Abstract

Hyperspherical close-coupling method is used to calculate the elastic, positronium formation and excitation cross sections for positron collisions with atomic hydrogen at energies below the H(n=4) threshold for the J=2 partial wave. The resonances below each inelastic threshold are also analyzed. The adiabatic hyperspherical potential curves are used to identify the nature of these resonances.

1. Introduction

The scattering between a positron and an atomic hydrogen is one of the simplest-looking quantum mechanical three-body problems. Yet it poses major challenge for theorists as well as for experimentalists over the years. The difficulty of formulating a satisfactory theoretical approach which accounts for all the possible inelastic transitions, including excitation, positronium formation, and ionization processes in a broad energy range is responsible for the slow progress in this field.

In the past, positron-hydrogen atom scattering has been treated theoretically using the standard methods generalized from electron-atom scattering, such as the close cou-
pling method [1-6], the R-matrix method [7], and the variational method [8-9]. There are some successes, especially in the lower energy region where few channels are open. As the collision energy increases the number of open inelastic channels increases rapidly and there are few results in the higher energy region where all the possible final channels are addressed.

An alternative approach, developed in the last few years for treating positron-hydrogen atom scattering, is the hyperspherical close coupling (HSCC) method. The HSCC has been initially developed for two-electron atomic systems [10], but has since been generalized to any three-body systems recently by Igarashi and Toshima [11], and by Zhou and Lin [12]. The basic formulation is similar to the earlier work of Archer et al [13] but the recent success of the HSCC method owes much to the improvement in the numerical accuracy which makes the detailed studies of this collision system possible.

The HSCC method has been used to study in details the J=0 and J=1 partial waves in $e^+ + H$ collisions in the energy region below the H(n=4) threshold [14]. Partial cross sections to each final state and the resonances below and near each inelastic threshold were examined. There are few inelastic cross sections available for comparison in the higher energy region except some recent ones from the close coupling method [3]. For the resonance parameters, calculations based on the complex coordinate rotation method [15,16] have been carried out for a number of states and they compare well with the results from the HSCC method [14]. The HSCC has also been used to show that there are no resonances in the positronium formation channel at energies above the ionization threshold [17]. This is a subject of great controversies [4,6,11,18-21]. The HSCC method also has been applied to calculate and compare resonances in the collision systems: $e^- + H$, $e^+ + H$ and $e^- + Ps$ [22]. In carrying out these calculations, the same set of codes are used since the HSCC method has been developed for the general three-body systems.
In this paper we report new results for the J=2 partial wave for the positron-hydrogen atom scattering using the HSCC method. The HSCC method is briefly reviewed in Section 2 and recent numerical implementations are addressed. The results for the calculated inelastic scattering cross sections and resonance parameters are presented in Section 3. Adiabatic hyperspherical potential curves are used to assist the interpretation of the calculated resonances. A final summary is given in Section 4.

2. The Hyperspherical Close Coupling Method

First we define the Jacobi coordinates of the three particles. There are three possible choices of the Jacobi coordinates, as depicted in Fig. 1. From each set of Jacobi coordinates, $\vec{\rho}_1$ and $\vec{\rho}_2$, a set of hyperspherical coordinates can be defined. In hyperspherical coordinates, the wavefunctions $\Psi$ are shown to satisfy

$$(-\frac{\partial^2}{\partial R^2} + H_{ad} - 2\mu E)\Psi(R, \phi, \hat{\Omega}) = 0,$$

where $R$ is the hyperradius, $\phi$ is the hyperangle and $\hat{\Omega}$ denotes collectively the four orientation angles of vectors $\vec{\rho}_1$ and $\vec{\rho}_2$. The adiabatic Hamiltonian $H_{ad}$ is the total Hamiltonian of the system in the center-of-mass frame evaluated at a constant value of the hyperradius and $\mu$ is a scaled mass.

In the HSCC approach, the hyperradius is divided into two regions at $R=R_0$. In the inner region $R \leq R_0$ where all the three particles interact with each other, the wavefunctions are to be expressed in terms of hyperspherical coordinates. In the outer region, the three-body system breaks into a single particle and a pair of particles in some bound states. In this outer region, the wave functions are appropriately expressed in terms of Jacobi coordinates for each arrangement.

