Properties of the bound S states ($L = 0$) in Coulomb three-body systems with unit charges

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Various energetic, geometric, and other properties for the ground and first vibrationally excited S states ($L = 0$) of Coulomb three-body systems having unit charges are obtained by means of accurate exponential wave functions. The mass dependence of the properties for these systems has a relatively smooth form for the ground states. The results presented should be useful as a basis for further investigation of these three-body systems. The prethreshold (weakly bound) exotic nonsymmetric systems ($d^+t^+p^-$, $\mu^+\pi^+\mu^-$, and $\mu^+\pi^+\pi^-$) considered have sharp cluster structures, i.e., the lighter positive ion moves in the field of the neutral pair (e.g., d^+ in $d^+t^+p^-$ moves in the field of t^+p^-).

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I. INTRODUCTION

In our previous study [1] of the Coulomb three-body systems with unit charges we considered the problem of the stability of the various bound states in such systems and in particular focused on the determination of the boundaries of the regions of stability. Similar and related problems have been studied in other papers (see, e.g., [2–9]). Here we consider various energetic, geometric, and other properties of such systems. Without loss of generality, we shall designate the systems as $X^+Y^+Z^-$, where X^+, Y^+, and Z^- are point particles with unit charges and masses m_X, m_Y, and m_Z, respectively. In general the $X^+Y^+Z^-$ system has bound state spectra which contain (i) a finite number of bound states, (ii) only one bound state, (iii) no bound states (empty spectrum), or (iv) an infinite number of bound states. We shall consider only cases (i) and (ii). An arbitrary state in such a system can be designated by two quantum numbers, i.e., the rotational quantum number L and the vibrational quantum number ν. We restrict ourselves to consideration of only the ground and the first vibrationally excited states, i.e., the (0,0) and (0,1) states in terms of the (L,ν) classification scheme. In another paper [10] we considered the bound $P(L = 1)$ and $D(L = 2)$ states of the muonic molecular ions.

For the Coulomb three-body systems with unit charges it is useful to introduce the dimensionless variables v_X, v_Y, and v_Z [1]

$$v_X = \frac{m_X}{m_X + m_Y + m_Z},$$
$$v_Y = \frac{m_Y}{m_X + m_Y + m_Z}, \tag{1}$$
$$v_Z = \frac{m_Z}{m_X + m_Y + m_Z},$$

instead of m_X, m_Y, and m_Z. Obviously, $0 \le v_i \le 1$, where $i = X, Y, Z$. Without loss of generality, we can further choose $m_X \ge m_Y$, i.e., $v_X \ge v_Y$. Since $v_X + v_Y + v_Z = 1$, only two of the v's are independent, e.g., v_X and v_Z, and for simplicity we assume that m_Z is the minimal mass.

We shall use the quasiatomic units in which $\hbar = 1, e = 1$, and $m_{\min} = m_Z = 1$. In these units the Hamiltonian of the Schrödinger equation for the $X^+Y^+Z^-$ system takes the form (in terms of the variables v_X and v_Z)

$$H(v_X, v_Z) = -\frac{v_Z}{2v_X}\nabla_X^2 - \frac{v_Z}{2(1 - v_X - v_Z)}\nabla_Y^2 - \frac{1}{2}\nabla_Z^2 - \frac{1}{r_{XZ}} - \frac{1}{r_{YZ}} + \frac{1}{r_{YZ}}. \tag{2}$$

Since all coefficients before the ∇_i^2 and $\frac{1}{r_{jk}}$ operators $(i, j, k = 1, 2, 3$ and $j \ne k)$ in this equation are analytical functions of v_X and v_Z, its solutions must be, in principle, analytical functions of these two variables. For the symmetric systems $X^+X^+Z^-$, $v_X = 1 - v_X - v_Z = \frac{1}{2}(1 - v_Z)$. Therefore, the Hamiltonian is

$$H(\lambda) = -\frac{\lambda}{2}\nabla_X^2 - \frac{\lambda}{2}\nabla_Y^2 - \frac{1}{2}\nabla_Z^2 - \frac{1}{r_{XZ}} - \frac{1}{r_{YZ}} + \frac{1}{r_{YZ}}, \tag{3}$$

where $\lambda = \frac{m_Z}{m_X} = \frac{v_Z}{v_X}$ is the single dimensionless variable. The other cases when $m_X \ge m_Z \ge m_Y$ and $m_Z \ge m_X \ge m_Y$ can be treated in an analogous man-

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ner. In this paper we consider the six muonic molecular ions (mesomolecules for short) $pp\mu$, $pd\mu$, $pt\mu$, $dd\mu$, $dt\mu$, and $tt\mu$ and seven exotic systems: four symmetric ones $t^+t^+p^-, d^+d^+p^-, \pi^+\pi^+\mu^-$, and $\mu^+\mu^+\pi^-$ and three nonsymmetric ones $d^+t^+p^-, \mu^+\pi^+\pi^-$, and $\mu^+\pi^+\mu^-$.

The ground state with $L=0$ [(0,0) states or S states] is bound for each of the muonic molecular ions, while excited S states exist only in the three heaviest systems: $dd\mu$, $dt\mu$, and $tt\mu$. Thus there are, in total, nine bound S states for the muonic molecular ions. The energy spectra for each of the considered exotic systems contains just one bound S state.

