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LETTER TO THE EDITOR

On the non-existence of resonances above the ionization threshold in positron–hydrogen scattering

Yan Zhou and C D Lin
Department of Physics, Kansas State University Manhattan, KS 66506, USA

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Abstract. The hyperspherical close-coupling method is applied to obtain both the elastic and positronium-formation cross sections for positron collisions with atomic hydrogen at energies above the ionization threshold for the $J = 0$ and $J = 1$ partial waves. In contrast to many previous results from the standard close-coupling calculations, no resonance structures were found in the present results and the cross sections were found to vary smoothly with collision energies. A possible explanation for the occurrence of 'resonances' in previous calculations is also proposed.

The scattering of positrons on atomic hydrogen has long been a subject of great theoretical interest. It is a simple Coulomb three-body system where rearrangement processes can be studied. Many theoretical tools that have been shown to be useful in electron–atom collisions have been extended to study positron–hydrogen atom scatterings. For the low-energy region, where only a small number of channels are open, it has been shown that variational methods (Humberston 1986) and large-scale close-coupling calculations (Mitroy 1995) are capable of obtaining accurate cross sections for elastic scattering and positronium-formation to the ground state. Similar accurate results have also been obtained using the hyperspherical close-coupling method (see, for example, Archer *et al* (1990), Igarashi and Toshima (1994) and Zhou and Lin (1994)).

In recent years, there have been many papers addressing the unexpected resonance structures in the positronium-formation cross section at energies above the ionization threshold in positron–hydrogen atom collisions. A resonance at about 35.6 eV was 'discovered' originally by Higgins and Burke (1991) in the s-wave cross section in the positronium-formation channel using the R-matrix method. This resonance was 'confirmed' in the close-coupling calculation by Hewitt *et al* (1991) using the close-coupling method in momentum space and also by Gien (1994) using the algebraic variational method. Similar calculations were extended to higher partial waves by Higgins and Burke (1993) and Mitroy (1994) and more 'resonances' were found in these calculations.

Despite the repeated 'confirmation' of these 'resonances', their origin is always under suspicion. The positions and widths of the 'resonances' change rapidly as the basis-set size is enlarged. In most of the close-coupling calculations, only the H (1s,2s,2p) and Ps (1s,2s,2p) states are included in the basis expansion. In others, some limited number of pseudostates were included to simulate the polarization effect. In the most complete close-coupling calculation to date, Kernoghan *et al* (1994) includes H (1s,2s,$\overline{3}$s,$\overline{4}$s,2p,$\overline{3}$p,$\overline{4}$p,$\overline{3}$d,$\overline{4}$d) and Ps

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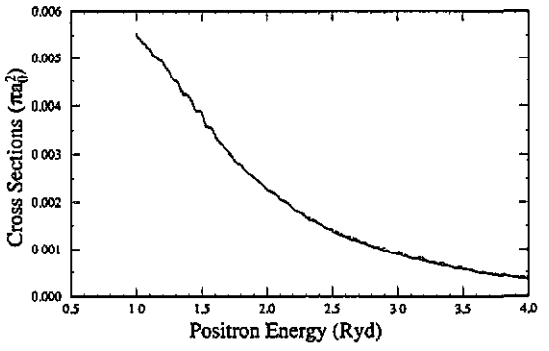

Figure 1. Positronium-formation cross sections to Ps (1s) state in positron–hydrogen scattering in the s-wave. The number of hyperspherical channels used in the calculations are 30 (broken curve) and 40 (full curve).

(1s,2s,$\overline{3s}$,$\overline{4s}$,2p,$\overline{3p}$,$\overline{4p}$,$\overline{3d}$,$\overline{4d}$) basis functions (the bars refer to pseudostates) in an 18-state close-coupling scheme. Their results indicate that these 'resonances' disappear for $J = 0$ and $J = 1$, but many structures are still evident in the $J = 2$ calculation. They attributed that the 'resonances' in earlier calculations are the result of neglecting the ionization channels in the close-coupling expansion. This interpretation, while plausible, is still unsatisfactory. The ionization cross section in the energy region considered is expected to be a smooth function as energy is varied. While the lack of ionization channels in the basis set can change the magnitude of the positronium formation cross sections, the influence is expected to vary smoothly with collision energies without any sharp features.

