PAPER

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Phys. Scr. **85** (2012) 065305 (3pp) doi:10.1088/0031-8949/85/06/065305

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S Bhattacharyya[1], J K Saha[2], P K Mukherjee[3,4] and T K Mukherjee[2]

[1] Acharya Prafulla Chandra College, New Barrackpore, Kolkata 700 131, India
[2] Narula Institute of Technology, Agarpara, Kolkata 700 109, India
[3] Department of Mathematics, Visva Bharati, Santiniketan, West Bengal, 731 235, India
[4] Ramakrishna Mission Vivekananda University, Belur Math, West Bengal, 711 202, India

E-mail: sukhamoy.b@gmail.com

Received 22 December 2011
Accepted for publication 15 May 2012
Published 7 June 2012
Online at stacks.iop.org/PhysScr/85/065305

Abstract
The ground state energy eigenvalues of the symmetric three-body exotic negative ions $p^+\pi^-\pi^-$ and $p^+K^-K^-$ have been determined variationally for the first time using an explicitly correlated Hylleraas basis set. Ground state energies of Ps^- and $p^+\mu^-\mu^-$ were also determined to check the accuracy of the present methodology by comparing those results to a few accurate earlier results for these systems.

PACS numbers: 31.15ac, 31.15ve, 36.10Dr, 36.10Gv

1. Introduction

The quantum mechanical description of Coulombic three-body exotic systems has drawn considerable attention in recent years as the x-rays emitted from such systems provide useful information about nuclear structure ([1] and references therein) and the muon-catalyzed fusion process [1–3] in stellar bodies. These exotic complexes may be formed in experiments during the passage of hadrons through matter or dense plasma, although they have low lifetimes [3–5]. The estimation of the ground state energy eigenvalue of three-body exotic systems was started long ago by Hylleraas [6], Cohen *et al* [7] and Kolos *et al* [8], and afterwards, many workers have investigated the structure of such three-body exotic systems by using different theoretical methods [9–26] over the last few decades. In this study, we have focused on a number of exotic three-body negative ions under Coulomb interaction. These include $p^+X^-X^-$, where X^- is a π^- or a K^- (first calculations of such), as well as $X^- = \mu^-$, which is done to compare our results to previous results for this system. Additionally, we consider Ps^- for such comparison purposes. Specifically, we calculate the ground state energy for each of these four three-body systems.

Knowledge of the ground state energies and wave functions of these exotic, negative three-body systems is a necessary part of what is needed when calculating their formation rates as well as their photon emission rates and wavelengths. Such three-body systems are usually expected to be formed through collision and capture processes in highly excited states which may relax to the ground state emitting a cascade of photons. The $X^- + H$ collision exhibits some interesting features which are different from those of electron or proton impacts as the masses of the negative X^- ions under consideration (i.e. μ^-, π^- and K^-) are appreciably high. The adiabatic Born–Oppenheimer situation characterized by the Fermi–Teller radius $R_{FT} = 0.639$ au [27, 28] is important, which indicates that the electronically bound states become absent if the radial distance between H and (X^-) is less than R_{FT}. When the center-of-mass translational energy is less than the ionization threshold (13.6 eV), the electron emission takes place during capture of X^-, giving rise to the formation of the two-body system p^+X^- [28],

$$X^- + H(1s) \rightarrow p^+X^- + e^-. \quad (1)$$

This two-body system p^+X^- can further capture a negatively charged third particle (X^-) during its passage through matter by the collision process to form a three-body system. The stability of the three-body system may vary depending upon the mass of the particle (X^-). It is true that hadronic hydrogen atoms pX^- ($X^- = \pi^-$ and K^-) in the 1s state have a very short lifetime ($\sim 10^{-16}$ s for $p\pi^-$ and $\sim 10^{-18}$ s for pK^-) due to prompt nuclear absorption via the strong interaction. But the three-body ion $p^+X^-X^-$ is energetically more bound than the corresponding two-body subsystem p^+X^- although the lifetimes of these three-body systems are sufficiently small. Recent advances in optical technologies and laser sources make it possible to produce extreme ultraviolet light pulses as short as 80 attoseconds [29–32]. Thus, the direct exploration of the electronic dynamics in atoms, molecules and solids in

Table 1. Non-relativistic energy eigenvalues $-E$ (au) of three-body systems Ps^- and $p^+X^-X^-$ ($X = \mu, \pi$ and K). ρ_1, ρ_2 are the nonlinear parameters and N is the dimension of the triple exponent correlated wave function.

