Hyperfine-structure splitting in the triplet states of carbon muonic ions

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Hyperfine-structure splittings in the $2^3S(L=0)$ state of the six-body carbon muonic $^{11}C^{6+}\mu^-e_4^-$, $^{12}C^{6+}\mu^-e_4^-$, $^{13}C^{6+}\mu^-e_4^-$, and $^{14}C^{6+}\mu^-e_4^-$ ions are determined numerically with the use of variational wave functions. The variational wave functions for each of these carbon muonic ions are constructed with the use of six-body Gaussoids which explicitly depend upon all 15 relative coordinates $r_{12}, r_{13}, \ldots, r_{56}$ defined in an arbitrary six-body system.

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I. INTRODUCTION

Numerical analysis of the hyperfine structure splitting in light muonic atoms and ions has a long history. First evaluations of the hyperfine structure splitting in the helium muonic atoms were performed 30 years ago [1–6]. Both the $^3He^{2+}\mu^-e^-$ and $^4He^{2+}\mu^-e^-$ atoms have extensively been studied in a number of later works (see, e.g., [7–10]). In general, the knowledge of hyperfine structure splitting allows one to obtain some additional information about magnetic nuclear properties (see, e.g., [11,12]). Moreover, experimental studies of light muonic atoms can be used to increase the accuracy of current experimental measurements for light nuclei (see, e.g., [13] and references therein). Therefore, it is important to expand our considerations to the lithium muonic, beryllium muonic, boron muonic, and more complicated muonic-atomic systems. The hyperfine structure splittings in some such atoms and ions have been discussed in several of our recent papers [14,15]. Note that in all few-electron muonic atoms and ions, we always have a very significant contribution from electron-electron correlations. Such a correlation does not exist in one-electron helium muonic atom, but in many-electron muonic atoms and ions, the electron-electron interactions provide substantial corrections to the bound-state energies. Moreover, in any muonic atom and ion, one finds some additional (or muonic) contributions into electron-nucleus correlations. The source of such contributions follows from the overlap of muonic wave function with the nuclear wave function at very short distances $r \approx \alpha^2 a_0$ and with atomic (or many-electron) wave function at relatively large distances $r \approx a_0$.

Theoretical and experimental investigations of the structure and properties of various muonic atoms and ions started in the middle of 1960s [16–20]. The current bibliography for muonic atoms and ions includes more than 1000 publications. A large number of interesting effects can be found in each muonic atom. Briefly, these effects can be separated into a few groups: (1) recoil effects; (2) retardation effects; (3) analysis of interparticle correlations; (4) vacuum polarization, self-energy, and anomalous magnetic moment; (5) nuclear deformations analysis; (6) nuclear polarization and isomeric shifts; (7) polarization of muons. A separate group of problems is related with the study of muonic atoms with unstable nuclei which have finite lifetimes [21,22]. Analysis of the bound-state properties of muonic atoms (and ions) allows one to evaluate the overall contribution of each of these effects in the total energy and bound-state structure.

In this work, we consider the hyperfine structure of the bound triplet $2^3S(L=0)$ states of carbon muonic ions $^{11}C^{6+}\mu^-e_4^-$, $^{12}C^{6+}\mu^-e_4^-$, $^{13}C^{6+}\mu^-e_4^-$, and $^{14}C^{6+}\mu^-e_4^-$. We assume that in each of these carbon muonic ions, there are magnetic interactions between the nuclear, muon, and total electron spins. In those cases where the nuclear spin equals zero identically, the magnetic interaction includes only one term, corresponding to the magnetic interaction between the muon spin and total electron spin. In general, such an interaction between three spins produces a very interesting hyperfine structure. Below, we want to determine the energy differences between the energy levels which represent the hyperfine structure. It is clear that an accurate evaluation of the hyperfine splitting in these six-body ions will require numerical computation of three two-particle delta functions (muon-nuclear, electron-nuclear, and electron-muon delta functions). In turn, such computations can be performed only with the use of accurate six-body wave functions explicitly written in the 15 relative coordinates r_{12}, r_{13}, r_{14}, r_{15}, r_{16}, r_{23}, r_{24}, r_{25}, r_{26}, r_{34}, r_{35}, r_{36}, r_{45}, r_{46}, and r_{56}. The trial wave functions must correspond to the triplet permutation symmetry between four identical electrons.

The study of the hyperfine structure splitting in carbon muonic, nitrogen muonic, and oxygen muonic atoms and ions is of interest for several reasons. First, in such systems, the radius of the muonic orbit is approximately equal to the radius of the central nucleus. In other words, the muon moves almost on the surface of the nucleus. This means that in all these atoms and ions, we can observe an actual interaction between the motion of muon μ^- and various surface-type excitations of the nucleus. Second, such an interaction can produce very substantial differences in the hyperfine structure splitting for different nuclear isomers (i.e., for the excited nuclear states) of the same nucleus. Some isomers (with excitation energies from 50 up to 200–300 keV) in light nuclei are stable for a relatively long time which can be sufficient to measure the hyperfine structure splitting. Third, the formulas known from the general theory of hyperfine structure splitting must be corrected, since the negatively charged muon cannot be considered as a truly point particle in carbon muonic and heavier atoms and ions. A different reason is the study of electron-electron correlations in carbon muonic, nitrogen muonic, and oxygen muonic ions. The

presence of various interparticle correlations in these six-body systems drastically complicates highly accurate computations.

