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Positron-hydrogen scattering: internal consistency and threshold behaviour for excited states

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Abstract. The positron-hydrogen collision system is considered with the one- and two-centre convergent close-coupling methods with a particular focus on initial excited states. The previous limitation on the two-centre method, restricting the Laguerre basis size, has been removed allowing for larger bases, which is necessary for the examination of the near-threshold cross section behaviour for three-body breakup. Excellent agreement with the Wannier–Klar predictions for these systems is found for initial states with principal quantum number $n \leq 3$. The accuracy of the presented cross sections is supported by demonstrating internal consistency of the one- and two-centre calculations.

1 Introduction

We appreciate the opportunity to contribute to the special issue in tribute to Professor Michael Brunger. It was with great sadness that we learned of Michael's serious illness and untimely passing. He has been a stalwart of our field since his Ph.D. days at Flinders University during the mid 1980s. One of us (I.B.) has known him as both a friend and collaborator soon after arriving at Flinders in 1985. Michael was an extraordinary individual who was single-minded and very goal-oriented. His great focus on achievement has resulted in an extraordinary publication list with a very diverse set of coauthors and topics. His ability to keep progress on track to ensure timely contributions from all concerned was particularly effective. His dedication to students and academic values was admirable. We are forever grateful to have known Michael, and he will be sorely missed. One area where Michael made a substantial contribution is the area of positron scattering. We dedicate the following positron scattering work to his memory.

The three-body e^+-H and the equivalent Ps-p^+ systems have been recently studied extensively theoretically by fully quantal and classical methods [1–7]. The fully quantal, two-centre convergent close-coupling method of [8], was utilised across the full energy range considered, including the most challenging region of just above the three-body breakup threshold. In order to establish convergence in this region large Laguerre bases are required for the generation of sufficiently many low positive-energy pseudostates in the target expansion, before solving the arising close-coupling equations. While this is not a problem in the case of the one-centre convergent close-coupling (CCC) calculations of electron or positron scattering, the two-centre positron scattering requires very complicated matrix elements whose evaluation required special analytical techniques in order to make the calculations tractable [8]. This created the limitation that the Laguerre basis size $N_\ell \leq 30$, whether for the atomic or the Ps orbital angular momentum ℓ. While this was not a substantial problem for the ground state [2,7], the application to excited states did not result in sufficiently accurate results for near-threshold breakup cross sections [7].

Here we report the removal of the analytical limitations in the original two-centre positron scattering CCC implementation [8], and provide cross sections for near threshold behaviour, which can be demonstrated to agree with the predictions of the Wannier threshold theory [9] as implemented by [10] for the positron projectiles. Furthermore, we check the new two-centre calculations by comparison with their single-centre counterparts and thereby demonstrate the internal consistency of the CCC formalism for excited states, as well as the ground state done previously [11,12].

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2 Convergent close-coupling theory

The CCC theory was initially developed for the electron-hydrogen collision system [13]. Briefly, the atomic target wave-functions are obtained via diagonalisation of the target Hamiltonian in a Laguerre basis. With increasing basis size N_ℓ, where ℓ is the target state orbital angular momentum, the negative-energy states converge to the true discrete eigenstates, while the positive-energy pseudostates provide an increasingly dense discretisation of the target continuum. Collectively, the usage of the Laguerre basis induces a quadrature rule for the infinite sum over the discrete subspace and an integration over the target continuum. Convergence is obtained by simply increasing $\ell_{\max}$ and N_ℓ for $0 \leq \ell \leq \ell_{\max}$.

The single-centre application to positron scattering on atomic hydrogen simply starts with the electron-impact implementation, changes the sign of the potentials, and drops the exchange matrix elements. The first such implementation [14] showed that low-energy phaseshifts were correctly reproduced so long as $\ell_{\max}$ was sufficiently large (up to 15). This followed by application at higher energies for the breakup cross section [15] resulting in support of one experiment over another. Together, these show the utility of the single-centre CCC approach to positron scattering, with the effects of positronium (Ps) formation being treated indirectly by the positive-energy pseudostates. However, there is the limitation that the method is unable to distinguish between the Ps-formation and breakup cross sections, and is unable to yield convergent cross sections in the small energy region (extended Ore gap) between the Ps-formation and breakup thresholds. It also is unable to yield the Ps($n\ell$)-H($n'\ell'$) rearrangement transitions, which are necessary for application to anti-hydrogen formation calculations, see [6] for example.

