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Resonances in positron scattering from Na and K

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Abstract. S-wave resonances in the positron-sodium and positron-potassium systems are calculated using the stabilization method. For the target atom, the interaction between the core and the outer electron is taken care by a model potential. Hylleraas-type wave functions are used to represent the correlation effects between the outer electron, the positron and the core. Resonance energies and widths for the resonances lying below the Ps($n = 2$) threshold are reported.

PACS. 34.85.+x Positron scattering – 03.65.Nk Scattering theory – 33.40.+f Multiple resonances (including double and higher-order resonance processes, such as double nuclear magnetic resonance, electron double resonance, and microwave optical double resonance)

1 Introduction

The study of resonance phenomena in positron-atom collisions is of fundamental interest. During the past several years, a good number of theoretical studies have been performed to search atomic resonances in positron-atom scattering ([1–11], and references therein), among which the positron-alkali atom scattering ([2,9], and references therein) has attracted considerable interest in view of the fact that positronium (Ps) formation is possible even for nearly zero-energy positrons. The alkali atom target can be treated as the system containing one active electron located outside a core of tightly bound electrons. However, positron-hydrogen scattering differs greatly from the positron-alkali scattering in many respects. The hydrogen target has degeneracy in its spectrum whereas alkali targets do not have such property. The pioneering theoretical investigations on resonance phenomena in positron-alkali systems were performed by the group at the York University [2] using close coupling approximation (CCA) in which the model potential has been used to represent the inert core of the alkali atom. In these calculations they used both the Hartree-Fock and model potential wave function to represent the motion of the active valence electron of the alkali atom. They have obtained the resonance energy E_r and the resonance width Γ by fitting the energy-dependent eigenphase sums to the well-known Briet-Wigner formula. Roy and Ho [9] has investigated S-wave and P-wave resonances in positron-lithium scattering using stabilization method and they have obtained resonances below the Ps($n = 2$) and Ps($n = 3$) thresholds. Reported resonance energies of Roy and Ho [9] below the Ps($n = 2$) threshold are in reasonable agreement with those of Ward et al. [2a] and McAlinden et al. [11]. In the course of their study in the couple-state calculations of positron scattering by lithium in the energy range 0.5–60 eV, McAlinden et al. (1994) have reported the existence of two resonances, but no widths were reported.

In the present work, efforts have been made to search S-wave resonances in the scattering of positron from atomic sodium and potassium. During past 25 years, a good number of theoretical studies ([2,12–18], and references therein), and a series of experimental investigations [19–23] have been performed in the positron-sodium and positron-potassium systems. Experimental information on the total and Ps formation cross sections for the positron-sodium system are in good agreement with those of theoretical predications. However most of theoretical studies in the scattering of positron from sodium and potassium atoms are associated mainly with the CCA method [2,15–17]. It is worthy to mention in this context is that Ryzhikh et al. [24] have predicted the electronic stability of the ground state for positronic sodium. However, besides these extensive studies in positron-Na and positron-K scattering, there is limited information on the resonance phenomena for the positron-sodium and positron-potassium systems except for the pioneering investigations of Ward et al. [2a].

In the present work, in a manner very similar to the recent calculations of Kar and Ho [10], we have calculated the resonance energy E_r and the resonance width Γ in positron-sodium and positron-potassium systems. S-wave resonance parameters (E_r, Γ) have been extracted by using the *stabilization* method proposed by Mandelsthan et al. [25]. This method needs only the diagonalization of real matrix elements with different box sizes (L). Plots

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of the various energies $E_n(L)$ versus the varying box size L lead to obtain the stabilization diagram, which provides the information for the large region of energy spectrum, as well as presenting some flat plateaus in the vicinity of avoided crossings that correspond to the occurrence of resonances. The physical origin of the flat region reveals the localization of resonance scattering wave functions at the short range, and as such, its energy is stabilized. To extract resonance parameters (E_r, Γ) with the help of a fitting procedure, one needs to calculate the density of resonance states in the vicinity of an avoided crossing of two energy levels in the stabilization plateaus. Details successful applications to this simple and powerful computational method to extract resonance parameters (E_r, Γ) can be found in the works of Ho and co-workers [6–10,26].

