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Accurate ground state wavefunctions for several three-body systems

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Abstract The angularly correlated basis functions proposed by Gasaneo and Ancarani (Phys Rev, A 77:012705, 2008) are used to construct approximated wavefunctions, satisfying all two-body cusp conditions, for several three-body systems. The focus here is on the study of the following negatively charged hydrogen-like ions: $^{\infty}H^-$, $^1H^-$, D^-, T^- and Mu^-, the negative positronium ion Ps^-, and the exotic systems $e^-e^-(nm_e)^+$ in which one of the particles is heavier than the other two. Accurate results for the mean of the ground state energy and of other radial quantities are compared with those given in the literature, when available.

Keywords Three-body systems · Cusp conditions

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1 Introduction

Two-electron atoms and ions are the simplest of all quantum systems in which electron-electron correlations have an important effect. The determination of bound states energies and wavefunctions of three-body systems can be separated into,

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essentially, three categories. A first one is based on highly sophisticated calculations (see, e.g., [2, 3]) built with thousands of variational parameters and leading to very accurate results for the energies. A second one provides simple functions with the correct functional structure and with a very low number of parameters [4–7]; the energies reported are, however, often not good enough to properly describe the systems. A third line of work deals with wavefunctions and energies which are of intermediate quality.

Following this third line of work, we apply here the Angular Correlated Configuration Interaction (ACCI) method, described in [1, 8, 9], to three-body systems with general masses. The form of the trial wavefunctions proposed is introduced in Section 2. In Section 3 we report the results of the calculations of the ground state energies and other mean values, for negatively charged hydrogen-like ions $^{\infty}H^-$, $^1H^-$, D^-, T^- and Mu^-, the negative positronium ion Ps^-, and the exotic systems $e^-e^-(nm_e)^+$. Atomic units are used throughout.

2 Theory

Let us consider atomic systems composed of three-particles with charges $z_1 < 0$, $z_2 < 0$, $z_3 > 0$, and respective masses m_1, m_2, m_3. Let $\mu_{ij} = \frac{m_i m_j}{m_i + m_j}$ $(i \neq j)$ be the reduced masses. We shall designate as particle 3 the heaviest particle, *i.e.* the nucleus of mass m_3 and charge z_3, and the two lighter particles, labeled 1 and 2, with masses m_1, m_2 and charges $z_1 = z_2 = -1$. The vectors $\mathbf{r}_{13}$ and $\mathbf{r}_{23}$ will denote the two light particles positions with respect to the nucleus, and $\mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1$ their relative position.

The C3-like basis functions proposed in [1] satisfy exactly all the two-body Kato cusp conditions [10]. Following the methodology proposed in [8, 9], each term of the basis set is multiplied by a power series which does not affect this property. In terms of the interparticle coordinates r_{ij} $(i \neq j)$, the trial wavefunctions with M linear variational parameters $c_{ijk}^{n_1 n_2 n_3}$, are constructed as

$$\Psi_{C3-M} = \sum_{n_1,n_2,n_3} \varphi_{n_1}(\mu_{13}, r_{13})\varphi_{n_2}(\mu_{23}, r_{23})\chi_{C3}(n_3, \mu_{12}, r_{12}) \times \sum_{ijk\neq 1} c_{ijk}^{n_1 n_2 n_3}\, r_{13}^i r_{23}^j r_{12}^k \tag{1}$$

where $\varphi_{n_i}(\mu_{i3}, r_{i3})$ are $l = 0$ hydrogenic functions of principal quantum numbers n_i $(i = 1, 2)$; $\chi_{C3}(n_3, \mu_{12}, r_{12}) = {}_1F_1(-n_3, 2, -2\mu_{12} z_1 z_2 r_{12}/n_3)$ with n_3 a positive integer is an angular correlation factor which diagonalizes the electron–electron Coulomb interaction [1, 11].