We begin our analysis from a brief consideration of the hyperfine structure splitting in the triplet states of carbon muonic ions, the general theory of which is described in Sec. II. Note that the hyperfine structure splittings in the carbon muonic ions and atoms have never been considered previously. The overall complexity of this problem makes its accurate solution extremely difficult. Numerical evaluation of the hyperfine splitting in the carbon muonic ions contains two difficult points: (1) antisymmetrization of each basis four-electron function and (2) effective optimization of a large number of nonlinear parameters in the trial wave functions. Construction of variational six-body wave functions for such systems and their proper antisymmetrization with respect to all electron coordinates are discussed in Sec. III. Section IV includes the results of numerical evaluations and concluding remarks can be found in Sec. V.

II. HYPERFINE-STRUCTURE SPLITTING

In the lowest-order approximation, the hyperfine structure splitting (below, hyperfine splitting, for short) in any light muonic atom and ion in its bound $S(L=0)$ states is described by the Fermi-Segré formula. In this study, we shall consider only the $S(L=0)$-electron states in the carbon muonic ions. The Fermi-Segré Hamiltonian which represents the hyperfine splitting in the S states of light muonic atoms and ions with $A-2$ $(A\geq 3)$ electrons is written in the form [23]

$$H_{HF} = -\mathcal{A}\delta(\mathbf{r}_{\mu N})(\mathbf{s}_\mu\cdot\mathbf{I}_N) - \mathcal{B}\left[\sum_{i=1}^{A-2}\delta(\mathbf{r}_{\mu i})\mathbf{s}_i\right]\cdot\mathbf{s}_\mu - \mathcal{C}\left[\sum_{i=1}^{A-2}\delta(\mathbf{r}_{iN})\mathbf{s}_i\right]\cdot\mathbf{I}_N, \tag{1}$$

where the sum is taken over all $A-2$ electrons in the system. For carbon muonic ions discussed in this study, $A=6$ (the total number of particles) and $A-2=4$ (the total number of electrons). The muon μ^- is a heavy particle which also has the negative charge. Three coupling constants $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ from Eq. (1) are defined below. Also, in this equation and everywhere below in this work, the vectors $\mathbf{s}_i$, $\mathbf{s}_\mu$, and $\mathbf{I}_N$ designate the spin vectors of the ith electron, muon, and carbon nucleus, respectively. Note that there are a number of restrictions in applications of the formula, Eq. (1), to various (light) muonic atoms and ions.

The hyperfine splitting in the bound $S(L=0)$ state of the light muonic atoms is described by the expectation value $\delta H_s=\langle H_{HF}\rangle$, which is taken over the spatial coordinates of all particles. The value δH_s is represented in the form [23]

$$\delta H_s = \langle H_{HF}\rangle = -\mathcal{A}\langle\delta(\mathbf{r}_{\mu N})\rangle(\mathbf{I}_N\cdot\mathbf{s}_\mu) - \mathcal{B}\langle\delta(\mathbf{r}_{e\mu})\rangle(\mathbf{S}_e\cdot\mathbf{s}_\mu) - \mathcal{C}\langle\delta(\mathbf{r}_{eN})\rangle(\mathbf{S}_e\cdot\mathbf{I}_N), \tag{2}$$

where $\delta(\mathbf{r}_{XY})=\delta_{XY}$ designates the two-particle delta function between particles X and Y. The notations $\delta(\mathbf{r}_{eN})$ and $\delta(\mathbf{r}_{e\mu})$ stand for the properly symmetrized electron-nucleus and electron-muon delta functions, respectively. The notation $\mathbf{S}_e$ in Eq. (2) means the total electron spin, i.e., it is the vector sum of all single-electron spin vectors, i.e., $\mathbf{S}_e=\Sigma_{i=1}^{A-2}\mathbf{s}_i$. This value is obtained with the use of the following formula for the electronic expectation values:

$$\left\langle\sum_{i=1}^{A-2}[\delta(\mathbf{r}_{ai})\mathbf{s}_i]\right\rangle = \langle\delta(\mathbf{r}_{ae})\rangle\sum_{i=1}^{A-2}\mathbf{s}_i = \langle\delta(\mathbf{r}_{ae})\rangle\mathbf{S}_e, \tag{3}$$

where $a=N$ and μ in our notations, while e designates the generalized electron coordinate.

Now, we can write the explicit expressions for the coupling constants $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ in Eqs. (1) and (2) (in atomic units where $\hbar=1$, $e=1$, and $m_e=1$)

$$\mathcal{A}=\frac{2\pi}{3}\alpha^2\frac{g_\mu g_N}{m_\mu m_p},\quad \mathcal{B}=\frac{2\pi}{3}\alpha^2\frac{g_e g_\mu}{m_e m_\mu},\quad \mathcal{C}=\frac{2\pi}{3}\alpha^2\frac{g_e g_N}{m_e m_p}, \tag{4}$$

where α is the fine-structure constant and m_e, m_μ, and m_p are the electron, muon, and proton masses, respectively. Also, in these equations $g_N=\mu_N/I_N$, where the nuclear magnetic moment (μ_N) is expressed in the nuclear magnetons $\frac{e\hbar}{2m_pc}=(m_e/m_p)\mu_0$, where μ_0 is the Bohr magneton. The maximal value of the nuclear moment μ_N (for each nucleus) can be found in tables of nuclear data (see, e.g., [24] and references therein). In atomic units, the Bohr magneton equals $\frac{1}{2}$ exactly.