In the so-called diabatic-by-sector method, the inner region is further divided into many small sectors. Within each sector, the wave function is expanded as
\[
\Psi(R, \phi, \hat{\Omega}) = \sum_\nu \sum_I F_{\nu I}(R) \Phi_{\nu I}(R_a; \theta, \phi) \tilde{D}_{I M_J}^J(\omega_1, \omega_2, \omega_3),
\]

(2)

where we have expressed the wave functions in the body-frame of the system, with the \(z'\)-axis chosen to be along the line connecting from the positron to the proton. The \(y'\)-axis is chosen to be perpendicular to the plane of the three particles and that the electron is always on the \(+x'\) side. In (2), the normalized \(D\)-function has good-parity [23], with the \(\omega\)'s being the Euler angles. The angle \(\theta\) is between the two vectors, \(\vec{\rho}_1\) and \(\vec{\rho}_2\), \(\phi\) is the hyperangle and \(\nu\) is the channel index. \(R_a\) is chosen at the midpoint of the sector, \(J\) is the total angular momentum, \(I\) is the absolute value of the projection of \(\vec{J}\) along the body frame's \(z'\) axis and running from 0 to \(J\) for \((-1)^J P = 1\) states and from 1 to \(J\) for \((-1)^J P = -1\) states, with \(P\) being the parity.

We solve the basis functions \(\Phi_{\nu I}(R_a; \theta, \phi)\) at \(R_a\) for a fixed \(I\) component on the \((\theta, \phi)\) plane using the finite-element method. The hyperradial function satisfies a set of coupled differential equations

\[
\left(-\frac{\partial^2}{\partial R^2} - \frac{1}{4R^2} - 2\mu E\right) F_{\mu I}(R) + \sum_{\nu J'} V_{\mu I, \nu J'}(R) F_{\nu J'}(R) = 0
\]

(3)

where the coupling matrix elements \(V\)'s are defined explicitly in Zhou and Lin [12].

In the practical implementation of the HSCC method, the set of hyperradial equations (3) are integrated within each sector. Starting with the innermost sector, the integration is continued until it reaches the boundary of the next sector. At this boundary, the total wave functions are expanded in terms of basis functions of the next sector from which integration within the next sector can be carried out. This procedure is continued from small hyperradius to \(R_0\) where the wave function is matched to an outside solution expressed in terms of independent electronic coordinates \(\vec{\rho}_1, \vec{\rho}_2\). From the matching, one can extract the K-matrix and the partial scattering cross sections.
\[ \sigma_{ij}^{(J)} = \frac{4\pi(2J+1)}{k^2} \left| \frac{K}{1 - iK} \right|_{ij}^2 \]  

where \( k \) is the momentum of the incident particle.

In order to be able to calculate excitation and positronium formation cross sections to excited states, the matching radius \( R_0 \) should be chosen at a relative large value, and the hyperspherical basis functions also have to be evaluated at large values of \( R \). In the large \( R \) region, the basis functions for the lower channels are located near the singularities of the potential surfaces. We improve the numerical accuracy by introducing two new angles which are more appropriate for describing the large \( R \) region, as discussed in Zhou and Lin [14]. Another complication due to the degenerate hydrogenic excited states is that the coupling among the different subshells in a given principal quantum number is quite large. To accommodate the interaction among the degenerate hydrogenic states, we use the dipole states of Gailitis and Damburg[24] and of Seaton[25]. The details of this transformation is also discussed in Ref. [14].

3. Results and Discussion

To obtain results for D wave scattering, the basis functions for the \( I=0, 1 \) and 2 components are first calculated. The matching radius is chosen at \( R_0=250.655 \) a.u. and 351 sectors are used in the inner region. Since we are interested in energies below the \( \text{H}(n=4) \) threshold, in the solution of hyperradial equations (3) we include 21 basis functions for \( I=0 \), 13 for \( I=1 \) and 9 for \( I=2 \). The basis set can be enlarged to achieve higher accuracy but at the expense of more computing time.

