# Coupled-channels optical calculation of positron–hydrogen resonances*

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An application of the coupled-channels optical method is given for the energy-dependent phenomena of positron–hydrogen resonances below the $n = 2$ excitation threshold. The equivalent local optical potential is used to account for the target polarization and positronium formation. The calculation includes 9 explicitly physical coupled channels. The lowest S-wave resonance energy position and new resonances are found. Angular dependence of the cross section in the resonance region are investigated.

**Keywords:** positron, hydrogen, resonance

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## 1. Introduction

Positron-atom scattering has been an important area of intense research in atomic and molecular physics and it also has extensive applications in many areas such as plasma physics and materials science.[1−3] Since Mittleman[4] predicted that an infinite sequence of resonances should exist below the $n = 2$ excitation threshold in positron–hydrogen scattering, there has been continuous interest in the study of resonance phenomena in positron–hydrogen systems over the past decades. A number of studies have demonstrated the existence of resonances below the excitation of the $n = 2$ threshold and a variety of theoretical approximations have been used to predict the positions and widths of the resonances,[5−17] even though there are not yet any reports of experimental observations. The close-coupling approach is one of the most widely used methods of studying the resonances in electron- and positron-atom scattering. An advantage in the method is that the numerical procedures used in close-coupling calculations allow computer codes to sweep through any energy region. Early close-coupling calculations[5] showed some of these resonances in the S- and P-waves with the lowest S-wave resonance lying at the 9.784 eV with a width of $1.13 \times 10^{-3}$ eV. In their calculations, only three hydrogen states (1s, 2s, 2p) and no positronium states were included. Recently, larger coupling scheme calculations of close-coupling, with positronium states explicitly coupled, have been carried out.[10−12,14,15] The most comprehensive investigation was performed by Mitroy[12] with 21 states, in which 6 physical channels (1s, 2s, 2p, 3s, 3p, 3d), 7 pseudo-states, the lowest 3 physical states of positronium (1s, 2s, 2p), and 5 pseudo-positronium levels were included. However, the position of the lowest S-wave resonant energy in these calculations lay near the H ($n = 2$) threshold and only two S-wave resonances could be found with this coupling scheme. No lower resonances were found in these calculations.[5−17] These calculations indicated that the existence of these resonances should be independent of the coupling scheme, and provided that it contains the degenerate 2s and 2p states, but different coupling schemes give different locations of resonant energies.[14,15] Therefore, a convergence calculation of close-coupling is necessary to have definite results.

In the present work, we report on new calculation results for the resonances below the H($n = 2$) excitation threshold in positron–hydrogen scattering, obtained by employing the coupled-channels optical method.[18] In this calculation, the lowest lying S-, P- and D-wave positions of resonant energies are found. The angular dependence of the cross section for elastic scattering in the resonance region is studied. The momentum space coupled-channels optical method (CCO) for electron–atom collisions given by McCarthy and Stelbovics[19] was used to calculate the energy dependence phenomenon in electron–hydrogen scattering[20] and negative-ion resonances in

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an electron–sodium system.[21] Good agreements were achieved with experimental data and other theoretical calculations. In the present method, an equivalent local polarization potential is used to describe the positron formation rearrangement channels.[18] This method can take all reaction channels into account.[18] The method is used to calculate various scattering cross sections (positronium formation cross section, ionization cross section, integral cross section and total scattering cross section) for a positron-atom system and satisfactory results are obtained in comparison with experimental data and other theoretical calculation results.[18,22] In this paper, we use the method to investigate the energy dependence phenomenon in elastic positron–hydrogen scattering. To the best of our knowledge, such resonance structures in differential cross sections have not been reported yet.

## 2. Model and method

The position of resonance energy can be determined by calculating the elastic cross section for positron–hydrogen scattering. In the present problem the elastic cross section for positron–hydrogen collision is calculated by solving coupled integral equations in momentum space

$$\begin{aligned}&\langle \boldsymbol{k}i|T_{\rm S}|0\boldsymbol{k}_0\rangle\\ =\ &\langle \boldsymbol{k}i|V_{\rm S}^{(Q)}|0\boldsymbol{k}_0\rangle\\ &+\sum_{j\in P}\int {\rm d}^3q\frac{\langle \mathbf{k}i|V_{\rm S}^{(Q)}|j\mathbf{q}\rangle\langle \mathbf{q}j|T_{\rm S}|0\mathbf{k}_0\rangle}{E^{(+)}-\epsilon_j-q^2/2},\end{aligned}\quad(1)$$