For the sodium and potassium atoms, the loosely bound valance electron is involved in the transitions. Furthermore, for the energy region below the excited positronium formation thresholds, the e^+–Na and e^+–K systems can be modeled by a three-body system that consists of a frozen core, a positron and an electron. In our calculation, we have used an accurate model potential to represent the interaction between the core and the outermost active electron. Hylleraas-type basis functions have been used to incorporate the correlation effect between the outer electron, the positron and the core.

2 Theory

The Hamiltonian H for the core, the e^- and the e^+ (in Rydbergs) of the proposed systems is given by

$$H = -\nabla_1^2 - \nabla_2^2 + V^{(e^-)}(r_1) + V^{(e^+)}(r_2) + \frac{2}{r_{12}}, \tag{1}$$

where the subscripts 1 and 2 denote the coordinates of the outer electron and the positron, respectively; r_{12} is the relative distance between the electron and the positron. In equation (1), $V^{(e^-)}$ and $V^{(e^+)}$ are, respectively, the model potentials used to represent the interactions between the outer electron, and the positron with the core. An accurate model potential for the active electron and the core, in the explicit form, is given by

$$V^{(e^-)}(r) = -\frac{2}{r}\left[1 + (Z-1)\exp(-c_1 r) + c_2 r \exp(-c_3 r)\right], \tag{2}$$

where c_1, c_2 and c_3 are the variational parameters; $Z = 11$ for Na and $Z = 19$ for K. For e^+–Na scattering, we set $c_1 = 7.902$, $c_2 = 23.51$, and $c_3 = 2.688$ as suggested by Hanssen et al. [27] and Schweizer et al. [28]. For e^+–K scattering, we set $c_1 = 3.491$, $c_2 = 10.591$, and $c_3 = 1.730$ as suggested by Schweizer et al. [28]. Using the model potential given in equation (2), we have calculated the ground and excited states of the Na and K atoms by diagonalizing the Hamiltonian with Slater-type orbital (STOs):

$$\varphi_{nlm} = r^{n+l}\exp(-\lambda r)Y_{lm}(\theta,\phi), \quad n = l, l+1, ... \tag{3}$$

In equation (3), the parameters λ has units of a_0^{-1}, with a_0 being the Bohr radius. The ground and excited states energies are nicely comparable with the experimental results [29] for the sodium atom but these are quite reasonable in the case of potassium. The results are shown in Table 1 for sodium and potassium. Hanssen et al. [27] have used this model potential for Na during their model potential calculations of the Na–He systems. Hewitt et al. [16] have also used the similar type of model potential in course of their study of positron collisions with alkali atoms at the low and intermediate energies. We have not explicitly included any terms to represent the polarization of the core and the active electron.

Table 1. Comparison of calculated eigen-energies of the model potential for Na and K with experiment. All energies are in Rydbergs. Experimental energies are converted to Rydberg units.

Na		
states	present	experiment [29]
$3s$	−0.37772	−0.37772
$4s$	−0.14334	−0.14316
$3p$	−0.22304	−0.22318
$4p$	−0.10204	−0.10188
K		
states	present	experiment [29]
$4s$	−0.31653	−0.3190
$5s$	−0.12726	−0.12878
$4p$	−0.19870	−0.20062
$5p$	−0.09373	−0.09272

For the positron, the interaction $V^{(e^+)}$ is same as that for $V^{(e^-)}$, but with an opposite sign for the same c_1, c_2 and c_3, i.e.,

$$V^{(e^+)}(r) = -V^{(e^-)}(r), \tag{4}$$

where $V^{(e^-)}(r)$ is given by equation (2). The correlation effect between the electron, the positron and the core can be considered by employing the Hylleraas-type wave functions:

$$\Psi = \sum_{l+m+n \leq \omega} C_{lmn} r_{12}^l r_1^m r_2^n e^{-\alpha(r_1+r_2)}, \tag{5}$$

where ω, l, m and n are positive integers or zero and ω will determine the basis size N in the basis expansion of the equation (5) through the relation $N = (\omega+1)(\omega+2)(\omega+3)/6$. The coordinates r_1 and r_2 are for the positron and electron relative to the nucleus, and r_{12} is the relative distance between them. The scaling factor α in the wave functions (5), with units of a_0^{-1}, is related to the reciprocal range of a *soft* wall [6–10,26]. More details discussion is available in the very recent work of Kar and Ho [10]. The convergence of the results has been examined with increasing number of terms in the basis expansion (5).

