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Variational calculation of some S-states of Coulomb three-body systems

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Abstract. A generalized Hylleraas-type basis set with three nonlinear parameters is proposed to study three-body systems interacting *via* coulomb forces within the framework of non-relativistic quantum mechanics. This basis set improves the rate of convergence with respect to previous ones, specially for non-symmetric systems and excited states of two electron atoms. Accurate binding energies and other properties for S-states of helium-like ions, muonic molecules and the positronium negative ion are reported.

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1 Introduction

Accurate determination of bound state properties of three body systems is currently the focus of much research. Since the pioneering work of Hylleraas [1] including explicitly the interparticle distance in the wave function, the variational method using a basis set expansion has been widely employed. For S-states of atomic systems the most precise eigenvalues have been obtained by including logarithmic terms in the basis set [2,3] or by using the *double* basis set of Drake and collaborators [4,5]. For molecular systems such as H_2^+ and some other three body systems with a wide range of mass ratio of the constituent particles, different analytical parameterizations of the basis functions have been proposed to obtain binding energies and other properties [6–23]. Other techniques such as the finite-element method [25,26] and the hyperspherical harmonic method [27,28] have been also used for those systems providing very accurate results.

One of the most used basis sets is that of Pekeris [29], who worked with the isoperimetric coordinates introduced by Coolidge and James [30], and which consists on the product of three Laguerre polynomials multiplied by an exponential. The main advantage of this basis set is that the number of nonzero matrix elements is linear with the dimension of the basis, *i.e.* this basis is quasi-orthogonal, which allows one to work in double precision even for large values of the dimension of the truncated basis. This basis set has been recently twofold modified to include one [9,31,32] and two [14] variational parameters in the exponential. Both generalizations greatly improve the convergency of the basis set, being the second one specially appropriate to study those systems of a molecular nature, *i.e.* those systems for which one mass is much lighter than the other two.

The aim of this work is twofold. First we introduce a generalization of the Pekeris basis set that includes a third non linear parameter to study different three-body Coulomb systems. This generalization was previously introduced in [33] to study S-wave resonances of helium, although the variational parameters were not chosen completely free. This modification will keep the quasi-orthogonal character of the basis set for systems with three non-identical particles. However, this property will not be fulfilled for the rest of three-body systems because of the antisymmetry of the wave function.

Secondly, the performance of this basis set is studied in a wide range of three body systems by comparing the rate of convergence with those of the basis sets with one and two non-linear free parameters. As we shall see later, the basis set used in this work improves the convergence specially in the case of non-symmetric three body systems, *i.e.* those with all the particles different. Besides we shall calculate different global properties, such as the expectation values $\langle r_{ij}^k\rangle$, and some local properties, such as the expectation values $\langle\delta(r_{ij})\rangle$, which play an important role for any few-body system in the calculation of relativistic corrections, hyperfine structure, quantum electrodynamic and weak interaction effects [34,35].

The scheme of the present work is the following. In the next section we shall introduce the basis set used in this work. In Section 3 a study of the convergence is performed in terms of the number of non-linear variational parameters. We shall also present the best results provided by this basis set as compared with the most accurate values known in the literature for the systems above mentioned. Finally some conclusions can be found in Section 4.

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$$\begin{aligned}H = &-\frac{2}{m_1(u+v)(v+w)}\left[uw\left(\frac{\partial^2}{\partial u^2}+\frac{\partial^2}{\partial w^2}-\frac{\partial^2}{\partial u\partial w}\right)+v(u+v+w)\frac{\partial^2}{\partial v^2}+(w-u)\left(\frac{\partial}{\partial u}-\frac{\partial}{\partial w}\right)+(u+2v+w)\frac{\partial}{\partial v}\right]\\ &-\frac{2}{m_2(u+v)(u+w)}\left[vw\left(\frac{\partial^2}{\partial v^2}+\frac{\partial^2}{\partial w^2}-\frac{\partial^2}{\partial v\partial w}\right)+u(u+v+w)\frac{\partial^2}{\partial u^2}+(w-v)\left(\frac{\partial}{\partial v}-\frac{\partial}{\partial w}\right)+(2u+v+w)\frac{\partial}{\partial u}\right]\\ &-\frac{2}{m_3(u+w)(v+w)}\left[uv\left(\frac{\partial^2}{\partial u^2}+\frac{\partial^2}{\partial v^2}-\frac{\partial^2}{\partial u\partial v}\right)+w(u+v+w)\frac{\partial^2}{\partial w^2}+(v-u)\left(\frac{\partial}{\partial u}-\frac{\partial}{\partial v}\right)+(u+v+2w)\frac{\partial}{\partial w}\right]\\ &+\frac{2q_1q_2}{v+w}+\frac{2q_1q_3}{u+w}+\frac{2q_2q_3}{u+v}\end{aligned} \tag{1}$$