where $i$ and $j$ represent target states, $P$ projects a finite set of target states including the ground state 0, and $Q$ projects the continuum and the positronium formation channels. The subscript S indicates the total spin. $V_{\rm S}^{(Q)}$ has two parts, the channel-coupling potential $V_{\rm S}$ and the complex, nonlocal polarization potential $W_{\rm S}^{(Q)}$, i.e.,

$$V_{\rm S}^{(Q)}=V_{\rm S}+W_{\rm S}^{(Q)},\quad(2)$$

$$W_{\rm S}^{(Q)}=W_{\rm I}^{(Q)}+W_{\rm PS}^{(Q)}.\quad(3)$$

Here, $W_{\rm I}^{(Q)}$ and $W_{\rm Ps}^{(Q)}$ denote parts of the polarization potential which describe the ionization continuum and the positronium formation rearrangement processes respectively.

The form used for the matrix element of the polarization potential $W_{\rm I}^{(Q)}$ describing ionization is

$$\begin{aligned}&\langle \boldsymbol{k}'i|W_{\rm I}^{(Q)}|j\boldsymbol{k}\rangle\\ =\ &\sum_{n\in Q}\langle \boldsymbol{k}'i|V|\chi_n^{(-)}\rangle\frac{1}{E^{(+)}-E_n}\langle\chi_n^{(-)}|V|j\boldsymbol{k}\rangle,\end{aligned}\quad(4)$$

where $|\chi_n^{(-)}\rangle$ represents the distorted wave function for the reaction starting in channel $n$. The notation $n$ is a discrete notation for the three-body continuum channel. For the ionization state the extreme screening approximation is used

$$|\chi_n^{(-)}\rangle=|\psi^{(-)}(\boldsymbol{q}_<),\boldsymbol{q}_>\rangle,\quad(5)$$

where $\boldsymbol{q}_<$ and $\boldsymbol{q}_>$ are the momenta of the outgoing particles with greater and smaller absolute values respectively. Ionization is described in the independent particle model, where $\langle \boldsymbol{r}|\psi^{(-)}(\boldsymbol{q}_<)\rangle$ is a Coulomb wave orthogonalized to the orbital from which the electron is removed. $\langle \boldsymbol{r}|\boldsymbol{q}_>\rangle$ is a plane wave.

The model used for positronium formation is

$$|\chi_n^{(-)}\rangle=|c\phi_\mu\boldsymbol{Q}\rangle,\quad(6)$$

where $\phi$ is the bound state of positronium, and $\boldsymbol{Q}=\boldsymbol{k}_{\rm Ps}$ is the momentum of the positronium centre of mass. The plane wave $\langle \boldsymbol{R}|\boldsymbol{Q}\rangle$ represents the motion of the positronium, since only short-range terms in the positronium-ion potential survive.

The optical potential for positronium formation is

$$\begin{aligned}&\langle \boldsymbol{k}'i|W_{\rm Ps}^{(Q)}|j\boldsymbol{k}\rangle\\ =\ &\sum_\mu\langle \boldsymbol{k}'i|V|\tilde{\chi}_n^{(-)}\rangle\\ &\times\frac{1}{E^{(+)}-\epsilon_\mu-\frac{1}{4}k_{\rm Ps}^2}\langle\tilde{\chi}_n^{(-)}|V|j\boldsymbol{k}\rangle.\end{aligned}\quad(7)$$

Here,

$$|\tilde{\chi}_\mu^{(-)}\rangle=(1-\sum_n|n\rangle\langle n|)|\chi_\mu^{(-)}\rangle.\quad(8)$$

A half-on shell equivalent-local approximation is made for the positronium formation potential, and the optical potential matrix element is calculated only at about ten points in the variable $K$, where

$$K=|\boldsymbol{k}-\boldsymbol{k}'|,\ \frac{1}{2}k^2=E-\epsilon_j.\quad(9)$$

The equivalent-local complex potential is calculated by a multidimensional method using Cartesian momentum variables.[23]