	$-E$ (au)			
	$e^+e^-e^-$	$p^+\mu^-\mu^-$	$p^+\pi^-\pi^-$	$p^+K^-K^-$
N	$\rho_1 = 0.5713$ $\rho_2 = 0.1982$	$\rho_1 = 92.538\,29$ $\rho_2 = 202.046\,99$	$\rho_1 = 235.462\,45$ $\rho_2 = 64.609\,45$	$\rho_1 = 780.504\,17$ $\rho_2 = 152.445\,83$
21	0.261 922 367 52	97.561 145 45	124.682 660 67	330.735 158 77
39	0.261 987 953 27	97.566 459 42	124.689 230 31	330.785 807 88
66	0.262 002 465 63	97.566 926 21	124.690 480 20	330.799 405 15
102	0.262 004 800 83	97.566 971 97	124.690 602 16	330.800 369 33
150	0.262 005 035 95	97.566 980 68	124.690 652 64	330.800 578 96
210	0.262 005 064 05	97.566 983 12	124.690 665 04	330.800 627 66
285	0.262 005 068 09	97.566 983 99	124.690 670 39	330.800 634 36
375	0.262 005 069 25	97.566 984 36	124.690 672 56	330.800 635 84
483	0.262 005 069 74	97.566 984 52	124.690 673 58	330.800 636 47
609	0.262 005 069 97	97.566 984 59	124.690 674 07	330.800 636 77
	0.262 005 070 23[a]	97.374 760 7[c]		
	0.262 005 068[b]	97.566 983 4[d]		
affinity	0.012 005	4.646 575	5.808 481	14.285 793

[a] Drake *et al* [14].
[b] Saha *et al* [15].
[c] Ancarani *et al* [21].
[d] Frolov*et al* [22].

this time domain is gradually coming within reach. Therefore the experimental measurement of the structural properties of such three-body systems having very small lifetimes may be possible in future.

2. Methodology

Here we designate the proton as particle 3 and the two X^- as particles 1 and 2. The translational invariance of the Hamiltonian of the three-body system makes it possible to describe the motion of the system with respect to their center of mass in six co-ordinates. Among these six co-ordinates, r_1, r_2 and r_{12} are the sides of the triangle formed by the particles with the proton position being where r_1 and r_2 intersect, particle 1 at the other end of r_1 and particle 2 at the other end of r_2. The remaining three coordinates are the Eulerian angles defining the orientation of the triangle in space. For the spherically symmetric ground state, the three-body general variational equation [33] for arbitrary angular momentum reduces to

$$\delta \int \left[\frac{1}{2}\left(\frac{1}{m_1}+\frac{1}{m_3}\right)\left(\frac{\partial\Psi}{\partial r_1}\right)^2 + \frac{1}{2}\left(\frac{1}{m_2}+\frac{1}{m_3}\right)\left(\frac{\partial\Psi}{\partial r_2}\right)^2 + \frac{1}{2}\left(\frac{1}{m_1}+\frac{1}{m_2}\right)\left(\frac{\partial\Psi}{\partial r_{12}}\right)^2 + \frac{1}{m_1}\frac{r_1^2-r_2^2+r_{12}^2}{2r_1r_{12}}\left(\frac{\partial\Psi}{\partial r_1}\right)\left(\frac{\partial\Psi}{\partial r_{12}}\right) + \frac{1}{m_2}\frac{r_2^2-r_1^2+r_{12}^2}{2r_2r_{12}}\left(\frac{\partial\Psi}{\partial r_2}\right)\left(\frac{\partial\Psi}{\partial r_{12}}\right) + \frac{1}{m_3}\frac{r_1^2+r_2^2-r_{12}^2}{2r_1r_2}\left(\frac{\partial\Psi}{\partial r_1}\right)\left(\frac{\partial\Psi}{\partial r_2}\right) + (V-E)\Psi^2 \right] \mathrm{d}v_{r_1,r_2,r_{12}} = 0, \quad (2)$$

where the masses are $m_1 = m_2 = m_X = \{m_\mu, m_\pi, m_K\}$ depending on the system under study with $m_\mu = 206.768\,262 * m_e$, $m_\pi = 273.132\,426 * m_e$, $m_K = 966.101\,6949 * m_e$ and $m_3 = m_p = 1836.152\,6675 * m_e$, where m_e is the mass of an electron. It should be mentioned here that m_e is taken to be 1 as we have considered atomic units throughout. The three-body potential V is expressed as

$$V = -\frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}}. \quad (3)$$

We have considered the correlated wave function in triple exponent Hylleraas-type basis as

$$\Psi(r_1, r_2, r_{12}) = \sum_{l\geqslant 0}\sum_{m\geqslant 0}\sum_{n\geqslant 0}[C^{(1)}_{lmn}\left(r_1^l r_2^m + r_1^l r_2^m\right) r_{12}^n \eta_1(1)\eta_1(2) + C^{(2)}_{lmn}\{r_1^l r_2^m \eta_1(1)\eta_2(2) + r_1^m r_2^l \eta_1(2)\eta_2(1)\} r_{12}^n + C^{(3)}_{lmn}\left(r_1^l r_2^m + r_1^m r_2^l\right) r_{12}^n \eta_2(1)\eta_2(2)]. \quad (4)$$