II. CALCULATIONS

A. Wave functions

In all calculations we have used the exponential variational expansion in relative (Hylleraas) coordinates r_{31}, r_{32}, and r_{21} for the wave function. In the case of bound states with $L=0$ [i.e., $(0,\nu)$ states or S states] they take the form [11–16]

$$\psi_{L=0}(r_{32}, r_{31}, r_{21}) = (1+\delta P_{21}) \sum_{i=1}^{N} C_i \exp(-\alpha_i r_{32} - \beta_i r_{31} - \gamma_i r_{21}), \quad (4)$$

where δ equals 1 for symmetric systems and 0 for nonsymmetric systems and P_{21} is the permutation operator for the identical particles (2 and 1). The linear parameters $C_i (i=1,2,\ldots,N)$ are determined from variational calculations. The nonlinear parameters α_i, β_i, and γ_i are selected quasirandomly [11,12,17] from three positive intervals $[0,A], [0,B]$, and $[0,C]$,

$$\alpha_i = \langle\langle \tfrac{1}{2} i(i+1)\sqrt{2}\rangle\rangle A, \quad (5)$$

$$\beta_i = \langle\langle \tfrac{1}{2} i(i+1)\sqrt{3}\rangle\rangle B, \quad (6)$$

$$\gamma_i = \langle\langle \tfrac{1}{2} i(i+1)\sqrt{5}\rangle\rangle C, \quad (7)$$

where $\langle\langle x\rangle\rangle$ is the fractional part of x. The values of the constants A, B, and C have been chosen as 1.377 13, 1.455 81, and 2.047 47, respectively (see [7]) for the mesomolecules (in muon atomic units $m_\mu = 1, \hbar = 1$, and $e=1$) and as 1.051, 0.717, and 0.674 for the exotic nonsymmetric systems (in quasi atomic units $m_{\min} = 1, \hbar = 1$, and $e=1$). In view of the number (N) of terms used, no further optimization of α, β, and γ has been carried out.

For the symmetric exotic systems $d^+d^+p^-, t^+t^+p^-$, $\pi^+\pi^+\mu^-$, and $\mu^+\mu^+\pi^-$ a more general choice of α_i, β_i, and γ_i was used. They were generated from the intervals $[0,A_2], [B_{1,i}, B_2]$, and $[G_{1,i}, G_2]$ as

$$\alpha_i = \langle\langle \tfrac{1}{2} i(i+1)\sqrt{2}\rangle\rangle A_2, \quad (8)$$

$$\beta_i = \langle\langle \tfrac{1}{2} i(i+1)\sqrt{3}\rangle\rangle (B_2 - B_{1,i}) + B_{1,i}, \quad (9)$$

$$\gamma_i = \langle\langle \tfrac{1}{2} i(i+1)\sqrt{5}\rangle\rangle (G_2 - G_{1,i}) + G_{1,i}. \quad (10)$$

To choose the values of $B_{1,i}$ and $G_{1,i}$ for each i, we used the prescription

$$B_{1,i} = -k\alpha_i = -0.075\alpha_i,$$
$$G_{1,i} = -\kappa \min(\alpha_i, \beta_i) = -0.375 \min(\alpha_i, \beta_i) \quad \text{if} \quad \beta_i \geq 0,$$
$$G_{1,i} = -\beta_i \quad \text{if} \quad \beta_i < 0.$$

This means that the parameters β_i and γ_i can be negative, but to guarantee square integrability the following three sums must always be positive: $\alpha_i + \beta_i > 0$, $\alpha_i + \gamma_i > 0$, and $\beta_i + \gamma_i > 0$. For the lightest symmetric exotic systems $\pi^+\pi^+\mu^-$ and $\mu^+\mu^+\pi^-$ the constants A, B, and C were taken to be 1.157, 0.783, and 0.819, respectively, while for the $d^+d^+p^-$ and $t^+t^+p^-$ systems the values taken were 1.334, 1.259, and 1.391. It should be noted that this approach is a simplified version of the integral transform (generator coordinate) method [11,12,17,18].

B. Values of the physical constants

In all our calculations of the bound S states we used the following particle masses relative to the electron mass m_e: $m_\mu/m_e = 206.768\,262$, $m_p/m_e = 1836.152\,701$, $m_d/m_e = 3670.483\,014$, $m_t/m_e = 5496.921\,58$, and $m_\pi/m_e = 273.126\,95$.

The conversion factor m_μ was used to convert the total energies from muon atomic units ($m_\mu = 1, \hbar = 1$, and $e=1$) to the usual hartree atomic units ($m_e = 1, \hbar = 1$, and $e=1$). To convert energies to hartree atomic units the conversion factor $E_h \approx 27.211\,396\,1$ eV was applied. All values of the particle masses were taken from CODATA 1986 (see, e.g., [19]). The numerical calculations for the muonic molecular ions, as well as for the systems containing one muon, have been made in muon atomic units. The bound states in $d^+d^+p^-, t^+t^+p^-$, and $d^+t^+p^-$ were computed in proton atomic units ($m_p = 1, \hbar = 1$, and $e=1$).

