The hyperfine structure of the ground states in the helium
muonic atoms

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Abstract

The hyperfine structures of the ground states in the $^3\text{He}^{2+}\mu^-e^-$ and $^4\text{He}^{2+}\mu^-e^-$ helium-muonic atoms are investigated with the use of highly accurate variational wave functions. The differences between corresponding levels of hyperfine structure (i.e. hyperfine splittings) are determined to very high numerical accuracy. In particular, we have found that the hyperfine structure splitting in the ground state of the $^4\text{He}^{2+}\mu^-e^-$ atom is $\Delta\nu \approx 4464.55454(3) \ MHz$, while analogous splitting for the $^3\text{He}^{2+}\mu^-e^-$ atom is $\Delta\nu \approx 4166.43547(3)$.  

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I. INTRODUCTION

In this study we report the results of highly accurate calculations of the ground $S(L = 0)$-states in the helium-muonic $^3\text{He}^2^+\mu^-e^-$ and $^4\text{He}^2^+\mu^-e^-$ atoms. Our recently improved methods for highly accurate variational computations allow us to construct extremely accurate variational wave functions for these three-body helium-muonic atoms. Such wave functions can be used to obtain essentially exact expectation values of various bound state properties of these systems. In particular, the expectation values of all interparticle delta-functions $\delta_{ij}$ can now be determined to very high numerical accuracy. By using these expectation values one can finally solve the long standing problem of hyperfine structure splitting in the $^3\text{He}^2^+\mu^-e^-$ and $^4\text{He}^2^+\mu^-e^-$ atoms [1] - [7].

In this study we reconsider the problem of highly accurate computations of the helium-muonic $^3\text{He}^2^+\mu^-e^-$ and $^4\text{He}^2^+\mu^-e^-$ atoms. For simplicity, below we restrict ourselves to the analysis of the ground $S(L = 0)$-states in such systems. The ground state in the helium-muonic atom is designated as the $1s_\mu1s_e$-state. Analogous electron-excited states (or $1s_\mu2s_e$-state) in the helium-muonic atoms were discussed in our earlier study [7]. Our main goal is to determine the hyperfine structure splitting in each of these atoms by using the results of most recent highly accurate computation of the expectation values of interparticle delta-functions. The computed values of the hyperfine structure splitting in each helium muonic atom must be compared with the known experimental results [8]. For the ground states in the helium-muonic atoms such experiments were performed in 1970’s. Analogous experimental observations and measurements of the hyperfine structure splitting for the electron-excited states in the helium-muonic atoms are difficult to perform.

For the ground states in the $^3\text{He}^2^+\mu^-e^-$ and $^4\text{He}^2^+\mu^-e^-$ helium-muonic atoms the hyperfine structure splittings have been measured to very good accuracy (see references and discussions in [8]). The known experimental values of the hyperfine structure splitting of the ground states in these two atoms are 4166.41 MHz and 4464.95 MHz, respectively [8]. A large number of theoretical investigations of muonic-helium atoms have been conducted since the middle of 1970’s. In many of these works the main goal was to produce highly accurate evaluation of the hyperfine structure splitting for the ground states of the $^3\text{He}^2^+\mu^-e^-$ and $^4\text{He}^2^+\mu^-e^-$ atoms. In general, to obtain the actual hyperfine structure and evaluate the hyperfine structure splittings one needs to determine the expectation values of all three in-
terparticle delta-functions. The main computational troubles of earlier studies were related with the expectation values of the electron-muonic delta-function. Another complication was related to a slow convergence rate observed in numerical computations of the expectation values of the electron-nucleus delta-function. In general, it was very hard to determine the electron-muonic and electron-nucleus delta-functions to the accuracy better than $1 \cdot 10^{-6}$ a.u. For the electron-nucleus delta-function such a ‘limiting’ accuracy was $\approx 2 \cdot 10^{-7}$ a.u. Finally, it was almost impossible to evaluate the hyperfine structure splitting in the helium-muonic atoms to good numerical accuracy. A substantial progress has been achieved only in our work [7] where we have applied a special Fortran pre-translator MPFUN written by David H.Bailey [9], [10]. By using this pre-translator we determined the hyperfine structure splitting $4166.392 \text{ MHz}$ for the ground state in the $^3\text{He}^{2+}\mu^{-}e^{-}$ atom and $4464.555 \text{ MHz}$ for the ground state in the $^4\text{He}^{2+}\mu^{-}e^{-}$ atom [7]. The absolute uncertainties in both cases are less than 10 kHz. It appears that these values were very close to the known experimental values of the hyperfine structure splitting measured for these atoms, which equal 4166.41 MHz and 4464.95 MHz, respectively [8].