In this letter we present results of elastic and positronium formation to Ps ($n = 1$) cross sections for $J = 0$ and 1 in the energy region above the ionization threshold using the hyperspherical close-coupling method. The method has been applied to the lower-energy region to study excitation and positronium-formation cross sections (Zhou and Lin 1995). We extend the method to the energy region above the ionization threshold to illustrate that there are no 'resonances' in our results, independently of how many hyperspherical basis functions are used in the calculation. Our results are in agreement with the earlier work of Igarashi and Toshima (1994) where they performed calculations using a smaller basis set and much coarser energy meshes. They did not observe any 'resonances' in their calculation either.

The hyperspherical close-coupling method used in the present work has been described previously (Zhou and Lin 1994). The hyperradius is separated into two regions: an inside region where the wavefunctions are expanded in hyperspherical coordinates and an outside region where the wavefunctions are expressed in terms of Jacobi coordinates of the two arrangements, i.e. $e^+ + H$ and $p^+ + Ps$. In the inside region we use the diabatic-by-sector method, where the basis functions within each sector are the adiabatic hyperspherical surface functions at the midpoint of the sector. In the outside region, the basis functions are hydrogenic and positronium states as used in the close-coupling calculation.

In figure 1 we show the calculated positronium-formation cross section in the energy range of 1–4 Rydbergs for the $J = 0$ partial wave. The matching radius was set at R_0= 76.655 au and we have performed calculations using 20, 30 and 40 channels in the inside region. In the outer region, we include H (1s,2s,2p,3s,3p,3d) and Ps (1s,2s,2p) states. *It is clear that the cross section drops smoothly with increasing energies.* There are small ripples (of a few % in relative magnitude) but they are believed to be due to the lack of basis functions representing the ionization channels in the outside region. Calculations are underway to include ionization channels using pseudostates in the outer region. We have also checked the cross sections by doing the matching at a larger hyperradius, but the cross sections are always stable to within a few %. For this process, resonances were reported by Higgins and Burke (1993), Gien (1994) and Mitroy and Stelbovics (1994).

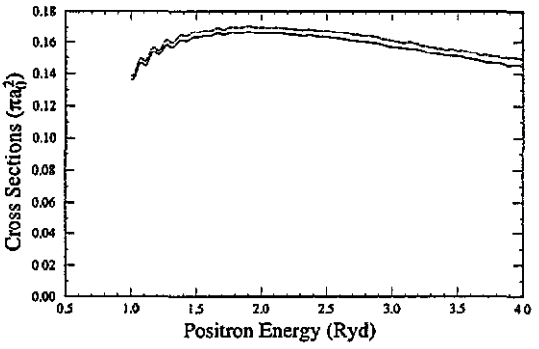

Figure 2. Elastic-scattering cross section in positron–hydrogen scattering in the s-wave. The number of hyperspherical channels used are 30 (broken curve) and 40 (full curve).

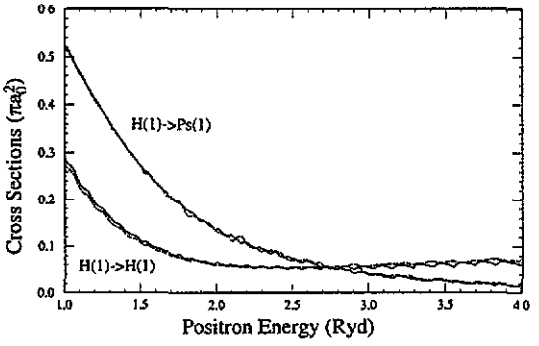

Figure 3. P-wave elastic and positronium-formation to Ps (1s) cross sections in positron–hydrogen-atom scattering. The number of hyperspherical channels used are 25 (broken curves) and 34 (full curves).

