.891834956719\times10^{-9}$	$0.8603698107765\times10^{-9}$	$0.7693556850118\times10^{-9}$
$\langle (\mathbf{r}_{31}\cdot\mathbf{r}_{32})\rangle$	$0.6481923017012\times10^{-6}$	$0.4760056176442\times10^{-6}$	$-0.3165376621716\times10^{-7}$
$\langle (\mathbf{r}_{32}\cdot\mathbf{r}_{21})\rangle$	$0.1823920955250\times10^{-4}$	$0.1807521784888\times10^{-4}$	$0.1757423757056\times10^{-4}$
$\langle (\mathbf{r}_{31}\cdot\mathbf{r}_{21})\rangle$	3.000907144943	3.000655487779	2.999857684042
τ_{21}	$0.7949897389\times10^{-4}$	$0.5736626942044\times10^{-4}$	$-0.1030210584369\times10^{-4}$
τ_{31}	$0.2429269699\times10^{-2}$	$0.2429079347733\times10^{-2}$	$0.2428529279259\times10^{-2}$
τ_{32}	0.9999874898390	0.9999877108127	0.9999883739697
$\langle f\rangle$	$0.6240646280282\times10^{-3}$	$0.6185391074597\times10^{-3}$	$0.6016502857779\times10^{-3}$
$\langle -\nabla_2\cdot\nabla_3\rangle$	−158836.012273384	−161714.388101948	−171012.450045429
$\langle -\nabla_1\cdot\nabla_3\rangle$	−0.968050038563694	−0.976746235435464	−1.00433918647835
$\langle -\nabla_1\cdot\nabla_2\rangle$	−0.0316792133619937	−0.0230667712584065	0.00426059055935379
$\langle -\frac{1}{2}\nabla_1^2\rangle$	0.4998646259628	0.4999065033469	0.5000392979595
$\langle -\frac{1}{2}\nabla_2^2\rangle$	79418.02197630	80857.20558436	85506.22289242
$\langle -\frac{1}{2}\nabla_3^2\rangle$	79418.49016171	80857.68242409	85506.72719231
$\langle \delta_{21}\rangle$	0.313681896	0.313760812	0.314002531
$\langle \nu_{21}\rangle$	0.994773280	0.994934677	0.999486447
$\overline{\nu_{21}}$ [a]	0.9951869453478	0.995186453478	0.995186453478
$\langle \delta_{31}\rangle$	0.320611819	0.320631162	0.320697954
$\langle \nu_{31}\rangle$	−2.0007595	−1.9980667	−1.9994278
$\overline{\nu_{31}}$ [a]	−1.999636157582	−1.999725850875	−2.0
$\langle \delta_{32}\rangle$	20149938.827	20700137.343	22510841.038
$\langle \nu_{32}\rangle$	−398.5424086	−402.1373156	−413.5365311
$\overline{\nu_{32}}$ [a]	−398.5424113627	−402.1373165919	−413.5365240000
$\langle \delta_{321}\rangle$	$0.641422\times10^{+7}$	$0.658999\times10^{+7}$	$0.716904\times10^{+7}$
η	0.4741×10^{-14}	0.5157×10^{-14}	0.4037×10^{-14}
E_{tr}	−398.542411362650112	−402.137316591922656	−413.536524000000000

[a]The exact value from Eq. (5).

make only a few following remarks. In all formulas given below and also in Table II, the notations 1 and 2 refer to the electron and muon, respectively. The notation 3 designates the helium nucleus. δ_{31}, δ_{21}, and δ_{321} stand for the two- and three-particle Dirac δ functions, respectively. The two-body cusp is determined in a traditional manner [15,16]:

$$\langle \nu_{ij} \rangle = \frac{\left\langle \delta(\mathbf{r}_{ij}) \dfrac{\partial}{\partial r_{ij}} \right\rangle}{\langle \delta(\mathbf{r}_{ij}) \rangle}, \tag{4}$$

where $\delta_{ij} = \delta(\mathbf{r}_{ij})$ is the appropriate Dirac δ function and $(ij) = (21)$ and (31). The exact value $\overline{\nu}_{ij}$ of the two-particle Coulomb cusp equals [15]

$$\overline{\nu}_{ij} = q_i q_j \frac{m_i m_j}{m_i + m_j}, \tag{5}$$

where q_i and q_j are the charges and m_i and m_j the masses of the particles.