III. PROPERTIES

The S-state properties are listed in Tables I–VI. In each table N is the number of basis functions used for the property values reported. The number of digits presented is such that they are unchanged by using a basis of N–100 functions and, to this extent, the values are converged. The total energies E in Table I and the binding energies ε are more accurate than those previously reported in the literature (in [7,16,18] different masses were used). The kinetic energy $\langle T\rangle$ is reported as well as the virial factor η, defined by

$$\eta = \left| 1 + \frac{2\langle T\rangle}{\langle V\rangle} \right|, \quad (11)$$

where $\langle V\rangle$ is the expectation value of the potential energy. The deviation of this parameter from zero is an indication of the quality of the wave functions used (see,

TABLE I. The total energies (E) in muon atomic units ($m_\mu = 1, \hbar = 1$, and $e = 1$) for the ground and excited (*) S states ($L = 0$) of the mesomolecules and for the ground S states ($L = 0$) of the exotic systems. N is the number of basis functions used.

Symmetric systems					
N	$pp\mu$	$dd\mu$	$tt\mu$	$dd\mu^*$	$tt\mu^*$
500	-0.49438682024790	-0.531111135395	-0.546374225477	-0.479706380352	-0.496762893748
600	-0.49438682024833	-0.531111135400	-0.546374225581	-0.479706380364	-0.496762894246
700	-0.49438682024858	-0.531111135402	-0.546374225598	-0.479706380368	-0.496762894248

Nonsymmetric systems					
N	$pd\mu$	$pt\mu$	N	$dt\mu$	$dt\mu^*$
800	-0.5127117964991	-0.5198800897792	1000	-0.538594975052	-0.488065357819
900	-0.5127117965003	-0.5198800897811	1100	-0.538594975056	-0.488065357833
1000	-0.5127117965008	-0.5198800897819	1200	-0.538594975058	-0.488065357841

Symmetric exotic systems					
N	$d^+d^+p^-$	$t^+t^+p^-$	N	$\pi^+\pi^+\mu^-$	$\mu^+\mu^+\pi^-$
500	-0.3526256795580	-0.4000369456694	600	-0.2991166915327	-0.2976892640165
600	-0.3526256795598	-0.4000369456709	700	-0.2991166915335	-0.2976892640175
700	-0.3526256795603	-0.4000369456721	800	-0.2991166915342	-0.2976892640182

Nonsymmetric (weakly bound) exotic systems			
N	$d^+t^+p^-$	$\mu^+\pi^+\mu^-$	$\mu^+\pi^+\pi^-$
1100	-0.381190901672	-0.286302242013	-0.33101694736
1200	-0.381190901682	-0.286302244854	-0.33101701177
1300	-0.381190901688	-0.286302245644	-0.33101717037

TABLE II. The expectation values in muon atomic units ($m_\mu = 1, \hbar = 1$, and $e = 1$) of some properties for the ground S states ($L = 0$) of the symmetric mesomolecules.

System / Particles	$pp\mu$ 123	$dd\mu$ 123	$tt\mu$ 123
N	700	700	700
ε	-253.150192	-325.070689	-362.906555
$\langle T \rangle$	0.494386820245	0.531111135391	0.54637422552
η	0.334×10^{-11}	0.114×10^{-10}	0.815×10^{-10}
α	0.57352	0.75803	0.92417
$\langle \frac{1}{2}\nabla_1^2 \rangle$	0.286758809199	0.37901760388	0.442086314
$\langle \frac{1}{2}\nabla_3^2 \rangle$	0.429803280369	0.48840895645	0.5131158217
$\langle r_{21} \rangle$	3.29948618437	2.8344517660	2.652824760
$\langle r_{31} \rangle$	2.38566658563	2.1199316476	2.017373311
$\langle r_{21}^2 \rangle$	12.3904084642	8.8767546423	7.662138325
$\langle r_{31}^2 \rangle$	7.76950381445	5.9462232199	5.312898701
Δr_{21}	0.37166240852	0.3238555956	0.297929139
Δr_{31}	0.60425930037	0.5684317830	0.552671914
τ_{21}	0.151678044543	0.18110529165	0.1948528255
τ_{31}	0.544146849143	0.53407920314	0.5293921144
$\tau_{r_{21}}$	0.2026254984	0.2535804397	0.2789116867
$\tau_{r_{31}}$	0.6146062688	0.5988509681	0.5905292070
$\tau_{p_{31}}$	0.0637714384	0.0693629628	0.070499849
$\tau_{p_{21}}$	0.0547556040	0.0535388714	0.050777164
$\langle \delta_{31} \rangle$	0.131500864	0.15873897	0.17036215
$\langle \delta_{21} \rangle$	0.39372×10^{-4}	0.24395×10^{-5}	0.2187×10^{-6}
$\langle \delta_{321} \rangle$	0.5549×10^{-4}	0.4280×10^{-5}	0.422×10^{-6}
$\langle \nu_{31} \rangle$	-0.8987883	-0.946676	-0.9637495
$\langle \nu_{31} \rangle^a$	-0.8987879287820	-0.9466714310522	-0.9637483334950
$\langle \nu_{21} \rangle$	4.4392	8.8692	12.986
$\langle \nu_{21} \rangle^a$	4.440122200669	8.875837564471	13.29246937327

[a]The exact value from Eq. (19).

e.g., [20,21]). In the present mesomolecule calculations η never deviated from zero by more than 1×10^{-10}.