In figure 2 we show the s-wave elastic-scattering cross sections above the ionization threshold. The dependence on the number of channels used in the inner region is more sensitive and the ripples are removed only when the number of basis functions is above 30, but again *there is no indication of any resonances*; while Higgins and Burke (1991), Hewitt *et al* (1991), Gien (1994) and Mitroy (1994) observed resonant structures in this region.

In figure 3 we show the p-wave elastic and positronium-formation cross sections in the energy region above the ionization threshold. The matching radius was chosen again at 76.655 au, and 25 and 34 channels in the inside region were used, while in the outer region we included H (1s,2s,2p,3s,3p,3d) and Ps (1s,2s,2p) states. *Both cross sections show smooth variation with energy except of the small ripples as noted previously.* Resonances were observed in the R-matrix calculations of Higgins and Burke (1993).

'Resonances' have also been observed in scattering from the Ps ground state by protons in the p-wave, as predicted in the calculation of Mitroy and Stelbovics (1994). In figure 4 we show the elastic-scattering cross section for such a collision process using a similar basis set (only the $N = 34$ for the inside region is shown). Clearly there is no structure in the whole energy region covered.

From the results discussed above, we believe that there are no resonances of any type for positron scattering on atomic hydrogen at energies above the ionization threshold in any elastic or inelastic channels. From the hyperspherical point of view, there are no adiabatic potential curves which show potential barriers way above the ionization threshold. The 'resonances' which appeared in all the two-centre close-coupling calculations are likely to be spurious results. They are not the results of numerical errors, but are the consequence of the method itself. As to why the 'resonances' appear in these calculations, we offer the

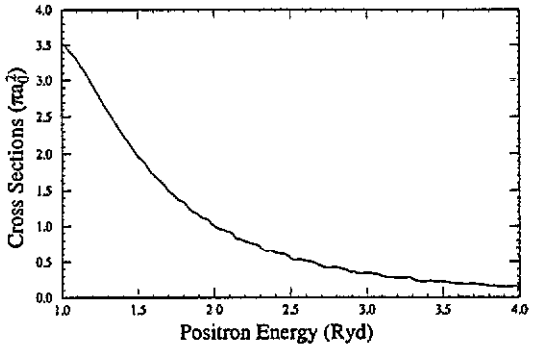

Figure 4. P-wave elastic-scattering cross section for protons colliding with Ps (1s). The results shown are from calculations using 34 hyperspherical channel functions.

following plausible interpretation.

In the close-coupling calculation, atomic orbitals on both centres (meaning H and Ps pairs) are employed in the basis set. These orbitals are not orthogonal at any finite separation of the system. In the region where the particles are close together, atomic orbitals from one centre appear to be like pseudostates (bound states in the continuum) with respect to the other centre. The 'resonances' found in the close-coupling calculations may be due to 'Feshbach resonances' associated with these pseudostates. When the basis set is enlarged, the positions of the pseudostates are shifted and thus the 'resonances' are displaced as well. In this way, the 'resonances' observed in the calculations are similar to those seen in earlier close-coupling calculations for electron–atom collisions when pseudostates are used in the basis functions. In the latter, the energies of the pseudostates are known and pseudoresonances are easily identified. In positron–atom scattering, the energies of the pseudostates vary with the separation between the proton and the positron, as well as with the basis set included. By increasing the number of states on the two centres (including pseudostates), additional new resonances may appear at higher energies. One should be able to show that 'resonances' appear *only* when atomic states on both centres are used in the expansion. We believe that any single centre expansion would not result in 'resonances' in the elastic and direct excitation cross sections above the ionization threshold.

In summary, we show that the cross sections for elastic and positronium-formation cross sections above the ionization threshold are smooth functions of collision energies. We employed the hyperspherical close-coupling method to obtain these cross sections and no 'resonances' were observed. We speculate that the 'resonances' obtained in all the close-coupling calculations are most likely due to the two-centre basis functions which are not orthogonal, and the basis set from one centre may appear as pseudostates in another resulting in resonances which are pseudoresonances in nature.

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