In presenting the results, we first mention that the thresholds, in increasing order, for \( \text{Ps}(n=1) \), \( \text{H}(n=2) \), \( \text{Ps}(n=2) \), \( \text{H}(n=3) \) and \( \text{H}(n=4) \) are located at 0.5, 0.75, 0.875, 0.8889 and 0.9375 Ryd, respectively, above the ground state of \( \text{H} \). There are resonances below each threshold.
3.1. Elastic and Ps(n=1) formation cross sections

In Fig. 2 we show the D-wave elastic and Ps(n=1) formation cross sections for positron scattering with atomic hydrogen in the energy region between 0.7 and 0.94 Ryd. Both cross sections change little in the whole energy region shown. There are resonance structures below each inelastic threshold, but pronounced ones are observed only below the H(n=2) threshold. In the figure we also show the close coupling results of Mitroy and Ratnavelu[3] where they performed close coupling calculations using six atomic states on each center. Their calculation will be denoted as CC(6,6). The results from the two calculations are in quite reasonable agreement.

The agreement in the elastic and Ps(n=1) formation cross sections between the two calculations, however, does not imply that the predicted resonance positions are identical. Both have calculated one Feshbach resonance below the H(n=2) threshold. The position and the width of this resonance are listed in Table 1. Note that the CC(6,6) results are quite different from the HSCC results. In similar comparison for the S- and P-waves results, the CC(6,6) results also show large discrepancies from the HSCC results in the resonance parameters. In those cases, the HSCC results are in good agreement with those obtained variationally using the complex coordinate rotation method[15,16]. The CC(6,6) results were different. We tend to believe that our results here are more accurate than those from the CC(6,6) calculations.

The HSCC method allows one to analyze qualitatively and semiquantitatively the resonance structures. In Fig. 3 we show the three adiabatic potential curves that converge to the H(n=2) threshold. Only one curve is attractive which can support Feshbach resonances. The position of the calculated resonance is shown as dotted lines in the figure. Note that one would expect an infinite series of resonances associated with the lowest curve since this potential approaches the threshold as $-0.81/R^2$. Such
a dipole potential can support an infinite number of resonances, but all the higher ones are very close to the threshold and were not examined.

3.2. Excitation cross sections to the 2s and 2p states

We show in Fig. 4 the D-wave excitation cross sections to 2s and 2p states. The results from the CC(6,6) calculations are also shown. Note that the results from the two calculations are again quite close, except in the resonance region. We have examined three resonances below the Ps(n=2) threshold. The positions and the widths are listed in Table 1 and the results for the first two are compared to the CC(6,6) results. Again the discrepancy is quite significant.

Our calculations show small structures near the H(n=2) threshold. We suspect that these structures are due to the relatively small basis functions used in this calculation.

We also show in Fig. 5 the three adiabatic potential curves that converge to the Ps(n=2) threshold. Note that the lowest curve is rather attractive. In fact, it behaves as $-17.49/R^2$ asymptotically. Note that the second curve in Fig. 5 has a small attractive part in the inner region, but the potential well is not strong enough to support a resonance.

3.3. Ps(n=2) formation cross sections

The cross sections for the positronium formation cross sections to 2s and 2p states are shown in Fig. 6. These cross sections are quite small, about 0.5% of the cross sections for the elastic and the Ps(n=1) cross sections, and about 10% of the n=2 excitation cross sections. The resonances are quite pronounced in these small channels. The resonance positions and widths below the H(n=3) threshold are studied and the results are shown in Table 1. There are no other calculations available for comparison in this energy range.

3.4. Excitation cross sections to n=3 states
The excitation cross sections to H(n=3) states have also been calculated. The results are shown in Fig. 7. These cross sections are about a factor of two smaller than the Ps(n=2) cross sections in the same energy region. The resonances are quite pronounced at energies below the H(n=4) threshold and the positions and widths of the five lowest resonances are shown in Table 1.

