S-, P- and D-wave resonances in positronium-sodium and positronium-potassium scattering

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Abstract

Scattering of positronium (Ps) by sodium and potassium atoms has been investigated employing a three-Ps-state coupled-channel model with Ps(1s,2s,2p) states using a time-reversal-symmetric regularized electron-exchange model potential fitted to reproduce accurate theoretical results for PsNa and PsK binding energies. We find a narrow S-wave singlet resonance at 4.58 eV of width 0.002 eV in the Ps-Na system and at 4.77 eV of width 0.003 eV in the Ps-K system. Singlet P-wave resonances in both systems are found at 5.07 eV of width 0.3 eV. Singlet D-wave structures are found at 5.3 eV in both systems. We also report results for elastic and Ps-excitation cross sections for Ps scattering by Na and K.

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Recent successful high precision measurements of positronium (Ps) scattering by H₂, N₂, He, Ne, Ar, C₄H₁₀, and C₅H₁₂ [1,2] have enhanced theoretical activities [3–6] in this subject. We suggested [7] a regularized, symmetric, nonlocal electron-exchange model potential and used it in the successful study of Ps scattering by H [8], He [7,9–11], Ne [11], Ar [11], H₂ [12] and Li [13]. Our results were in agreement with experimental total cross sections [1,2], specially at low energies for He, Ne, Ar and H₂. Moreover, these studies yielded correct results for resonance and binding energies for the S wave electronic singlet state of Ps-H [4,8] and Ps-Li [13] systems in addition to experimental pick-off quenching rate in Ps-He [10] scattering.

In the present work we use the above exchange potential to study Ps-Na and Ps-K scattering using the three-Ps-state coupled channel method. We find resonances in the singlet channel at low energies in S, P and D waves of both systems near the Ps(2) excitation threshold. We also report angle-integrated elastic and Ps-excitation cross sections for both systems.

The appearance of resonances in electron-atom [14] and positron-atom [15] scattering, and in other atomic processes in general, is of great interest. Several resonances in the electron-hydrogen system have been found in the close-coupling calculation and later reconfirmed in the variational calculation [16]. Resonances have also been found in the close-coupling calculation of electron scattering by Li, Na and K [17]. These resonances provide the necessary testing ground for a theoretical formulation, which can eventually be detected experimentally. Detailed dynamical description of the important degrees of freedom in a theoretical formulation is necessary for the appearance of these resonances. The ability of the present exchange potential to reproduce the resonances in diverse Ps-atom systems [8,13] assures its realistic nature.

The theory for the coupled-channel study of Ps scattering with the regularized model potential has already appeared in the literature [7,8,11] and we quote the relevant working equations here. For target-elastic scattering we solve the following Lippmann-Schwinger scattering integral equation in momentum space

\[ f^\pm_{\nu',\nu}(k', k) = B^\pm_{\nu',\nu}(k', k) - \sum_{\nu''} \frac{1}{2\pi^2} \frac{B^\pm_{\nu',\nu''}(k', k'') f^\pm_{\nu'',\nu}(k'', k)}{k''^2/4 - k''^2/4 + i0} \]

where the singlet (+) and triplet (−) “Born” amplitudes, \( B^\pm \), are given by \( B^\pm_{\nu',\nu}(k', k) = g^D_{\nu',\nu}(k', k) \pm g^E_{\nu',\nu}(k', k) \), where \( g^D \) and \( g^E \) represent the direct and exchange Born amplitudes and the \( f^\pm \) are the singlet and triplet scattering amplitudes, respectively. The quantum
states are labeled by the indices $\nu$, referring to the Ps atom. The variables $k$, $k'$, $k''$ etc denote the appropriate momentum states of Ps; $k_{\nu',\nu}$ is the on-shell relative momentum of Ps in the channel $\nu''$. We use atomic unit (a.u.) where $\hbar = m = 1$ with $m$ is the electron mass.

