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Resonance States of Hadronic Three-Body Ions: Stabilization Method

Research Article

S. Dutta[1], J. K. Saha[*2], S. Bhattacharyya[3] and T. K. Mukherjee[4]

[1] *Belgharia Texmaco Estate School, Belgharia, Kolkata 700056, India*
[2] *Department of Physics, Aliah University, IIA/27, Newtown, Kolkata 700156, India*
[3] *Department of Physics, Acharya Prafulla Chandra College, New Barrackpore, Kolkata 700131, India*
[4] *Department of Physics, Narula Institute of Technology, Agarpara, Kolkata 700109, India*
[*] **Corresponding author:** jsaha84@gmail.com

Abstract. Bound and resonance states of symmetric three-body exotic pXX negative atomic ions ($X = \mu^-, \pi^-, K^-$) as well as exotic ppX positive molecular ions for total angular momentum $J = 0$, are studied in details under the framework of Stabilization method. The resonance states under consideration lie below $N = 2$ ionization threshold of the corresponding pX atom. The wave-function is expanded in correlated multi-exponent Hylleraas type basis set for explicit incorporation of p-p, μ-μ, π-π or K-K correlations. The methodology has been tested by estimating the parameters of the resonance states of $(p\mu\mu)^-$, $(pp\mu)^+$, $(p\pi\pi)^-$ and $(pp\pi)^+$ and comparing with the results existing in the literature. The interparticle interactions for all the systems under consideration are purely Coulombic.

Keywords. Three-body systems; Stabilization method; Hylleraas coordinate; Resonance state; Correlation

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1. Introduction

The non-separability of the dynamical equation of motion of three body systems in both classical and quantum mechanics, draws a considerable attention by the researchers around the globe [9, 35]. From the very beginning of quantum mechanics various approximation methods had been used to study the structural properties of such systems. Being a quintessential quantum mechanical three body system, the non-relativistic upper bound energy eigenvalue of helium atom was estimated by Hylleraas [17] in the year 1929, using variational approach.

In this work [17] Hylleraas used a new coordinate system to expand the wavefunction in terms of inter-particle (electron-nucleus and electron-electron) distances. After this pioneering work of Hylleraas [17], different variants of this correlated variational framework has been evolved [12,13,16,17,20,21,27,29,32,33] which adequately account for the effect of inter-particle correlation in the basis set.

Quantum mechanical three body system with arbitrary comparable masses bounded via Coulomb interaction also drags considerable attention in recent years. In general, there are two class of energy levels for these systems: the bound states lying below the first ionization threshold ($N = 1$) and the resonant states embedded in the continuum. Thus the bound states are stable against autoionization, while the resonant states decays to an neutral atomic configuration by ejecting particle due to the autoionizing process and thus posses a finite lifetime. It has been observed that when massive negatively charged particles, such as antiprotons ($\bar{p}$), kaons (K), pions (π), and muons (μ), enters into matter, they slow down as they excite and ionize the atoms or molecules of the matter and at the end the particles being captured by the positive ions present in the medium, form the bound or resonance states of exotic atoms [2, 11, 30, 36]. Thus during the decay of these three-body ions, X-rays are emmited during bound-bound transition or one of the particle is ejected from it via Augey process [30]. Such investigations are going into full swing in case of muonic-, pionic- and kaonic-hydrogen atoms [1, 3, 15, 25, 26, 31].

Although the structural properties of bound states of these systems have extensively been studied by adopting various quantum chemical methods [5, 7, 8, 10, 14, 18, 22, 24], but the same for the resonance states are rather considerably less in number [18, 19]. In the present work, we have made an attempt to estimate the energy eigenvalues of ground states and the parameters (position and width) of first three resonant states of ppX positive molecular ions and first two resonant states of pXX negative atomic ions ($X = \mu^-, \pi^-, K^-$), below the $2s$ threshold of pX atom. For this purpose, we have expanded the basis set in the explicitly correlated multi-exponent Hylleraas type basis set and carried out calculations under the framework of Stabilization method [28, 34]. In order to check the consistency of the present methodology, we have compared the resonance parameters (position and width) with few existing theoretical data [18, 19].