For computation we make a partial-wave expansion of $T$ and $V^{(Q)}$ matrix elements, defining the partial matrix elements

$$\langle k'n'l'L'\parallel T_J\parallel Llnk\rangle\quad(10)$$

for the total orbital angular momentum quantum number $J$ by

$$\langle \boldsymbol{k}' i|T|j\boldsymbol{k}\rangle = \sum_{L,M,L',M',J,K} \langle \hat{\boldsymbol{k}}'|L''M''\rangle C^{M'm'K}_{L'l'J} \langle k'n'l'L' \parallel T_J \parallel Llnk\rangle C^{MmK}_{LlJ} \langle LM|\hat{\boldsymbol{k}}\rangle, \tag{11}$$

where

$$\langle \hat{\boldsymbol{k}}|LM\rangle \equiv Y_{LM}(\hat{\boldsymbol{k}}), \tag{12}$$

and $C^{Mmk}_{LlJ}$ is a Clebsch–Gordan coefficient. The definition of

$$\langle k'n'l'L' \parallel V^{(q)}_J \parallel Llnk\rangle \tag{13}$$

is analogous to expression (11), with $V^{(Q)}$ substituted for $T$.

The energies and widths of resonances for particular values of $J$ are found by fitting the Breit–Wigner form with a liner background

$$\sigma_{\rm R} = aE + b + \frac{c + id}{E - E_{\rm R} + 0.5i\gamma_{\rm R}} \tag{14}$$

to the partial cross section $\sigma$ for each resonance over the resonant energy range, where $E$ is the incident energy, $a$, $b$, $c$, and $d$ are the fitting parameters, $E_{\rm R}$ is the resonant energy, and $\gamma_{\rm R}$ is the width.

## 3. Results and discussion

In the present calculation, 9 discrete states of hydrogen are included in $P$ space for convergence. They are 1, 2, 3, 4s; 2, 3, 4p and 3, 4d. The optical potential that represents the formation of positronium in its $n = 1$ and $n = 2$ bound states is explicitly included in the coupling 1s–1s. The optical potential that represents the continuum is included in the couplings 1s–1s, 1s–2s and 1s–2p. In the present case, only the real part of the potential that represents polarization of the target is explicitly coupled, since incident energies are less than the ionization threshold of hydrogen. We swept through the energy range from 9.0 eV to the $n = 2$ excitation threshold at 10.2 eV with the coupled-channels optical calculations to hunt for resonances of positron–hydrogen scattering at energy intervals of 0.1 meV.

The positions and the widths of the resonances found in the present calculation are listed in Table 1, and compared with the results of 21-state close coupling calculation of Mitroy,[12] the complex-coordinate rotation approach of Ho and Yan,[16] and the 3-state close coupling calculation of Seiler *et al.*[5] Three S-wave resonances have been found below the $n = 2$ excitation threshold. The lowest S-wave resonance is located at 9.428 eV and has a width of $2.76 \times 10^{-3}$ eV. To the best of our knowledge, it is the lowest-lying resonant energy that has been found so far. The second S-wave resonance position is located at 10.158 eV. We identify these two resonances to be those that have already been identified by Seiler *et al.*,[5] which correspond to positions at 9.784 and 10.178 eV, respectively. The lowest-lying S-wave resonance positions in the calculations given by Mitroy[12], and Ho and Yan[16] were at 10.108 eV and 10.094 eV, respectively. The lowest resonance reported here is farther from the $n = 2$ threshold of hydrogen than those in Refs. [5], [12] and [16], which is probably due to the fact that this work includes more physical channels in the coupling scheme, thereby making the positions of resonance energy shift away from the threshold. The third S-wave resonance found in the present calculation, lying at the energy position 10.202 eV, accords well with the results of the 3-state close-coupling calculation,[5] and the 21-state close-coupling calculation,[12] and is close to the result of the complex-coordinate rotation calculation.[16] Note that only two resonances have been found by their calculations.[12,16] Three P-wave resonances are identified in our calculation. The resonance lying at 9.682 eV is the lowest-lying P-wave resonance. We also identify that this resonance should be the one that has already been located at 9.991 eV by Seiler *et al.*,[5] while the resonance at 10.187 eV possibly corresponds to the resonance at position 10.151 eV obtained by Mitroy's[12] calculation and 10.138 eV obtained by Ho and Yan's[16] calculation. The P-wave resonance at 10.203 eV is in very good agreement with the results of both close coupling calculations of Mitroy[12] and Seiler *et al.*[5] Only one P-wave resonance has been found in the calculation of Ho and Yan.[16] A possible D-wave resonance is found at the position of resonant energy 10.078 eV in the present calculation, while Mitroy[12] obtained a D-wave resonance located at the energy 10.203 eV.