To avoid complication of calculating exchange potential with a many-electron wave function, we consider a frozen-core one-electron approximation for the targets Na and K. Such wave functions have been successfully used for scattering of alkali metal atoms in other contexts and also for positronium scattering by Li [5]. The Na(3s) and K(4s) frozen-core hydrogen-atom-like wave functions are taken as

$$\phi_{Na}(r) = \frac{1}{9\sqrt{3}} \frac{1}{\sqrt{4\pi a_0^3}} (6 - 6\rho + \rho^2)e^{-\rho/2}$$

$$\phi_{K}(r) = \frac{1}{96\sqrt{4\pi a_0^3}} (24 - 36\rho + 12\rho^2 - \rho^3)e^{-\rho/2}$$

where $\rho = 2r\alpha$ with $\alpha = 1/(n\alpha_0)$. Here $n = 3$ for Na and $n = 4$ for K and $\alpha_0 = (2n^2E_i)^{-1}a_0$ with $E_i$ the ionization energy of the target in a.u. and $a_0$ the Bohr radius of H. Here we use the following experimental values for ionization energies for Na and K, respectively: 5.138 eV and 4.341 eV [18].

The direct Born amplitude of Ps scattering is given by [7,9]

$$g_{\nu',\nu}^D(k_f, k_i) = \frac{4}{Q^2} \int \phi^*(r) [1 - \exp(iQ\cdot r)] \phi(r) dr$$

$$\times \int \chi^\nu_\nu(t) 2i \sin(Q\cdot t/2) \chi^\nu_\nu(t) dt,$$

where $\phi(r)$ is the target wave function and $\chi(t)$ is the Ps wave function. The exchange amplitude corresponding to the model potential is given by [8]

$$g_{\nu',\nu}^E(k_f, k_i) = \frac{4(-1)^{l+l'}}{D} \int \phi^*(r) \exp(iQ\cdot r) \phi(r) dr$$

$$\times \int \chi^\nu_\nu(t) \exp(iQ\cdot t/2) \chi^\nu_\nu(t) dt$$

with

$$D = (k_i^2 + k_f^2)/8 + C^2[\alpha^2 + (\beta^2 + \beta'^2)/2]$$

where $l$ and $l'$ are the angular momenta of the initial and final Ps states and $C$ is the only parameter of the exchange potential. The initial and final Ps momenta are $k_i$ and $k_f$, $Q = k_i - k_f$, and $\beta_i$ and $\beta_f$ are the binding energies of the initial and final states of Ps in a.u., respectively. It has been demonstrated for the Ps-H system that at high energies the
model-exchange amplitude (5) reduces to [19] the Born-Oppenheimer exchange amplitude [20]. This exchange potential for Ps scattering is considered [7] to be a generalization of the Ochkur-Rudge exchange potential for electron scattering [21].

After a partial-wave projection, the system of coupled equations (1) is solved by the method of matrix inversion. Forty Gauss-Legendre quadrature points are used in the discretization of each momentum-space integral. The calculation is performed with the exact Ps wave functions and frozen-core orbitals (2) and (3) for Na and K ground state. We consider Ps-Na and Ps-K scattering using the three-Ps-state model that includes the following states: Ps(1s)Na(3s), Ps(2s)Na(3s), Ps(2p)Na(3s), and Ps(1s)K(4s), Ps(2s)K(4s), Ps(2p)K(4s), for Na and K, respectively. The parameter $C$ of the potential given by (5) and (6) was adjusted to fit the accurate theoretical results [22] for PsNa and PsK binding energies which are 0.005892 a.u. and 0.003275 a.u., respectively. We find that $C = 0.785$ fits both binding energies well in the three-Ps-state model and this value of $C$ is used in all calculations reported here. The proper strength of the model potential is obtained by fitting the binding energies of the Ps-Na and Ps-K systems, and it is expected that this choice of $C$ would lead to a good overall description of scattering in these systems. We recall that this value of $C$ also reproduced the accurate variational result of PsH resonance energy in a recent five-state model for Ps-H scattering [8]. A similar variation of the parameter $C$ from unity also led to a good overall description of the total scattering cross section in agreement with experiment [2] in the Ps-He system in the energy range 0 eV to 70 eV [9].

The Ps-Na and Ps-K systems have an effective attractive interaction in the electronic singlet channel as in Ps-H [8] and Ps-Li [13] systems. The targets of these systems have one active electron outside a closed shell. In the present three-Ps-state calculation we find resonances in the singlet channel in both systems. No resonances appear in the triplet channel possibly because of a predominantly repulsive interaction in this channel. For the resonances to appear, the inclusion of the excited states of Ps is fundamental in a coupled-channel calculation. The static-exchange model with both the target and Ps in the ground state does not lead to these resonances. A detailed study of these resonances in coupled-channel study of Ps-H [4,8] and Ps-Li [13] systems in the singlet channel has appeared in the literature.

