Calculation of the ground-state energy and average distance between particles for the nonsymmetric muonic ^{3}He atom

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A calculation of the ground-state energy and average distance between particles in the nonsymmetric muonic ^{3}He atom is given. We have used a wave function with one free parameter, which satisfies boundary conditions such as the behavior of the wave function when two particles are close to each other or far away. In the proposed wave function, the electron-muon correlation function is also considered. It has a correct behavior for r_{12} tending to zero and infinity. The calculated values for the energy and expectation values of r^{2n} are compared with the multibox variational approach and the correlation function hyperspherical harmonic method. In addition, to show the importance and accuracy of approach used, the method is applied to evaluate the ground-state energy and average distance between the particles of nonsymmetric muonic ^{4}He atom. Our obtained results are very close to the values calculated by the mentioned methods and giving strong indications that the proposed wave functions, in addition to being very simple, provide relatively accurate values for the energy and expectation values of r^{2n}, emphasizing the importance of the local properties of the wave function.

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I. INTRODUCTION

Muonic helium ($^3\mathrm{He}^{+2}\mu^- e^-$) is an exotic atom, consisting of a $^3\mathrm{He}^{+2}$, a negative muon, and an electron. In the ground state, the orbital radius of the muon is about 400 times smaller than that of the electron due to their mass ratio and different charge screening. Therefore, in the simplest approximation, the muonic helium atom can be considered to be hydrogenlike with a pseudonucleus $(^3\mathrm{He}^{+2}\mu^-)^+$. This system ($^3\mathrm{He}^{+2}\mu^- e^-$) is of great interest to atomic physicists, for the following reasons. (i) It is a pure atomic three-body system, which is quite unusual since all three particles are not identical, have very different masses, and no Pauli principle applies.

(ii) The atom is produced in the reaction of capture of the negative muon by the positive helium ion. It is one of the products in the process of muon catalyzed fusion, and therefore its spectroscopic properties have to be studied carefully to understand the fusion reactions properly. (iii) It is the simplest system for observing the electromagnetic interactions of the electron and negative muon, since the interaction between the spin magnetic moments of the muon and electron can be determined through precise measurement of the ground-state hyperfine structure interval $\Delta\nu$.

In general, the properties of muonic helium atoms have received great deal of attention since the early days of quantum mechanics. Energy eigenfunctions for these systems have been developed from many approaches with varying degrees of sophistication and accuracy. These calculations are generally based on the variational approach with a large number of variational parameters [1–3]. It is of considerable interest to develop wave functions that illustrate some of the important properties such as the behavior of the wave function, when two particles are close to each other or far away. These local properties have been found [4–6] to be very useful in developing simple wave functions.

To show the importance and accuracy of the method used, we use the mentioned local properties here to calculate the ground-state energy and average distance between the particles of the ($^3\mathrm{He}^{+2}\mu^- e^-$) atom. In Sec. II, some general properties of the wave functions are reviewed. In Sec. III, the nonrelativistic Hamiltonian for the muonic ^{3}He atom is written and a simple wave function based on local properties is introduced, the ground-state energy and average distance between the particles are calculated, and the obtained results are compared with other methods, followed by a discussion and conclusion.

II. SOME GENERAL PROPERTIES OF THE WAVE FUNCTIONS

A. Cusp condition for wave functions

The nonrelativistic Hamiltonian for a three-particle system is given by

$$H = \sum_{i=1}^{3} \frac{p_i^2}{2m_i} + \sum_{i<j}^{3} \frac{q_i q_j}{\mathbf{r_{ij}}}, \qquad (1)$$

where m_i, q_i, and $\mathbf{r_{ij}} = \mathbf{r_i} - \mathbf{r_j}$ are the mass, charge, and the interparticle distance, respectively. Let us, consider the manifold of configurations in which particles i and j are within an arbitrarily small distance ϵ of each other $(0 \leqslant r_{ij} \leqslant \epsilon)$ and other distances well separated $(r_{ik}$ or $r_{jk} \geqslant \epsilon)$. The only singular point of this manifold is for $r_{ij}=0$. In this state, two terms in the Hamiltonian, i.e, the Coulomb interaction and the kinetic energy between these particles, will dominate. In the center of mass frame of these two particles, we have