In this study we substantially improved the overall accuracy of our computations. The overall quality of our wave functions has also been improved. The current accuracy of the expectation values of interparticle delta-functions can now be evaluated as $\pm 7 \cdot 10^{-11}$ a.u. (or even better). Right now, we can determine the hyperfine structure splittings in both helium muonic atoms to much better accuracy than it was possible in [7].

II. THREE-BODY VARIATIONAL WAVE FUNCTION

Our computational goal in this study is to determine the highly accurate solutions of the non-relativistic Schrödinger equation

$$H \Psi(r_e, r_\mu, r_{\text{He}}) = E \Psi(r_e, r_\mu, r_{\text{He}}),$$

where $E < 0$ is the numerical parameter (energy) and $H$ is the following Hamiltonian

$$H = -\frac{\hbar^2}{2m_e} \left[ \nabla^2_e + \left( \frac{m_e}{m_\mu} \right) \nabla^2_\mu + \left( \frac{m_e}{M_{\text{He}}} \right) \nabla^2_{\text{He}} \right] + \frac{e^2}{r_{e\mu}} - \frac{2e^2}{r_{e\text{He}}} - \frac{2e^2}{r_{\mu\text{He}}}$$

(1)

where $\hbar, m_e$ and $e$ are the reduced Planck constant, electron mass and absolute value of the electric charge of the electron. Everywhere below in this study, we shall use only atomic units, where $\hbar = 1, m_e = 1$ and $e = 1$. In these units one finds

$$H = -\frac{1}{2} \left[ \nabla^2_e + \left( \frac{1}{m_\mu} \right) \nabla^2_\mu + \left( \frac{1}{M_{\text{He}}} \right) \nabla^2_{\text{He}} \right] + \frac{1}{r_{e\mu}} - \frac{2}{r_{e\text{He}}} - \frac{2}{r_{\mu\text{He}}}$$

(2)
where masses of the muon \( m_\mu = 206.768262 \ m_e \) and helium nuclei \( M_{3\text{He}} = 5495.8852 \ m_e \) and \( M_{4\text{He}} = 7294.2996 \ m_e \) must be expressed in the electron mass \( m_e \).

To simplify all formulas below we designate the electron, muon and helium nucleus as particles 1, 2 and 3, respectively. For the considered ground \( S(L = 0) \)–states in the three-body \( ^3\text{He}^{2+} \mu^- e^- \) and \( ^4\text{He}^{2+} \mu^- e^- \) muonic atoms the wave function depends upon three scalar interparticle coordinates, i.e. \( \Psi(r_e, r_\mu, r_{\text{He}}) = \Psi(r_{21}, r_{31}, r_{32}) \). This unknown wave function \( \Psi \) can be approximated to very high accuracy by using different variational expansions. In particular, in this work we apply the exponential variational expansion in three-body relative coordinates \( r_{21}, r_{31} \) and \( r_{32} \). For the \( S(L = 0) \)–states in the helium-muonic atoms this expansion takes the form

\[
\Psi_{LM} = \sum_{i=1}^{N} C_i \exp\left(-\alpha_i r_{21} - \beta_i r_{31} - \gamma_i r_{32}\right) \tag{3}
\]

where \( C_i \) are the linear (or variational) parameters, while \( \alpha_i, \beta_i, \gamma_i \) are the non-linear parameters. In general, the exponential variational expansion has significantly more complex form even for the \( S(L = 0) \)–states \[11\]. First, it is convenient to write such an expansion in the three perimetric coordinates \( u_1, u_2, u_3 \) which are completely independent and each of them varies between 0 and \( +\infty \). In this case all non-linear parameters \( \alpha_i, \beta_i, \gamma_i \) must be positive. Second, for some three-body systems it is necessary to use the complex values for these parameters. It is allows one to accelerate the overall convergence rate of this variational expansion, e.g., for adiabatic and/or weakly-bound systems. Here we do not want to discuss all advantageous of exponential variational expansions for three-body systems. Note only that the expansion, Eq.\( (3) \), provides a simple method \[11\] to construct extremely accurate variational wave functions for an arbitrary three-body systems (and different states in such systems). The overall quality of the final wave function, Eq.\( (3) \) is very good, and it can be used to determine all expectation values needed for analysis of the given three-body system. In particular, such a wave function generates very accurate expectation values of all interparticle delta-functions which are of great interest for this study (see the next Section).
III. SPIN-SPIN CONTACT INTERACTION BETWEEN TWO PARTICLES