3 Results

To show the dependency on the total number M of linear parameters of the proposed trial wavefunction, we have considered two approximated wavefunctions Ψ_{C3-M},

Table 1 The mean energy and the mean of several radial quantities for the ground state of several negatively charged hydrogen-like three-body systems, obtained using the Ψ_{C3-14} and Ψ_{C3-18} approximated wavefunctions, are compared with the numerically "exact" values of [3]

		Mu^-	$^1H^-$	D^-	T^-	$^\infty H^-$
$\langle -E \rangle$	Ψ_{C3-14}	0.52373	0.52613	0.52628	0.52633	0.52644
	Ψ_{C3-18}	0.52464	0.52703	0.52719	0.52724	0.52734
	Exact	0.52505	0.52744	0.52760	0.52765	0.52775
$\langle r_{i3} \rangle$	Ψ_{C3-14}	2.56767	2.5552	2.55441	2.55415	2.55362
	Ψ_{C3-18}	2.67316	2.65922	2.65833	2.65804	2.65744
	Exact	2.72718	2.71209	2.71114	2.71082	2.71018
$\langle r_{i3}^2 \rangle$	Ψ_{C3-14}	9.88098	9.7846	9.77849	9.77646	9.77238
	Ψ_{C3-18}	11.1969	11.0769	11.0693	11.0668	11.0617
	Exact	12.0742	11.9317	11.9227	11.9197	11.9137
$\langle r_{12} \rangle$	Ψ_{C3-14}	4.13923	4.12060	4.11942	4.11903	4.11824
	Ψ_{C3-18}	4.33763	4.31619	4.31483	4.31437	4.31346
	Exact	4.43928	4.41569	4.41419	4.41369	4.41269
$\left\langle \frac{1}{r_{12}} \right\rangle$	Ψ_{C3-14}	0.32140	0.32292	0.32302	0.32305	0.32312
	Ψ_{C3-18}	0.31259	0.31417	0.31427	0.31430	0.31437
	Exact	0.30920	0.31081	0.31092	0.31095	0.31102

To allow for a direct comparison with these values, we have taken the same masses values which were taken from [12]

with $M = 14$ and 18 (the M coefficients are available from the authors upon request). They both can be represented by the general formula:

$$
\begin{aligned}
\Psi_{C3-M} = {} & N e^{-Z(\mu_{13} r_{13} + \mu_{23} r_{23})} \\
& \Big\{ \chi_{C3}(1, \mu_{12}, r_{12}) \Big[c_{000}^{111} + c_{200}^{111}(r_{13}^2 + r_{23}^2) + c_{220}^{111} r_{13}^2 r_{23}^2 + c_{300}^{111}(r_{13}^3 + r_{23}^3) \\
& + c_{002}^{111} r_{12}^2 + c_{320}^{111}(r_{13}^3 r_{23}^2 + r_{13}^2 r_{23}^3) + c_{202}^{111}(r_{13}^2 r_{12}^2 + r_{23}^2 r_{12}^2) \\
& + c_{302}^{111}(r_{13}^3 r_{12}^2 + r_{23}^3 r_{12}^2) + c_{402}^{111}(r_{13}^4 r_{12}^2 + r_{23}^4 r_{12}^2) + c_{222}^{111} r_{13}^2 r_{23}^2 r_{12}^2 \Big] \\
& + \chi_{C3}(2, \mu_{12}, r_{12}) \Big[c_{000}^{112} + c_{200}^{112}(r_{13}^2 + r_{23}^2) + c_{220}^{112} r_{13}^2 r_{23}^2 + c_{300}^{112}(r_{13}^3 + r_{23}^3) \\
& + c_{002}^{112} r_{12}^2 + c_{320}^{112}(r_{13}^3 r_{23}^2 + r_{13}^2 r_{23}^3) + c_{202}^{112}(r_{13}^2 r_{12}^2 + r_{23}^2 r_{12}^2) \\
& + c_{302}^{112}(r_{13}^3 r_{12}^2 + r_{23}^3 r_{12}^2) + c_{402}^{112}(r_{13}^4 r_{12}^2 + r_{23}^4 r_{12}^2) + c_{222}^{112} r_{13}^2 r_{23}^2 r_{12}^2 \Big] \Big\}
\end{aligned}
\tag{2}
$$