There are no other calculations available for comparison. The small structures near the threshold are likely due to the small number of hyperspherical channels used in the present calculation.

Careful analysis of the resonances at the higher thresholds is more difficult due to the numerous avoided crossings. For example, we show in Fig. 8 some of the adiabatic curves that converge to the H(n=3) threshold. We also show that the uppermost curve which converges to the Ps(n=2) limit has many avoided crossings with the H(n=3) curves.

4. Summary

In this paper we present D-wave results for the excitation and positronium formation cross sections in positron-hydrogen atom collisions at energies below the H(n=4) threshold using the hyperspherical close coupling method. There are few calculations available for comparison in the higher energy region considered in this paper. Together with our previous results for the S- and P-wave, we illustrated that the hyperspherical close coupling method provides a very powerful method for treating general rearrangement collisions. Calculations including the ionization channels are underway which would allow the HSCC method to be extended to the higher energy region. The method can be generalized to collisions between positrons and alkali atoms by employing a model potential description of the target atom.
Acknowledgements

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Table 1. Positions and widths of D-wave resonances below different inelastic thresholds for the $e^+ + H$ collision system. The present results are from the HSCC calculation, while the CC(6,6) results are from the close coupling calculation of Mitroy and Ratnavelu [3]. The energies and half widths are in units of Rydbergs.

|                      | present                  | CC(6,6)              |
|----------------------|--------------------------|----------------------|
|                      | E(Ryd)                   | $\frac{1}{2}\Gamma$(Ryd) | E(Ryd) | $\frac{1}{2}\Gamma$(Ryd) |
| Below H(N=2) Threshold | -0.250031 1.65(-6)       | -0.25006 3.9(-4)     |
| Below Ps(N=2) Threshold | -0.143429 1.66(-4)       | -0.13715 1.25(-4)    |
|                      | -0.128529 6.66(-5)       | -0.12765 3.3(-4)     |
|                      | -0.12503 6.32(-6)        |                      |
| Below H(N=3) Threshold | -0.114529 4.79(-4)       |                      |
|                      | -0.111630 7.89(-5)       |                      |
| Below H(N=4) Threshold | -0.075582 6.27(-5)       |                      |
|                      | -0.069775 6.76(-5)       |                      |
|                      | -0.066940 4.70(-5)       |                      |
|                      | -0.064103 1.39(-5)       |                      |
|                      | -0.063855 2.74(-5)       |                      |
Figure Captions

Fig. 1. Three sets of Jacobi coordinates for the three particle system.

Fig. 2. D-wave elastic and Ps(n=1) formation cross sections for positron scattering with atomic hydrogen. Elastic cross sections: solid lines, present results; dotted lines, from CC(6,6)[3]. Ps(n=1) formation cross sections: long dashed lines, present results; dash-dotted lines, CC(6,6). The two results for the Ps(n=1) formation are almost indistinguishable. The sharp structures are due to the resonances below each inelastic threshold.

Fig. 3. D-wave adiabatic potential curves that converge to the H(n=2) threshold. The position of the lowest Feshbach resonance is indicated by the dotted lines.

Fig. 4. D-wave excitation cross sections to 2s and 2p states for positron scattering with atomic hydrogen. Excitation to 2s: solid line, present result; dotted lines, CC(6,6)[3]. Excitation to 2p: long dashed lines, present results; dash-dotted lines, CC(6,6).

Fig. 5. D-wave adiabatic potential curves that converge to the Ps(n=2) threshold. The position of the first Feshbach resonance is indicated by the dotted lines.

Fig. 6. D-wave positronium formation cross sections to 2s and 2p states for positron scattering with atomic hydrogen obtained from the present calculation: solid line for Ps(2s) and dotted lines for Ps(2p).

Fig. 7. D-wave excitation cross sections to H(3s), H(3p) and H(3d) states for positron scattering with atomic hydrogen. Solid line: excitation to 3s; dotted lines: excitation to 3p; dashed lines: excitation to 3d.

Fig. 8. D-wave adiabatic potential curves that converge to the H(n=3) threshold. The uppermost curve converging to Ps(n=2) is also shown.
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