Unnatural parity resonance states in positron-excited hydrogen scattering*

Ma Jia(马 佳), Zhou Ya-Jun(周雅君)†, and Wang Yuan-Cheng(王远成)

Center for Theoretical Atomic and Molecular Physics, Academy of Fundamental and Interdisciplinary Sciences, Harbin Institute of Technology, Harbin 150081, *China*

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The coupled-channels optical method for positron scattering has been applied to investigate resonance states with unnatural parities in a positron-excited hydrogen system. The positronium formation channels and continuum channel are included via a complex equivalent local potential. Resonance states with angular momenta $L = 1$ to $L = 2$ and parities $(-1)^{L+1}$ are calculated. Resonance energies and widths are reported and compared with other theoretical calculations. We found that the opening positronium formation channels play an important role in forming nondipole Feshbach resonances.

Keywords: positrons, excited-hydrogen atom, unnatural parity resonances, positronium, coupled-channels optical method

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1. Introduction

During recent decades, there has been continuous interest in theoretical investigations of resonances in positron–hydrogen scattering.[1−15] The resonances in positron–hydrogen scattering play an important role in the production of anti-hydrogen atoms through the rearrangement scattering of positronium by antiprotons.[16] In addition to the resonances of natural parities, resonance states with unnatural parity are of particular interest.[17] However, comparing with a number of theoretical studies for resonances with natural parity in positron–hydrogen system, only limited theoretical methods have focused on the investigation of resonances with unnatural parities.[18−20] Recently, Yan and Ho[18] presented an investigation of resonances with unnatural parities in a positron–hydrogen system by using the complex-coordinate rotation method,[18] in which the coordinations of positronium formation have been included via Hylleraas wave functions. Resonance parameters of unnatural parity states with angular momenta $L = 1$ to $L = 5$ have been reported. They indicated that there are dipole series and nondipole unnatural parity resonance states and occurrence of the latter is due to the excited states of positronium interacting with hydrogen via a large attractive polarization potential. Another work for investigating unnatural parity resonance states in positron–hydrogen systems is the hyperspherical close-coupling calculation (HSCC).[19] A remarkable theoretical advantage of the approach is the use of the hyper-radius to represent positron and electron collectively. It allows a part of the correlation effects to be described efficiently. Both complex rotation[18] and HSCC[19] studies demonstrated that Ps channels play an important role in forming unnatural parity states. Such resonances cannot be obtained by positron scattering with the ground-state hydrogen atom, but they can be accessed by the positron scattering with an excited-state hydrogen.

In the present paper, we report the new results for resonance states with unnatural parities in positron excited hydrogen collisions obtained employing the momentum space coupled channels optical method (CCO) for positron–atom scattering.[21] In the present method, the Ps formation rearrangement channels have been included via an equivalent local potential that is an *ab initio* complex potential. The method has been applied to calculations of scattering cross sections (positronium formation cross section, ionization cross section, integrate cross section, and total cross section) for a positron-ground state hydrogen system and obtained satisfactory results compared with experimental data and other theoretical calcu-

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†Corresponding author. E-mail: yajunzhou2003@yahoo.com.cn

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lation results.[21] The method has also been applied to study energy dependence in positron–hydrogen, helium and alkali atom collisions.[22–26]

Now this method is extended to study resonance states with unnatural parity in the positron scattering by the excited hydrogen. In the present work, 13 states (2, 3, 4, 5, 6p; 3, 4, 5, 6s; 3, 4, 5, 6d) of hydrogen are explicitly coupled (P space); the target continuum and Ps formation in their $n = 1$, $n = 2$, and $n = 3$ states are included in the channel couplings 2p–2p, 2p–3s, 3s–3s.