In this study, we consider the ^{11}C, ^{12}C, ^{13}C, and ^{14}C nuclei which have nuclear spins $I_N=\frac{3}{2},0,\frac{1}{2}$, and 0, respectively. The ^{12}C and ^{13}C carbon nuclei are stable, while the ^{14}C nucleus decays with the emission of a β^- particle (electron) $(T_{1/2}\approx 5715$ yr). Analogously, the ^{11}C nucleus decays with the emission of a β^+ particle (positron) $(T_{1/2}\approx 20.3$ min). The atomic masses of the corresponding carbon atoms relative to $^{12}\mathrm{C}=12.000$ (exactly) are

$$M(^{11}\mathrm{C}) = 11.011\ 434,\quad M(^{12}\mathrm{C}) = 12.000\ 00,$$

$$M(^{13}\mathrm{C}) = 13.003\ 354\ 838,\quad M(^{14}\mathrm{C}) = 14.003\ 241\ 989.$$

The mass of the bare neutron in these units is $M_n=1.008\ 664\ 916$. The same (neutron) mass in atomic units is $M_n=1838.683\ 662m_e$. This gives us the corresponding conversion coefficient $x=1822.888\ 486\ 4$. This number must be multiplied by the mass of carbon nuclei expressed in carbon units, i.e., mass units relative to $^{12}\mathrm{C}=12.000$.

The fine-structure constant α, masses of the muon m_μ and proton M_p, and g factors used in our present calculations were chosen from [24,25],

$$\alpha = 7.297\ 352\ 568\times 10^{-3},\quad m_p = 1836.152\ 672\ 61,$$

$$m_\mu = 206.768\ 283\ 8m_e,\quad m_e = 1,$$

$$g_e = -2.002\ 319\ 304\ 371\ 8,\quad g_\mu = -2.002\ 331\ 839\ 6,$$

$$g_N(^{11}\mathrm{C}) = -0.9640\times\left(\tfrac{2}{3}\right) = -0.785\ 07,$$

$$g_N(^{13}\mathrm{C}) = 0.702\,41 \times 2 = 1.404\,82.$$

For the ^{12}C and ^{14}C nuclei, $g_N(^{12}\mathrm{C})=0.0$ and $g_N(^{14}\mathrm{C})=0.0$. The hyperfine splitting is traditionally expressed in MHz. To convert the energies from a.u. to MHz, the conversion factor $6.579\,683\,920\,61\times10^9$(MHz/a.u.) has been used.

Now, one can determine the $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ coupling constants from Eq. (3) for each of the isotope-substituted carbon muonic ions considered in this work. First, note that for the ^{12}C and ^{14}C nuclei, the coupling constants $\mathcal{A}$ and $\mathcal{C}$ equal zero identically. The coupling constant $\mathcal{B}$ equals 14 229.176 563 556 MHz for all carbon muonic ions. Numerical values of the constants $\mathcal{A}$ and $\mathcal{C}$ for the ^{11}C and ^{13}C nuclei are

$$\mathcal{A}(^{11}\mathrm{C}) = 3.038\,407\,551\,330\,6\ \ \mathrm{MHz},$$

$$\mathcal{C}(^{11}\mathrm{C}) = 628.242\,381\,853\,71\ \ \mathrm{MHz},$$

$$\mathcal{A}(^{13}\mathrm{C}) = -5.436\,987\,397\,633\,6\ \ \mathrm{MHz},$$

$$\mathcal{C}(^{13}\mathrm{C}) = -1124.189\,515\,426\,3\ \ \mathrm{MHz}. \tag{5}$$

Note that these coefficients have different signs for ^{11}C and ^{13}C nuclei.

The total electron spin $S_e=|\mathbf{S}_e|$ of any triplet state equals 1, while the muon spin $s_\mu=|\mathbf{s}_\mu|=\frac{1}{2}$ in all cases. As mentioned above, the hyperfine splitting for the $2^3S(L=0)$ state of the ^{12}C and ^{14}C carbon muonic ions is determined only by the magnetic interaction between the muon and total electron spins. Such an interaction produces the actual splitting between the doublet $F=\frac{1}{2}$ and quartet $F=\frac{3}{2}$ states. In the 2^3S states of the ^{11}C and ^{13}C carbon muonic ions, the situation is more complicated (see below). Here and everywhere below in this work, $\mathbf{F}$ designates the total spin of the carbon muonic ion, i.e., $\mathbf{F}=\mathbf{I}_N+\mathbf{s}_\mu+\mathbf{S}_e$, in our present notations. Possible values of F for each of the carbon muonic ions are discussed in Sec. IV. In fact, for all light muonic atoms and ions with $I_N\geq\frac{1}{2}$, it is very useful (see below) to introduce the total spin $\mathbf{K}$ of the central muonic quasinucleus, i.e., $\mathbf{K}=\mathbf{I}_N+\mathbf{s}_\mu$ and $|\mathbf{K}|=I_N\pm\frac{1}{2}$.

III. VARIATIONAL WAVE FUNCTIONS

To evaluate the hyperfine splitting in actual carbon muonic four-electron ions, one needs to compute the expectation values of all two-particle delta functions which are included in Eq. (2). Such calculations are performed with the use of variational six-body wave functions. In turn, these wave functions are determined from the corresponding Schrödinger equation $H\Psi=E\Psi$ for bound states. The Hamiltonian H of an arbitrary A-particle carbon muonic ion takes the form (in atomic units)

$$H = -\frac{1}{2}\left[\sum_{i=1}^{A-2}\nabla_i^2 + \frac{1}{m_\mu}\nabla_{A-1}^2 + \frac{1}{M}\nabla_A^2\right] + \sum_{i=1}^{A-2}\sum_{j=2(>i)}^{A-1}\frac{1}{r_{ij}} - \sum_{i=1}^{A-1}\frac{Q}{r_{iA}}, \tag{6}$$

where the largest index A always designates the nucleus, the index $A-1$ stands for the negatively charged muon, and indices $1,\ldots,A-2$ mean the electrons. Also, in this equation, $\boldsymbol{\nabla}_i=(\frac{\partial}{\partial x_i},\frac{\partial}{\partial y_i},\frac{\partial}{\partial z_i})$ is the gradient operator of the ith particle $(i=1,2,\ldots,A)$. The notation r_{ij} stands for the (ij)-relative coordinate $r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|=r_{ji}$, where $\mathbf{r}_i$ are the Cartesian coordinates of the ith particle.