The expectation values of the two interparticle cosine functions are determined traditionally:

$$\tau_{ij} = \langle \cos(\mathbf{r}_{ik} \cdot \mathbf{r}_{jk}) \rangle = \left\langle \frac{\mathbf{r}_{ik} \cdot \mathbf{r}_{jk}}{r_{ik} \cdot r_{jk}} \right\rangle, \tag{6}$$

where $(i,j,k) = (1,2,3)$. The quantity $\langle f \rangle$ is expressed in terms of the relative coordinates (r_{31}, r_{32}, r_{21}) or perimetric coordinates (u_1, u_2, u_3) [where $u_i = \frac{1}{2}(r_{ij} + r_{ik} - r_{jk})$, and $(i,j,k) = (1,2,3)$] as follows:

$$\langle f \rangle = \left\langle \psi \left| \frac{u_1}{r_{32}} \frac{u_2}{r_{31}} \frac{u_3}{r_{21}} \right| \psi \right\rangle = \int \int \int |\psi(u_1, u_2, u_3)|^2 u_1 u_2 u_3 du_1 du_2 du_3. \tag{7}$$

The value $\langle f \rangle$ can be calculated directly or by applying τ_{ij}. The equalities

$$\tau_{21} + \tau_{32} + \tau_{31} = 1 + 4\langle f \rangle \tag{8}$$

hold for arbitrary three-body nonsymmetric systems. The virial factor η is determined as follows:

$$\eta = \left| 1 + \frac{\langle V \rangle}{2\langle T \rangle} \right|, \tag{9}$$

where $\langle T \rangle$ and $\langle V \rangle$ are the expectation values of the kinetic and potential energy, respectively. The deviation of the factor η from zero indicates the quality of the wave function used. The appropriate binding energies ε are given in eV (1 Ry = 27.2113961 eV). Note also that in Table II only stable figures from calculations with the higher values of N are presented.

Note that some expectation values in Table II can be expressed as the linear combinations of other properties. For instance, for the three relative vectors $\vec{r}_{32}$, $\vec{r}_{31}$, and $\vec{r}_{21}$ we have

$$\vec{r}_{32} - \vec{r}_{31} + \vec{r}_{21} = 0. \tag{10}$$

Therefore, the three following equalities $[(i,j,k) = (1,2,3)]$

$$\vec{r}_{ik} \cdot \vec{r}_{jk} = \frac{1}{2}(r_{ik}^2 + r_{jk}^2 - r_{ij}^2) \tag{11}$$

hold in any case. For the appropriate expectation values one finds (see Table II)

$$\langle \vec{r}_{ik} \cdot \vec{r}_{jk} \rangle = \frac{1}{2}(\langle r_{ik}^2 \rangle + \langle r_{jk}^2 \rangle - \langle r_{ij}^2 \rangle). \tag{12}$$

Analogously, since $\vec{p}_1 + \vec{p}_2 + \vec{p}_3 = 0$, then we write

$$\vec{p}_i \cdot \vec{p}_j = \frac{1}{2}(p_k^2 - p_i^2 - p_j^2) \tag{13}$$

and

$$\langle \vec{p}_i \cdot \vec{p}_j \rangle = \frac{1}{2}(\langle p_k^2 \rangle - \langle p_j^2 \rangle - \langle p_i^2 \rangle), \tag{14}$$

respectively $[(i,j,k) = (1,2,3)]$. Moreover, if the three $\vec{p}_i$ are determined by the relations $\vec{p}_i = (-\imath)\vec{\nabla}_i$ in Cartesian coordinates, then one finds

$$\langle -\vec{\nabla}_i \cdot \vec{\nabla}_j \rangle = \left\langle -\frac{1}{2}\nabla_k^2 \right\rangle - \left\langle -\frac{1}{2}\nabla_i^2 \right\rangle - \left\langle -\frac{1}{2}\nabla_j^2 \right\rangle, \tag{15}$$

where $(i,j,k) = (1,2,3)$. The expectation values from both sides of this equality can be found in Table II. Note, however, that the last three equalities are obeyed only in Cartesian coordinates and only if $\vec{p}_i = (-\imath)\vec{\nabla}_i$. In the present study such a choice is used, and therefore, $\langle -\vec{\nabla}_i \cdot \vec{\nabla}_j \rangle$ can be expressed through $\langle -\frac{1}{2}\nabla_i^2 \rangle$ and vice versa.