The two-centre CCC implementation [8] for positron scattering has an explicit inclusion of Ps states, and thereby eliminates the above-mentioned limitations of the single-centre CCC approach. However, the Ps-H matrix elements are particularly complicated, see Sect. IIC of [8]. To make things computationally tractable, analytical expansions of the Laguerre basis were utilised. However, as is often the case with analytical expansions, the expansion coefficients become large and oscillate in sign, potentially leading to precision loss. For this reason, explicit coding was done only for Laguerre bases with $N_\ell \leq 30$. While this was not a major limitation in general, the study of near-threshold breakup requires a sufficiently large number of positive-energy states to ensure convergence, see [2] for example. This issue becomes particularly problem-

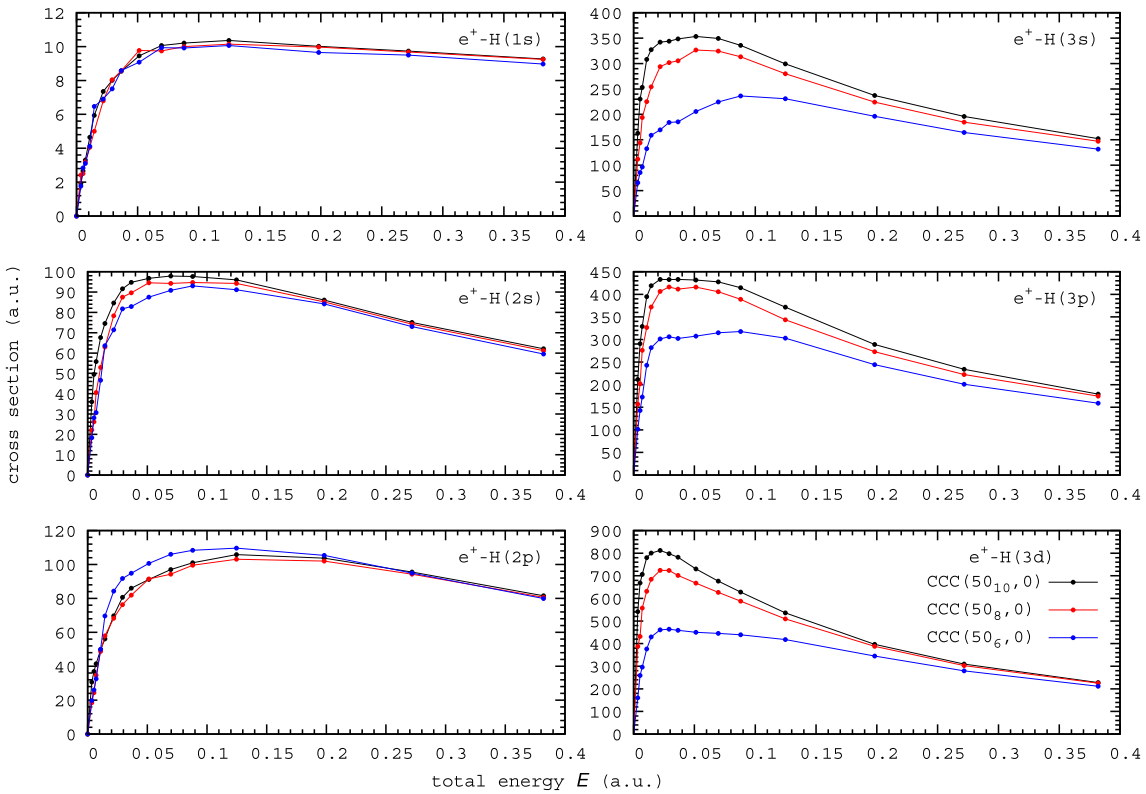

Fig. 1 Positron-impact total electron-loss (breakup plus Ps-formation) cross sections arising in single-centre CCC calculations, see text for details. The calculations have been performed at the total energies specified by the dots, which have been connected by straight lines to help guide the eye. A single CCC calculation at a total energy E yields the presented results for all of the specified initial states

atic in the case of excited initial states, where the range of validity of Wannier-like behaviour is diminished [7].