Our first computational goal here is to produce highly accurate bound-state solutions of the Schrödinger equation $H\Psi=E\Psi$, where $E<0$ and Ψ are the corresponding energy and wave function and $\|\Psi\|=1$. An accurate six-body wave function can be approximated by using the variational expansion written in 15-dimensional Gaussoids of the relative coordinates $r_{12},r_{13},r_{14},r_{15},r_{16},\ldots,r_{56}$ defined in an arbitrary six-body system. For the bound $S(L=0)$ states of the carbon muonic ions, this variational expansion takes the form

$$\Psi_{L=0}(\{r_{ij}\}) = \mathcal{P}_s\sum_{i=1}^{\mathcal{N}} C_k \exp\left(-\sum_{ij}\alpha_{ij}^{(k)} r_{ij}^2\right), \tag{7}$$

where $\{r_{ij}\}$ designates the set of 15 relative coordinates

$$r_{12},r_{13},r_{14},r_{15},r_{16},r_{23},r_{24},r_{25},r_{26},r_{34},r_{35},r_{36},r_{45},r_{46},r_{56}$$

which are needed for complete description of an arbitrary spatial point in six-body systems. The notation N in Eq. (7) means the total number of variational functions, while the second summation in Eq. (7) is taken over all possible different pairs of particles. The projector $\mathcal{P}_s$ produces the trial wave function with the correct permutation symmetry between all (four) electrons.

Let us describe the explicit construction of this projector $\mathcal{P}_s$. Note that all computations below are performed with the use of only one-electron spin function $\chi_1=(\alpha\beta-\beta\alpha)\alpha\alpha$ which corresponds to the $S=1$ and $S_z=1$ values. The two other (electronic) spin functions $\chi_0=(\alpha\beta-\beta\alpha)(\alpha\beta+\beta\alpha)$ and $\chi_{-1}=(\alpha\beta-\beta\alpha)\beta\beta$ correspond to the $S=1$, $S_z=0$ and $S=1$, $S_z=-1$ values, respectively. These three spin functions χ_1,χ_0,χ_{-1} form a regular triplet. In this work, we restrict ourselves to the use of one (electron) spin function $\chi_1=(\alpha\beta-\beta\alpha)\alpha\alpha$ only.

Now, we need to obtain the spatial part of the total wave function with the correct permutation symmetry between all identical particles, i.e., between particles 1, 2, 3, and 4 (electrons). The corresponding spatial projector can be obtained by calculating the explicit expression for the following spin expectation value:

$$\mathcal{P} = \mathcal{C}\langle(\alpha\beta-\beta\alpha)\alpha\alpha|\hat{\mathcal{A}}|(\alpha\beta-\beta\alpha)\alpha\alpha\rangle, \tag{8}$$

where $\mathcal{C}$ is the normalization factor, while $\hat{\mathcal{A}}$ is the complete four-particle (or four-electron) antisymmetrizer

$$\hat{\mathcal{A}} = \hat{e} - \hat{P}_{12} - \hat{P}_{13} - \hat{P}_{23} - \hat{P}_{14} - \hat{P}_{24} - \hat{P}_{34} + \hat{P}_{123} + \hat{P}_{132} + \hat{P}_{124} + \hat{P}_{142} + \hat{P}_{134} + \hat{P}_{143} + \hat{P}_{234} + \hat{P}_{243} - \hat{P}_{1234} - \hat{P}_{1243} - \hat{P}_{1324} - \hat{P}_{1342} - \hat{P}_{1423} - \hat{P}_{1432} + \hat{P}_{12}\hat{P}_{34} + \hat{P}_{13}\hat{P}_{24} + \hat{P}_{14}\hat{P}_{23}. \quad (9)$$

Here, $\hat{e}$ is the identity permutation, while $\hat{P}_{ij}$ is the permutation of the ith and jth identical particles. Analogously, the operators $\hat{P}_{ijk}$ and $\hat{P}_{ijkl}$ are the permutations of three identical particles (i, j, and k) and four identical particles (i, j, k, and l), respectively. After some algebra, one finds the following explicit formula for the corresponding spatial projector:

$$\mathcal{P} = \frac{1}{2\sqrt{6}}(2\hat{e} + 2\hat{P}_{12} - \hat{P}_{13} - \hat{P}_{23} - \hat{P}_{14} - \hat{P}_{24} - 2\hat{P}_{34} - 2\hat{P}_{12}\hat{P}_{34} - \hat{P}_{123} - \hat{P}_{124} - \hat{P}_{132} - \hat{P}_{142} + \hat{P}_{134} + \hat{P}_{234} + \hat{P}_{243} + \hat{P}_{143} + \hat{P}_{1432} + \hat{P}_{1234} + \hat{P}_{1243} + \hat{P}_{1342}) \quad (10)$$

associated with the triplet states. This projector creates the spatial part of the total (triplet) wave function with the correct permutation symmetry between all four identical particles (electrons).