2. Model and method

The position of resonance energy can be determined by solving the coupled Lippmann–Schwinger equations in the momentum space:

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

where i, j represent target states, P projects a finite set of target states including the initial state $|0\rangle$ (in the present case, in its 2p state), and Q projects the continuum and the positronium formation channels. $V^{(Q)}$ has two parts, the channel-coupling potential V and the complex equivalent local polarization potential $W^{(Q)}$,

$$V^{(Q)} = V + W^{(Q)}, \quad (2)$$

$$W^{(Q)} = W_{\mathrm{I}}^{(Q)} + W_{\mathrm{Ps}}^{(Q)}. \quad (3)$$

Here $W_{\mathrm{I}}^{(Q)}$ and $W_{\mathrm{Ps}}^{(Q)}$ stand for the parts of the polarization potential that describe the ionization continuum and positronium formation rearrangement process, respectively. The model used for the matrix element of the polarization potential $W_{\mathrm{I}}^{(Q)}$ describing the continuum was given by McCarthy and Stelbovics.[27]

The positronium formation channel is described by the model:

$$|\chi_\mu^{(-)}\rangle = |\phi_\mu \boldsymbol{Q}\rangle, \quad (4)$$

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

The optical potential matrix for positronium formation channels is

$$\begin{aligned}&\langle \boldsymbol{k}'i|W_{\mathrm{Ps}}^{(Q)}|j\boldsymbol{k}\rangle \\ =\ &\sum_\mu \langle \boldsymbol{k}'i|V|\tilde{\chi}_\mu^{(-)}\rangle \frac{1}{E^{(+)}-\epsilon_\mu - k_{\mathrm{Ps}}^2}\langle \tilde{\chi}_\mu^{(-)}|V|j\boldsymbol{k}\rangle.\end{aligned}\quad (5)$$

Here

$$|\tilde{\chi}_\mu^{(-)}\rangle = \left(1-\sum_n |n\rangle\langle n|\right)|\chi_\mu^{(-)}\rangle. \quad (6)$$

$|\tilde{\chi}_\mu^{(-)}\rangle$ is orthogonalized to the 2p state of hydrogen, from which the electron is captured. A detailed calculation of the potential matrix element for positronium formation can be found in Ref. [21].

An 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

$$K = |\boldsymbol{k} - \boldsymbol{k}'|, \quad \frac{1}{2}k^2 = E - \epsilon_0. \quad (7)$$

The equivalent-local complex potential is calculated by a multidimensional method using Cartesian momentum variables.[27]

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

$$\langle k'n'l'L'||T_J||Llnk\rangle \quad (8)$$

for the total orbital angular momentum quantum number J by

$$\begin{aligned}&\langle \boldsymbol{k}'i|T|j\boldsymbol{k}\rangle \\ =\ &\sum_{L,M,L',M',J,K}\langle \hat{\boldsymbol{k}}'|L''M''\rangle C_{L'l'J}^{M'm'K} \\ &\times \langle k'n'l'L'||T_J||Llnk\rangle C_{LlJ}^{MmK}\langle LM|\hat{\boldsymbol{k}}\rangle,\end{aligned}\quad (9)$$

where

$$\langle \hat{\boldsymbol{k}}|LM\rangle \equiv Y_{LM}(\hat{\boldsymbol{k}}), \quad (10)$$

and C_{LlJ}^{Mmk} is a Clebsch–Gordan coefficient. The definition of $\langle k'n'l'L'||V_J^{(Q)}||Llnk\rangle$ is analogous to expression (8) with $V^{(Q)}$ substituted for T.

We consider J as implying two parity states: natural and unnatural states. In the present case, the initial state of target is in the 2p state of hydrogen, we may have n-parity (natural) $\Pi(L+l) = \Pi(J)$ or unnatural parity $\Pi(L+l) = \Pi(J+1)$. In the present work, we only calculated unnatural parity resonances.

