Positron-impact ionisation of hydrogen near the threshold

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Abstract. The near-threshold behavior for positron-impact ionization (breakup) of hydrogen is considered. The two-centre convergent close-coupling method is used. We find that convergence in the cross section is only practically obtained if two near-complete expansions are used, one centred around H and the other around Ps. The contribution to the breakup cross section becomes the same for both centres as the threshold is approached. The calculations are found to be in good agreement with the threshold law predicted by Ihra et al. [Phys. Rev. Lett. 78, 4027 (1997)].

1. Introduction
Following the work of Wannier [1], electron-impact ionisation threshold laws have been studied extensively in semi-classical [2, 3, 4] and fully quantum-mechanical [5, 6] approaches. However, the corresponding positron-impact ionisation problem has received relatively little attention. Klar [7] extended the Wannier theory to the positron-hydrogen case quite some time ago. This semi-classical work was broadened by Ihra et al. [8] employing the hidden crossing theory for application over a larger energy range. The first fully quantum mechanical study has been presented [9] only very recently, utilising a two-centre convergent close-coupling (CCC) method. Here we give an overview of these results and provide some extra detail.

2. Convergent close-coupling method
The implementation of the CCC method to positron-hydrogen collisions was given by Kadyrov and Bray [10]. There full calculations were presented over a broad energy range and compared with various experiments. One of these was the measurement of the total breakup cross section by Jones et al. [11]. This cross section denotes the process where after the collision the three particles remain free, i.e. it excludes Ps-formation. In the two-centre CCC method this cross section arises from excitation of the positive-energy H- and Ps-states. A question of fundamental interest is how do these two contributions behave depending on the choice of the close-coupling (CC) expansion.

Historically, owing to computational limitations, the CC expansions included just a few lowest lying target states. This precluded calculation of ionisation processes. Two-centre expansions are computationally even more demanding and one of the earliest was reported by Higgins and Burke [12] using just the ground state for each centre. This exposed some unexpected resonance phenomena and the question of convergence in the close-coupling expansion became of increasing
interest. Presently, we are able to utilise near-complete expansions on both centres and examine the nature of convergence in some detail.

As for electron-hydrogen scattering the convergence of the CC expansions may be readily studied within the S-wave model [13], which retains just the target expansion s-states for the zeroth partial wave of the total orbital angular momentum.

We begin with the presentation in Fig. 1 of the major result of Ref. [9]. The CCC(H+Ps) curve denotes the S-wave breakup cross section that is convergent with respect to the usage of complete s-state expansions on both centres. We see that there is good agreement with the threshold laws derived by Klar [7] and Ihra et al. [8] below around 1 eV. This may be contrasted with electron-impact ionisation which does not yield the correct threshold law within the S-wave model, see Ref. [9] for discussion. Additionally, we see that the CCC(Ps+Ps) curve, which is simply the doubling of the Ps-contribution to the cross section, is in good agreement with CCC(H+Ps) also at energies below 1 eV. This indicates that the H- and Ps-contributions become the same in this region.

![Figure 1.](image)

**Figure 1.** (Colour online) Total $e^+\text{-}H$ S-wave model breakup cross section as a function of excess energy calculated using the two-center CCC method. The argument to the CCC label indicates which center’s positive-energy states were used. The Wannier-like threshold laws are due to Klar [7] and Ihra et al. [8]

The CCC calculations denoted by CCC(H+Ps) require immense computational resources due to the large number of states, typically 35, for each centre. Furthermore, using two near-complete expansions leads to highly ill-conditioned linear equations. Given that we are using square-integrable expansions there is no overlap between the two centres at infinite separations and hence there is no formal problem. However, the ill-conditioning means greater accuracy is required and hence more computation.

One way to avoid this is to restrict one of the centres to just the bound eigenstates, and let the other centre span the continuum in addition to its own bound states. This certainly reduces the computational complexity and, one might hope, covers all of the possible collision processes. In Fig. 2 we give an example of two such calculations. The two CC calculations have 35 states on one centre and just the lowest three eigenstates on the other. Only the positive-energy states from the set of 35 contribute to the breakup cross section. CC(35, 3) calculation has 1s, 2s, and 3s Ps-states, and shows substantial pseudoresonance problems over an extended range. These pseudoresonances depend on the states used on both centres. A different result is obtained if the 1s, 2s, and 3s are the H-states and it is the Ps centre that is expanded using the 35
states. Though it may be that for large-enough expansions such approaches would converge, for the model considered this is less practical than having two near-complete expansions on both centres.

Also shown in Fig. 2 are the results of an S-wave calculation that includes s-, p- and d-states of Ps and H. Owing to the computational difficulty we have to reduce the number of states for each \( l \) from 35 to around 13 – \( l \). As a consequence we were unable to go below 1 eV since the population of the pseudostates became sparser. However, the result shows the same qualitative threshold behavior as previously, and even quantitatively similar at energies above 10 eV. This behaviour is quite different to the electron-scattering case, where adding p-states leads to a major quantitative and qualitative change in the cross sections. Clearly, explicit incorporation of Ps-formation takes into account the electron-positron correlations.

Summarising, we have considered near-threshold behavior of the S-wave cross section for positron-impact ionisation of hydrogen atom taking into account only s- as well as s-, p- and d-states of hydrogen and positronium. We have found that the correct threshold behaviour is observed only if complete expansions are used on both the atomic and positronium centres. The separate contributions to the breakup cross section from both centers are found to become equal as the threshold is approached.

All the classical and semiclassical threshold laws mentioned in this work were also obtained for the lowest partial wave in the ionization cross section as calculated in this work. According to Rost’s and Heller’s [14] semiclassical theory all partial waves should have the same energy dependence near the threshold. A question that remains to be answered is whether Rost’s and Heller’s prediction holds in a fully quantum-mechanical treatment? Higher partial waves require even greater computational resources and such calculations are currently underway.

**Figure 2.** (Colour online) The same as in Fig. 2, but the CC(35,3) and CC(3,35) results are obtained using one pseudobasis around one centre and a few eigenstates for the other. The second curve labelled CCC are the present results with s-, p- and d-states

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