In order to exhibit the existence of these resonances, we plot the partial wave phase shift as a function of energy near a resonance for each resonance case in Figs. 1–3. From the variation of the phase shift, we can obtain a more complete description of the resonant behaviour. From these figures, we can see that the rapid transit of the phase shift through $\pi$ radians corresponds to the behaviour of the elastic cross section by the appearance of sharp structure. We hope that the positions and the widths of these resonances determined by this calculation could be confirmed by the experimental data in the near future.

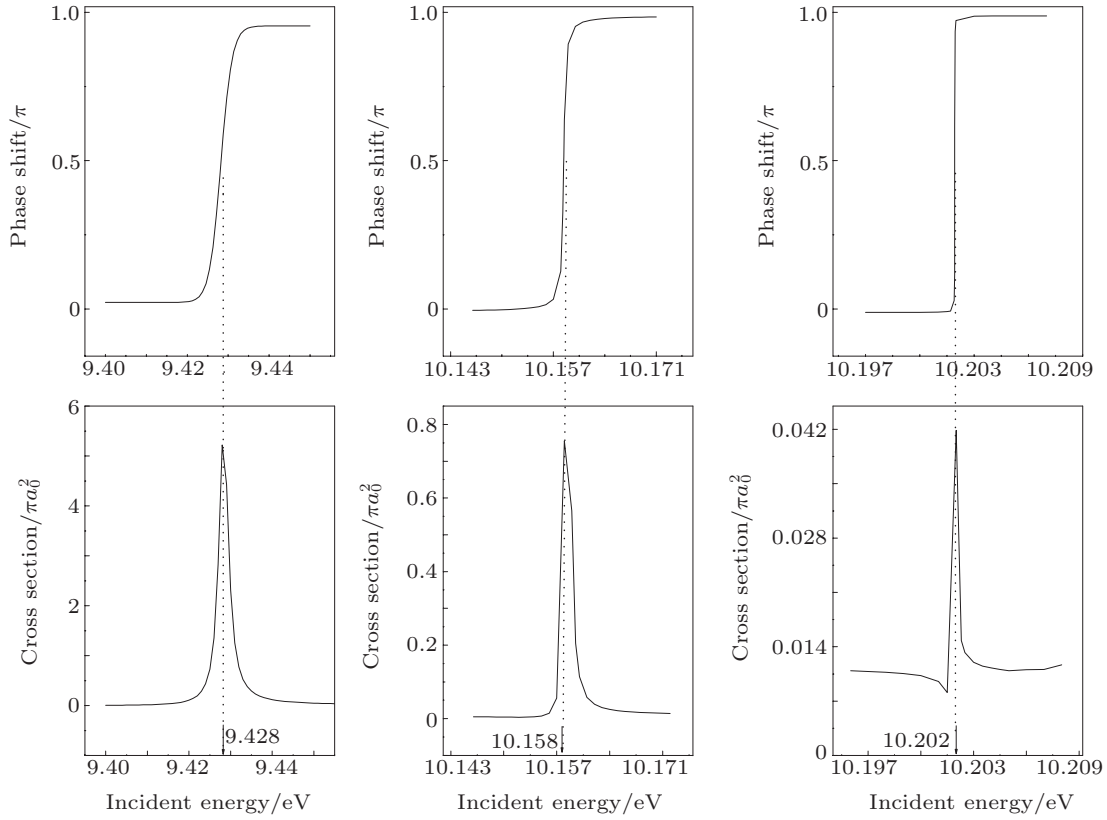



**Fig. 1.** S-wave phase shifts near a resonance (top portion) and resulting shapes of the elastic cross section near a resonance (bottom portion).