2 Wave functions and densities

The Hamiltonian of a three body Coulomb system in a state of S-type can be written, once subtracted the center of mass motion, in terms of the three relative distances among the particles. In this work we shall use the so called isoperimetric coordinates defined as $u = -r_{12} + r_{13} + r_{23}$, $v = r_{12} - r_{13} + r_{23}$ and $w = r_{12} + r_{13} - r_{23}$, introduced by Coolidge and James [30], being the range of each one of them from zero to infinity. Here r_{ij} is the distance between the particles i and j. The Hamiltonian of a three-body Coulomb system in terms of these coordinates, in units $\hbar = e = 1$, is

see equation (1) above

where m_i and q_i, $i = 1, 2, 3$, are the mass and the charge, respectively, of the particle i.

The basis functions used in this work are

$$L_k(\alpha u)L_l(\beta v)L_m(\gamma w)\mathrm{e}^{-\alpha u/2}\mathrm{e}^{-\beta v/2}\mathrm{e}^{-\gamma w/2} \tag{2}$$

where $L_k(x)$ is the Laguerre polynomial of degree k, and α, β and γ are non-linear variational parameters. Most of the overlap matrix elements are zero in such a way that there will be no numerical problems in making the diagonalization for any number of states in the basis in a double precision calculation. For systems with three different particles, the wave function will be expanded as follows

$$\begin{aligned}\Psi(u,v,w) = &\,\mathrm{e}^{-[\alpha u+\beta v+\gamma w]/2}\\ &\times\sum_{k,l,m} C_{klm}L_k(\alpha u)L_l(\beta v)L_m(\gamma w).\end{aligned} \tag{3}$$

where $k + l + m \le N$. In the case that the system under study has two identical particles, the expression of the Hamiltonian reduces to a simpler one as can be seen, for example, in [14]. The wave function used to describe the ^{1}S states of these systems is given by

$$\begin{aligned}\Psi(u,v,w) = &\,\mathrm{e}^{-\gamma w/2}\\ &\times\sum_m\sum_{k\le l} C_{klm}\Big[\mathrm{e}^{-\alpha u/2}L_k(\alpha u)\mathrm{e}^{-\beta v/2}L_l(\beta v)\\ &+\mathrm{e}^{-\beta u/2}L_l(\beta u)\mathrm{e}^{-\alpha v/2}L_k(\alpha v)\Big]L_m(\gamma w)\end{aligned} \tag{4}$$

since for singlet states the spatial wave function must be symmetric for the two identical particles, which will be labeled 2 and 3 hereafter. It must be also mentioned that in the case $\alpha \ne \beta$ the quasi-orthogonality presented above is greatly reduced due to the symmetrization. This basis generalizes the one proposed by Pekeris [29] who used $\alpha = \beta = \gamma/2$, being α the square root of minus the binding energy of the corresponding eigenstate. Later α was taken as a variational parameter [31,32], increasing the rate of convergence. The basis set with only a non-linear variational parameter has worked very well for atomic systems providing accurate results with short expansions. However the rate of convergence is reduced when is used to study systems of molecular nature such as H_2^+ [13,14,19]. The inclusion of a second non-linear variational parameter has allowed to increase the convergence without losing the quasi-orthogonality ($\alpha = \beta$, γ) [14].