Here $\eta_i(j) = e^{-\rho_i r_j}$ and ρ are the nonlinear parameters. The different ρ in the Slater-type orbitals incorporate the effect of radial correlation in the wave function, whereas the angular correlation effect is taken care of through different powers of r_{12}. In a multi-exponent basis set, if there are p number of nonlinear parameters, the number of terms in the radially correlated basis is $\frac{p(p+1)}{2}$ and therefore the dimension of the full basis (N) including angular correlation will be $[\frac{p(p+1)}{2} \times q]$, where q is the number of terms involving r_{12}. For example, as we have used two nonlinear parameters, the number of terms in the radially correlated basis is 3 and with seven terms involving different powers of r_{12}, the dimension of the full basis (N) becomes 21. The linear variational parameters $C^{(1)}$, $C^{(2)}$, $C^{(3)}$ used in equation (4) along with energy eigenvalue E are determined by solving the

generalized eigenvalue equation [34]

$$\underline{\underline{H}}\,\underline{C} = E\,\underline{\underline{S}}\,\underline{C}, \tag{5}$$

where $\underline{\underline{H}}$ is the Hamiltonian matrix, $\underline{\underline{S}}$ is the overlap matrix, $\underline{C}$ is the column matrix consisting of linear variational parameters and E is the energy eigenvalue. The nonlinear parameters (ρ) are determined by the optimization procedure using the Nelder–Mead algorithm [35]. All computations are carried out in quadruple precision to ensure better numerical stability for extended multiple exponent Hylleraas basis sets.

3. Results and discussion

To check the consistency of the present methodology we have calculated the ground state energy of the positronium ion (Ps^-) for which accurate theoretical estimates are available [6, 7, 16–20]. The Ps^- ion can be visualized keeping the positron at the origin with two electrons being the other two identical particles and is subject to the same potential expressed in equation (3). The computational data obtained from our calculation are displayed in table 1. The total number of terms (N) in the correlated wave function is given in the first column of table 1. In the second column, we have listed the energy eigenvalues of the ground state of the Ps^- ion with the increasing number of terms (N) in the wave function along with a few other theoretical results [14, 15]. A good convergence for the ground state energy eigenvalues of the Ps^- ion is achieved and our results agree fairly well with other results, as is evident from table 1. It is important to note that better results for the ground state energy of Ps^- ion may be produced from the present method by increasing the number of nonlinear parameters in the correlated wave function. But the aim of this paper is not to produce the best variational upper bound of ground state energy of Ps^-. Instead, we are interested in estimating the ground state energies of other three-body systems $p^+\mu^-\mu^-$, $p^+\pi^-\pi^-$ and $p^+K^-K^-$ whose respective two-body subsystems exist. The ground state energy eigenvalues of the Ps^- ion obtained from the present variational method certainly assures us about the desired level of accuracy for the present purpose. The ground state energy eigenvalues of $p^+\mu^-\mu^-$, $p^+\pi^-\pi^-$ and $p^+K^-K^-$ ions are listed in subsequent columns in table 1. The corresponding optimized nonlinear parameters are also given in respective columns. To check the convergence of the energy values we have increased the number of terms (N) in the wave function up to 609 parameters ($l+m+n=11$) in a systematic manner. It is evident from table 1 that the energy eigenvalues converge at least up to the fifth decimal place for all the systems under investigation. A few theoretical results for the ground state energy of $p^+\mu^-\mu^-$ exist, some of which are listed [21, 22] in the table for a comparison with the present results. Our result for the ground state energy of $p^+\mu^-\mu^-$ is the lowest as yet obtained, as is evident from table 1.

The ground state energy eigenvalues of the hydrogen-like two-body subsystems $p^+\mu^-$, $p^+\pi^-$ and p^+K^- are −92.920 409, −118.882 193 and −316.514 844 au, respectively. At the end of table 1, we have given the exotic affinities (electron affinity in the case of Ps^-) defined as the difference between the ground state energy eigenvalues of two-body and three-body systems. From the numbers obtained as exotic affinity it appears that it increases almost linearly with an increase in the reduced mass of the two-body subsystem. It will be highly interesting to observe the behavioral change in exotic affinities of such systems under an external environment such as plasma. Our findings may serve as a benchmark reference for future investigations in related disciplines.

Acknowledgments

The authors are grateful for support from the Department of Atomic Energy, Government of India under grant no. 2011/37P/15/BRNS/0074. PKM acknowledges support from the Department of Science and Technology, Government of India under grant no. SR/S2/LOP- 22/2008.

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