2. Method

Here we use the designation of two identical particles (pp or XX) as particle 3 and the non-identical one (p or X) as particle 3. Due to translation symmetry of the Hamiltonian of three-body system, it is possible to describe the motion of the system with respect to their center of mass in six co-ordinates. If the distances of the particles 1 and 2 with respect to the 3rd particle are r_1 and r_2 and the distance between particles 1 and 2 is r_{12}, then r_1, r_2 and r_{12} form the sides of a triangle. Besides these three coordinates (r_1, r_2 and r_{12}), the remaining three coordinates are the Eulerian angles [4] defining the orientation of the triangle in space. For the spherically symmetric ground state ($^1S^e$), the three-body general variational equation [23] reduces to

$$\delta \int \left[\frac{1}{2} \left(\frac{1}{m} + \frac{1}{M} \right) \left\{ \left(\frac{\partial \Psi}{\partial r_1} \right)^2 + \left(\frac{\partial \Psi}{\partial r_2} \right)^2 \right\} + \frac{1}{m} \left(\frac{\partial \Psi}{\partial r_{12}} \right)^2 + \frac{1}{M} \cos(r_1, r_2) \frac{\partial \Psi}{\partial r_1} \cdot \frac{\partial \Psi}{\partial r_2} \right.$$

$$+\frac{1}{m}\left\{\cos(r_2,r_{12})\frac{\partial\Psi}{\partial r_2}\cdot\frac{\partial\Psi}{\partial r_{12}}+\cos(r_1,r_{12})\frac{\partial\Psi}{\partial r_1}\cdot\frac{\partial\Psi}{\partial r_{12}}\right\}+(V-E)\Psi^2\Bigg]d\tau=0 \tag{2.1}$$

where the volume element is $d\tau = r_1 r_2 r_{12} dr_1 dr_2 dr_{12}$ and the potential is given by

$$V=-\frac{1}{r_1}-\frac{1}{r_2}+\frac{1}{r_{12}} \tag{2.2}$$

and we have defined

$$\cos(r_i,r_j)=\frac{r_i^2+r_j^2-r_k^2}{2\,r_i\,r_j} \tag{2.3}$$

where, the indices $(i,j,k)\equiv(1,2,12)$ and the m and M are the masses of the identical and non-identical particles respectively. The masses (in a.u.) of p and X ($X=\mu^-,\pi^-,K^-$) particles are taken as $m_p = 1836.152\ 6675$, $m_\mu = 206.768\ 262$, $m_\pi = 273.132\ 426$ and $m_K = 966.101\ 6949$ respectively. The trial radial wave function $\Psi(r_1,r_2,r_{12})$ can be written as,

$$\Psi(r_1,r_2,r_{12})=\sum_{k=1}^{s} r_1^{l_k}\, r_2^{m_k}\, r_{12}^{n_k}\left[\sum_{i=1}^{p} C_{kii}\eta_i(1)\eta_i(2)+\sum_{i=1}^{p}\sum_{j=1}^{p} C_{kij}\eta_i(1)\eta_j(2)\right]. \tag{2.4}$$

In the second sum $i<j$ and $\eta_i(m)=e^{-\rho_i r_m}$, ρ being the non-linear parameter. p denotes the number of non-linear parameters which are taken in a geometrical sequence following $\rho_i=\rho_{i-1}\gamma$; γ being the geometrical sequence. The function $g(1,2)$ containing correlation terms, is expanded into Hylleraas basis set as follows, the effect of the radial correlation is incorporated through different ρ's in the wave function whereas, the angular correlation effect is taken care of through different powers of r_{12}. The dimension of the full multi-exponent basis (N) is $\left[\frac{p(p+1)}{2}\times s\right]$, where s is the number of terms involving r_{12} and p is the number of exponents. For a fixed number of basis, p and s should be chosen in such a manner that the effect of radial as well as angular correlation is properly incorporated in the wavefunction.

After choosing the proper trial radial wave function, the energy eigenvalues are obtained by solving the generalized eigenvalue equation involving the Hamiltonian and overlap matrices given by

$$\underline{\underline{H}}\;\underline{C}=E\underline{\underline{S}}\;\underline{C}, \tag{2.5}$$

where $\underline{\underline{H}}$ and $\underline{\underline{S}}$ are Hamiltonian and overlap matrices respectively. The necessary basis integrals of the form

$$A(m,n,l;a_1,a_2)=\int_{r_1=0}^{\infty}\int_{r_2=0}^{\infty}\int_{|r_1-r_2|}^{r_1+r_2} r_1^m r_2^n r_{12}^l e^{-a_1 r_1-a_2 r_2}dr_1 dr_2 dr_{12} \tag{2.6}$$

with the condition, $m\geq 0$, $n\geq 0$, $l\geq 0$ and $a_1,a_2>0$. This integral has been evaluated following Calais and Lowdin [6]. All calculations are carried out in quadruple precision in order to have a better numerical accuracy. Repeated diagonalization of the Hamiltonian matrix in the Hylleraas basis set of 675 parameters is done in the present work for 200 different values of γ. The plot of each energy eigenroot versus γ produces the stabilization diagram. The density of resonance states is then calculated from the stabilization diagram and by fitting with a Lorentzian profile we have estimated the parameters of a particular resonance state.