With the best eigenfunction one can calculate analytically the different interparticle densities and related properties such as their radial moments. In the general case of non-symmetric systems, we can consider three different interparticle distributions. These, $\rho_{ij}(\mathbf{r})$, with $i, j = 1, 2, 3$ ($i \ne j$) are defined by

$$\rho_{ij}(\mathbf{r}) = \int \mathrm{d}\mathbf{r}_{12}\mathrm{d}\mathbf{r}_{13}\delta(\mathbf{r}-\mathbf{r}_{ij})|\Psi(r_{12}, r_{13}, r_{23})|^2 \tag{5}$$

and give us the probability density of finding the particle i separated by the vector $\mathbf{r}$ from the particle j. These three functions are spherically symmetric for all the states and systems here studied, so they will be hereafter denoted by $\rho_{ij}(r)$.

Using the wave function given by equation (3), it is possible to evaluate analytically all the integrals required to build the densities. For non-symmetric systems it is obtained

$$\rho_{ij}(r) = \mathrm{e}^{-2\alpha_i r}\sum_{k=-1}^{2N} a_{ij,k}r^k + \mathrm{e}^{-2\alpha_j r}\sum_{k=-1}^{2N} b_{ij,k}r^k \tag{6}$$

with $a_{ij,-1} = -b_{ij,-1}$, $\alpha_1 = \gamma$, $\alpha_2 = \beta$, $\alpha_3 = \alpha$ valid when $\alpha_i \ne \alpha_j$. Let note that ρ_{ij} is not divergent at the origin because the restriction $a_{ij,-1} = -b_{ij,-1}$. In the case $\alpha_i = \alpha_j$ the expression becomes

$$\rho_{ij}(r) = \mathrm{e}^{-2\alpha_i r}\sum_{k=0}^{2N+2} d_{ij,k}r^k. \tag{7}$$

Table 1. Convergence study of the basis sets with one, two and three non-linear variational parameters. The results are in atomic units except the $\pi^+\mu^+\pi^-$ and $d^+t^+\mu^{-*}$ for which muonic units have been used. For each value of the parameter N there are three entries corresponding to the basis with one [1], two [2] and three [3] non linear parameters. We also show the best ground state eigenvalues of the systems from references [8,14,21,38], and this work, respectively.

$N[B]$	H^-		H_2^+	$3^1\mathrm{S}$ He
5[1]	−0.527 401 963		−0.583 234 64	−1.957 535 36
5[2]	−0.527 402 591		−0.591 836 06	−1.964 156 04
5[3]	−0.527 428 556		−0.591 941 03	−2.060 930 02
12[1]	−0.527 445 850		−0.594 672 48	−2.060 854 77
12[2]	−0.527 445 851		−0.596 993 55	−2.060 910 35
12[3]	−0.527 445 866		−0.597 005 34	−2.060 988 81
15[1]	−0.527 445 876 636		−0.596 006 26	−2.060 981 68
15[2]	−0.527 445 876 647		−0.597 124 43	−2.060 982 06
15[3]	−0.527 445 878 154		−0.597 124 75	−2.060 989 03
Exact	−0.527 445 881 114		−0.597 139 063 123	−2.060 989 082 352
$N[B]$	$e^-e^+e^-$	$N[B]$	$\pi^+\mu^+\pi^-$	$d^+t^+\mu^{-*}$
5[1]	−0.261 957 584	5[1]	−0.329 920 916	−0.484 357 04
5[2]	−0.261 957 585	5[2]	−0.329 926 422	−0.487 287 42
5[3]	−0.261 996 705	5[3]	−0.330 701 092	−0.487 332 20
12[1]	−0.262 005 012 935	8[1]	−0.330 829 436	−0.487 904 45
12[2]	−0.262 005 012 937	8[2]	−0.330 834 671	−0.488 043 33
12[3]	−0.262 005 046 760	8[3]	−0.331 002 275	−0.488 046 82
15[1]	−0.262 005 068 847	12[1]	−0.330 998 375	−0.488 063 44
15[2]	−0.262 005 068 848	12[2]	−0.330 999 709	−0.488 065 13
15[3]	−0.262 005 069 384	12[3]	−0.331 016 414	−0.488 065 22
Exact	−0.262 005 070 232 975 7		−0.331 017 308	−0.488065 357 8