Here we should mention that by using equation (4) for the positron interacting with the core, the exchange effect between the positron and the electron was included. With such an approximation, the $V^{(e^+)}$ used here is more ‘repulsive’ than the real physical situation. Therefore when we interpret our final results, we should keep in mind that our reported energies may lie somewhat higher than the true resonance energies. A more realistic potential for $V^{(e^+)}$ can be considered in future investigations. For example, a direct potential acting on the positron along could be obtained by using a Hartree-Fock wave function. Such an approach is worthwhile to try.

We should mention that in constructing the $3s$ state of the Na atom using the Slater orbital (Eq. (3)), we have also obtained the lower-lying $1s$ and $2s$ states. While we have not projected out such ‘artificial’ states (see [17,24] for example), it would not affect our resonance investigation, as resonances are located in scattering continua. In bound state investigations, it would be important to project out the lower lying ‘artificial’ states. For example, there has been some interest to investigate the binding of the e^+–Na (or Ps–Na$^+$) system [17,24,30]. In [24], the authors were able to project out the lower-lying artificial states, and obtained a bound state for the e^+–Na system. However, in our present work, projecting out the lower-lying “artificial” states using the Hylleraas basis is not straightforward. It is outside the scope of our present work to investigate the bound states for the e^+–Na and e^+–K systems.

3 Results and discussions

It has been discussed, so far, that we have used the stabilization method to extract resonance energies and widths by calculating the density of resonance states. Energy levels $E_n(\alpha)$ have been computed by diagonalization of the Hamiltonian (1) with Hylleraas-type basis functions (5). Figures 1a to 5a show the stabilization plots of energy eigenvalues with the scaling parameter α. The change of the scaling factor α leads to the identification of stabilized energy eigenvalues, and from which resonance energies and widths can be deduced.

3.1 Na results

We have computed the energy eigenvalues for 1501 different α values within the range 0.15 to 0.8 with a mesh size of 0.0005. We have performed calculations for $\omega = 15$, 16, 17 and 18 corresponding to 816, 969, 1140 and 1330 basis terms, respectively.

To extract the resonance energy E_r and the resonance width Γ, we have calculated the density of the resonance states for two energy levels at the avoided crossing with the help of the following formula,

$$\rho_n(E) = \left| \frac{E_n(\alpha_{i+1}) - E_n(\alpha_{i-1})}{\alpha_{i+1} - \alpha_{i-1}} \right|^{-1}_{E_n(\alpha_i)=E}, \qquad (6)$$

where the index i is the ith value of α. After calculating the density of resonance states $\rho_n(E)$ with the above formula (6), we fit it to the following Lorentzian form that yields the resonance energy E_r and the total width Γ, with

$$\rho_n(E) = y_0 + \frac{A}{\pi} \frac{\Gamma/2}{(E - E_r)^2 + (\Gamma/2)^2}, \qquad (7)$$