The analysis of the computed properties for helium-muonic atoms indicates clearly that they have two-shell cluster structure, as expected. This means that the muon moves at very short distances from the nucleus. The radius of the muonic shell is ≈ 413.5 times smaller than the radius of the outside, electron shell. The electron and muon velocities are quite comparable to each other. However, the correlation between electron and muon motions in the helium-muonic atoms is significantly smaller than the electron-electron correlation in the usual helium atom. In order to show the principal difference between our previous [4] and present wave functions, let us introduce the following parameter, which is very useful in few-body bound-state computations:

$$\chi = 10^3 \sqrt{\frac{1}{3} \sum_{(ij)} \left(\frac{\langle \nu_{ij} \rangle}{\overline{\nu}_{ij}} - 1 \right)^2}. \tag{16}$$

Here, $\langle \nu_{ij} \rangle$ and $\overline{\nu}_{ij}$ are the computed and expected (i.e., predicted) cusp values. The summation is to be extended over all different pairs of particles in the N-body system, i.e., $i \neq j = 1, \ldots, N$ and also $(ij) = (ji)$. In particular, for the three-body systems (where $N = 3$) one finds (ij)

=(32),(31),(21). The parameter χ indicates the cusp quality of the wave function determined in calculations. For the exact wave function this parameter equals zero exactly. In the general case, the smaller values of the χ parameter correspond to more accurate wave functions. The wave function used in Ref. [4] gives $\chi \approx 4.0028447$. Our present wave functions have a significantly better cusp quality, since, e.g., for the $^3He^{2+}\mu^- e^-$ atom $\chi \approx 0.40329858$. It should be mentioned, however, that cusps as well as other geometrical and dynamical properties (see, e.g., Table II) are the so-called secondary properties. The only primary property is the bound-state energy. The main point to be emphasized is that any improvement of the secondary properties is real if and only if the same wave function provides also the better bound-state energy. A separate improvement of the secondary properties, and in particular, an artificial ''cusp-improvement'' has no sense. Furthermore, such an artificially corrected cusp does not indicate the better quality of the computed δ function.

Now, let us discuss the hyperfine splitting calculations for the helium-muonic atoms in detail. The hyperfine perturbation of the ground $S(L=0)$ state is given by the expectation value of the following operator:

$$H_{HF} = -\frac{8\pi}{3}\vec{\mu}_\mu \cdot \vec{\mu}_N \delta(\mathbf{r}_{\mu N}) - \frac{8\pi}{3}\vec{\mu}_\mu \cdot \vec{\mu}_e \delta(\mathbf{r}_{e\mu}) - \frac{8\pi}{3}\vec{\mu}_e \cdot \vec{\mu}_N \delta(\mathbf{r}_{eN}), \tag{17}$$

where $\vec{\mu}_e$, $\vec{\mu}_\mu$, and $\vec{\mu}_N$ are the magnetic moments of the electron, muon, and nucleus, respectively. The Dirac δ function $\delta(\mathbf{r}_{ij})$ is determined traditionally, i.e., $\delta(\mathbf{r}_{ij}) = \delta(\mathbf{r}_i - \mathbf{r}_j)$. For the considered $S(L=0)$ states the nonrelativistic wave function factorizes into a product of coordinate-space and spin-space parts. Following Ref. [6] it can be shown that the spin-space expectation value $\langle H_{HF} \rangle$ (i.e., spin operator) can be represented in the form

$$\delta H_s = \langle H_{HF} \rangle = -a\vec{s}_\mu \cdot \vec{I}_N - b\vec{s}_e \cdot \vec{s}_\mu - c\vec{s}_e \cdot \vec{I}_N, \tag{18}$$