Analytical formulas for all matrix elements needed in bound-state computations of four-electron atomic systems are presented in our previous publication [26] (see also [27]) and are not repeated here (formulas for the two-particle delta functions are discussed below). We use the same basis set as in [26]. For discussion of optimization of the nonlinear parameters in the radial-wave functions, the reader is also referred to [26].

To conclude this section, let us derive the explicit analytical formulas for expectation values of the two-particle delta functions in arbitrary six-body systems. For basis set Eq. (7), we introduce the following compact notation [26]:

$$\langle\alpha| = \langle\alpha^{(k)}| = \exp\left(-\sum_{i>j=1}^{A} \alpha_{ij}^{k} r_{ij}^{2}\right) \quad (11)$$

and

$$|\beta\rangle = |\beta^{(\ell)}\rangle = \exp\left(-\sum_{i>j=1}^{A} \beta_{ij}^{\ell} r_{ij}^{2}\right), \quad (11)$$

where A is the total number of particles in the system. In our present case, $A=6$. In this notation, the overlap matrix element $\langle\alpha|\beta\rangle$ takes the form

$$\langle\alpha|\beta\rangle = \int\int\int\int\int \exp(-a_{12}r_{12}^2 - a_{13}r_{13}^2 - a_{14}r_{14}^2 - a_{15}r_{15}^2 - a_{16}r_{16}^2 - a_{23}r_{23}^2 - a_{24}r_{24}^2 a_{25}r_{25}^2 - a_{26}r_{26}^2 - a_{34}r_{34}^2 - a_{35}r_{35}^2 - a_{36}r_{36}^2 - a_{45}r_{45}^2 - a_{46}r_{46}^2 - a_{56}r_{56}^2) d^3\mathbf{r}_1 d^3\mathbf{r}_2 d^3\mathbf{r}_3 d^3\mathbf{r}_4 d^3\mathbf{r}_5 = \langle\alpha^{(k)}|\beta^{(\ell)}\rangle = \pi^{3\cdot(A-1)/2} D^{-3/2}, \quad (12)$$

where $\mathbf{r}_i = \mathbf{r}_{i6}$ $(i=1,3,4,5)$, $a_{ij} = \alpha_{ij} + \beta_{ij}$, and D is the determinant of the $(A-1)\times(A-1)$ matrix $\hat{B}$ with the matrix elements

$$b_{ii} = \sum_{j\neq i}^{A} (\alpha_{ii}^{k} + \beta_{ii}^{\ell}), \quad i = 1,2,\ldots,A-1,$$

$$b_{ij} = -(\alpha_{ij}^{k} + \beta_{ij}^{\ell}), \quad i \neq j = 1,2,\ldots,A-1. \quad (13)$$

In particular, in the case of $A=6$, an arbitrary matrix element of the $\hat{B}$ matrix is a 5×5 matrix. Analytical and/or numerical computation of the determinant of this matrix is straightforward.

Now let us obtain the analytical formula for expectation values of two-particle delta functions in the basis Eq. (7). For simplicity, consider the $\delta_{12} = \delta(\mathbf{r}_{12})$ delta function, i.e., the $\langle\alpha|\delta(\mathbf{r}_{12})|\beta\rangle$ matrix element. By using the formula Eq. (12), one finds

$$\langle\alpha|\delta(\mathbf{r}_{12})|\beta\rangle = \int\int\int\int \exp[-(a_{13}+a_{23})r_{13}^2 - (a_{14}+a_{24})r_{14}^2 - (a_{15}+a_{25})r_{15}^2 - (a_{16}+a_{26})r_{16}^2 - a_{34}r_{34}^2 - a_{35}r_{35}^2 - a_{36}r_{36}^2 - a_{45}r_{45}^2 - a_{46}r_{46}^2 - a_{56}r_{56}^2] d^3\mathbf{r}_1 d^3\mathbf{r}_3 d^3\mathbf{r}_4 d^3\mathbf{r}_5. \quad (14)$$

This integral exactly coincides with the corresponding overlap integral for the four-body system (particles 1, 3, 4, and 5). To make such a coincidence 1:1, we need to introduce the nonlinear parameters $\tilde{a}_{13} = a_{13} + a_{23}$, $\tilde{a}_{14} = a_{14} + a_{24}$, $\tilde{a}_{15} = a_{15} + a_{25}$, $\tilde{a}_{16} = a_{16} + a_{26}$. Then the four particles in such a system must be renumbered. In any case, the answer is clear and can be written in the form

$$\langle\alpha|\delta(\mathbf{r}_{12})|\beta\rangle = \pi^{3\cdot(A-2)/2} D_4^{-3/2}, \quad (15)$$

where D_4 is the determinant of the corresponding 4×4 matrix. Note that the explicit form of this matrix element exactly coincides with the corresponding matrix element of the overlap known for the $(A-1)$-body system. The last formula and its generalizations to other two-particle delta functions allow one to compute the matrix elements of all two-particle delta functions needed in our computations.

IV. NUMERICAL VALUES

By using the methods described in the previous section, we have determined the expectation values of the electron-nuclear, muon-nuclear, and electron-muon delta functions. The total energies of all carbon muonic ions considered in this study can be found in Table I. Table I also contains all expectation values of the r_{ij}^{-2}, r_{ij}^{-1}, and r_{ij} distances and $\langle\delta(\mathbf{r}_{N\mu})\rangle$, $\langle\delta(\mathbf{r}_{Ne})\rangle$, and $\langle\delta(\mathbf{r}_{\mu e})\rangle$ expectation values. Here and below, the notation N stands for nucleus. In our calculations, we have used the variational expansion Eq. (7) with 600 and 700 basis functions. Numerical coincidence between the results obtained for 600 and 700 basis functions has been used as a criterion of our accuracy. The total number of varied nonlinear parameters in such wave functions is up to 10 500. Numerical optimization of these nonlinear parameters is described in detail in [26]. Such an optimization provided sufficient numerical accuracy for all expectation values computed with our trial wave functions.