In the case of systems with two identical particles, we shall follow the notation used in atomic systems [36], calling $\rho_{12}(r) = \rho_{13}(r) \equiv \rho(r)$, single-particle density and $\rho_{23}(r) \equiv h(r)$, intracule density. These functions are given by

$$\rho(r) = \mathrm{e}^{-2\gamma r} \sum_{k=-1}^{2N} a_k r^k + \mathrm{e}^{-2\alpha r} \sum_{k=-1}^{2N} b_k r^k + \mathrm{e}^{-2\beta r} \sum_{k=-1}^{2N} c_k r^k + \mathrm{e}^{-(\alpha+\beta) r} \sum_{k=-1}^{2N} d_k r^k \quad (8)$$

with $a_{-1} = -(b_{-1} + c_{-1} + d_{-1})$, and

$$h(r) = \mathrm{e}^{-2\alpha r} \sum_{k=-1}^{2N} f_k r^k + \mathrm{e}^{-2\beta r} \sum_{k=-1}^{2N} g_k r^k + \mathrm{e}^{-(\alpha+\beta) r} \sum_{k=0}^{2N+2} s_k r^k \quad (9)$$

with $f_{-1} = -g_{-1}$ and we have considered $\alpha \neq \beta$. It must be stressed that all the coefficients involved can be analytically evaluated once the linear coefficients C_{klm} which determine the variational wave function have been obtained.

3 Results

For each calculation we shall consider $k + l + m \leq N$ (the so called Pekeris shell), so N will limit the dimension of the basis. For non-symmetric systems this dimension is 56, 165, 455, 680, 969, 1 330, 1 771 and 2 300 for $N = 5$, 8, 12, 14, 16, 18, 20 and 22, respectively and for symmetric ones the dimension is 34, 252, 444, 715, 1 078, 1 729 and 2 856 for $N = 5$, 12, 15, 18, 21, 25 and 30 respectively.

We have used the following particle masses in atomic units: $m_\mu = 206.768262$, $m_p = 1\,836.152701$, $m_d = 3\,670.483\,014$, $m_t = 5\,496.921\,58$, $m_{\mathrm{He}^{2+}} = 7\,294.299\,62$ and $m_\pi = 273.126\,95$. Here we shall present the results for the atomic systems, the positronium negative ion and the hydrogen molecular ion in atomic units, for the exotic system $d^+t^+p^-$ in proton atomic units ($m_p = 1$, $\hbar = 1$ and $e = 1$) and for the muonic molecular ions we have used the muon atomic units ($m_\mu = 1$, $\hbar = 1$ and $e = 1$).

To assess the impact of the third parameter on the rate of convergence of the basis set we have studied systems with two identical particles. In this analysis we have also considered the basis set with only one non-linear parameter. We have selected the ground state of both the hydrogen atomic ion H^- and the hydrogen molecular ion H_2^+, which can be considered as prototype of those systems with atomic or molecular character, respectively. We have also considered the $3^1\mathrm{S}$ state of the helium atom and the ground state of the positronium negative ion. In Table 1 the energy is shown for these systems, in atomic units, in term of the parameter N, *i.e.* the dimension of the basis used. As we can see the rate of convergence for the atomic systems and even for the positronium negative ion is practically unchanged when a second non-linear

Table 2. Ground state energy in atomic units of the negative two-electron ions of hydrogen, deuterium, tritium and $e^-e^+e^-$. A dimension of 2856 ($N = 30$) has been used.