We have now removed the requirement of analytic expansions when evaluating Eqs. (48) and (49) in Sect. IIC of [8]. Instead, the two equations are calculated on a very large momentum p grid, for all of the required quantum numbers, while taking care of the analytical behaviour as $p \to 0$, and $p \to \infty$. Subsequently, a five point interpolation rule is utilised to extract an accurate result at all required values of p. High accuracy is required in the calculation of the two-centre matrix elements as the subsequent close-coupling equations are particularly ill-conditioned. The new implementation is similar in the amount of computer time it requires, and the level of precision is sufficient. The numerical implementation also has the benefit of allowing the usage of bases other than the Laguerre one, such as the box basis, already used for calculating electron-impact breakup cross sections of atomic hydrogen [2].

3 Results

Even though the single-centre calculations do not have explicit inclusion of Ps formation, such calculations allow us to establish internal consistency with two-centre calculations, which do include Ps formation explicitly. For example, above the breakup threshold the sum of the cross sections for excitation of the positive-energy states in the single-centre CCC should converge to the sum of Ps-formation and breakup (electron-loss) cross sections. We begin our presentation by looking at the convergence of single-centre calculations, which are labeled as CCC($N_{\ell_{\max}}$, 0), indicating that $0 \le \ell \le \ell_{\max}$ and $N_\ell = N_{\ell\max} - \ell$, and that there are zero Ps states explicitly included.

In Fig. 1 the positron-impact total electron-loss cross sections are presented, for $n \le 3$ initial states H($n\ell$), as functions of total energy E (positron energy plus the energy of the initial target state). These are the sum of cross sections for all open positive-energy pseudostates, and correspond to the physical process of breakup (sometimes referred to as direct ionization) together with Ps formation. As the true breakup cross section is zero at the $E = 0$ threshold, in the energy region just above the threshold the single-centre CCC cross sections yield predominantly Ps formation. In other words, as the Laguerre bases N_ℓ and $\ell_{\max}$ are increased, the sum of the positive-energy cross sections should converge to a step-function at the $E = 0$ threshold, with the height of the step being the Ps-formation cross section. Though with finite bases it is not possible to reproduce a step-function, we do see a rapid rise in the cross sections past the threshold. There is clear convergence with increasing $\ell_{\max}$, though slower