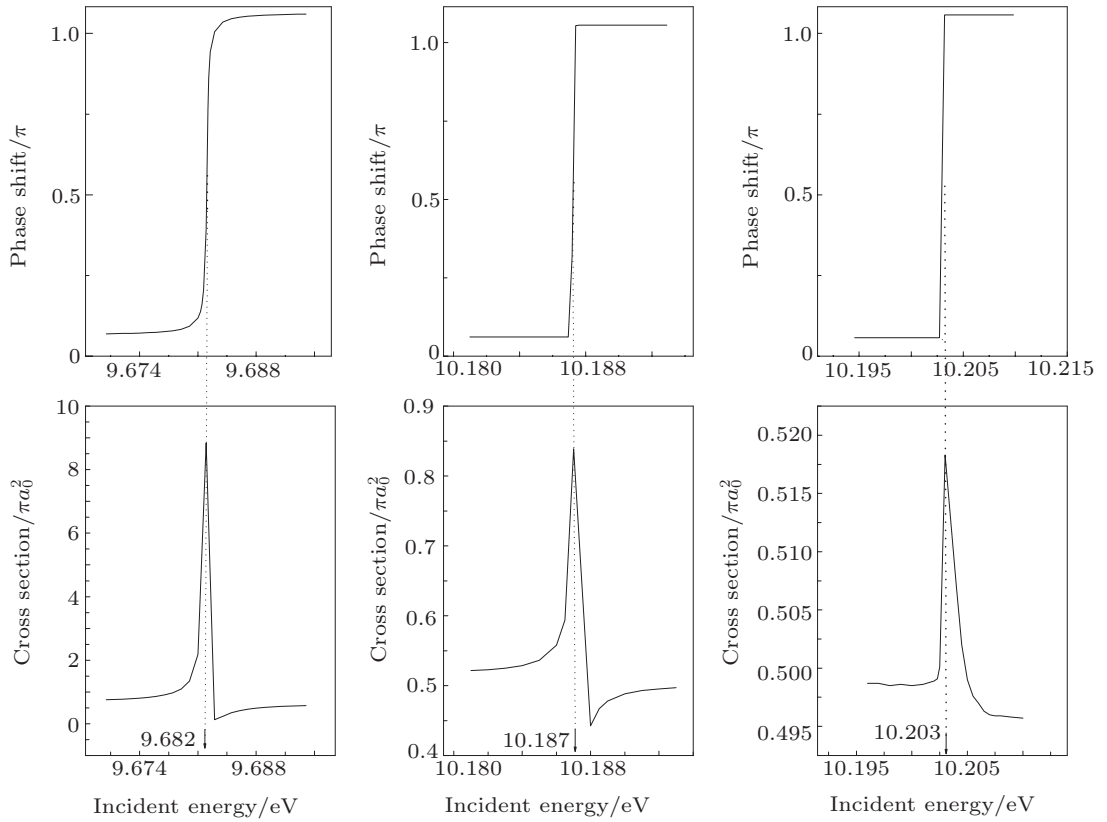



**Fig. 2.** P-wave phase shifts near a resonance (top portion) and resulting shapes of the elastic cross section near a resonance (bottom portion).

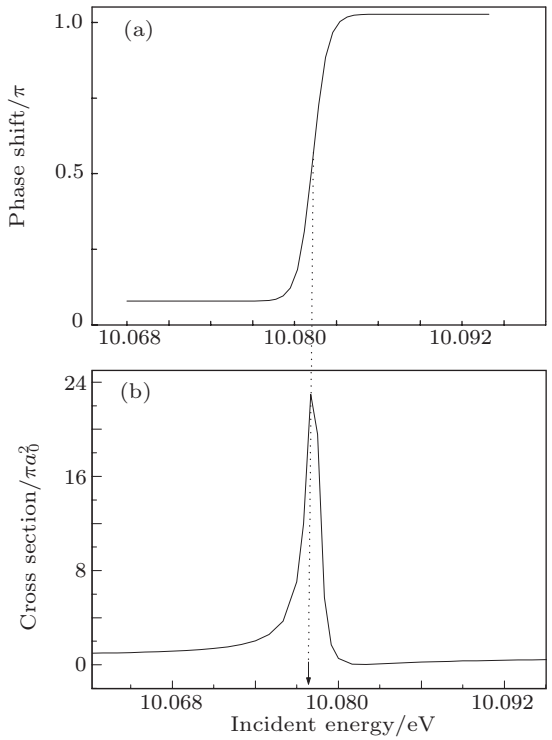



**Fig. 3.** D-wave phase shift near a resonance (a) and resulting shape of the elastic cross section near a resonance (b).

In order to demonstrate more details of the characteristics of the resonance in positron–hydrogen scattering, we present the study of the angular dependence of the cross sections for elastic scattering in the resonance region. Since no theoretical and experimental investigations have been reported on the angular behaviour of the cross section in the resonance region, we compare the present result with angular behaviour of resonances in electron–hydrogen scattering.[24] The elastic scattering spectra at 33°, 54°, 70° and 90° are shown in Fig. 4. The energies of these resonance features are given in Table 1.