3. Results and Discussions

A portion of the stabilization diagram for $^1S^e$ states originating from two negatively charged kions (K) of exotic pKK ion is given in Figure 1. In this diagram we have plotted first 40

eigenroots of $^1S^e$ symmetry of exotic pKK ion for 200 different values of γ ranging from 0.63058 a.u. to 0.74954 a.u. From Figure 1, one can see that there exist two classes of states:

(1) There exists only one energy level below $N = 1$ ionization threshold of pK at -316.515 a.u., formed due to ground state $(1s^2)$ configuration remains invariant with the variation in γ. The energy eigenvalue of this level is -330.800637 which is consistent with the value obtained by Dutta et al. [10] using 990 terms in the multi-exponant Hylleraas type basis set.

(2) Roots lying above $N = 1$ but below $N = 2$ ionization threshold of pK at -79.129 a.u. are sensitive with the variation in γ and give rise to flat plateau in the vicinity of avoided crossings of the energy eigenroots for some particular energy value which is a clear signature of resonance states.

Similar classes of states are also observed for the other exotic systems like $p\mu\mu$, $pp\mu$, $p\pi\pi$, $pp\pi$ and ppK. The ground state energies of atomic $(pXX)^-$ ion and molecular $(ppX)^+$ ion $[X = \mu, \pi, K]$ are given in Table 1 and the present results are compared with the lowest energy eigenvalues available in literature [5, 10, 18].

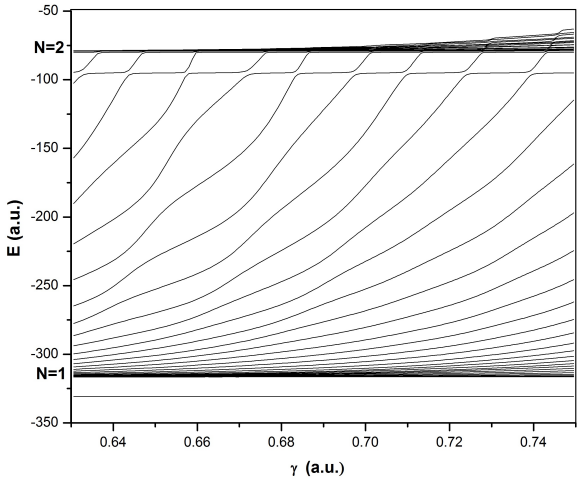

Figure 1. Stabilization diagram for $^1S^e$ states of exotic pKK ion

Table 1. Bound states energies ($-E$ in a.u.) of atomic $(pXX)^-$ ion and molecular $(ppX)^+$ ion below pX $(1s)$ threshold $E_{pX} = -\frac{\lambda}{2}$ a.u.; λ being the reduced mass of the exotic pX atom

$E_{p\mu} = -92.920\ 408$		$E_{p\pi} = -118.882\ 182$		$E_{pK} = -316.514\ 843$	
$p\mu\mu$	$pp\mu$	$p\pi\pi$	$pp\pi$	pKK	ppK
97.566 983	102.223 503	124.690 678	129.718 076	330.798 993	334.575 390
97.566 984 59[a]	102.223 503 6[b]	124.690 674[c]	129.718 073[c]	330.800 637[c]	334.575 377[c]

[a] [5]; [b] [18]; [c] [10]

Enlarged view of the stabilization diagram (Figure 1) for $^1S^e$ state of exotic pKK ion in the energy range -100 a.u. to -78.5 a.u. is given in Figure 2. From a closer look at Figure 2, one can see that for a short range of γ each eigenroot becomes almost flat in the vicinity of avoided crossings in the neighborhood of a particular resonance state. The density of states $\rho_n(E)$ is

calculated by evaluating the inverse of the slope at a number of points near the flat plateau of each energy eigenroot using the formula [28, 34] given by:

$$\rho_n(E) = \left| \frac{\gamma_{i+1} - \gamma_{i-1}}{E_n(\gamma_{i+1}) - E_n(\gamma_{i-1})} \right|_{E_n(\gamma_i)=E_i} . \tag{3.1}$$