Since particle masses are always under revision, we also report values of the mass shift (mass gradient) parameters α and β defined by

$$E_{\rm new} = E_{\rm our} + \alpha \left(\frac{m_{Z,\rm new}}{m_{X,\rm new}} - \frac{m_{Z,\rm our}}{m_{X,\rm our}} \right) + \beta \left(\frac{m_{Z,\rm new}}{m_{Y,\rm new}} - \frac{m_{Z,\rm our}}{m_{Y,\rm our}} \right) \quad (12)$$

and

$$E_{\rm new} = E_{\rm our} + \alpha \left(\frac{m_{Z,\rm new}}{m_{X,\rm new}} - \frac{m_{Z,\rm our}}{m_{X,\rm our}} \right) \quad (13)$$

for the $X^+Y^+Z^-$ and $X^+X^+Z^-$ systems, respectively, and $m_{\rm min} = m_z$. The subscript "our" designates the values used (obtained) by us, while the subscript "new" stands for the new values which can be available in the future. The numerical values of α and β were determined by fitting energies from separate calculations. The other property we list is $\frac{1}{2}\langle \nabla_i^2 \rangle$.

The following geometric properties are supplied: $\langle r_{ij} \rangle$, $\langle r_{ij}^2 \rangle$, and Δr_{ij}; the latter is the dimensionless Pearson correlation coefficient and takes the form

$$\Delta r_{ij} = \frac{\sqrt{[\langle r_{ij}^2 \rangle - \langle r_{ij} \rangle^2]}}{\langle r_{ij} \rangle}. \quad (14)$$

This coefficient can be used as a measure of the uncertainty in the expected geometrical structure [18]. The statistical angular correlation coefficients τ_{ij} were determined by

$$\tau_{ij} = \langle \hat{\mathbf{r}}_{ik} \cdot \hat{\mathbf{r}}_{jk} \rangle \quad (15)$$

where $\hat{\mathbf{r}}_{ij} = \mathbf{r}_{ij}/r_{ij}$.

In addition, we have calculated two other statistical

TABLE III. The expectation values in muon atomic units ($m_\mu = 1, \hbar = 1$, and $e = 1$) of some properties for the ground S states ($L = 0$) of the nonsymmetric mesomolecules.

System / Particles	$pd\mu$ 123	$pt\mu$ 123	$dt\mu$ 123
N	1000	1000	1200
ε	-221.547672	-213.838543	-319.136967
$\langle T \rangle$	0.512711796494	0.519880089775	0.53859497499
η	0.605×10^{-11}	0.625×10^{-11}	0.628×10^{-10}
α	0.36756	0.39898	0.44797
β	0.28062	0.28182	0.41717
$\langle \frac{1}{2}\nabla_1^2 \rangle$	0.28061919520	0.28181756747	0.391076475
$\langle \frac{1}{2}\nabla_2^2 \rangle$	0.36746090398	0.39898243020	0.421883781
$\langle \frac{1}{2}\nabla_3^2 \rangle$	0.46041133627	0.47313691355	0.500695298
$\langle r_{21} \rangle$	3.1007104035	3.0365243209	2.747914133
$\langle r_{31} \rangle$	2.4514875888	2.4612768385	2.117912247
$\langle r_{32} \rangle$	2.0876991487	2.0020112758	2.023720496
$\langle r_{21}^2 \rangle$	10.829021113	10.347734315	8.28732531
$\langle r_{31}^2 \rangle$	8.0334941737	8.0316257610	5.88185390
$\langle r_{32}^2 \rangle$	5.8965262741	5.4044336503	5.39705712
Δr_{21}	0.35543346178	0.34965053612	0.31226424
Δr_{31}	0.58028810034	0.57080101390	0.55793250
Δr_{32}	0.59404000719	0.59024999327	0.563754889
τ_{21}	0.165076398580	0.17029438462	0.187625971
τ_{32}	0.600402600413	0.61701775054	0.550815275
τ_{31}	0.477226952552	0.45600843004	0.512758399
$\tau_{\mathbf{r}21}$	0.2226126908	0.2298534862	0.2652371
$\tau_{\mathbf{r}32}$	0.6873944867	0.7059509348	0.6190988
$\tau_{\mathbf{r}31}$	0.5196872193	0.4901256907	0.5701776
$\tau_{\mathbf{p}21}$	0.0790214884	0.0792439004	0.07112494
$\tau_{\mathbf{p}32}$	0.0376459140	0.0349782304	0.04412236
$\tau_{\mathbf{p}31}$	0.0516163164	0.0539451532	0.05451457
$\langle \delta_{32} \rangle$	0.1734562	0.1893821	0.1745146
$\langle \delta_{31} \rangle$	0.11770973	0.1136388	0.1545255
$\langle \delta_{21} \rangle$	0.146174×10^{-4}	0.89750×10^{-5}	0.8871×10^{-6}
$\langle \delta_{321} \rangle$	0.22833×10^{-4}	0.1452×10^{-4}	0.1628×10^{-5}
$\langle \nu_{32} \rangle$	-0.9466715	-0.963748	-0.963746
$\langle \nu_{32} \rangle^{\rm a}$	-0.9466714310522	-0.9637483334950	-0.9637483334950
$\langle \nu_{31} \rangle$	-0.898789	-0.898789	-0.946674
$\langle \nu_{31} \rangle^{\rm a}$	-0.8987879287820	-0.8987879287820	-0.9466704702882
$\langle \nu_{21} \rangle$	5.9186	6.6565	10.640
$\langle \nu_{21} \rangle^{\rm a}$	5.919183313052	6.656690661360	10.64418670485

[a]The exact value from Eq. (19).