The energies and widths of resonances for particular values of J have been found by fitting the Breit–Wigner form with a linear background

$$\sigma_{\rm R} = |aE + b + \frac{c + {\rm i}d}{E - E_{\rm R} + {\rm i}\Gamma_{\rm R}/2}|^2, \qquad (11)$$

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

3. Results and discussion

In the present work, resonance states with unnatural parities have been calculated for positron-excited hydrogen scattering over the energy region 0.06 eV–3.4 eV below the $n = 2$ ionization threshold of hydrogen at energy intervals of 0.0001 eV. The numerical results are shown in Tables 1 and 2, along with the results obtained by the method of complex-coordinate rotation of Yan and Ho[18] and the coupled-channel scheme in the hyperspherical coordinate system of Shimamura *et al.*[19] The lowest unnatural resonance state is located at energy position −0.1271 (Ry) with a width 1.4×10^{-5} (Ry) lying below the Ps ($n = 2$) threshold, which is very close to the result found by using the complex-coordinate method as well as hyperspherical close-coupling calculation. It has been pointed out that the unnatural parity resonance state is not a result of

Table 1. Energies $E_{\rm R}$ (Ry) and widths $\Gamma_{\rm R}$ (Ry) of $^{\rm e}{\rm P}$ resonances in e^+–H scattering. $x[y] = x \times 10^y$. $E_{\rm th}$ represents the threshold energy.

Threshold, $E_{\rm th}$	CCO[a]	Complex rotation[b]	HSCC[c]
	$E_{\rm R}$, $\Gamma_{\rm R}$	$E_{\rm R}$, $\Gamma_{\rm R}$	$E_{\rm R}$, $\Gamma_{\rm R}$
Ps ($n = 3$), −0.055556			
H ($n = 4$), −0.062466			
			−0.06256, 2.6[–6]
	−0.06301, 1.9[–5]	−0.06291, 1.4[–5]	−0.06286, 1.0[–6]
	−0.06500, 2.6[–5]	−0.06430, 3.8[–5]	−0.06422, 3.8[–5]
		−0.07116, 9.2[–5]	−0.07104, 9.2[–5]
H ($n = 3$), −0.11105			
	−0.1111, 2.5[–5]		−0.1111, 1.1[–7]
	−0.1121, 5.0[–7]	−0.1117, 2.4[–6]	−0.1116, 2.4[–6]
Ps ($n = 2$), −0.12500			
	−0.1271, 1.4[–5]	−0.1273, 8.2[–6]	−0.1273, 8.6[–6]
H ($n = 2$), −0.24986			

[a] Present calculation, [b] Ref. [18], [c] Ref. [19].

Table 2. Energies $E_{\rm R}$ (Ry) and widths $\Gamma_{\rm R}$ (Ry) of $^{\rm o}{\rm D}$ resonances in e^+–H scattering. $x[y] = x \times 10^y$. $E_{\rm th}$ represents the threshold energy.

Threshold, $E_{\rm th}$	CCO[a]	Complex rotation[b]	HSCC[c]
	$E_{\rm R}$, $\Gamma_{\rm R}$	$E_{\rm R}$, $\Gamma_{\rm R}$	$E_{\rm R}$, $\Gamma_{\rm R}$
Ps ($n = 3$), −0.055556			
H ($n = 4$), −0.062466			
	−0.06279, 5.9[–5]	−0.06275, 1.0[–5]	−0.06270, 3.4[–6]
	−0.06335, 2.3[–5]	−0.06323, 4.3[–5]	−0.06308, 4.0[–5]
	−0.06384, 7.1[–6]	−0.06379, 2.0[–5]	−0.06372, 2.0[–5]
		−0.06984, 6.0[–5]	−0.06970, 6.0[–5]
	−0.1051, 8.6[–4]		
	−0.1109, 7.3[–5]		
H ($n = 3$), −0.11105			
	−0.1111, 2.3[–7]	−0.1111, 2.0[–6]	−0.1111, 7.6[–6]
Ps ($n = 2$), −0.12500			
H ($n = 2$), −0.24986			

[a] Present calculation, [b] Ref. [18], [c] Reference [19].

dipole interaction due to the degenerate excited target states, while in this case it is most likely a result of an electron in its 2p positronium state interacting with the positively charged and infinitely massive proton[18] and the results of Shimamura *et al.*[19] show that the e^+H potential approaching the threshold Ps ($n = 2$) has a minimum and supports a bound state, which turns into a Feshbach resonance. The present calculation can provide strong evidence to support the viewpoint, since when we omitted the 2p positronium state in the optical potential, the resonance feature disappeared.