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$$[-(2m_{ij})^{-1}\nabla_{ij}^2 + q_i q_j r_{ij}^{-1} + O(\epsilon^0)]\psi = 0, \quad (2)$$

where $m_{ij}=m_i m_j/(m_i+m_j)$ is the reduced mass of the two-particle subsystem and $O(\epsilon^n)$ implies terms of order n in r_{ij}. Thus, the most general bounded solution of Eq. (2) can be written in the form

$$\psi = \sum_{l,m} K_{lm}(r_{ij}) Y_l^m(\theta_{ij}, \phi_{ij}). \quad (3)$$

Substituting Eq. (3) into Eq. (2) and projecting out an lm state, we get

$$\frac{d^2}{d^2 r_{ij}}[r_{ij}K_{lm}(r_{ij})] - \frac{l(l+1)}{r_{ij}}K_{lm}(r_{ij}) - 2m_{ij}q_i q_j K_{lm}(r_{ij}) = O(r_{ij}^{l+1}). \quad (4)$$

Use of expansion

$$K_{lm}(r_{ij}) = r_{ij}^l(c_0 + c_1 r_{ij} + \cdots) \quad (5)$$

in Eq. (4) leads to

$$c_1 = \frac{m_{ij}q_i q_j}{(l+1)}c_0, \quad (6)$$

which may be described as the cusp or coalescence property of the wave function.

B. Asymptotic conditions for wave functions

The Schrödinger equation for a three-particle system is given by

$$H\psi = E\psi. \quad (7)$$

The ground-state eigenfunction of Hamiltonian H in Eq. (7) can be expanded in terms of the one-particle energy eigenfunctions [4,7]:

$$\psi = \sum_n u_n(\mathbf{r_{ij,k}})\phi_\mathbf{n}(\mathbf{r_{ij}}), \quad (8)$$

$$\left(-\frac{\nabla_{ij}^2}{2m_{ij}} + \frac{q_i q_j}{r_{ij}}\right)\phi_n = E_n^{(1)}\phi_n, \quad (9)$$

where

$$m_{ij} = \frac{m_i m_j}{m_i + m_j}. \quad (10)$$

Substituting the expression for ψ into Eq. (7), and projecting out the state ϕ_n, for $r_{ij,k}$ tending to infinity, we get

$$\left[\frac{p_{ij,k}^2}{2m_{ij,k}} + \frac{q_k(q_i+q_j)}{r_{ij,k}}\right]u_n = -\epsilon_n u_n \quad (11)$$

and

$$\epsilon_n = E_n^{(1)} - E. \quad (12)$$

The asymptotic form of u_n is given by

$$u_n \to r_{ij,k}^{[-q_k(q_i+q_j)(m_{ij,k/2\epsilon_n})^{1/2}-1]} e^{-(2m_{ij,k}\epsilon_n)^{1/2} r_{ij,k}}, \quad \text{for } r_{ij,k} \to \infty, \quad (13)$$

so that for $n=0$ state, the wave function is

$$\psi \to r_{ij,k}^b e^{-ar_{ij,k}}\phi_0(r_{ij}), \quad (14)$$

where

$$a = (2m_{ij,k}\epsilon_0)^{1/2}, \quad (15)$$

$$b = -\frac{q_k(q_i+q_j)m_{ij,k}}{a} - 1, \quad (16)$$

$$\mathbf{r_{ij,k}} = \mathbf{r_{kj}} - \frac{m_i}{m_i + m_j}\mathbf{r_{ij}}, \quad (17)$$

and

$$m_{ij,k} = \frac{(m_i + m_j)m_k}{m_i + m_j + m_k}. \quad (18)$$

Expanding $r_{j,k}$ in inverse powers of r_{kj}, we get

$$\psi \to r_{kj}^b \exp\left(-ar_{kj} + a\left[\frac{m_i}{(m_i+m_j)}\right] \times \left[\frac{r_{kj}\cdot r_{ij}}{\mathbf{r_{kj}}}\right]\right)\phi_0(r_{ij}), \quad \text{for } r_{kj\to\infty}. \quad (19)$$

In the next section, we use the obtained result in Eq. (19) for the introduced wave function for $({}^3\mathrm{He}^{+2}\mu^- e^-)$ atom in asymptotic conditions.