angular correlation coefficients

$$\tau_{\mathbf{r}_{ij}} = \frac{2\langle \mathbf{r}_{ik} \cdot \mathbf{r}_{jk} \rangle}{\langle \mathbf{r}_{ik}^2 \rangle + \langle \mathbf{r}_{jk}^2 \rangle} \tag{16}$$

and

$$\tau_{\mathbf{p}_{ij}} = \frac{2\langle \boldsymbol{\nabla}_i \cdot \boldsymbol{\nabla}_j \rangle}{\langle \nabla_i^2 \rangle + \langle \nabla_j^2 \rangle} = \frac{\langle \boldsymbol{\nabla}_i \cdot \boldsymbol{\nabla}_j \rangle}{\langle \frac{1}{2}\nabla_i^2 \rangle + \langle \frac{1}{2}\nabla_j^2 \rangle}. \tag{17}$$

These values as well as τ_{ij} are bounded between $+1$ and -1. If $\tau_{ij} = +1$ there is perfect positive correlation where the position vectors of particles i and j (i.e., $\mathbf{r}_{ik}$ and $\mathbf{r}_{jk}$) are expected to coincide and if $\tau_{ij} = -1$ there is perfect negative correlation where particles i and j are expected to be at diametrical positions with respect to the third particle k. It should be noted that $\tau_{ij}(\tau_{\mathbf{r}_{ij}})$ assesses angular correlation primarly for small (intermediate) separations of the third particle from i and j. $\tau_{\mathbf{p}_{ij}}$ assesses angular correlation for intermediate momenta $\mathbf{p}_{ij}$. All these measures of angular correlation for the electrons in the ground S states of heliumlike ions (H^-, He, Li^+, Be^{2+}, etc.) have been found to be negative (see, e.g., [22]), while for the Ps^- ion ($e^+e^-e^-$) they are positive [23]. In fact, for the series of two electron ions with the "nucleus" Z^+, which includes H^-, Mu^- ($e^-\mu^+e^-$), and Ps^-, there is an intermediate value of m_Z for each of these quantities such that τ_{21} vanishes, i.e., it is expected that there is orthogonality between the position vectors of the electrons or the electrons are completely independent of each other. The latter is not possible for the species discussed here.

Finally, expectation values of the Dirac delta functions δ_{ij} and δ_{321} are given, where appropriate, as well as the two-body cusp ratio

$$\nu_{ij} = \frac{\langle \delta(\mathbf{r}_{ij}) \times \frac{\partial}{\partial r_{ij}} \rangle}{\langle \delta(\mathbf{r}_{ij}) \rangle}, \tag{18}$$

TABLE IV. The expectation values in muon atomic units ($m_\mu = 1, \hbar = 1$, and $e = 1$) of some properties for the excited S states ($L = 0$) of the mesomolecules.

System	$dd\mu$	$tt\mu$	$dt\mu$
Particles	123	123	123
N	700	700	1200
ϵ	-35.844247	-83.770727	-34.834446
$\langle T \rangle$	0.479706380346	0.49676289423	0.48806535776
η	0.274×10^{-10}	0.152×10^{-10}	0.586×10^{-10}
α	0.77168	1.08229	0.50136
β			0.38364
$\langle \frac{1}{2}\nabla_1^2 \rangle$	0.3588445914	0.5411473341	0.383632748
$\langle \frac{1}{2}\nabla_2^2 \rangle$			0.500357609
$\langle \frac{1}{2}\nabla_3^2 \rangle$	0.4362350359	0.4560520737	0.447633191
$\langle r_{21} \rangle$	5.694739220	4.453656634	5.16122895
$\langle r_{31} \rangle$	3.616306082	2.965847588	3.93323568
$\langle r_{32} \rangle$			2.73875105
$\langle r_{21}^2 \rangle$	37.41878622	22.47682796	30.631299
$\langle r_{31}^2 \rangle$	20.54097550	12.88610526	22.397192
$\langle r_{32}^2 \rangle$			11.760494
Δr_{21}	0.3922123115	0.364947856	0.38716615
Δr_{31}	0.7554408014	0.681875424	0.66914142
Δr_{32}			0.75359642
τ_{21}	0.099259216895	0.11743429490	0.107147791
τ_{32}	0.535810156225	0.53992533101	0.643593833
τ_{31}			0.430245915
$\tau_{\mathbf{r}_{21}}$	0.089167255	0.012786573	0.10323846
$\tau_{\mathbf{r}_{32}}$	0.645599380	0.635604174	0.77822311
$\tau_{\mathbf{r}_{31}}$			0.47166207
$\tau_{\mathbf{p}_{21}}$	0.019412094	0.020957125	0.020474422
$\tau_{\mathbf{p}_{32}}$	0.017536030	0.024610949	0.016185218
$\tau_{\mathbf{p}_{31}}$			0.023842927
$\langle \delta_{32} \rangle$			0.1787572
$\langle \delta_{31} \rangle$	0.1371458	0.1481590	0.1072330
$\langle \delta_{21} \rangle$	0.16752×10^{-5}	0.24247×10^{-6}	0.7428×10^{-6}
$\langle \delta_{321} \rangle$	0.295×10^{-5}	0.470×10^{-6}	0.14×10^{-5}
$\langle \nu_{32} \rangle$			-0.963741
$\langle \nu_{32} \rangle^a$	-0.9466714310522	-0.9637483334950	-0.9637483334950
$\langle \nu_{31} \rangle$	-0.946670	-0.963752	-0.946670
$\langle \nu_{31} \rangle^a$	-0.9466714310522	-0.9637483334950	-0.9466714310522
$\langle \nu_{21} \rangle$	8.8758	13.314	10.60
$\langle \nu_{21} \rangle^a$	8.874539991861	13.29246937327	10.64418670485