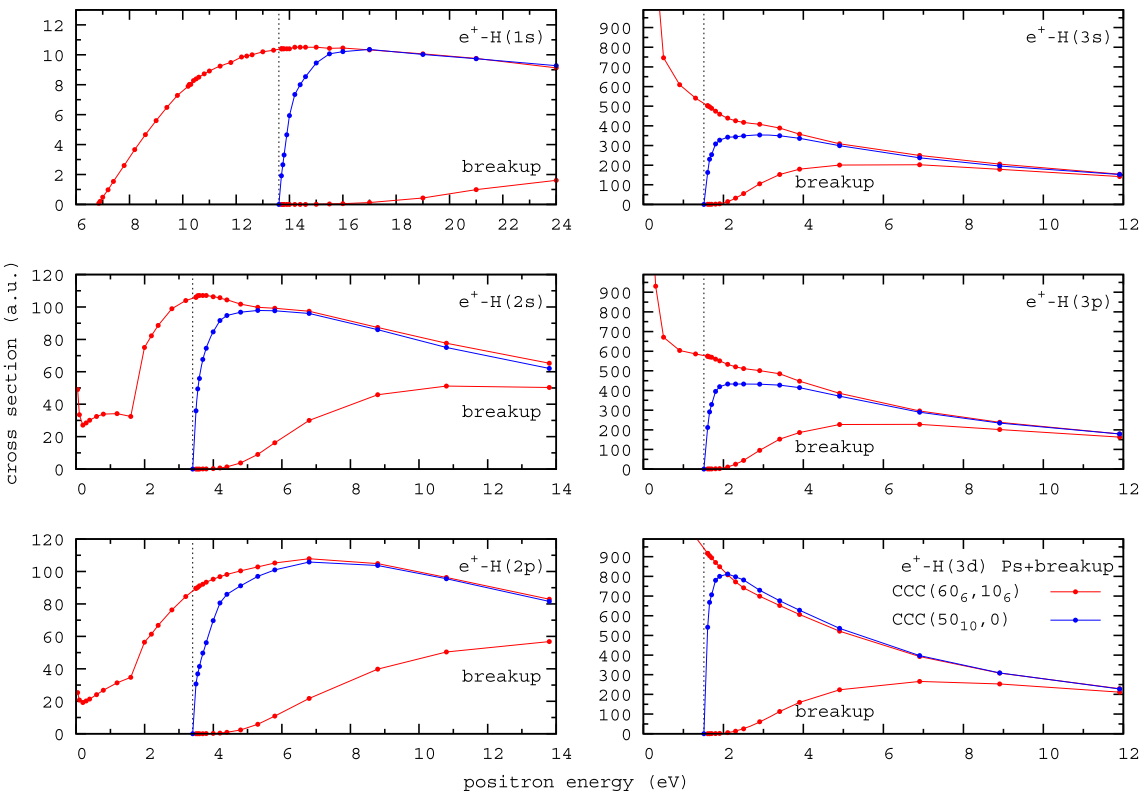

Fig. 2 Electron-loss (Ps-formation plus breakup) cross sections for positron-hydrogen scattering obtained from the CCC(50_{10}, 0) and CCC(60_6, 10_6) calculations, see text. The breakup component in the CCC(60_6, 10_6) calculation is given separately. The vertical dashed line indicates the breakup threshold