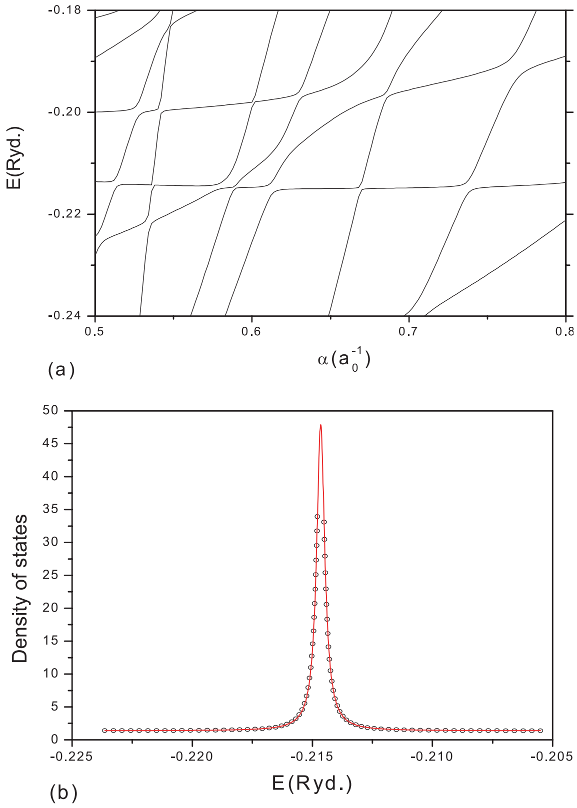

Fig. 1. (a) Stabilization plot for the S-wave e^+–Na system. (b) The fitting of the density of resonance states (circles) to the Lorentzian form of equation (7) for the S-wave e^+–Na system.

where y_0 is the baseline offset, A is the total area under the curve from the base line, E_r is the center of the peak and Γ denotes the full width of the peak of the curve at half height. Figures 1b to 5b show the nature of the density of resonance states $\rho_n(E)$ with varying eigenenergy E for the lowest resonance below the Ps($n = 2$) threshold. The circles are the results of the actual calculations of the density of resonance states using the formula (6) and the solid line is the fitted Lorentzian form of the corresponding $\rho_n(E)$. Here, for all the figures presented in this work, the results were obtained using 1330-term wave functions.

The stabilization diagrams in Figures 1a to 3a clearly show the stabilization character near the energy $E_r = -0.21$, $E_r = -0.15$ Ryd and $E_r = -0.13$ Ryd respectively, which are believed to be associated with and lying below the Ps($n = 2$) positronium formation threshold energy $E_t = -0.125$ Ryd.

Figure 1b shows the density of the resonance states $\rho_n(E)$ for the lowest resonance approaching the excited Ps($n = 2$) threshold. From the fit, we have obtained a resonance energy of $E_r = -0.21465$ Ryd (2.219 eV) and a resonance width $\Gamma = 0.00041$ Ryd (5.58 meV). Here and hereafter, the resonance energy E_r and the resonance width Γ expressed in eV is relative to the ground state Na($3s$) atom. Figures 2b and 3b show the density of the resonance states $\rho_n(E)$ for the second and third resonances, respectively, approaching the excited Ps($n = 2$) threshold. Figure 2b shows a resonance

Table 2. Convergence behavior for the resonance energy E_r and resonance width Γ (in Rydbergs) below the Ps($n = 2$) excitation threshold.

	$N = 816$ $\omega = 15$	$N = 969$ $\omega = 16$	$N = 1140$ $\omega = 17$	$N = 1330$ $\omega = 18$
S(1)	$E_r = -0.20924$ $\Gamma = 0.00022$	$E_r = -0.21117$ $\Gamma = 0.00029$	$E_r = -0.21318$ $\Gamma = 0.0043$	$E_r = -0.21465$ $\Gamma = 0.00041$
S(2)	$E_r = -0.15060$ $\Gamma = 0.00066$	$E_r = -0.15113$ $\Gamma = 0.00079$	$E_r = -0.15148$ $\Gamma = 0.00082$	$E_r = -0.15164$ $\Gamma = 0.00086$
S(3)	$E_r = -0.13087$ $\Gamma = 0.00010$	$E_r = -0.13114$ $\Gamma = 0.00052$	$E_r = -0.13161$ $\Gamma = 0.00045$	$E_r = -0.13182$ $\Gamma = 0.00062$