[a]The exact value from Eq. (19).

where $\delta(\mathbf{r}_{ij})$ is the appropriate Dirac delta function and $(ij) = (21), (31)$, and (32). The exact value of ν_{ij} equals [24]

$$\nu_{ij} = q_i q_j \frac{m_j m_j}{m_j + m_j}, \tag{19}$$

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

It may be noted that the quantity $\langle f \rangle$ [23] in 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 $(i, j, k) = (1, 2, 3)$

$$\langle f \rangle = \langle \psi \mid f \mid \psi \rangle = \left\langle \psi \left| \frac{u_1}{r_{32}} \frac{u_2}{r_{31}} \frac{u_3}{r_{21}} \right| \psi \right\rangle = \iiint \mid \psi(r_{31}, r_{32}, r_{21}) \mid^2 \frac{u_1}{r_{32}} \frac{u_2}{r_{31}} \frac{u_3}{r_{21}} r_{31} r_{32} r_{21} dr_{31} dr_{32} dr_{21}$$
$$= \iiint \mid \psi(u_1, u_2, u_3) \mid^2 u_1 u_2 u_3 du_1 du_2 du_3, \tag{20}$$

can be calculated directly or from the τ_{ij}. The equality

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

holds for an arbitrary three-body Coulomb system. For the symmetric systems it takes the form

$$\tau_{21} + 2\tau_{31} = 1 + 4\langle f \rangle, \tag{22}$$

where 1 and 2 are the identical particles.

A. Mesomolecules

Our results for the bound S states of the mesomolecules are listed in Tables I–IV. From these tables we have established that the final accuracy achieved for the binding energies ε in these mesomolecules is $\approx 3 \times 10^{-9}$ eV for $pp\mu$, $\approx 1.5 \times 10^{-8}$ eV for $pd\mu$, $\approx 2 \times 10^{-8}$ eV for $pt\mu$, $\approx 3 \times 10^{-8}$ eV for $dd\mu$, $\approx 1 \times 10^{-7}$ eV for $dt\mu$, and $\approx 3 \times 10^{-7}$ eV for $tt\mu$ in the case of the ground S states.

TABLE V. The expectation values in quasiatomic units ($m_{\min} = 1, \hbar = 1$, and $e = 1$, where $m_{\min}$ is the mass of the lightest particle) of some properties for the ground S states ($L = 0$) of the symmetric exotic systems.

System / Particles	$d^+d^+p^-$ (1 2 3)	$t^+t^+p^-$ (1 2 3)	$\pi^+\pi^+\mu^-$ (1 2 3)	$\mu^+\mu^+\pi^-$ (1 2 3)
N	700	700	800	800
ε	-966.684055	-1260.778512	-81.849859	-73.818505
$\langle T \rangle$	0.352625679551	0.400036945651	0.29911669156	0.2976892644
η	0.128×10^{-10}	0.265×10^{-10}	0.825×10^{-10}	0.885×10^{-10}
α	0.24739	0.75803	0.17083	0.17527
$\langle \frac{1}{2}\nabla_1^2 \rangle$	0.1241936515753	0.164343585105	0.08763308712	0.854120857
$\langle \frac{1}{2}\nabla_3^2 \rangle$	0.228370366058	0.29024461432	0.16643303571	0.1675802442
$\langle r_{21} \rangle$	5.7977797454	4.7948136985	7.24928710	7.7144121
$\langle r_{31} \rangle$	3.8480889333	3.2564605723	4.71133202	4.9047327
$\langle r_{21}^2 \rangle$	41.459494488	27.716241473	66.215585	76.585643
$\langle r_{31}^2 \rangle$	22.570533433	15.616944272	34.989971	39.225379
Δr_{21}	0.48310499645	0.45339347139	0.50989931	0.53562192
Δr_{31}	0.72403999959	0.68750746508	0.75918557	0.79407737
τ_{21}	0.064524476149	0.090505407362	0.0375229150	0.002714413
τ_{31}	0.574807453303	0.565432012537	0.58497158687	0.599015336
$\tau_{\mathbf{r}_{21}}$	0.08155705292	0.11262277084	0.05379194	0.02377434
$\tau_{\mathbf{r}_{31}}$	0.64750080288	0.63960775088	0.65426828	0.66129840
$\tau_{\mathbf{p}_{21}}$	0.03436376394	0.04343558663	0.02239316	0.00260748
$\tau_{\mathbf{p}_{31}}$	0.03574268102	0.04539891354	0.02447338	0.00757899
$\langle \delta_{31} \rangle$	0.05010598	0.07242510	0.03078332	0.03042574
$\langle \delta_{21} \rangle$	0.25780×10^{-3}	0.23798×10^{-3}	0.217154×10^{-3}	0.28457×10^{-3}
$\langle \delta_{321} \rangle$	0.13108×10^{-3}	0.17672×10^{-3}	0.67585×10^{-4}	0.8810×10^{-4}
$\langle \nu_{31} \rangle$	-0.666557	-0.749607	-0.569136	-0.56914
$\langle \nu_{31} \rangle^a$	-0.6665563520030	-0.7496066955496	-0.5691387268936	-0.5691387268936
$\langle \nu_{21} \rangle$	0.99941	1.49664	0.66032	0.499884
$\langle \nu_{21} \rangle^a$	0.9995037482452	1.496858506650	0.6604663292087	0.5

[a]The exact value from Eq. (19).