Here to study the resonances, first we calculate the S-, P- and D-wave elastic phase shifts and cross sections in the singlet channel of the Ps-Na and Ps-K systems using the 3-Ps-state model. In figure 1 we show the low-energy singlet S-wave cross sections. The singlet S-wave phase shifts near the resonance energies are shown in the off-set of figure 1. The Ps-Na system has a resonance at 4.58 eV of width 0.002 eV. The resonance in the Ps-K
system appears at 4.77 eV and has a width 0.003 eV. The phase shift curves clearly show
the resonances where the phase shifts jump by $\pi$.

In figure 2 we show the singlet P-wave Ps-Na and Ps-K elastic phase shifts; the cor-
responding singlet P-wave cross sections are shown in the off-set. Both systems possess
resonances at 5.07 eV of width of 0.3 eV. The cross sections clearly exhibit these resonances.
In figure 3 we plot the D-wave singlet elastic cross sections for Ps-Na and Ps-K systems at
low energies. There is a structure in both systems at 5.3 eV which is more diffuse than in S
and P waves.

Next we calculate the different partial cross sections of Ps-Na and Ps-K scattering. The
convergence of the cross sections with respect to partial waves is slower in this case than in
the case of Ps-H scattering. At a incident Ps energy of 50 eV, 40 partial waves were used to
achieve convergence of the partial-wave scheme. In figures 4 and 5 we plot different angle-
integrated partial cross sections of Ps-Na and Ps-K scattering, respectively. Specifically, we
plot the elastic, Ps(2s) and Ps(2p) excitation cross sections using the three-Ps-state model.
For comparison we also plot the elastic cross section obtained with the static-exchange
model. The elastic cross section is large at low energies in both systems. The effect of the
inclusion of highly polarizable Ps(2) states in the coupling scheme could be considerable,
specially at low energies. The local minima in the three-Ps-state elastic cross section for
both systems at about 4 ~ 5 eV are manifestations of the P- and D-wave resonances in this
energy region. Similar minima found in electron scattering by alkali-metal atoms are also
consequences of resonances [17].

To summarize, we have performed a three-Ps-state coupled-channel calculation of Ps-Na
and Ps-K scattering at low energies using a regularized symmetric nonlocal electron-exchange
The only parameter of the model potential was adjusted to fit accurate theoretical result for
PsNa and PsK binding [22]. We present the results of angle-integrated partial cross sections
at different Ps energies. We find resonances in S, P and D waves near the Ps(2) excitation
threshold. In this study we have used a three-Ps-state model. Similar resonances have
been observed in the coupled-channel study of electron-H [16], electron-Na, electron-K [17],
positron-hydrogen [15], Ps-H [4,8] and Ps-Li [13] systems. In most cases, a more complete
calculation and (in some cases) experiments have reconfirmed these resonances. Hence we
do not believe that the appearance of resonances in the present three-state calculation to be
so peculiar as to have no general validity. On the contrary, in view of the correlation found
between resonance and binding energies in the singlet Ps-H system [8], it is expected that
the reproduction of correct binding energies of the Ps-Na and Ps-K systems in the present
model should lead to correct resonance energies in these systems. However, the resonance
energies might change slightly after a more complete calculation (with accurate many-body
wave functions of the target and including the excited states of the target) and it would be
interesting to study the present resonances using more complete theoretical models in the
future in addition to compare the present results with future experiments.

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REFERENCES


   Yan Z C and Ho Y K 1999 Phys. Rev. A 59 2697
   Yan Z C and Ho Y K 1999 Phys. Rev. A 60 5098


    Shimamura I 1971 J. Phys. Soc. (Japan) 31 852
Figure Caption:

1. Singlet S-wave elastic cross sections at different Ps energies for Ps-Na (dashed line) and Ps-K (full line) scattering. The corresponding phase shifts near resonance are shown in the off-set.

2. Singlet P-wave elastic phase shifts at different Ps energies for Ps-Na (dashed line) and Ps-K (full line) scattering. The corresponding cross sections are shown in the off-set.

3. Singlet D-wave elastic cross sections at different Ps energies for Ps-Na (dashed line) and Ps-K (full line) scattering.

4. Partial cross sections for Ps-Na scattering at different Ps energies: three-Ps-state elastic (full line), three-Ps-state Ps(2s) (dashed-dotted line), three-Ps-state Ps(2p) (short-dashed line), static-exchange elastic (long-dashed line).

5. Same as in figure 4 for Ps-K scattering.