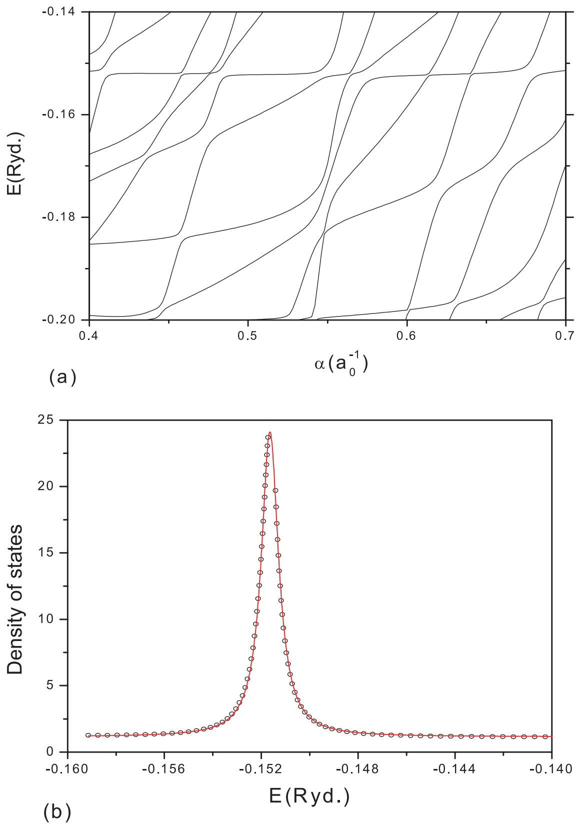

Fig. 2. (a) Stabilization plot for the S-wave e^+–Na system. (b) The fitting of the density of resonance states (circles) to the Lorentzian form of equation (7) for the S-wave e^+–Na system.

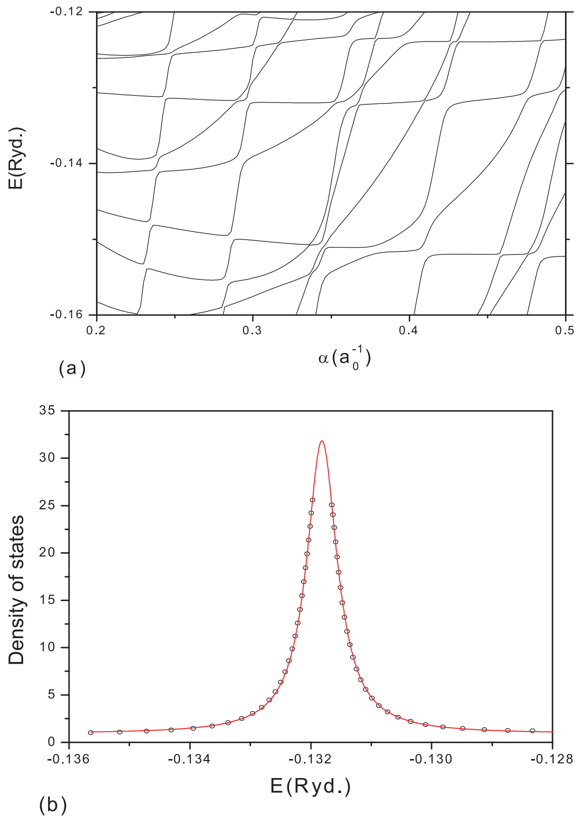

Fig. 3. (a) Stabilization plot for the S-wave e^+–Na system. (b) The fitting of the density of resonance states (circles) to the Lorentzian form of equation (7) for the S-wave e^+–Na system.

energy of $E_r = -0.15164$ Ryd (3.076 eV) and resonance width $\Gamma = 0.00086$Ryd (11.7 meV). From Figure 3b, we have obtained the resonance energy $E_r = -0.13182$ Ryd (3.346 eV) and resonance width $\Gamma = 0.00086$ Ryd (8.44 meV).