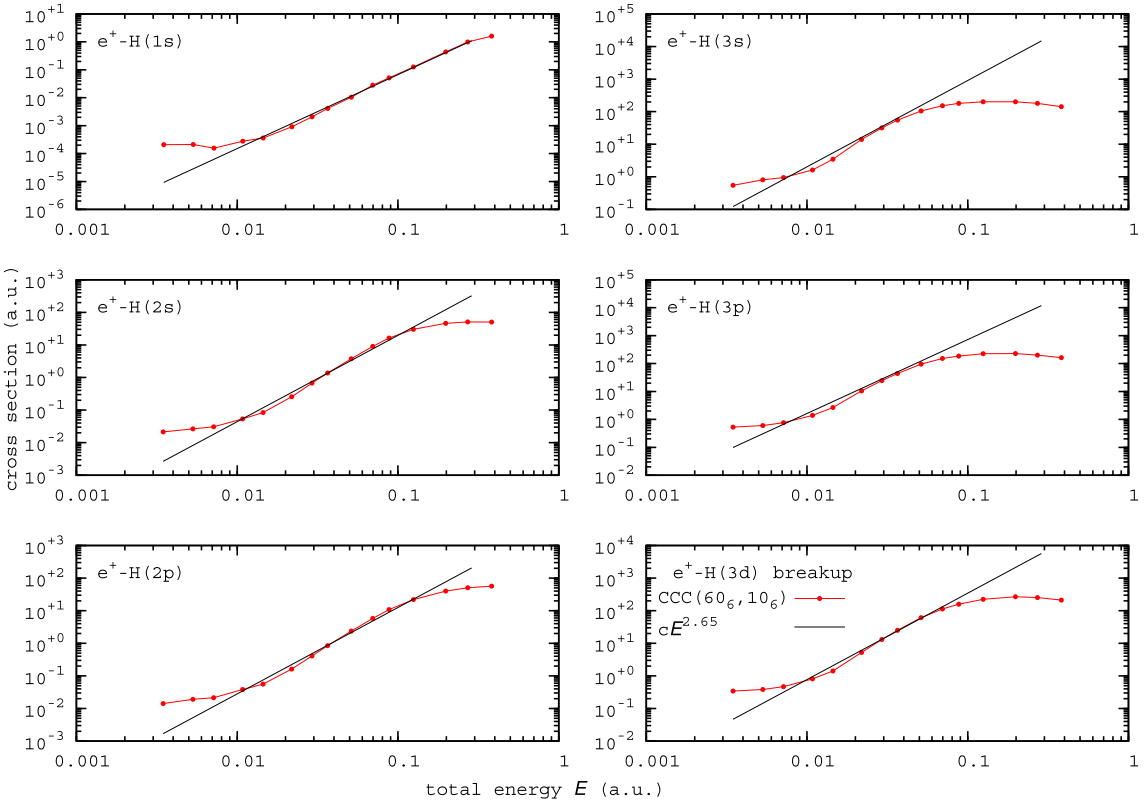

Fig. 3 The total breakup cross section in positron scattering on hydrogen for the specified initial states arising in CCC$(60_6, 10_6)$ calculations, see text. Comparison with the $E^{2.65}$ behaviour predicted by [10] is presented, with the constant of proportionality c chosen by best visual fit for each initial state

for the excited states, which are required to adequately model Ps formation in the single-centre CCC calculations. We shall use the largest, CCC$(50_{10}, 0)$, calculation for the internal consistency check of the two-centre calculations.

Our goal in performing the two-centre positron-hydrogen calculations is to obtain convergent results in the near-threshold region for the breakup cross section, and to compare this to the Wannier-like $E^{2.65}$ behaviour predicted by [10]. As such cross sections are particularly small, the challenge to calculate them accurately is immense. We found that the most computationally stable way of obtaining such cross sections is to take a large Laguerre basis on the H centre, as in single-centre calculations, and a box-basis on the Ps centre while keeping only the negative-energy states. The box basis size R_0 was varied to obtain sufficiently many negative-energy states to establish convergence in the breakup cross sections for comparison with the $E^{2.65}$ behaviour. We found $R_0 = 300$ to be sufficient for our purpose, resulting in $10 - \ell$ negative-energy Ps states, with the final results coming from calculations labeled as CCC$(60_6, 10_6)$.

In the CCC$(60_6, 10_6)$ positron-hydrogen calculations, Ps-formation cross sections arise from the excitation of the included Ps states, while the breakup cross section is obtained from the cross sections for excitation of the positive-energy hydrogen states. The sum of the separate Ps-formation and breakup cross sections can be compared with the total ionisation (electron loss) cross section arising in the single-centre calculations, as a check of internal consistency. Note also, that since such calculations are equivalent to Ps$(n\ell)$-p^+ scattering, we also obtain the Ps$(n\ell)$ breakup cross sections in exactly the same way, from the positive-energy hydrogen states. These can also be checked for Wannier-like behaviour.

Before considering the breakup cross sections individually, in Fig. 2 we compare the CCC$(50_{10}, 0)$ and CCC$(60_6, 10_6)$ calculations for the electron-loss cross sections. We see that, away from the breakup threshold there is good agreement between the two calculations for all initial states. From the smallness of the breakup cross sections in the near threshold regions we see that the single-centre results correspond to predominantly Ps formation. At the highest energies considered we see that breakup dominates Ps formation. Note that below the breakup threshold only the two-centre calculation is able to obtain Ps-formation cross sections. In this energy region single-centre calculations only yield (non-convergent) hydrogen excitation and elastic scattering cross sections.

We are now in a position to check the breakup cross sections arising in the CCC$(60_6, 10_6)$ calculations against the $E^{2.65}$ behaviour predicted by [10]. We begin with the positron-impact breakup of hydrogen, pre-