where the coefficients $c_{320}^{11n_3}$, $c_{302}^{11n_3}$ and $c_{402}^{11n_3}$ are set to zero for $M = 14$, while $c_{222}^{11n_3} = 0$ for $M = 18$. Note also that when the two light particles are identical (our case), the coefficients satisfy the following symmetry relation $c_{ijk}^{n_1 n_2 n_3} = c_{jik}^{n_1 n_2 n_3}$.

Tables 1 and 2 give the calculated mean values of the ground state energy and several radial quantities for weakly bound systems with $z_3 = 1$: negatively charged hydrogen-like ions (Table 1), the negative positronium ion Ps^- and the exotic systems $e^- e^- (nm_e)^+$ with $n > 1$ (Table 2). The positronium is the first of a list of systems of the form $e^- e^- (nm_e)^+$ where $(nm_e)^+$ refers to exotic particles whose masses are n times the mass of the electron, but with the charge of the positron (+).

Table 2 The mean energy for the ground state of exotic systems $e^-e^-(nm_e)^+$, obtained using the Ψ_{C3-14} and Ψ_{C3-18} approximated wavefunctions, are compared with the numerically "exact" values of [2]

n	$-E_{C3-14}$	$-E_{C3-18}$	$-E_{Frolov}$
1	0.260484	0.261393	0.262005
2	0.346577	0.347743	0.348372
3	0.390335	0.391537	0.392141
5	0.434773	0.43594	0.436497
6	0.447618	0.448763	0.449303
8	0.464862	0.465968	0.466483
10	0.47591	0.476987	0.477484
20	0.499796	0.500797	0.501254
40	0.512741	0.513696	0.514309
50	0.515418	0.516363	0.516793
70	0.518515	0.519449	0.519872
90	0.520253	0.52118	0.521601
100	0.520864	0.521789	0.522209
200	0.523635	0.524549	0.524964
1000	0.525875	0.52678	0.527191
∞	0.526438	0.527341	0.527751

In view of the moderate number of terms, all results can be considered as good. It should be mentioned that, at the cost of an increasing number M of coefficients, systematic improvement can be easily achieved by including (i) more configurations (n_1, n_2, n_3) and (ii) more terms (i, j, k) in the polynomial expansion. The limited number of terms can be useful to the collisional community; as far as we know, except for the infinite nuclear mass systems, for all other three-body systems investigated here, no wavefunctions as accurate and simple as those presented here, have been explicitly given in the literature.

For the exotic systems $e^-e^-(nm_e)^+$ we have followed the method proposed by Frolov [3] to obtain semi-analytical expressions for the energies and mean radial quantities as functions of the heaviest particle's mass, m_3. As an example, we have found the following expression:

$$\left\langle E\left({}^{m_3}H^-\right)\right\rangle = \left\langle E\left({}^{\infty}H^-\right)\right\rangle + \frac{0.561565}{m_3} - \frac{0.652826}{m_3^2} + \frac{0.81148}{m_3^3} - \frac{0.951078}{m_3^4} + \frac{0.785261}{m_3^5} - \frac{0.288451}{m_3^6} \tag{3}$$

relating analytically the finite to infinite mass systems of H^-.

4 Summary

We have used the C3-like basis set introduced in [1] in combination with the method proposed in [8, 9], to construct accurate Angular Correlated Configuration Interaction trial wavefunctions, with a moderate number of linear coefficients and satisfying all two-body Kato cusp conditions. The efficiency of the method has been illustrated by considering the ground state of several three-body systems with two electrons and a heavier particle with positive charge $z_3 = 1$ and variable mass m_3. Good agreement for the energy and other mean physical values is found for all cases.

The successful application of the method to other systems with larger values of z_3, and with either equal or unequal light particles, will be presented elsewhere. Moreover, the extension to excited states is part of our current investigations.

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