where $\vec{s}_e$, $\vec{s}_\mu$, and $\vec{I}_N$ are the spin vectors of the electron, muon, and nucleus, respectively. In this formula the constants a, b, and c have the following values (in atomic units):

$$a = A\langle \delta(\mathbf{r}_{\mu N}) \rangle = \frac{2\pi}{3}\alpha^2 \frac{g_\mu g_N}{m_\mu m_p}\langle \delta(\mathbf{r}_{\mu N}) \rangle, \tag{19}$$

$$b = B\langle \delta(\mathbf{r}_{e\mu}) \rangle = \frac{2\pi}{3}\alpha^2 \frac{g_e g_\mu}{m_e m_\mu}\langle \delta(\mathbf{r}_{e\mu}) \rangle, \tag{20}$$

$$c = C\langle \delta(\mathbf{r}_{eN}) \rangle = \frac{2\pi}{3}\alpha^2 \frac{g_e g_N}{m_e m_p}\langle \delta(\mathbf{r}_{eN}) \rangle, \tag{21}$$

where α is the fine structure constant, m_e, m_μ, and m_p are the electron, muon, and proton masses, respectively. Here, we used the fact that in atomic units the Bohr magneton equals $\frac{1}{2}$ exactly. The fine structure constant α, proton mass m_p, and g factors used in calculations were chosen from [13], [17], and [18]

$$\alpha = 7.29735308 \times 10^{-3}, \quad m_p = 1836.152701,$$

$$g_e = 2.002319304386, \quad g_\mu = 2.002331846,$$

$$g_N(^3\mathrm{He}) = 4.2552496, \quad g_N(^4\mathrm{He}) = 0.$$

In fact, the hyperfine splitting is traditionally expressed in MHz. To recalculate the energies from a.u. to MHz the following conversion factor $6.57968392061 \times 10^9$ (MHz / a.u.) [17] has been used. Now, one can easily calculate the A, B, and C constants

$$A(^3\mathrm{He}) = 16.468831488009 \ \text{MHz}, \quad A(^4\mathrm{He}) = 0,$$

$$B(^3\mathrm{He}) = 14229.180106055 \ \text{MHz},$$

$$B(^4\mathrm{He}) = 14229.180106055 \ \text{MHz},$$

$$C(^3\mathrm{He}) = 3405.2103352634 \ \text{MHz}, \quad C(^4\mathrm{He}) = 0.$$

Thus, the main problem is now to compute the expectation values of the appropriate Dirac δ functions. In fact, the numerical computation of all δ functions does not contain any principal difficulties. However, in contrast with the bound-state energies, there is no maximum-minimum principle for the δ function expectation values. Briefly, this means that the results of such calculations may oscillate around the exact values when the total number of basis functions grows. The typical situation is shown in Table III where the ''convergence'' of the three δ functions is presented for the $^3He^{2+}\mu^- e^-$ and $^4He^{2+}\mu^- e^-$ atoms. By using the results of our present calculations we have determined the following expectation values for the appropriate δ functions:

$$\langle \delta_{32} \rangle(^3\mathrm{He}) = 20149938.85 \pm 1 \times 10^{-2},$$

$$\langle \delta_{32} \rangle(^4\mathrm{He}) = 20700137.35 \pm 1 \times 10^{-2},$$

$$\langle \delta_{31} \rangle(^3\mathrm{He}) = 0.32061195 \pm 1 \times 10^{-7},$$

$$\langle \delta_{31} \rangle(^4\mathrm{He}) = 0.32063105 \pm 1 \times 10^{-7},$$

$$\langle \delta_{21} \rangle(^3\mathrm{He}) = 0.3136818 \pm 1 \times 10^{-7},$$

$$\langle \delta_{21} \rangle(^4\mathrm{He}) = 0.3137605 \pm 1 \times 10^{-7},$$

where the subscript 1 denotes the electron, the subscript 2 designates muon μ^-, and subscript 3 stands for the helium nucleus. Here, the expectation values for all δ functions are taken from the results of calculations with the maximal number of basis functions, i.e., $N=700$. In Table III for each expectation value only ten significant figures are presented. The appropriate uncertainties have been determined from comparison with the results of calculations with a smaller number of basis functions (see, e.g., Table III for the $^3He^{2+}\mu^- e^-$ and $^4He^{2+}\mu^- e^-$ atoms).