For the excited S state the results are $\approx 5 \times 10^{-8}$ eV for $dd\mu$, $\approx 3 \times 10^{-7}$ eV for $dt\mu$, and $\approx 5 \times 10^{-8}$ eV for $tt\mu$. This shows that our results are the best so far for the S states of the mesomolecules. Earlier calculations with the same particle masses were made by Kamimura [25] for only the $dt\mu$ ion. Other references to previous work on mesomolecule calculations can be found in [26].

Tables II–IV contain the results for calculations of the expectation values of some mesomolecular properties, most of which have not been calculated before. Where there are earlier calculations (see, e.g., [17] and [27] and references therein) there is essential agreement. It follows from these tables that, since the parameter $\varepsilon/E \leq 0.119$, the ground and first excited S states in all mesomolecules are relatively weakly bound. The analysis of the "averaged geometries" shows that these mesomolecules have a cluster structure, i.e., the lighter nucleus (e.g., Y^+) moves in the field of the two-body neutral cluster $X^+\mu^-$. As expected, the excited states of $dd\mu$, $dt\mu$, and $tt\mu$ have a much sharper cluster structure than the ground states. For the ground and excited states in symmetric systems such as $X^+X^+\mu^-$ we can say that the degree of clustering of their structure decreases as the parameter $\frac{m_X}{m_\mu}$ increases.

Both muon-nucleon and nucleon-nucleon distances increase as the nucleon masses decrease, since as the nucleon masses become heavier the molecules become more compact. As expected, the distances are larger for the excited states than in the ground state [18]. For the symmetric systems $(X^+X^+\mu^-)$ the appropriate distances coincide in the limit $\frac{m_X}{m_\mu} = \infty$ with the parameters for the adiabatic three-body system $(^\infty H^+)\mu^-(^\infty H^+)$ (or the ion $^\infty H_2{}^+$ in muon atomic units), i.e., $\langle r_{21} \rangle = R \approx 2$, and

TABLE VI. The expectation values in quasiatomic units ($m_{\min} = 1, \hbar = 1$, and $e = 1$, where $m_{\min}$ is the mass of the lightest particle) of some properties for the ground S states ($L = 0$) of the nonsymmetric (weakly bound) exotic systems.

System Particles	$d^+t^+p^-$ (1 2 3)	$\mu^+\pi^+\mu^-$ (1 2 3)	$\mu^+\pi^+\pi^-$ (1 2 3)
N	1300	1300	1300
ε	-319.149522	-9.749980	-4.409405
$\langle T \rangle$	0.3811909012	0.286302243	0.331020
η	0.565×10^{-9}	0.683×10^{-8}	0.460×10^{-5}
α	0.2244	0.1379	0.1972
β	0.0699	0.0239	0.0194
$\langle \frac{1}{2}\nabla_1^2 \rangle$	0.0690228400	0.023876	0.0193
$\langle \frac{1}{2}\nabla_2^2 \rangle$	0.22440894619	0.137927	0.1972
$\langle \frac{1}{2}\nabla_3^2 \rangle$	0.2717023734	0.158009	0.2144
$\langle r_{21} \rangle$	6.533299192	13.205	17.1
$\langle r_{31} \rangle$	5.822464263	12.447	16.7
$\langle r_{32} \rangle$	2.5359591808	3.14210	2.542
$\langle r_{21}^2 \rangle$	57.6218387	274.	490.
$\langle r_{31}^2 \rangle$	52.3560224	265.	490.
$\langle r_{32}^2 \rangle$	9.369594677	14.492	9.27
Δr_{21}	0.592016179	0.757	0.835
Δr_{31}	0.737827529	0.843	0.878
Δr_{32}	0.675766743	0.684	0.659
τ_{21}	0.007667841923	0.033378	0.02124
τ_{32}	0.7765842184	0.85599	0.9083
τ_{31}	0.3406293325	0.26775	0.1970
$\tau_{r_{21}}$	0.066484202	0.019332	0.00845
$\tau_{r_{31}}$	0.218466904	0.081669	0.00613
$\tau_{r_{32}}$	0.914804719	0.973130	0.9907
$\tau_{r_{21}}$	0.044100140	0.018289	0.0078
$\tau_{r_{31}}$	0.031129118	0.130749	0.0288
$\tau_{r_{32}}$	0.013537403	0.003461	0.00046
$\langle \delta_{32} \rangle$	0.1035725	0.0495356	0.0826
$\langle \delta_{31} \rangle$	0.02650205	0.00720	0.00667
$\langle \delta_{21} \rangle$	0.197210×10^{-3}	0.11021×10^{-3}	0.130×10^{-3}
$\langle \delta_{321} \rangle$	0.12210×10^{-3}	0.284×10^{-4}	0.51×10^{-4}
$\langle \nu_{32} \rangle$	-0.749600	-0.5692	-0.6607
$\langle \nu_{32} \rangle^a$	-0.74960669555	-0.56913872689	-0.66046632921
$\langle \nu_{31} \rangle$	-0.666546	-0.49991	-0.5700
$\langle \nu_{31} \rangle^a$	-0.66655635200	-0.5	-0.56913872689
$\langle \nu_{21} \rangle$	1.1981	0.5683	0.567
$\langle \nu_{21} \rangle^a$	1.19863668428	0.56913872689	0.56913872689