TABLE I. The expectation values in atomic units ($m_e=1$, $\hbar=1$, $e=1$) of some properties for the triplet 2^3S states of the ${}^{M}C^{6+}\mu^-e_4^-$ ions, where $M=11$, 12, 13, and 14. Below, the symbol N designates the nucleus, μ stands for muon, while e means electron.

	${}^{11}C^{6+}\mu^-e_4^-$	${}^{12}C^{6+}\mu^-e_4^-$	${}^{13}C^{6+}\mu^-e_4^-$	${}^{14}C^{6+}\mu^-e_4^-$
E	−3707.568055	−3719.662548	−3713.330854	−3715.610549
$\langle r_{N\mu}\rangle$	0.00122155	0.00122052	0.00121964	0.00121889
$\langle r_{Ne}\rangle$	1.420894	1.420931	1.420963	1.420992
$\langle r_{\mu e}\rangle$	2.113732	2.113689	2.113653	2.113625
$\langle r_{ee}\rangle$	2.950095	2.950095	2.950093	2.950089
$\langle r_{N\mu}^{-1}\rangle$	1227.944	1228.975	1229.864	1230.624
$\langle r_{Ne}^{-1}\rangle$	3.425555	3.425481	3.425418	3.425363
$\langle r_{\mu e}^{-1}\rangle$	1.795582	1.795513	1.795453	1.795403
$\langle r_{ee}^{-1}\rangle$	0.887227	0.887344	0.887445	0.887532
$\langle r_{N\mu}^{-2}\rangle$	3015236.2	3020306.9	3024675.3	3028413.4
$\langle r_{Ne}^{-2}\rangle$	33.58359	33.58309	33.58265	33.58225
$\langle r_{\mu e}^{-2}\rangle$	11.43341	11.43330	11.43321	11.43314
$\langle r_{ee}^{-2}\rangle$	3.595495	3.596245	3.596891	3.597444
$\langle \delta_{N\mu}\rangle$	4.5728735×10^8	4.5840530×10^8	4.5936890×10^8	4.6019382×10^8
$\langle \delta_{Ne}\rangle$	14.196110	14.191460	14.187461	14.184042
$\langle \delta_{\mu e}\rangle$	13.98921	13.99027	13.99115	13.99190

It is clear *a priori* that the radius of the muonic orbit in any light muonic atom is significantly smaller than the appropriate radii of electronic shells. For our expectation values, this means that $\langle r_{N\mu}\rangle \ll \langle r_{Ne}\rangle$ and $\langle r_{N\mu}\rangle \ll \langle r_{\mu e}\rangle$. Analogous relations are true for higher powers of interparticle distances, e.g., $\langle r_{N\mu}^2\rangle \ll \langle r_{Ne}^2\rangle$ and $\langle r_{N\mu}^2\rangle \ll \langle r_{\mu e}^2\rangle$. For the correct expectation values of delta functions, one finds the following (inverse) inequalities $\langle \delta_{N\mu}\rangle \gg \langle \delta_{Ne}\rangle$ and $\langle \delta_{N\mu}\rangle \gg \langle \delta_{\mu e}\rangle$. All these inequalities are obeyed for expectation values from Table I. Moreover, it can be shown that expectation values of electron-carbon and electron muonic delta functions are approximately equal to each other, but for light muonic atoms and ions, we have $\langle \delta_{Ne}\rangle > \langle \delta_{\mu e}\rangle$. This inequality is obeyed for carbon muonic ions.

As mentioned above, the expectation values of delta functions from Table I can be used to determine the hyperfine splitting in each of these carbon muonic ions (${}^{11}C^{6+}\mu^-e_4^-$, ${}^{12}C^{6+}\mu^-e_4^-$, ${}^{13}C^{6+}\mu^-e_4^-$, and ${}^{14}C^{6+}\mu^-e_4^-$). First, consider the ${}^{12}C^{6+}\mu^-e_4^-$ and ${}^{14}C^{6+}\mu^-e_4^-$ ions. The nuclear spin I_N equals zero in both these carbon nuclei. The total spin $\mathbf{F}$ in these ions equals $\mathbf{F}=\mathbf{S}_e+\mathbf{s}_\mu$. Since $S_e=1$ for the triplet electronic states and $s_\mu=\frac{1}{2}$, then there are two possible values of F, i.e., $F=\frac{1}{2}$ (doublet states) and $F=\frac{3}{2}$ (quartet states). The hyperfine splitting in the ${}^{12}C^{6+}\mu^-e_4^-$ and ${}^{14}C^{6+}\mu^-e_4^-$ ions is written in the form

$$\Delta E = \mathcal{B}\langle \delta(\mathbf{r}_{\mu e})\rangle s_\mu(2S_e+1) = \frac{3}{2}\mathcal{B}\langle \delta(\mathbf{r}_{\mu e})\rangle, \qquad (16)$$

where $s_\mu=\frac{1}{2}$ and $S_e=1$ for the triplet state. The expectation value of the electron-muon delta function for the ${}^{12}C^{6+}\mu^-e_4^-$ ion is ≈13.990 27, while for the ${}^{14}C^{6+}\mu^-e_4^-$ ion it is ≈13.991 90. Therefore, the hyperfine splitting in the ${}^{12}C^{6+}\mu^-e_4^-$ ion is ≈298 605.0 MHz and in the ${}^{14}C^{6+}\mu^-e_4^-$ ion is ≈298 639.7 MHz. Our estimates for uncertainties in these values are bounded between ≈3 and ≈10 MHz. These values equal the difference between the energies of the set of degenerate doublet states ($F=\frac{1}{2}$) and the set of degenerate quartet states ($F=\frac{3}{2}$) in these ions. Note that such differences are ≈75 times larger than the analogous difference in the muonic-helium atom ${}^4He^{2+}\mu^-e^-$ (ground state) which has the same hyperfine structure.