III. THEORETICAL CALCULATIONS

The nonrelativistic Hamiltonian for the nonsymmetric muonic ^{3}He atom is written as

$$H = -\frac{1}{2m_1}\nabla_{r_1}^2 - \frac{1}{2m_2}\nabla_{r_2}^2 - \frac{1}{M_h}\nabla_{r_1}\cdot\nabla_{r_2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{|\mathbf{r_1} - \mathbf{r_2}|}, \quad (20)$$

where

$$m_1^{-1} = M_e^{-1} + M_h^{-1}, \quad (21)$$

$$m_2^{-1} = M_\mu^{-1} + M_h^{-1}, \quad (22)$$

and M_μ, M_e, and M_h are the masses of muon, electron, and helium nucleus $({}^3\mathrm{He}^{+2})$, respectively. In addition r_1, r_2 are the coordinates of the electron and muon relative to the helium nucleus. All quantities are expressed in atomic units (a.u., $\hbar = e = M_e = 1$). The mass polarization part appears in the Hamiltonian since Jacobian coordinates are not being used. We consider the wave function which is separated into two parts:

$$\psi(r_1, r_2, r_{12}) = \phi(r_1, r_2)f(r_{12}), \quad (23)$$

where the first part is a radial function and the second is the correlation function and only a function of r_{12}. Before introducing the total wave function for the $({}^3\mathrm{He}^{+2}\mu^- e^-)$ atom, let us briefly review the local properties for this system.

When r_1 goes to zero, two terms of Coulomb interaction and kinetic energy for two particles dominate. With respect to Eq. (5), the total wave function of the $({}^3\mathrm{He}^{+2}\mu^- e^-)$ system for the S-state is given by

$$\psi \to f_0(r_2)(1 - 2m_1 r_1), \quad \text{for } r_1 \to 0. \tag{24}$$

Similarly,

$$\psi \to f_0(r_1)(1 - 2m_2 r_2), \quad \text{for } r_2 \to 0. \tag{25}$$

If r_{12} is very small relative to r_1 and r_2, the r_{12}^{-1} term will dominate. It is shown that [8]

$$\left.\frac{\partial \hat{\psi}}{\partial r_{12}}\right|_{r_{12}=0} = \frac{M_e M_\mu}{M_e + M_\mu} q_e q_\mu \psi(r_{12} = 0). \tag{26}$$

Therefore, the wave function at small r_{12} is given by

$$\psi \to \phi(r_1, r_2)\left(1 + \frac{M_e M_\mu}{M_e + M_\mu} r_{12} + \cdots\right), \quad \text{for } r_{12} \to 0. \tag{27}$$

From Eq. (27) it follows that the simplest correlation function for this system is

$$f(r_{12}) = 1 + \frac{M_e M_\mu}{M_e + M_\mu} r_{12}. \tag{28}$$

This correlation function does not have the desired property at $r_{12}=\infty$; therefore, the correlation function that has the desired properties at $r_{12}=0$ and $r_{12}=\infty$ is introduced [9]:

$$f(r_{12}) = 1 - \frac{1}{1 + 2\lambda} e^{-\lambda r_{12}}, \tag{29}$$

where λ is a variational parameter. Its small r_{12} expansion is

$$f(r_{12}) = \frac{2\lambda}{1 + 2\lambda}\left(1 + \frac{1}{2} r_{12} - \frac{\lambda}{4} r_{12}^2 + \cdots\right), \tag{30}$$

so that it satisfies the cusp condition of Eq. (26). On the other hand, as r_{12} becomes large, the function Eq. (29) has the desirable feature that it increases monotonically to unity.

Finally, when the electron is far away, according to Eq. (19), the total wave function is written as

$$\psi \to r_1^b \exp\left(-a r_1 + a\left[\frac{M_\mu}{M_\mu + M_h}\right]\left[\frac{r_1 \cdot r_2}{r_{12}}\right]\right)\phi_0(r_2), \quad \text{for } r_1 \to \infty, \tag{31}$$

where

$$a = (2m_{\mu h,e}\epsilon_0)^{1/2}, \tag{32}$$

$$b = \frac{-q_e(q_\mu + q_h)m_{\mu h,e}}{a} - 1, \tag{33}$$

$$m_{\mu h,e} = \frac{(M_\mu + M_h)M_e}{M_\mu + M_h + M_e}, \tag{34}$$

and $\phi_0(r_2)$ is the wave function of the residue system, $({}^3\mathrm{He}^{+2} - \mu^-)$. When muon is far away, we have.

$$\psi \to r_2^{b'} \exp\left(-a' r_2 + a'\left(\frac{M_e}{M_e + M_h}\right)\times\left(\frac{r_1 \cdot r_2}{r_{12}}\right)\right)\phi_0(r_1), \quad \text{for } r_2 \to \infty, \tag{35}$$

where

$$a' = (2m_{eh,\mu}\epsilon'_0)^{1/2}, \tag{36}$$

$$b' = \frac{-q_\mu(q_e + q_h)m_{eh,\mu}}{a'} - 1, \tag{37}$$

and

$$m_{eh,\mu} = \frac{(M_e + M_h)M_\mu}{M_\mu + M_h + M_e}, \tag{38}$$

where $\phi_0(r_1)$ is the wave function of the residue system, $({}^3\mathrm{He}^{+2} - e^-)$.