The calculated density of resonance states $\rho_n(E)$ is then fitted to the following Lorentzian form [28, 34],

$$\rho_n(E) = y_0 + \frac{A}{\pi} \frac{\Gamma_r/2}{(E-E_r)^2 + (\Gamma_r/2)^2} , \tag{3.2}$$

where y_0 is the baseline background, A is the total area under the curve from the baseline, E_r gives the position of the centre of the peak of the curve and Γ_r represents the full width of the peak of the curve at half height. Among different fitting curves for each eigenroot corresponding to a particular resonance state, the fitting curve with least χ^2 and the square of correlation closer to unity leads to the desired resonance energy (E_r) and width (Γ) as mentioned in ref. [28]. For example, from the stabilization plot of Figure 2 for the first $^1S^e$ resonance state below $N = 2$ ionization threshold of pK, we have calculated the inverse of the slope by using (3.1) at different points near the flat plateau of 24th eigenvalues in the interval of $\gamma = 0.724 - 0.738$.

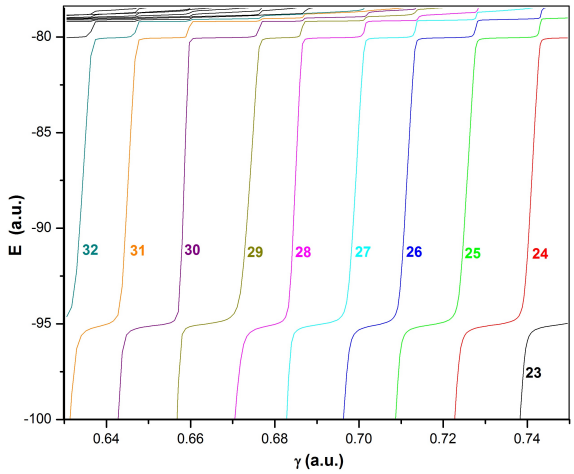

Figure 2. Enlarged view of the Stabilization diagram for $^1S^e$ states of exotic pKK ion below $N = 2$ ionization threshold of pK

The corresponding fitted curve is obtained by using (3.2) and is shown in Figure 3. The circles in Figure 3 are the calculated values of $\rho_n(E)$ while the solid line (red) corresponds to the fitted curve. Repeated calculations of $\rho_n(E)$ near the flat plateau of each of the eigenroot for first $^1S^e$ resonance state resulted Lorentzian fitted curve similar to that of Figure 3. Among all this fitting curve, we have found that 24th eigenroot corresponds to the best fit and from which $-E_r = 95.06738$(a.u.) and $\Gamma_r = 0.31004$(a.u.) are obtained. Similarly, the best fits for the second and third $^1S^e$ resonance states are shown in Figure 4 and 5, respectively.

Table 2 shows all the resonance energies (E_r in a.u.) and widths (Γ_r in a.u.) of $^1S^e$ states of exotic atomic $(pXX)^-$ ions and molecular $(ppX)^+$ ions [$X = \mu, \pi, K$] below $N = 2$ ionization threshold of pX atom. The results are being compared with those available in literature [18, 19] for $(pXX)^-$ and $(ppX)^+$ [$X = \mu, \pi$] ions. The comparison shows that resonance energies and widths are in very good agreement with the available results [18, 19]. To the best of our

knowledge the present calculated resonance energies and widths of $(pKK)^-$ and $(ppK)^+$ ions are given for the first time in the literature. Table 2 shows that the widths of the negative ions (pXX) are higher than the corresponding three body positive counterpart (ppX), which indicates that the resonance states of the molecular $(ppX)^+$ ions are more long lived than that of the atomic $(pXX)^-$ ions.

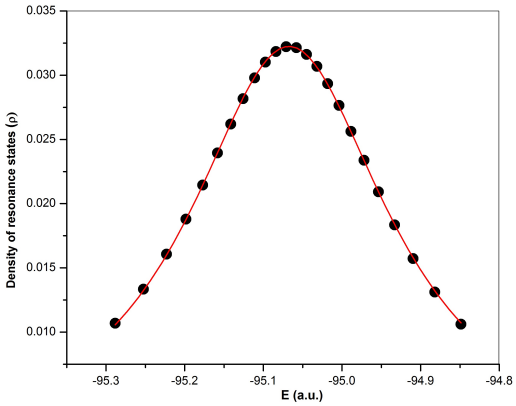

Figure 3. Calculated density (circles) and the fitted Lorentzian (solid line in red) for the ${}^1S^e$ resonance state [$-E_r = 95.06738$(a.u.) and $\Gamma_r = 0.31004$(a.u.)] of exotic pKK ion