Let us assume that we have two particles \( a \) and \( b \) which have non-zero spins \( s_a \) and \( s_b \), respectively. The non-relativistic Hamiltonian of the spin-spin interaction takes the form

\[
H_{ss} = -\frac{\mu_a}{s_a} s_a \cdot H_b = -\frac{\mu_a}{s_a} c \left( s_a \cdot \int \frac{n \times j_b}{r^2} dV \right)
\]  

(4)

where \( c \) is the speed of light in vacuum, \( n = \frac{r}{r} \) is the unit vector which corresponds to the radius-vector \( r \) and \( j_b \) is the current generated by the particle \( b \) with spin \( s_b \). For this current we can write

\[
j_b = \frac{\mu_b}{s_b} c \left( \nabla \times (\Psi^* s_b \Psi) \right) = \frac{\mu_b}{s_b} c \left( \frac{d\Psi^2(r)}{dr} \right) (n \times s_b)
\]  

(5)

The magnetic field \( H_b \) generated by this spin current \( j_b \) takes the form

\[
H_b = \frac{\mu_b}{s_b} \int_0^\infty \frac{d\Psi^2(r)}{dr} dr \oint \left( n \times (n \times s_b) \right) do = \frac{\mu_b}{s_b} \Psi^2(0) \frac{8\pi}{3} s_b
\]  

(6)

Therefore, the Hamiltonian of the spin-spin interaction of the particles \( a \) and \( b \) is

\[
H_{ss} = -\frac{8\pi \mu_a \mu_b}{3 s_a s_b} (s_a \cdot s_b) \langle \delta(r_{ab}) \rangle
\]  

(7)

where \( \delta(r_{ab}) = \delta(r_a - r_b) \) is the delta-function between two particles (\( a \) and \( b \)). The interparticle interaction which contains the corresponding delta-function is called the contact interaction.

In atomic systems all magnetic moments are traditionally measured in Bohr magnetons \( \mu_B \). In atomic units \( \hbar = 1, m_e = 1, e = 1 \) the value of the Bohr magneton equals \( \frac{1}{2} \) exactly. In these units the formula Eq.(7) takes the form

\[
H_{ss} = -\frac{2\pi \mu_a \mu_b}{3 s_a s_b} \langle \delta(r_{ab}) \rangle (s_a \cdot s_b)
\]  

(8)

In a few-body system the total Hamiltonian of the spin-spin interaction equals to the sum of different two-particle Hamiltonians, Eq.(8). In the general case, in \( A \)-body system one finds \( \frac{A(A-1)}{2} \) spin-spin terms, Eq.(8), in the total Hamiltonian which describes the hyperfine interactions. In reality, many actual few-body systems contain identical particles and, therefore, the total number of terms in the Hamiltonian of spin-spin interaction is less than the number of interparticle interactions \( \frac{A(A-1)}{2} \).
IV. THE HYPERFINE STRUCTURE OF THE HELIUM-MUONIC ATOMS

It follows from here that the general formula for the Hamiltonian of hyperfine structure \((\Delta H)_{\text{h.s.}}\) of an arbitrary three-body system is written as the sum of the three following terms. Each of these terms is proportional to the product of the factor \(\frac{2\pi}{3} \alpha^2\) and expectation value of the corresponding (interparticle) delta-funtion. The third (additional) factor contains the corresponding \(g\)–factors (or hyromagnetic ratios) and scalar product of the two spin vectors. For instance, for the \(^3\text{He}^{2+}\mu^-e^-\) atom this formula takes the form (in atomic units) (see, e.g., [12], (see also [7]))

\[
(\Delta H)_{\text{h.s.}} = \frac{2\pi}{3} \alpha^2 \frac{g_N g_\mu}{m_p m_\mu} \langle \delta(\mathbf{r}_{32}) \rangle (\mathbf{I}_N \cdot \mathbf{s}_\mu) + \frac{2\pi}{3} \alpha^2 \frac{g_N g_e}{m_p m_e} \langle \delta(\mathbf{r}_{31}) \rangle (\mathbf{I}_N \cdot \mathbf{s}_e) + \frac{2\pi}{3} \alpha^2 \frac{g_e g_\mu}{m_e m_\mu} \langle \delta(\mathbf{r}_{21}) \rangle (\mathbf{s}_e \cdot \mathbf{s}_\mu)
\]

where \(\alpha = \frac{e^2}{\hbar c}\) is the fine structure constant, \(m_\mu\) and \(m_p\) are the muon and proton masses, respectively. The notation \(N\) stands for the nucleus \(^3\text{He}\). The factors \(g_\mu, g_e\) and \(g_N\) are the corresponding \(g\)–factors. The expression for \((\Delta H)_{\text{h.s.}}\) is, in fact, an operator in the total spin space which has the dimension \((2s_N + 1)(2s_\mu + 1)(2s_e + 1) = 8\). In our calculations we have used the following numerical values for the constants and factors from Eq. (9):