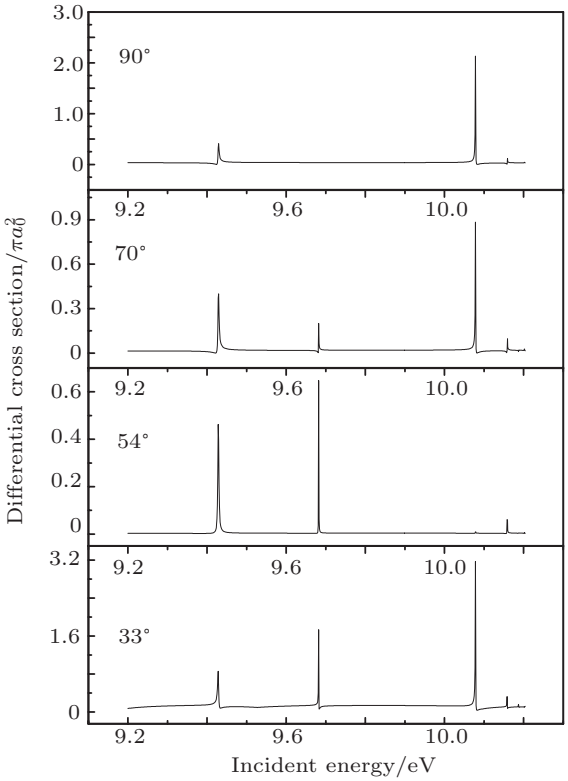



**Fig. 4.** Resonance structures of differential cross section in resonance region at scattering angles of 33°, 54°, 70° and 90°.

**Table 1.** Positions and widths for resonances of the $e^+$–H system. The notation $x^y$ implies $x \times 10^y$.

| J | $E_R$/eV | | $(\gamma_R/2)$/eV | |
|---|---|---|---|---|
| | Present work | Other work | Present work | Other work |
| S(1) | 9.428 | (9.784)[a] | $2.76^{-3}$ | $(1.13^{-3})$[a] |
| S(2) | 10.158 | (10.178)[a] | $4.0^{-4}$ | $(6.52^{-5})$[a] |
| | | (10.108)[b] | | $(2.12^{-3})$[b] |
| | | (10.094)[c] | | $(9.0^{-4})$[c] |
| S(3) | 10.202 | (10.203)[a] | $8.31^{-6}$ | $(3.50^{-7})$[a] |
| | | (10.199)[b] | | $(1.07^{-4})$[b] |
| | | (10.189)[c] | | $(5.0^{-5})$[c] |
| P(1) | 9.682 | (9.991)[a] | $3.6^{-4}$ | $(2.68^{-4})$[a] |
| P(2) | 10.187 | (10.151)[b] | $3.0^{-5}$ | $(2.15^{-4})$[b] |
| | | (10.138)[c] | | $(1.1^{-4})$[c] |
| P(3) | 10.203 | (10.203)[a] | $1.52^{-5}$ | $(1.64^{-6})$[a] |
| | | (10.202)[b] | | $(6.12^{-6})$[b] |
| D(1) | 10.078 | | $1.06^{-3}$ | |
| | | (10.203)[b] | | $(3.89^{-4})$[b] |

[a] 3-state close coupling (Seiler *et al.*[5]), [b] 21-state close coupling (Mitroy[12]),

[c] complex-coordinate rotations (Ho and Yan[16]).

The lowest energy resonance state at 9.428 eV exhibits S-wave behaviour, presented at all angles of calculations, but has different amplitudes and widths. The second resonance state at 9.682 eV exhibits P-wave behaviour, it is visible at all angles except 90 °. The third resonance state at 10.078 eV exhibiting D-wave behaviour has a very weak peak at 54°. The elastic scattering spectra present the same behaviour as that of electron–hydrogen scattering.[24] It is evident that the existence of the resonances due to the longer-range $r^{-2}$ attractive potential will not change even if the positronium formation channels are included.

## 4. Conclusions

We use the coupled-channels optical method to investigate energy-dependent phenomena, positron–hydrogen resonances in positron–hydrogen scattering, in which 9 states of target are included, the polarization of target and positronium formation channels are combined via an equivalent local optical potential. The lowest S-, P- and D-wave resonance locations and widths are found and new resonances are predicted. Angular dependence of the cross section is investigated. Our results show that larger close-coupling scheme can shift the positions of resonant energies away from opening channel threshold, and that angular behaviour of resonance in positron–hydrogen scattering is the same as that in electron–hydrogen scattering, even if the positronium formation channels are included. It is expected that the present work can be compared with experimental data in the near future.

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