TABLE III. The observed ''convergence'' for the δ function expectation values in atomic units for the ground states in the helium-3-muonic and helium-4-muonic atoms.

N^a	$\langle\delta_{32}\rangle$	$\langle\delta_{31}\rangle$	$\langle\delta_{21}\rangle$
400	0.2014993885×10^8	0.3206117828	0.3136817601
500	0.2014993884×10^8	0.3206117849	0.3136818352
550	0.2014993885×10^8	0.3206118465	0.3136817879
600	0.2014993885×10^8	0.3206118671	0.3136818350
700	0.2014993885×10^8	0.3206118514	0.3136818415
	$20149938.85\pm1\times10^{-2}$	$0.32061195\pm1\times10^{-7}$	$0.3136818\pm1\times10^{-7}$
N^a	$\langle\delta_{32}\rangle$	$\langle\delta_{31}\rangle$	$\langle\delta_{21}\rangle$
400	0.2070013736×10^8	0.3206309205	0.3137605171
500	0.2070013736×10^8	0.3206309726	0.3137605354
550	0.2070013735×10^8	0.3206310118	0.3137604991
600	0.2070013735×10^8	0.3206311011	0.3137605325
700	0.2070013735×10^8	0.3206311005	0.3137605147
	$20700137.35\pm1\times10^{-2}$	$0.32063105\pm1\times10^{-7}$	$0.3137605\pm1\times10^{-7}$

Now, for the a, b, and c coefficients in the $\delta\mathrm{H}_s$ operator we find

$$a(^3\mathrm{He})=331845941.65024\ \ \mathrm{MHz},\quad a(^4\mathrm{He})=0$$

$$b(^3\mathrm{He})=4463.4348281917\ \ \mathrm{MHz},$$

$$b(^4\mathrm{He})=4464.5461271580\ \ \mathrm{MHz}$$

$$c(^3\mathrm{He})=1091.7511257490\ \ \mathrm{MHz},\quad c(^4\mathrm{He})=0.$$

The diagonalization of the δH_s operator (in spin space) yields the three following eigenvalues:

$$\lambda_1=\frac{1}{4}(a+b+c)+\frac{1}{2}\sqrt{a^2+b^2+c^2-ab-ac-bc},$$

$$\lambda_2=\frac{1}{4}(a+b+c)-\frac{1}{2}\sqrt{a^2+b^2+c^2-ab-ac-bc},$$

$$\lambda_3=-\frac{1}{4}(a+b+c).$$

The hyperfine splitting equals $|\lambda_2-\lambda_3|$ for the $^3\mathrm{He}^{2+}\mu^-e^-$ atom and $|\lambda_1-\lambda_3|=b(^4\mathrm{He})$ for the $^4\mathrm{He}^{2+}\mu^-e^-$ atom, respectively. Now, by using the a, b, and c values presented above one easily finds that $|\lambda_2-\lambda_3|=4166.3894655$ MHz ≈4166.389 MHz (the hyperfine splitting for the $^3\mathrm{He}^{2+}\mu^-e^-$ atom) and $|\lambda_1-\lambda_3|=4464.5546647$ MHz ≈4464.555 MHz (the hyperfine splitting for the $^4\mathrm{He}^{2+}\mu^-e^-$ atom).