When the density of the resonance states $\rho_n(E)$ is fitted to the Lorentzian form, it has been observed that the χ^2 for each fitting is less than 0.1. All the results shown in Figures 1 to 3 are obtained using the 1330-term wave functions. However, the convergence has been reached from 1140 basis terms, as evident from Table 2. Three resonance energies S(1), S(2) and S(3) along with the corresponding widths in the unit of Rydbergs obtained from our calculations with 1330 basis terms of equation (5) are presented in Table 2. Table 2 also shows the numerical results of the resonance parameters E_r and Γ for 816, 969 and 1140 basis terms obtained from our calculations using the basis expansion of equation (5). Table 3 shows a comparison of our results with those of Ward et al. [2a]. Three resonances have been obtained from the present work at the energies 2.219, 3.076 and 3.346 eV with the corresponding widths 5.58, 11.7 and 8.44 meV. Ward et al. [2a] obtained three S-wave resonances at the energies 1.985, 3.195 and 3.62 eV. Table 3 shows that all the three resonance energies 1.985, 3.195 and 3.62 eV is comparable with those obtained from our calculations. The difference in widths may be due to the omission of the positronium formation channels in the CCA calculation [2a]. There are no other theoretical and experimental investigations on resonance phenomena in the scattering of positron from atomic sodium.

Table 3. Comparison of the S-wave resonance E_r and width Γ for the positron-sodium system with other calculations. The quoted values of resonance energy E_r in eV and the width Γ are in meV.

	Present	Ward et al. [2a]
S(1)	$E_r = 2.219$	$E_r = 1.985$
	$\Gamma = 5.58$	$\Gamma = 0.4$
	Na(3p) threshold ($E_t = 2.104$ eV)	
S(2)	$E_r = 3.076$	$E_r = 3.19$
	$\Gamma = 11.7$	$\Gamma = 0.2$
	Na(4s) threshold ($E_t = 3.189$ eV)	
S(3)	$E_r = 3.346$	$E_r = 3.62$
	$\Gamma = 8.44$	$\Gamma = 4$
	Ps($n = 2$) threshold ($E_t = 3.438$ eV)	
	Na(3d) threshold ($E_t = 3.616$ eV)	
	Na(4p) threshold ($E_t = 3.751$ eV)	

It should mention that in comparing the results of Ward et al. for the e^+–Na case and latter in the text for the e^+–K case, care has to be taken as the positronium channels were not included in their work [2a]. The good agreement between the present results and those in [2a] for some states may be coincidental. It has been shown that the convergence for the close coupling calculations could be very slow, as was demonstrated in an investigation of a bound state for the e^+–Li system. Bromley et al. [31] had to use angular momentum states with up to $L = 30$ in order to obtain a bound state for such a system.

The resonances reported in the present work are most likely the results of the A$^+$ ion (A = Na and K) attaching to the $N = 2$ threshold of the excited positronium atom. The induced dipole potential between the A$^+$ ion and the highly polarizable excited positronium is strong enough to support a number of quasi-bound states. Such quasi-bound states lying in the scattering continua would manifest themselves as resonances in e^+–A scattering. A discussion for the possible resonances in Ps–A$^+$ system was given in reference [32]. Calculations for a related system e^+–H has revealed a rich of resonances exist below various excited positronium thresholds [33].

3.2 K results

We have computed the energy eigenvalues for 2601 different α values within the range 0.2 to 1.5 with a mesh size of 0.0005. We have performed calculations for $\omega = 17$ and 18 corresponding to 1140 and 1330 basis terms, respectively. The stabilization diagrams in Figures 4a and 5a show the stabilization character near the energy $E_r = -0.21$ and $E_r = -0.16$ Ryd, respectively, which are believed to be associated with and lying below Ps($n = 2$) positronium formation threshold energy $E_t = -0.125$ Ryd.

Figure 4b shows the density of the resonance states $\rho_n(E)$ for the lowest resonance approaching the excited Ps($n = 2$) threshold. From the fit, we have obtained a resonance energy of $E_r = -0.20780$ Ryd (1.51 eV) and a resonance width $\Gamma = 0.00042$ Ryd (5.71 meV). Here and hereafter, the resonance energy E_r and the resonance width Γ expressed in eV is relative to the ground state K(4s) atom. Figure 5b shows the density of the resonance states $\rho_n(E)$ for the second resonance approaching the excited Ps($n = 2$) threshold. From a fit to equation (7), the results from Figure 5b give a resonance energy of $E_r = -0.15749$ Ryd (2.20 eV) and resonance width $\Gamma = 0.00103$ Ryd (14.0 meV).