\(\alpha = 7.2973525698 \cdot 10^{-3}\), \(m_p = 1836.152701 m_e\), \(m_\mu = 206.768262 m_e\), \(g_\mu = -2.0023318414\) and \(g_e = -2.002319304362\). The \(g\)–factor of the helium-3 nucleus is determined from the formula: \(g_N = \frac{\mathcal{M}_N}{I_N} = -4.2555016\), where \(\mathcal{M}_N = -2.1277508\) [13] is the magnetic moments (in nuclear magnetons) of the helium-3 nucleus. The spin of the helium-3 nucleus is designated in Eq. (9) as \(I_N = \frac{1}{2}\).

This means that in the ground state of the helium-3 muonic atom one finds eight spin states. They are separated into three different groups: (1) four spin states with \(J = \frac{3}{2}\), (2) two ‘upper’ spin states with \(J = \frac{1}{2}\), and (3) two ‘lower’ spin states with \(J = \frac{1}{2}\). Here and below the notation \(J\) (or \(J\)) stand for the total angular momentum \(J = L + S\). For the \(S(L = 0)\)–states we have \(J = S\), and therefore, \(J = S\). The energy of the group of four states with \(J = \frac{3}{2}\) is \(\approx 8.296777691701 \cdot 10^7\) \(MHz\), while the energy of the second group of two ‘upper’ spin states with \(J = \frac{1}{2}\) is \(\approx 8.296361048154 \cdot 10^7\) \(MHz\). The group of two ‘lower’ spin states with \(J = \frac{1}{2}\) has the energy \(\approx -2.488991643156 \cdot 10^8\) \(MHz\). The energy difference between the first and second groups of spin states is \(\approx 4166.43547(3)\) \(MHz\). Such a difference is called the hyperfine structure splitting of the ground state of the helium-3
muonic atom. To recalculate the energies expressed in atomic units into MHz we have used the following conversion factor $Ry = 6.579683920729 \cdot 10^9$.

The spin and magnetic moment of the helium-4 nucleus equals zero identically. Therefore, the hyperfine structure splitting in the ground state of the $^4\text{He}^{2+} \mu^- e^-$ atom is related with the electron-muon spin-spin interaction. Four spin state of the electron-muon pair are separated in the two groups with $J = 1$ (three states) and $J = 0$ (one state). The energy difference between these two groups of states is called the hyperfine structure splitting of the ground state in the $^4\text{He}^{2+} \mu^- e^-$ atom. With the constants mentioned above this hyperfine structure splitting is determined with the use of the formula

$$\Delta \nu = 14229.178083766834 \cdot \langle \delta(r_{e^-\mu^-}) \rangle$$

(10)

where $\langle \delta(r_{e^-\mu^-}) \rangle$ is the expectation value of the electron-muon delta-function. This formula produces the hyperfine structure splittings $\Delta \nu$ in MHz, if the expectation value of delta-functions is given in atomic units. By using this formula and our expectation value of the electron-muon delta-function from Table II we have found that $\Delta \nu(^4\text{He}^{2+} \mu^- e^-) = 4464.55454(3) \text{ MHz}$.

The uncertainties mentioned above have been determined from the corresponding uncertainties of the delta-functions. For instance, for the $^4\text{He}^{2+} \mu^- e^-$ atom one finds (from Table II) for the $\langle \delta(r_{e^-\mu^-}) \rangle$ expectation value $\langle \delta(r_{e^-\mu^-}) \rangle \approx 3.13760535825(7) \cdot 10^{-1}$ a.u. Now, by using three expectation values: $3.13760535825 \cdot 10^{-1}$, $3.13760535832 \cdot 10^{-1}$ and $3.13760535839 \cdot 10^{-1}$ we have evaluated the corresponding uncertainty in the $\Delta \nu(^4\text{He}^{2+} \mu^- e^-)$ value as $\approx 1 \cdot 10^{-5} \text{ MHz}$. By including the uncertainties known from modern experiments for the fine structure constant $\alpha$, conversion factor $Ry$, masses of the particles, etc one finds that our maximal uncertainty can be evaluated as $\approx 3 \cdot 10^{-5} \text{ MHz}$.