	α	β	γ	E
H^-	1.5824	1.0128	2.1319	−0.527 445 881 109
D^-	1.7966	1.1198	1.9715	−0.527 598 324 684
T^-	1.5300	1.0700	2.1900	−0.527 649 048 200
$e^-e^+e^-$	0.9681	0.5884	0.9380	−0.262 005 070 232 35

Table 3. Different properties of the ground state of the $p^+d^+\mu^-$ and $p^+t^+\mu^-$ molecules. Muon atomic unit are used. The notation $[x]$ means 10^x. A basis set with 1330 elements ($N = 18$) has been used.

	$p^+d^+\mu^-$	$p^+t^+\mu^-$
α	1.971 7	1.970 1
β	1.619 8	1.693 6
γ	1.970 1	1.947 6
E	−0.512 711 796 501 2	−0.519 880 089 782 7
E^a	−0.512 711 796 494	−0.519 880 089 775
η	−1.3 [−12]	−4.5 [−12]
$\langle r_{12}^{-1} \rangle$	0.369 096 391 8	0.374 961 122 74
$\langle r_{13}^{-1} \rangle$	0.641 146 371 6	0.633 391 625 57
$\langle r_{23}^{-1} \rangle$	0.753 373 613 2	0.781 329 676 74
$\langle r_{12} \rangle$	3.100 710 403 2	3.036 524 320 8
$\langle r_{13} \rangle$	2.451 487 588 5	2.461 276 838 3
$\langle r_{23} \rangle$	2.087 699 148 7	2.002 011 275 8
$\langle r_{12}^{2} \rangle$	10.829 021 108	10.347 734 313
$\langle r_{13}^{2} \rangle$	8.033 494 170 1	8.031 625 759 1
$\langle r_{23}^{2} \rangle$	5.896 526 273 4	5.404 433 650 1
$\langle r_{12}^{3} \rangle$	42.147 963 916	39.195 293 000
$\langle r_{13}^{3} \rangle$	32.267 859 867	31.925 834 966
$\langle r_{23}^{3} \rangle$	20.654 709 308	18.058 059 477
$\rho_{12}(0)$	1.461 712 7 [−5]	8.974 779 [−6]
$\rho_{13}(0)$	0.117 709 737 84	0.113 638 765
$\rho_{23}(0)$	0.173 456 214 30	0.189 382 104
ν_{12}	5.918 955	6.656 663 79
ν_{12}(exact)	5.919 183 31	6.656 690 66
ν_{13}	−0.898 788 597	−0.898 788 471
ν_{13}(exact)	−0.898 792 878	−0.898 792 878
ν_{23}	−0.946 672 672	−0.963 748 657
ν_{23}(exact)	−0.946 671 431	−0.963 648 333

[a] Bishop, Frolov, and Smith, (1995) [6].

Table 4. Different properties of the ground state and the first excited state of $d^+t^+\mu^-$ obtained with $N = 18$ for the former and $N = 22$ for the latter. Muon atomic unit are used. The notation $[x]$ means 10^x.

	$d^+t^+\mu^-$	$d^+t^+\mu^{-*}$
α	2.231 0	1.669 1
β	2.088 5	1.254 3
γ	1.811 3	1.230 2
E	−0.538 594 975 061	−0.488 065 357 850
E^a	−0.538 594 975 0	−0.488 065 357 8
η	4.6 [−13]	1.1 [−11]
$\langle r_{12}^{-1} \rangle$	0.403 825 669 07	0.243 933 337 6
$\langle r_{13}^{-1} \rangle$	0.722 700 008 53	0.514 688 754 3
$\langle r_{23}^{-1} \rangle$	0.758 315 610 66	0.705 375 299 0
$\langle r_{12} \rangle$	2.747 914 131 67	5.161 228 956 9
$\langle r_{13} \rangle$	2.117 912 246 54	3.933 235 695 9
$\langle r_{23} \rangle$	2.023 720 495 65	2.738 751 041 4
$\langle r_{12}^{2} \rangle$	8.287 325 300 53	30.631 300 03
$\langle r_{13}^{2} \rangle$	5.881 853 892 98	22.397 192 86
$\langle r_{23}^{2} \rangle$	5.397 057 113 85	11.760 494 07
$\langle r_{12}^{3} \rangle$	27.208 343 544 7	201.451 771 4
$\langle r_{13}^{3} \rangle$	19.740 231 101 7	154.628 511 7
$\langle r_{23}^{3} \rangle$	17.469 696 452 4	65.255 123 63
$\rho_{12}(0)$	8.871 194 77[−7]	7.411 555 8 [−7]
$\rho_{13}(0)$	0.154 525 544	0.107 232 991 7
$\rho_{23}(0)$	0.174 514 666	0.178 757 429 9
ν_{12}	10.643 4	10.656 0
ν_{12}(exact)	10.644 186 70	10.644 186 70
ν_{13}	−0.946 671 574	−0.946 671 427
ν_{13}(exact)	−0.946 671 431	−0.946 671 431
ν_{23}	−0.963 748 467 1	−0.963 748 254
ν_{23}(exact)	−0.963 748 333 5	−0.963 748 333 5