We now introduce the following total wave function for the atom, which satisfies mentioned boundary conditions. Based on the asymptotic conditions in Eqs. (31) and (35), the ground-state wave function is given by

$$\psi(r_1, r_2, r_{12}) = A[\phi_1(r_1)\phi_2(r_2) + \phi'_1(r_1)\phi'_2(r_2)]f(r_{12}), \tag{39}$$

$$\phi_1(r_1) = \exp\left(-a r_1 + a\left[\frac{M_\mu}{M_\mu + M_h}\right]\left[\frac{r_1 \cdot r_2}{r_{12}}\right]\right)(1 + c r_1)^{b,} \tag{40}$$

$$\phi_2(r_2) = \exp\left(\frac{-2M\mu M_h}{M_h + M_h} r_2\right). \tag{41}$$

Therefore,

$$\begin{aligned}\psi(r_1, r_2, r_{12}) = A\Bigg[&\exp\left(-a r_1 + a\left[\frac{M_\mu}{M_\mu + M_h}\right]\left[\frac{r_1 \cdot r_2}{r_{12}}\right]\right)\\ &\times\exp\left(\frac{-2M_\mu M_h}{M_\mu + M_h} r_2\right)(1 + c r_1)^b\\ &+\exp\left(-a' r_2 + a'\left[\frac{M_e}{M_e + M_h}\right]\left[\frac{r_1 \cdot r_2}{r_{12}}\right]\right)\\ &\times\exp\left(\frac{-2M_e M_h}{M_e + M_h} r_1\right)(1 + c' r_2)^{b'}\Bigg]f(r_{12}),\end{aligned} \tag{42}$$

where A is the normalization constant of wave function and the additional parameters c and c' are determined from the small r_1 and r_2 limiting behaviors. Thus, after expanding Eq. (42), for small r_1 and r_2, the muon-nucleus coalescence condition and the electron-nucleus coalescence according to Eqs (24) and (25) are satisfied only if

$$cb - a = -2m_1, \tag{43}$$

TABLE I. The calculated energy and average interparticle distances for muonic ^{3}He atom and its comparison with multibox variational approach and correlation function hyperspherical harmonic method.

Parameters	Our results	Multibox variational[a]	CFHH[b]
$-E$ (a.u.)	399.043 485 7	399.042 336 832 862 534 769 60	399.042 2728 33
$\langle r_{e-{}^3\mathrm{He}^{+2}}\rangle$	1.501 278 9		1.500 358 8
$\langle r_{\mu-{}^3\mathrm{He}^{+2}}\rangle$ (units of 10^3)	3.920 060 8		3.763 715 2
$\langle r_{e-\mu}\rangle$	1.501 288 1		1.500 364 7
$\langle (r_{e-{}^3\mathrm{He}^{+2}})^2\rangle$	3.026 535 8		3.001 440 7
$\langle (r_{\mu-{}^3\mathrm{He}^{+2}})^2\rangle$ (units of 10^6)	19.555 013 1		18.887 405 6
$\langle (r_{e-\mu})^2\rangle$	3.026 561 4		3.001 458 3

[a]Reference [11].
[b]Reference [12]; CFHH: correlation function hyperspherical harmonic.