[a]The exact value from Eq. (19).

both nucleons are stationary. We have found that the ground and first excited S states in mesomolecules exhibit positive angular correlation, i.e., $\tau_{ij} > 0$, $\tau_{\mathbf{r}_{ij}} > 0$, and $\tau_{\mathbf{p}_{ij}} > 0$ (in comparision with the negative values for the heliumlike ions; see, e.g., [22]). We note that our wave functions give accurate cusps ν_{31}, ν_{32}, and ν_{21}. These values coincide well with the exact values calculated from Eq. (19). In fact, the agreement between the calculated and exact cusp values is better than for any other functions in the literature (see the numerical comparision in [27] and references therein).

It is interesting [28] that in all mesomolecular S states the expectation value of the triple Dirac delta function $\langle\delta_{321}\rangle$ is greater than the expectation value of the two-body delta function $\langle\delta_{21}\rangle$ for the positively charged particles, i.e.,

$$\langle\delta_{321}\rangle = \langle\delta_{++-}\rangle \geq \langle\delta_{21}\rangle = \langle\delta_{++}\rangle. \tag{23}$$

B. Ground S states in the exotic three-body systems

The numerical results for a few of the so-called exotic three-body systems are shown in Tables I, V, and VI. The interaction potential between the particles in these exotic systems is the sum of the Coulomb potential and the potential of strong interaction. Obviously, the latter plays a significant role in such systems. However, to a first approximation we can neglect it and consider these systems as pure Coulomb three-body systems with unit charges. Table I includes the total energies of the exotic systems. The symmetric exotic systems are not extremely weakly bound in contrast to the nonsymmetric exotic systems considered. These nonsymmetric systems are close to the boundary of the stability region for three-body Coulomb systems with unit charges since the value of the parameter $\varepsilon/E \leq 0.02$ (for more details see, e.g., [1–3,29]). Such prethreshold systems have a sharp cluster structure, which can be modeled with good accuracy by a system where the lighter positive ion (e.g., Y^+) moves in the field of the pair X^+Z^- [29].

As may be seen from Table VI, the expected interparticle distance in the neutral cluster (X^+Z^-) is always significantly less than the other two distances, i.e.,

$$\langle r^k_{32}\rangle \ll \min\{\langle r^k_{31}\rangle, \langle r^k_{21}\rangle\}, \tag{24}$$

where $k = 1, 2$. We note that for the exotic systems, the inequality

$$\langle\delta_{++-}\rangle \ll \langle\delta_{++}\rangle \tag{25}$$

holds in contrast to that for the mesomolecules [Eq. (23)]. In conclusion, we observe that for all weakly bound (or prethreshold) systems $X^+Y^+Z^-$, the kinetic energy of the lightest positive ion is approximately equal to zero, i.e.,

$$T_1 = \frac{1}{m_1}\langle\tfrac{1}{2}\nabla^2_1\rangle \approx 0, \tag{26}$$

and T_1 is significantly smaller than T_2 and T_3. Following [30] we can prove Eq. (26), in the case of $L = 0$, for an arbitrary prethreshold (weakly bound) state in a Coulomb three-body system with unit charges.

It appears from the tables that the mass dependence of the properties for all mesomolecules and exotic systems has a relatively smooth form. This suggests that the expectation value of an arbitrary operator b can be presented as a series in v_X and v_Z, i.e.,

$$\langle b\rangle = \sum_{m,n} a_{mn} v^n_X v^m_Z \tag{27}$$

for the nonsymmetric $(X^+Y^+Z^-)$ systems, or as a series in λ, where $\lambda = \min\left(\frac{v_Z}{v_X}, \frac{v_X}{v_Z}\right)$,

$$\langle b\rangle = \sum_n a_n \lambda^n \tag{28}$$

for the symmetric $(X^+X^+Z^-)$ systems. The operator b in these equations corresponds to one of the properties presented. For instance, using the data in Table II, we can predict the following value for $\langle r^2_{d^+\pi^-}\rangle$ in the ground state of the $d^+d^+\pi^-$ system ($m_{\pi^-} = 273.126\,95 m_e$ [31]):

$$\langle r^2_{d^+\pi^-}\rangle \approx 6.540\,665\,5. \tag{29}$$

The direct value from the numerical calculations is $\approx$ 6.536 605. Thus, in this case and for a number of other properties the agreement is good.

IV. CONCLUSIONS

We have considered various properties of the S bound states in the Coulomb three-body systems with unit charges. Among the unexpected mesomolecular results we draw attention to the following: the angular correlation coefficients are positive and the inequality $\langle\delta_{++-}\rangle \geq \langle\delta_{++}\rangle$ holds true in all such systems. For the exotic nonsymmetric systems $d^+t^+p^-$, $\mu^+\pi^+\mu^-$, and $\mu^+\pi^+\pi^-$ we have found sharp cluster structures. The geometrical properties have a relatively smooth dependence on mass. These results should be valuable for further consideration of Coulomb three-body systems with unit charges.

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