[a] Ackermann, (1998) [26].

variational parameter is considered but it is appreciably improved when the third non-linear variational parameter is included. This behavior is very different in the molecular case: the main improvement is obtained with the inclusion of the second non-linear parameter, and the third one does not affect in an appreciable manner to the rate of convergence. So we can conclude that the basis with two non-linear variational parameters is enough to account for those systems with a molecular character because it can describe adequately the interparticle distribution of the two heavier particles [14]. However the basis with three non-linear variational parameters is specially adequate to study those three-body Coulomb systems with an atomic nature since the third parameter takes into account the different screening felt by the two electrons. This effect is enhanced for excited states of atomic systems as we can notice from Table 1. We have also included in this table two non-symmetric systems. For the $\pi^+\mu^+\pi^-$ system, the basis with three non-linear variational parameters is also more appropriate than any other with one or two non-linear variational parameter, as one should expect. However for the excited state $d^+t^+\mu^{-*}$, the basis with only two non linear variational parameters is enough to describe it adequately because predominates its nearly molecular character.

With the basis set proposed in this work we have studied some helium-like atomic ions of interest [10] and the positronium negative ion. For these systems the *double* basis set of [5] and the exponential expansion of [16,21] and [24] work with a great precision. We have also studied several three body systems such as the muonic molecular ions $p^+d^+\mu^-$, $p^+t^+\mu^-$ and $d^+t^+\mu^-$ (for the later we have also studied its excited state of S-type, denoted by $d^+t^+\mu^{-*}$) and some exotic, weakly bound, systems such as $\mu^+\pi^+\mu^-$, $\pi^+\mu^+\pi^-$ and $d^+t^+p^-$. All those systems have been extensively investigated, see *e.g.* [6,12,14,26,27].

In Table 2 we show very precise results for different isotopes of hydrogen ion and also for the positronium negative ion. They are calculated with $N = 30$ and confirm the *exact* estimate in reference [10] leading to a precise value of the electron affinity for the three first systems.

Table 5. Different properties of the $\mu^+\pi^+\mu^-$, $\mu^+\pi^+\pi^-$ and $d^+t^+p^-$ systems. We have worked with $N = 20$ for the first two systems and with $N = 22$ for the last one. Muon atomic unit are used for the two first systems and proton atomic units for the last one. The notation $[x]$ means 10^x.