The hyperfine structure splittings of the ${}^{11}C^{6+}\mu^-e_4^-$ ion and ${}^{13}C^{6+}\mu^-e_4^-$ ion are shown in Table II. To understand this structure, it is very useful to introduce the vector $\mathbf{K}=\mathbf{I}_N+\mathbf{s}_\mu$

TABLE II. The hyperfine structure levels E_{hp} and hyperfine splitting $\Delta E^K_{F,F\pm1}$ (in MHz) in the triplet 2^3S states in the carbon muonic ions ${}^{M}C^{6+}\mu^-e_4^-$. Here, $M=11$ and 13. Numerical uncertainties in the hyperfine splittings $\Delta E^K_{F,F\pm1}$ vary between ≈5 and ≈15 MHz.

$E_{hp}({}^{11}C^{6+}\mu^-e_4^-)$ (MHz)	K	F	$2F+1$	$\Delta E^K_{F,F\pm1}$
1.7368202945×10^9	1	2	5	
1.7367430603×10^9	1	1	3	77234.23
1.7367044407×10^9	1	0	1	38619.55
-1.0418996490×10^9	2	1	3	2.7786041×10^9
-1.0420125577×10^9	2	2	5	112908.63
-1.0421819084×10^9	2	3	7	169350.74

$E_{hp}({}^{13}C^{6+}\mu^-e_4^-)$ (MHz)	K	F	$2F+1$	$\Delta E^K_{F,F\pm1}$
6.2457886323×10^8	1	0	1	
6.2448730589×10^8	1	1	3	91557.34
6.2430416345×10^8	1	2	5	183142.45
-1.8731871994×10^9	0	1	3	2.4974914×10^9

which is the total spin of nucleus and muon, i.e., the total spin of central "quasinucleus." The differences between states which have different values of $K=|\mathbf{K}|$ are very large ($\geq 2.4\times 10^9$ MHz). Such cases can be detected *a priori* and they are not of interest in experiments. Therefore, it is not necessary to introduce a new index which labels levels with different K. Analogous differences between states with the same values of K are relatively small and can be measured in modern experiments. These levels represent the hyperfine structure splittings. In general, for each K and F, such differences can be designated as $\Delta E^K_{F,F-1}$ and/or $\Delta E^K_{F,F+1}$. In Table II, the $\Delta E^K_{F,F\pm 1}$ values are the differences between the energy located in a particular line [designated as the (K,F) level] and the energy from the line immediately above it. For the $^{13}C^{6+}\mu^- e_4^-$ ion, we have states with $K=1$ and $K=0$. The energy differences between states with $K=1$, i.e., $\Delta E^1_{0,1}\approx 91\ 557.3$ MHz and $\Delta E^1_{1,2}\approx 183\ 142.5$ MHz, form the hyperfine structure of the $^{13}C^{6+}\mu^- e_4^-$ ion. Analogously, for the $^{11}C^{6+}\mu^- e_4^-$ ion, one finds states with $K=1$ and $K=2$. Therefore, the hyperfine structure includes the four following energy differences: $\Delta E^1_{2,1}\approx 77\ 234.2$ MHz, $\Delta E^1_{1,0}\approx 38\ 619.5$ MHz and $\Delta E^2_{1,2}\approx 112\ 908.6$ MHz, $\Delta E^2_{2,3}\approx 169\ 350.7$ MHz. Our estimates of numerical uncertainties in these values vary between ≈ 5 and ≈ 15 MHz.

The computed numerical values of the hyperfine splitting can be confirmed in future experiments. Possible differences between the predicted and measured values in carbon muonic ions and atoms are of great interest for future theoretical and experimental development. Indeed, the radius of the $1s$ muonic orbit in carbon muonic, nitrogen muonic, and oxygen muonic ions and atoms ($r_\mu \approx \frac{a_0}{Q^2 m_\mu} \leq 7\times 10^{-13}$ cm) essentially coincides with the radius of the nucleus. Therefore, by studying the properties of such quasiatomic systems, we can obtain valuable information about various nuclear properties in many light nuclei. It is very likely that the first term in formula Eq. (1) used in this study to determine the hyperfine structure splitting must be corrected, since the negatively charged muon cannot be considered as a point particle in carbon muonic, nitrogen muonic, and oxygen muonic atoms and ions. In actual computations of hyperfine splitting in such systems, the muon-nuclear delta function must be replaced by some other function. This problem can be ignored for helium muonic atoms and ions. Another reason for possible discrepancies with experimental data is the absence of relativistic and lowest-order QED corrections in the present treatment.

V. CONCLUSIONS

The hyperfine structure splitting in the 2^3S states (electronic states) of some four-electron carbon muonic ions has been evaluated numerically. The predicted hyperfine splitting in the carbon muonic ions can, in principle, be measured in modern experiments and we hope that this work will stimulate some experimental activities in this direction. Based on the results of such experiments, one could then improve our computational methods to achieve better numerical accuracy for the corresponding delta functions by considering, e.g., the lowest-order relativistic and QED corrections to the hyperfine splitting.