The second lower-lying P^e resonance state located in energy position -0.1121 (Ry) with a width 5×10^{-7} (Ry), which lies slightly lower than the results of Yan and Ho[18] and Shimamura *et al.*,[19] which located at -0.1117 and -0.1116 (Ry) energy positions, respectively. We found a resonance state lying at -0.1111 (Ry). This result is in excellent agreement with the result of Shimamura *et al.*,[19] but this resonance state has not been shown in the calculation of Yan and Ho.[18] Below the $n = 4$ excited threshold of hydrogen, we identified two unnatural P^e resonance states lying at energy positions -0.065 (Ry) and -0.06301 (Ry), which are very close to both calculation results of -0.0643 (Ry) and -0.06291 (Ry) of Yan and Ho,[18] as well as -0.06422 (Ry) and -0.06286 (Ry) from calculation results of Shimamura *et al.*[19] We have not found the resonance features at -0.07116 (Ry) from Yan and Ho's calculation[18] and -0.07104 (Ry) and -0.06256 (Ry) from the calculation of Shimamura *et al.*[19] The resonances (P^e) below the H ($n = 4$) excited threshold and above Ps ($n = 2$) threshold are members of infinite dipole series, and occurrence of the resonances is due to the decouplings of p–d states of excited hydrogen. Our calculations show that Ps states do not affect the existence of such dipole resonances even though the positions and widths may be changed.

For the D^o resonance states, we obtained a narrow resonance feature at -0.1111 (Ry) energy position, which is in excellent agreement with the results of Yan and Ho[18] and Shimamura *et al.*[19] We also identified two peak structures at -0.1109 (Ry) and -0.1051 (Ry), which did not appeared in the calculations of Yan and Ho[18] and Shimamura *et al.*[19] Below the threshold of H ($n = 4$), we found two D^o resonance states lying in energy position -0.06384 (Ry) and -0.06279 (Ry), which are very close to the results of Yan and Ho[18] and Shimamura *et al.*[19] We have obtained another resonance structure at energy position -0.06335 (Ry) with a width 2.3×10^{-5} (Ry), which is corresponding to resonance energy position -0.06323 (Ry) with a width 4.4×10^{-5} (Ry) from calculation of Yan and Ho[18] and -0.06308 (Ry) with a width 4.0×10^{-5} (Ry) from calculation of Shimamura *et al.*[19] Similar to the P^e case, we suggest that this resonance is also due to the interaction of Ps ($n = 3$) states with positively-charged ion via an attractive polarization potential, since when we omitted Ps ($n = 3$) states, then the resonance feature disappeared, while the resonances D^o lying below H ($n = 4$) threshold and above Ps ($n = 2$) threshold belong to the dipole series.

Comparing with the complex-rotation[18] and hyperspherical[19] calculations, the present results for the resonance position and width of each located resonance state are closer to the results of the complex-rotation calculation,[18] as shown in Tables 1 and 2. The slight differences between the present results and the HSCC[19] results are attributed to the mass-polarization effect, since the nucleus was fixed in space in both of the present CCO and the complex-rotation calculations.[18]

4. Conclusion

In summary, we have reported resonances with unnatural parities in the positron-excited hydrogen collisions. The present results of resonance parameters are in excellent agreement with previous calculations. Our findings confirm that there are nondipole-independent Feshbach resonances caused by positronium states interaction with hydrogen atoms due to the polarizability of the excited states of positronium. This is different from the positron-ground state hydrogen system, where only dipole resonance exists, and the opening of the Ps channels is of a short-range effect, which will not affect the existence of such dipole resonances even though the positions and widths may be changed.

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