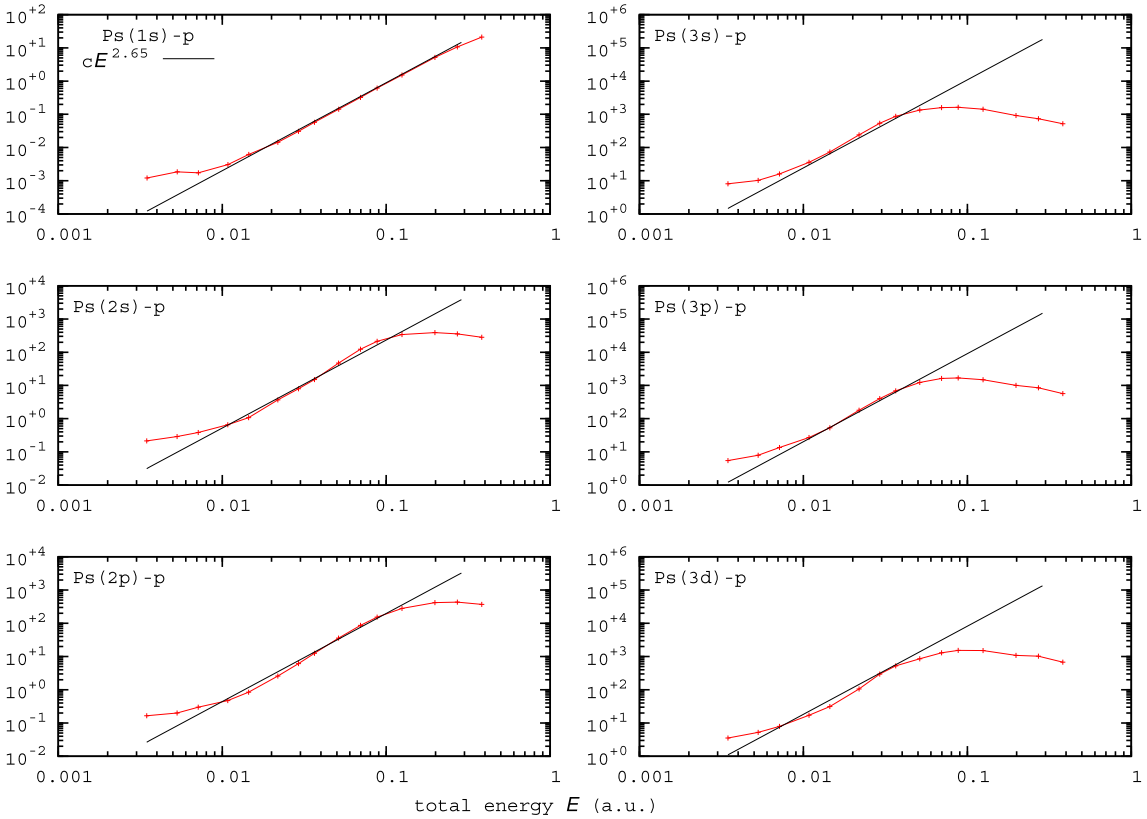

Fig. 4 The total breakup cross section for Ps($n\ell$)-p^+ scattering arising in CCC($60_6, 10_6$) calculations, see text. Comparison with the $E^{2.65}$ behaviour predicted by [10] is presented, with the constant of proportionality chosen by best visual fit for each initial state

sented in Fig. 3. These are the same cross sections presented in Fig. 2, except now on a log-log scale and against the total energy E. Comparison with the $E^{2.65}$ behaviour is very good for all initial states, and as stated by [7], the range of validity diminishes (as n^{-2}) with increasing n. Note that we also presented the problematic results at the lowest energies to demonstrate that there are limits to the accuracy of the calculations as $E \to 0$.

The CCC($60_6, 10_6$) calculations, simultaneously with the above, produce breakup cross sections for Ps($n\ell$)-p^+ scattering. These are given in Fig. 4, and compared with the $E^{2.65}$ behaviour. Once again we see excellent agreement, with the energy range of agreement diminishing with increasing n.

4 Conclusions

The two-centre CCC method for positron scattering has been enhanced by the removal of limits on the size, and type, of bases used in calculating the underlying atom-positronium matrix elements. This allowed us to perform sufficiently large calculations in the energy region just above the breakup threshold with sufficient accuracy to demonstrate agreement with the Wannier-like $E^{2.65}$ behaviour predicted by [10] for all initial states of H($n\ell$) and Ps($n\ell$) with $n \leq 3$. As expected, the range of validity of the $E^{2.65}$ behaviour diminishes with increasing n.

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Author contributions

The lead author performed the calculations and wrote the original manuscript, the others contributed ranging from assisting with code development, developing the underlying concepts through to reading and improving the manuscript.

Data Availability Statement This manuscript has no associated data or the data will not be deposited. [Authors' comment: Quantitative data presented in the figures may be obtained via an electronic scan, or requested from the lead author.]

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