It should be mentioned that our hyperfine structure splittings $\Delta \nu$ determined to very high accuracy in this study are very sensitive to variations of the basic physical constants, e.g., masses of particles, fine structure constant $\alpha$, etc. In the case of the fine-structure constant $\alpha$ the actual changes of the numerical values of $\Delta \nu$ are quadratic upon $\alpha$. This fact can be used to develop new experimental methods to measure the fine structure constant $\alpha$ and particle masses $m_\mu, M_\text{He}, M_4\text{He}$ to very high accuracy.
V. CONCLUSION

We have considered the hyperfine structures of the ground states of the helium-3 and helium-4 muonic atoms. Our predicted values of the hyperfine structure splittings for the helium-3 and helium-4 muonic atoms are 4166.43547(3) MHz and 4464.55454(3) MHz, respectively. They are very close to the known experimental values 4166.41 MHz and 4464.95 MHz, respectively [8]. Note that the corresponding experiments have been performed in 1970’s. Since then no new accurate measurements of the hyperfine splittings in these muonic atoms have been reported. In reality, such experiments are desperately needed to explain currently observed deviations between highly accurate theoretical and experimental results. For instance, the difference between theoretical and experimental results for the helium-3 muonic atom is $\approx 20$ times smaller than for the helium-4 atom. This has never been explained. On the other hand, the new experiments are also needed to predict and explain some new phenomena, e.g., to determine hyperfine structure splittings in the electron excited states of the helium-muonic atoms. Their predicted values can be found in [7].

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TABLE I: The convergence of the total energies in atomic units for the ground $1s_\mu 1s_e$ states in the helium-muonic atoms. $N$ is the total number of basis functions used in calculations.

| $N$ | $^{3}\text{He}^{2+}\mu^-e^-$ | $^{4}\text{He}^{2+}\mu^-e^-$ |
|-----|--------------------------------|--------------------------------|
| 3300 | -399.042 336 832 862 534 826 9920 -402.637 263 035 135 454 018 9238 | |
| 3500 | -399.042 336 832 862 534 826 9993 -402.637 263 035 135 454 018 9313 | |
| 3700 | -399.042 336 832 862 534 827 0052 -402.637 263 035 135 454 018 9373 | |
| 3840 | -399.042 336 832 862 534 827 0088 -402.637 263 035 135 454 018 9410 | |
| $P^{(a)}$ | -399.042 336 832 862 534 769 | -402.637 263 035 135 454 004 81 |

$^{(a)}$ The best results determined in earlier calculations [8].

TABLE II: Convergence of the expectation values of electron-muon and electron-nucleus delta-functions in atomic units for the ground $1s_\mu 1s_e$ states in the $^{3}\text{He}^{2+}\mu^-e^-$ and $^{4}\text{He}^{2+}\mu^-e^-$ helium-muonic atoms. The notation 1 means the electron $e^-$, the notation 2 stands for the muon $\mu^-$ and notation 3 designates the nuclues of the helium-3 and helium-4, respectively.

| $N$ ($^{3}\text{He}$) | $\langle \delta(r_{21}) \rangle$ | $\langle \delta(r_{31}) \rangle$ | $\langle \delta(r_{32}) \rangle$ | $\langle \delta(r_{321}) \rangle$ |
|----------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|
| 3300 | 3.13682319254·10^{-1} | 3.20611550947·10^{-1} | 2.0149938845207·10^{7} | 6.414000669·10^{6} |
| 3500 | 3.13682319389·10^{-1} | 3.20611550900·10^{-1} | 2.0149938845219·10^{7} | 6.414000959·10^{6} |
| 3700 | 3.13682319454·10^{-1} | 3.20611550894·10^{-1} | 2.0149938845223·10^{7} | 6.414000992·10^{6} |
| 3840 | 3.13682319465·10^{-1} | 3.20611550974·10^{-1} | 2.0149938845229·10^{7} | 6.414000801·10^{6} |

| $N$ ($^{4}\text{He}$) | $\langle \delta(r_{21}) \rangle$ | $\langle \delta(r_{31}) \rangle$ | $\langle \delta(r_{32}) \rangle$ | $\langle \delta(r_{321}) \rangle$ |
|----------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|
| 3300 | 3.13760535618·10^{-1} | 3.20631791336·10^{-1} | 2.07001373516980·10^{7} | 6.589975905·10^{6} |
| 3500 | 3.13760535756·10^{-1} | 3.20631791288·10^{-1} | 2.07001373516964·10^{7} | 6.589976203·10^{6} |
| 3700 | 3.13760535822·10^{-1} | 3.20631791281·10^{-1} | 2.07001373516999·10^{7} | 6.589976239·10^{6} |
| 3840 | 3.13760535832·10^{-1} | 3.20631791364·10^{-1} | 2.07001373517002·10^{7} | 6.589976038·10^{6} |