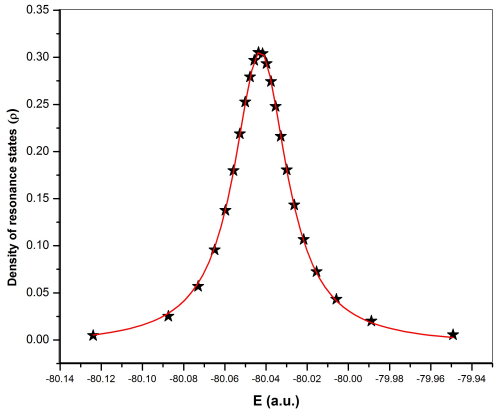

Figure 4. Calculated density (stars) and the fitted Lorentzian (solid line in red) for the ${}^1S^e$ resonance state [$-E_r = 80.0428$(a.u.) and $\Gamma_r = 0.03131$(a.u.)] of exotic pKK ion

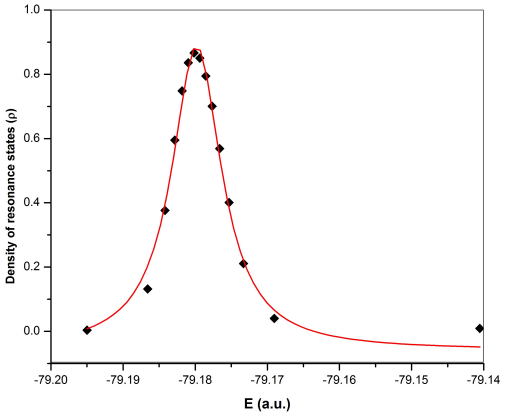

Figure 5. Calculated density (diamonds) and the fitted Lorentzian (solid line in red) for the ${}^1S^e$ resonance state [$-E_r = 79.1798$(a.u.) and $\Gamma_r = 0.0084$(a.u.)] of exotic pKK ion

Table 2. Resonance energies ($-E_r$ in a.u.) and widths (Γ_r in a.u.) of $L = 0$ states of atomic $(pXX)^-$ ion and corresponding ro-vibrational states of molecular $(ppX)^+$ ion below pX $(2s)$ threshold $E_{pX} = -\frac{\lambda}{8}$ a.u.; λ being the reduced mass of the exotic pX atom. Parameters are given for the best lorentzian fitting (*i.e.* for least χ^2) of the numerically estimated DOS of an energy eigen roots of the stabilization diagrams. The notation $P[\pm Q]$ stands for $P \times 10^{\pm Q}$

		$E_{p\mu} = -23.230\ 102$		$E_{p\pi} = -29.720\ 545$		$E_{pK} = -79.128\ 711$	
States	Parameters	$p\mu\mu$	$pp\mu$	$p\pi\pi$	$pp\pi$	pKK	ppK
1	$-E_r$	27.651 07	30.271 80	35.414 51	38.399 77	95.067 38	98.051 24
			30.271 841 23[a]		38.399 777 312 3[b]		
	Γ	27.608[-2]	5.963[-5]	30.258[-2]	9.220[-5]	31.004[-2]	8.68[-3]
			6.353[-5][a]		5.443[-5][b]		
2	$-E_r$	23.420 34	26.649 33	29.965 33	33.400 63	80.042 80	82.079 05
			26.649 428 350[a]		33.400 857 338[b]		
	Γ	1.902[-2]	1.030[-4]	2.788[-2]	3.274[-4]	3.131[-2]	4.35[-3]
			1.108[-4][a]		7.068[-5][b]		
3	$-E_r$		24.403 99		30.698 68	79.179 80	79.472 55
			24.404 608 394[a]		30.698 940 424 1[b]		
	Γ		2.065[-4]		2.153[-4]	8.40[-3]	6.486[-4]
			8.146[-5][a]		3.509[-5][b]		

[a] [18]
[b] [19]

4. Conclusion

In the present work we have adopted extended Hylleraas type basis set to estimate the ground state energy eigenvalues of exotic atomic $(pXX)^-$ ions and molecular $(ppX)^+$ ions $[X = \mu, \pi, K]$ below $N = 1$ ionization threshold of pX atom. Stabilization method is used to calculate the resonance energies and widths of the above mentioned exotic systems below $N = 2$ ionization threshold of pX atom. The present results consistent with those available in literature. The advantage of the present method lies in the fact that a single methodology enables us to predict reasonably accurate bound state energies and resonance parameters with much lesser number of terms in the basis set expansion thus minimizing the computational time. The resonance parameters for ppK and pKK ions are given for the first time in the literature. We hope the present results will be useful for the future references.

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Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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