$$c'b'-a'=-2m_2. \tag{44}$$

The proposed wave function ψ [Eq. (42)] with the correlation function $f(r_{12})$ [Eq.(29)] and the Hamiltonian [Eq. (20)] are used to calculate the energy of the muonic ^{3}He atom, according to

$$E=\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi}. \tag{45}$$

It should be noted that the parameter a in Eq. (32) or a' in Eq. (36) depends on E and is therefore determined iteratively. For the calculation of the energy, with assumed $a(a')$, and by λ variation, a minimum in the energy is achieved. To calculate the integrations in Eq. (45), Simpson's numerical method (breaking functions into many files and integrating each file separately) is used. For computing each term such as $I=\int_a^b f(x)dx$, we divided the interval $[a,b]$ in such a way that

$$a=x_0, \quad x_1<x_2<\cdots<x_N=b. \tag{46}$$

Let $P_{i,k}(x)$ $(i=1,\ldots,N)$, denote the polynomial of degree $\leqslant k$; by the rules of integration we know that

$$I(f)=\int_a^b f(x)dx=\sum_{i=1}^{N}\int_{x_{i-1}}^{x_i} f(x)dx\approx\sum_{i=1}^{N}\int_{x_{i-1}}^{x_i} P_{i,k}(x)dx. \tag{47}$$

We choose the $x_i's$ to be equally spaced, $x_i=a+ih$, with $h=(b-a)/N$; the Simpson approximation S_N can then written as [10]

$$S_N=\frac{h}{6}\left[f_0+f_N+2\sum_{i=1}^{N-1}f_i+4\sum_{i=1}^{N}f_{i-1}/2\right], \tag{48}$$

where $f_i=f(x_i)$. Here it should be mentioned that the integrations are expressed in spherical coordinates (r,θ,ϕ). The results of calculations for $N=100$ are given in Table I and the number of significant digit is 7. Expectation values of r^{2n} are calculated using the proposed wave function according to Eq. (42). The obtained results are given in Table I.

IV. CONCLUSION

Some general properties of the wave functions in specific spatial domains are analyzed. The wave functions have simple asymptotic structure when the electron or muon is far away, coalescence structure when they are close to the nucleus, and cusp property when the electron and muon are close to each other. We have developed a simple wave func-

TABLE II. The calculated energy and average interparticle distances of the muonic ^{4}He atom and its comparison with other methods.

Parameters	Our results	CFHH[a]	Variational[b]	Multibox variational[c]
$-E$ a.u..	402.636 637 8	402.640 908 323	402.640 941 351 835 3	402.637 269 632 190 074 50
$\langle r_{e-{}^4\mathrm{He}^{+2}}\rangle$	1.501 286 8	1.500 378 3	1.500 160 667 394	
$\langle r_{\mu-{}^4\mathrm{He}^{+2}}\rangle$ (units of 10^3)	3.870 262 0	3.730 033 1	3.730 035 226 601	
$\langle r_{e-\mu}\rangle$	1.501 291 7	1.500 159 6	1.500 166 571 854	
$\langle (r_{e-{}^4\mathrm{He}^{+2}})^2\rangle$	3.026 558 6	3.001 517 6		
$\langle (r_{\mu-{}^4\mathrm{He}^{+2}})^2\rangle$ (units of 10^6)	19.226 191 5	18.550 884 6		
$\langle (r_{e-\mu})^2\rangle$	3.026 583 8	3.000 627 0		

[a]Reference [14]; CFHH: correlation function hyperspherical harmonic.
[b]Reference [15].
[c]Reference [11].

tion with one free parameter for nonsymmetric muonic ^{3}He atom, which incorporates the local properties. With the use of the mentioned wave function, the ground-state energy and average distance between the particles are calculated. This results are compared with multibox variational approach [11] and correlation function hyperspherical harmonic method [12]. It is shown that the obtained values are very close to the values calculated by the mentioned methods. The calculated value for the energy agrees with 3.039×10^{-4} percent accuracy with the mentioned methods and emphasizes the importance of the local properties of the wave functions. In previous work, we performed such calculations for the symmetric muonic ^{4}He atom [13]. Our obtained results were very close to the values calculated by others. One can expect that the given wave function with a correlation function similar to that used in Eq. (29), with only a slight difference ($M_{^3\mathrm{He}^{+2}} \rightarrow M_{^4\mathrm{He}^{+2}}$), describes well the nonsymmetric muonic ^{4}He atom also. The results of the corresponding calculations are given in Table II. To assess the quality the reliability of given wave function, these results are compared with the multibox variational approach [11], the correlation function hyperspherical harmonic method [14], and other calculations [15]. Similar to the muonic ^{3}He atom, our obtained results for muonic ^{4}He atom are very close to the values calculated by other methods, giving strong indications that the proposed wave functions in general, in addition to being very simple, provides relatively accurate and reliable results, and can be used for calculation of lowest-order hyperfine splitting for the ground state of muonic helium atoms and is recommended for further studies.

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