The standard approach widely used in earlier papers is based on the fact that $a\gg b$ and $a\gg c$. In this approximation one easily finds that the hyperfine splitting equals $\Delta\nu=b$ for the $^4\mathrm{He}^{2+}\mu^-e^-$ atom and $\Delta\nu=\frac{3}{4}(b+c)$ for the $^3\mathrm{He}^{2+}\mu^-e^-$ atom. In other words, we have in this approximation

$$\Delta\nu(^4\mathrm{He})=14229.180061055\langle\delta(\mathbf{r}_{e\mu})\rangle\ \ \mathrm{MHz},$$

$$\Delta\nu(^3\mathrm{He})=10671.885079542\langle\delta(\mathbf{r}_{e\mu})\rangle+2553.9077514476\langle\delta(\mathbf{r}_{eN})\rangle\ \ \mathrm{MHz},\quad(22)$$

where $\langle\delta(\mathbf{r}_{e\mu})\rangle$ and $\langle\delta(\mathbf{r}_{eN})\rangle$ are the expectation values for the electron-muonic and electron-nucleus δ functions, respectively. From these formulas and our expectation values we find $\Delta\nu(^4\mathrm{He})\approx4464.555$ MHz and $\Delta\nu(^3\mathrm{He})\approx4166.383$ MHz. These values are very close to the experimentally known values for $\Delta\nu(^4\mathrm{He})\approx4464.95$ MHz [19] and $\Delta\nu(^3\mathrm{He})\approx4166.41$ MHz (for references and a review of experimental data see [6] and [10]). For the $\Delta\nu(^3\mathrm{He})$ value the observed agreement can be considered as excellent. Furthermore, we estimate the maximal numerical errors for the both theoretical $\Delta\nu$ values as a few kHz. The difference between the hyperfine splittings determined in the standard approach and by using the exact diagonalization of δH operator is also a few kHz.

The results of our present study can be also presented in the same form as in Ref. [7]:

$$\Delta\nu=\Delta\nu_{nr}(1+\epsilon^r),\quad(23)$$

where $\Delta\nu$ and $\Delta\nu_{nr}$ are the exact (or experimental) and computed nonrelativistic hyperfine splittings, respectively. ϵ^r is the total correction which includes relativistic, radiative, and radiative recoil contributions. The absolute value of ϵ^r is of principal interest for all future theoretical works. In Ref. [7] it was found that the factor $\epsilon^r\approx2\times10^{-3}$, since [7] the numerical value of the ϵ^r has been decreased significantly. In the present study the determined ϵ^r values are ≈300 times smaller than in Ref. [7] for the $^4\mathrm{He}^{2+}\mu^-e^-$ atom and even ≈3000 times smaller in the case of the $^3\mathrm{He}^{2+}\mu^-e^-$ atom. In fact, this means that all relativistic and radiative corrections are significantly smaller than was predicted in earlier works. In other words, the high-precision, nonrelativistic wave functions reproduce the hyperfine splitting for both helium-muonic atoms quite accurately. However, our computed values do not coincide with the known experimental

numbers exactly. Furthermore, the leading, lowest-order ($\sim\alpha^2$) self-energy and vacuum-polarization corrections to the hyperfine splitting must be evaluated accurately. Their total contribution can be approximated [5] by the known hydrogenic value [20], i.e., $\Delta\nu\alpha^2(\ln 2-2.5)\approx 0.39-0.41$ MHz, but the real lowest-order correction can be smaller. Actually, the new high-precision measurements of the hyperfine splitting should be performed for both helium-muonic atoms $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$. The results of such measurements are critically important to provide further progress in theoretical studies of such systems. Hopefully, this our work will stimulate further experimental activity to perform the high-precision measurements for the hyperfine splitting in the helium-muonic atoms.

The present approach can also be used to determine the hyperfine splitting for the positively charged $^6Li^{3+}\mu^-e^-$ and $^7Li^{3+}\mu^-e^-$ muonic ions. The appropriate analytical expressions can easily be found from Eqs. (17)–(23) mentioned above. The following values for the nuclear constants have been used in our present calcualtions: $M(^6\mathrm{Li})=10957.602m_e$, $g_N(^6\mathrm{Li})=1.64410$, $M(^7\mathrm{Li})=12780.885m_e$, and $g_N(^7\mathrm{Li})=6.51288$ [21–23]. Finally, the hyperfine splitting for the $^6Li^{3+}\mu^-e^-$ ion is $\approx$29311.4 MHz and for the $^7Li^{3+}\mu^-e^-$ ion it is $\approx$36790.8 MHz. These values to the best of our knowledge, have not been computed or measured previously.

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