TABLE III. The expectation values in atomic units ($m_e=1$, $\hbar=1$, $e=1$) of some properties for the triplet 2^3S states of the $^{10}B^{5+}\mu^- e_4^-$ atom and of the $^{14}N^{7+}\mu^- e_4^-$ and $^{16}O^{5+}\mu^- e_4^-$ ions. Below, the symbol N designates the nucleus, μ stands for muon, while e means electron.

	$^{10}B^{5+}\mu^- e_4^-$	$^{14}N^{7+}\mu^- e_4^-$	$^{16}O^{8+}\mu^- e_4^-$
E	−2569.9804254	−5060.4774031	−6619.3264317
$\langle r_{N\mu}\rangle$	0.00146734	0.00104476	0.00091325
$\langle r_{Ne}\rangle$	1.8186385	1.2307717	0.9809335
$\langle r_{\mu e}\rangle$	2.7149371	1.7672922	1.4460161
$\langle r_{ee}\rangle$	3.409419	2.582458	2.427053
$\langle r^{-1}_{N\mu}\rangle$	1022.251	1435.731	1642.480
$\langle r^{-1}_{Ne}\rangle$	2.624248	4.203401	4.789220
$\langle r^{-1}_{\mu e}\rangle$	1.352163	2.305344	2.687542
$\langle r^{-1}_{ee}\rangle$	0.795587	0.956779	1.254295
$\langle r^{-2}_{N\mu}\rangle$	2089701.2	4121887.4	5394769.7
$\langle r^{-2}_{Ne}\rangle$	20.20718	50.38942	66.29744
$\langle r^{-2}_{\mu e}\rangle$	6.863444	17.75158	23.96170
$\langle r^{-2}_{ee}\rangle$	2.884106	3.877054	7.969599

Note that the four-electron six-body muonic atoms and ions are interesting atomic systems for research. All such systems include one negatively charged muon, four electrons, and one light nucleus, e.g., B, C, N, O, etc. The total energies of such systems are the values of a few thousands of atomic units, while the corresponding pure electron energies are significantly (hundred times) smaller. All properties of light muonic atoms and ions, e.g., their dipole and magnetic moments, have two components: a muon component and an electron component. Neither the bound-state spectra nor other properties in these atoms and ions have been the subject of previous studies. The total energies of the triplet 2^3S states, expectation values of functions of various relative coordinates, and hyperfine structure splittings for the family of carbon muonic positive ions have been calculated in this study. These results are summarized in Tables I and II. Analogous expectation values determined for the $^{10}B^{5+}\mu^- e_4^-$ atom and $^{14}N^{7+}\mu^- e_4^-$, $^{16}O^{8+}\mu^- e_4^-$ ions (in their 2^3S states) can be found in Table III. As follows from Table III, the total energy of the four-electron six-body muonic atoms rapidly increases with the electric charge Q of the nucleus. The same conclusion is true for the expectation values of delta functions and some other properties. The 2^3S state in the $^{10}B^{5+}\mu^- e_4^-$ atom is a weakly bound state, since its total binding energy is less than 1% of its total energy.

Our calculations of the hyperfine structure splitting in muonic atoms and ions with different nuclear charge Q are essentially based on the formula, Eq. (1). In applications to the ground states of the $^3He\mu^- e^-$ and $^4He\mu^- e^-$ atoms, this formula gives excellent agreement with the experimental results for the hyperfine structure splitting. Theoretical (or predicted) values for these two systems are 4166.393 and 4464.555 MHz, respectively [10]. The corresponding experimental values are 4166.41 and 4464.95 MHz, respectively.

This indicates clearly that all corrections, including lowest-order relativistic and QED corrections, contribution of terms which represent the interaction with the quadrupole nuclear moment, etc., are very small in comparison to the leading term which is given by Eq. (1). It is very likely that the formula, Eq. (1), can be applied to the $S(L=0)$ states in arbitrary muonic atoms and ions with $Q \leq 10$. For sodium muonic atoms and ions ($Q=11$), the spatial radius of the muonic orbit essentially coincides with the radius of the nucleus. In this case, we can expect to observe large deviations between our results obtained for the hyperfine structure splitting [which follow from the formula, Eq. (1)] and real experimental values.

In this study, we consider the hyperfine splitting in the 2^3S states of four-electron carbon muonic ions ($Q=6$). The 2^3S states in the similar nitrogen muonic and oxygen muonic ions are also considered. We expect that the deviations between our results which follow from formula, Eq. (1), and experimental values of the hyperfine splitting in these ions will be small, but noticeable. An important source of additional corrections in all four-electron muonic atoms and ions is related with the electron-electron correlations. This effect cannot be observed in the helium muonic atoms. Unfortunately, the hyperfine structure splitting has never been measured experimentally for any of these four-electron muonic ions and atoms.

For muonic atoms and ions with $Q \geq 11$ (but for $Q \leq 20$), our formula, Eq. (1), produces only approximate evaluations of the hyperfine structure splitting. In muonic atoms and ions with $Q > 20$, the negative muon moves inside of atomic nucleus. In such cases, the formula, Eq. (1), cannot be used even in the first approximation. The hyperfine structure splitting in these muonic atoms and ions must be computed with the use of different theoretical approach. In particular, the magnetic moment of the muon must be coupled with the magnetic moments of nucleons outside closed shells. For each of the particles (muon, protons, and neutrons), the magnetic moment contains the two parts: spin part and orbital part. The explicit expressions for the corresponding gyromagnetic factors are presumably complicated and presently unknown.

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