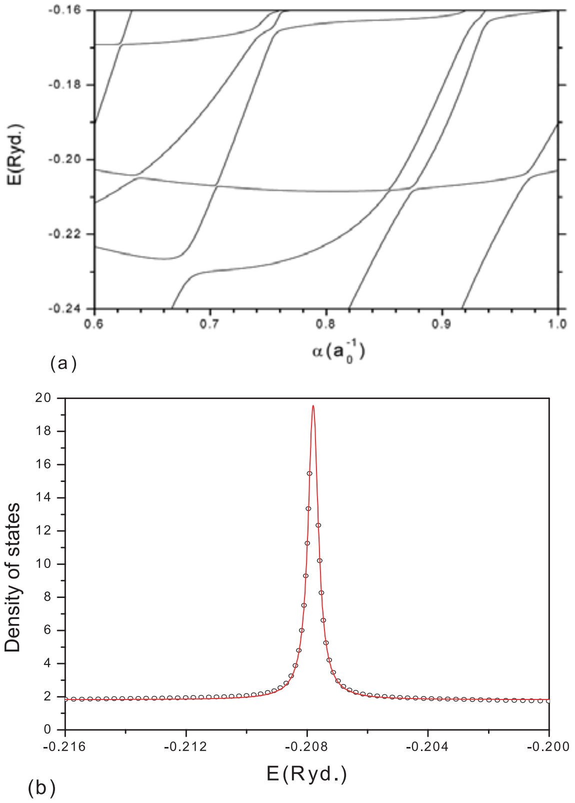

Fig. 4. (a) Stabilization plot for the S-wave e^+–K system. (b) The fitting of the density of resonance states (circles) to the Lorentzian form of equation (7) for the S-wave e^+–K system.

Again, when the density of the resonance states $\rho_n(E)$ is fitted to the Lorentzian form, it has been observed that the χ^2 for each fitting is less than 0.1. All the results shown in Figures 4 and 5 are obtained using the 1330-term wave functions. Two resonance energies S(1) and S(2) along with the corresponding widths in the unit of Rydbergs obtained from our calculations with 1330 basis terms of equation (5) are presented in Table 4 along with the numerical results of the resonance parameters E_r and Γ for 1140 basis terms of equation (5). We have constructed Table 5 to compare our results with those of Ward et al. [2a]. We have obtained from the present work two resonances located at the energies of 1.51 eV and 2.20 eV, with the corresponding widths 5.71 meV and 14.0 meV. Ward et al. [2a] obtained two S-wave resonances at the energies 1.5 eV and 2.45 eV. Table 5 shows a comparison between our results and those of reference [2a]. Again, the difference in width may be due to the fact that no Ps channels were included in reference [2a]. There are no other theoretical and

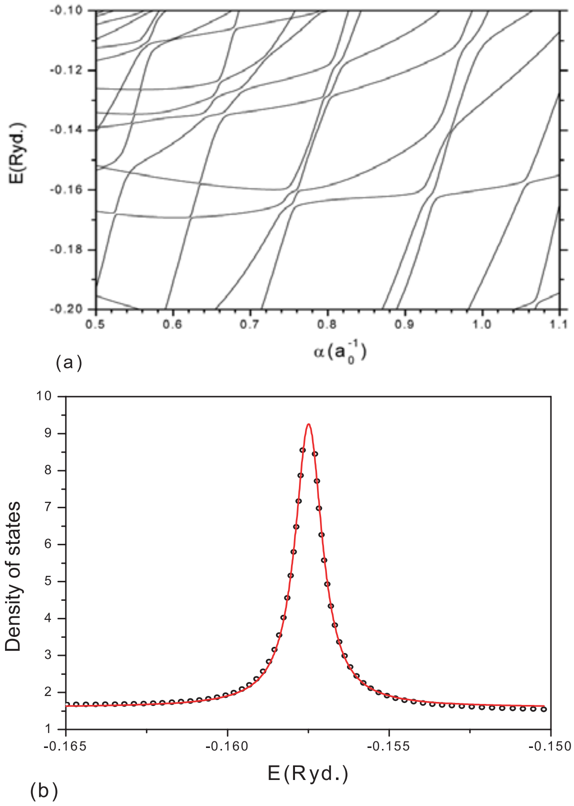

Fig. 5. (a) Stabilization plot for the S-wave e^+–K system. (b) The fitting of the density of resonance states (circles) to the Lorentzian form of equation (7) for the S-wave e^+–K system.