	$\mu^+\pi^+\mu^-$	$\mu^+\pi^+\pi^-$	$d^+t^+p^-$
α	0.666 2	0.630 5	1.020 8
β	0.267 0	0.219 8	0.574 1
γ	0.684 3	0.804 2	1.110 8
E	−0.286 302 245 938	−0.331 017 308 039	−0.381 190 901 668
E^a	−0.286 302 245 644	−0.331 017 170 37	−0.381 190 901 688
η	4.4 [−9]	2.9 [−8]	−3.8 [−11]
$\langle r_{12}^{-1} \rangle$	0.123 191 4	0.110 256 4	0.209 459 651
$\langle r_{13}^{-1} \rangle$	0.181 353 4	0.151 782 2	0.326 582 947
$\langle r_{23}^{-1} \rangle$	0.514 442 5	0.620 508 8	0.645 258 508
$\langle r_{12} \rangle$	13.206 497 9	17.285 475	6.533 298 463 11
$\langle r_{13} \rangle$	12.448 081 6	16.836 055	5.822 463 522 00
$\langle r_{23} \rangle$	3.142 001 875	2.541 693 2	2.535 959 189 75
$\langle r_{12}^2 \rangle$	274.296 385	514.465 76	57.621 789 995
$\langle r_{13}^2 \rangle$	265.209 703	509.112 52	52.355 973 542
$\langle r_{23}^2 \rangle$	14.492 1503	9.263 489 1	9.369 5947 383
$\langle r_{12}^3 \rangle$	8 293.45	22 752.438	676.620 179
$\langle r_{13}^3 \rangle$	8 193.69	22 681.597	645.746 251
$\langle r_{23}^3 \rangle$	92.811 59	46.334 165	46.657 100 50
$\rho_{12}(0)$	1.102 270 5 [−4]	1.302 018 9 [−4]	1.972 019 440 [−4]
$\rho_{13}(0)$	7.197 965 3 [−3]	6.650 678 0 [−3]	2.650 206 643 [−2]
$\rho_{23}(0)$	4.953 514 06 [−2]	8.263 907 6 [−2]	0.103 572 524
ν_{12}	0.568 338	0.566 932	1.198 403 09
ν_{12}(exact)	0.569 138 727	0.569 138 727	1.198 636 68
ν_{13}	−0.499 819 1	−0.568 020 9	−0.666 550 319
ν_{13}(exact)	−0.5	−0.569 138 727	−0.666 556 352
ν_{23}	−0.569 139 250	−0.660 465 790	−0.749 607 103
ν_{23}(exact)	−0.569 138 727	−0.660 466 329	−0.749 606 695

[a] Bishop, Frolov, and Smith, (1995) [6].

Different properties obtained from the best wave function are shown for the non-symmetric systems in Tables 3–5. In these tables the particles 1, 2, 3 coincide with those written in the first, second and third place, respectively. Some quantities there reported are the energy, E, of the system (using units that consider the mass of its lightest particle equal to one), and the virial factor η defined by

$$\eta = \frac{\langle V \rangle}{\langle T \rangle} + 2 \tag{10}$$

where $\langle V \rangle$ and $\langle T \rangle$ are the expectation values of the potential and kinetic energy, respectively. The difference with respect to zero (*i.e.* the exact value of η), is a measure of the quality of the solution found. Some other quantities are the expectation values

$$\langle r_{ij}^n \rangle = \int r_{ij}^n \rho_{ij}(r_{ij}) \mathrm{d}\mathbf{r}_{ij}; \quad n = -1, 1, 2, 3 \tag{11}$$

for the three different pairs and the values $\rho_{jk}(0)$ and $\nu_{jk} = \rho'_{jk}(0)/2\rho_{jk}(0)$. This last quantity is the two body cusp ratio for particles j and k, whose exact value, for a general three body Coulomb system of masses m_i and charges q_i, $i = 1, 2, 3$, is given by [37]

$$q_j q_k \frac{m_j m_k}{m_j + m_k} \cdot \tag{12}$$

An additional test for evaluating the quality of the solutions can be performed by studying how well the two body cusp ratios are satisfied. A comparison with other results in the literature (see Ref. [6] and references therein) shows an improvement in the values of the energy. This also appears for the other quantities as η and ν_{ij}.

4 Conclusions

We have introduced a new Hylleraas three-parameter basis set to study S bound states of three-body Coulomb systems. Although it can be utilized for studying any type of these Coulomb systems, the greatest improvement appears in studying excited states of atomic systems in which the electrons feel a different screening each one, and mainly in studying non-symmetric Coulomb systems, *i.e.* those in which all the particles are different. This basis allows us to obtain analytical expressions for the interparticle distribution functions and to perform calculations for any number of states of the basis. The results obtained for the eigenvalues are the most accurate in the literature for the non-symmetric systems here studied. This basis also provides accurate values for the cusps of the densities improving previous results.

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