Table 4. Convergence behavior for the resonance energy E_r and resonance width Γ (in Rydbergs) below the Ps($n = 2$) excitation threshold.

	$N = 1140$ $\omega = 17$	$N = 1330$ $\omega = 18$
S(1)	$E_r = -0.19866$	$E_r = -0.20780$
	$\Gamma = 0.00065$	$\Gamma = 0.00042$
S(2)	$E_r = -0.15753$	$E_r = -0.15749$
	$\Gamma = 0.00055$	$\Gamma = 0.00103$

Table 5. Comparison of the S-wave resonance E_r and width Γ for the positron-potassium system with other calculations. The quoted values of resonance energy $E_r$in eV and the width Γ are in meV.

	Present	Ward et al. [2a]
S(1)	$E_r = 1.51$	$E_r = 1.5$
	$\Gamma = 5.71$	$\Gamma = 1.7$
	K(4p) threshold ($E_t = 1.608$ eV)	
S(2)	$E_r = 2.20$	$E_r = 2.45$
	$\Gamma = 14.0$	$\Gamma = 0.54$
	K(5s) threshold ($E_t = 2.606$ eV)	
	Ps($n = 2$) threshold ($E_t = 2.639$ eV)	
	K(5p) threshold ($E_t = 3.062$ eV)	

experimental investigations on resonance phenomena in the scattering of positron from atomic potassium.

It is apparent from Table 1 that the ground and excited states energies of K calculated using the model potential (2) differ somewhat with the experimental values [29]. It seems that there are some uncertainties in our calculated resonance parameters for the positron-potassium systems. The uncertainty in the width for the second resonance S(2) is about 50% as the convergence is very slow. The uncertainty is about ±0.009 Ryd for the energy of S(1). It has already mentioned that we have used the values of c_1, c_2 and c_3 for the model potential (2) as reported by Schweizer et al. [28]. In the course of their study of the model potentials for the alkali metal atoms and Li-like ions, Schweizer et al. [28] have reported the parameters which represent the energy quite well with smallest averaged error in the energy, $\Delta E/E$, for the states with the principal quantum number ranging from 6–40. ΔE is the difference between the computation and the experimental results. In future investigations for the positron-potassium system, it would be of interest to use a model potential which can produce the K(4s) energy that is matched with the experimental value [29].

4 Summary and conclusions

This work presents calculations of S-wave resonances in e^+–Na and e^+–K scattering using the stabilization method, together with employing Hylleraas-type wave functions. For e^+–Na system, the resonances located at 2.219, 3.076 and 3.346 eV measured from the ground state of sodium atom, have been found, with the corresponding resonance widths shown in Table 5 (and in Tab. 4 but in Rydberg units). For e^+–K system, the resonances located at 1.51 and 2.20 eV measured from the ground state of potassium atom, have been found, with the corresponding resonance widths shown in Table 4 (and in Tab. 5 but in Rydberg units). The results, those are obtained from the present calculations have been compared in Table 3 for Na and Table 5 for K with the results available in the literature. The stabilization plots reveal that there are a few other very narrow resonances present in the positron-sodium system converging to the Ps($n = 2$) threshold. The extraction of such high-lying resonances is not an easy task at the level of computation we have performed so far. Presumably, if more extensive basis sets for the wave functions were used, resonance parameters would be less difficult to extract. But for practical reasons, the most extensive wave functions used in the present investigation are limited to 1330 terms.

There are several experimental investigations on the total and Ps formation cross sections in the positron-sodium systems [19–23]. With the recent advancement of the new technological breakthrough, mono-energetic positron beams are now available in different positron research laboratories around the globe [34–37]. We hope that our findings will stimulate experimental search for resonances in the positron-sodium and positron-potassium systems.

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