

## Calculation of the total and total ionization cross sections for positron scattering on atomic hydrogen

Igor Bray\*

*Electronic Structure of Materials Centre, The Flinders University of South Australia, G.P.O. Box 2100, Adelaide 5001, Australia*

Andris T. Stelbovics†

*Centre for Atomic, Molecular and Surface Physics, School of Mathematical and Physical Sciences, Murdoch University, Perth 6150, Australia*

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The total and total ionization cross sections for positron scattering on atomic hydrogen are calculated by applying the convergent close-coupling method to the model where positronium-formation channels are omitted. This model accurately describes the physics of the scattering whenever the positronium-formation cross section is negligible, in particular, above 100 eV for this system. The total ionization cross section results in this energy region are in excellent agreement with the recent measurements of Jones *et al.* [J. Phys. B **26**, L483 (1993)], and so lie below the earlier measurements of Spicher *et al.* [Phys. Rev. Lett. **64**, 1019 (1990)], and the recent calculations of Acacia *et al.* [Phys. Lett. (to be published)]. The total cross section is in very good agreement with the recent measurements of Zhou *et al.* (unpublished) down to 30 eV.

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The theoretical treatment of the  $e^-$ -H scattering system by the convergent-close-coupling (CCC) method [1], which expands the total wave function in a large set of square-integrable states obtained by diagonalizing the target Hamiltonian in a Laguerre basis, provides an essentially complete description of the scattering. In fact, we believe that we are able to solve the nonrelativistic time-independent Schrödinger equation for the  $e^-$ -H scattering problem without approximation, to an accuracy determined only by the size of the Laguerre basis. For the case of electron scattering the method has already been extensively tested by comparison with experiment and model problems. In this case the validity of the method is independent of the projectile energy. Its greatest successes include the ability to obtain quantitative agreement with the total ionization cross section and spin asymmetry for electron impact of atomic hydrogen [2], and the quantitative agreement with the Poet-Temkin model  $e^-$ -H problem that treats states with only zero orbital angular momentum [3]. The latter work demonstrated the important result that pseudoresonances, typically associated with square-integrable expansions of the continuum, diminish and disappear with increasing basis size. More recently, the method has been generalized to hydrogenlike atoms and ions [4], and has achieved excellent agreement with the very accurate spin-resolved measurements available for the  $e^-$ -Na scattering system. As such, we believe that the CCC method is the most accurate, generally applicable approach to electron scattering for the atomic targets of H, Li, Na, and K, as well as the multitude of ions that have the same isoelectronic se-

quence as any of these atoms. Its validity is independent of projectile energy or the transition of interest. As it is based on the close-coupling formalism it yields results for all included channels simultaneously, allowing for a check of a single calculation with a number of different experiments.

A full application of this method to the  $e^+$ -H system is complicated by the fact that dual-center expansions are necessary for the description of the additional positronium (Ps) -formation channels; see Hewitt, Noble, and Bransden [5], for example. At present such an implementation appears unlikely in the near future. However, the CCC method can be trivially extended to the model of the  $e^+$ -H system where the Ps channels are neglected. Such a model will provide an accurate description of the scattering, provided the Ps channels are closed, as occurs for low impact energy, or provided the energy is chosen in regions where the Ps-formation cross section is negligible. This has been tested at energies below the Ps-formation threshold [6], where quantitative agreement with the very accurate elastic phase shifts was obtained. Interestingly, this was only possible by expansion of the total wave function, with the hydrogen target states having orbital angular momentum up to  $l = 15$ . The large angular-momentum expansions were necessary in order to describe the effect of virtual Ps formation on the elastic phase shifts. Measurement of the Ps cross section for the  $e^+$ -H scattering system have been carried out by Sperber *et al.* [7], who found it to be negligible above 100 eV. We therefore consider the energy range above 100 eV, as well as below the Ps-formation threshold of 6.8 eV, to be the range where we can apply the model with confidence.

In this work we apply the CCC method to the calculation of the total and total ionization cross sections for positron impact of atomic hydrogen. Our motivation is

\*Electronic address: igor@esm.ph.flinders.edu.au

†Electronic address: stelbovi@atsibm.csu.murdoch.edu.au

to provide a resolution of conflicting experimental results. Recently, Jones *et al.* [8] measured this cross section, and found their results to be considerably lower than those of the earlier measurements of Spicher *et al.* [9]. The recent calculations of Acacia *et al.* [10,11] favor the Spicher *et al.* measurements. Though both sets of measurements and theory converge to the Born approximation, this only happens above 600 eV, with there being a factor of 2 difference between the two experiments at 200 eV. The Born approximation is in excellent agreement with the latest measurements across the entire energy range, which has to be seen as fortuitous, as this approximation is independent of the projectile charge and so predicts the same results for both positron and electron impact, which is not the case. There have also been recent measurements of the total cross section by Zhou *et al.* [12], which we will see are also helpful in the resolution of the above discrepancy.

The details of the CCC method for electron scattering on atomic hydrogen may be found in Ref. [1]. For positron scattering we simply drop exchange and change the sign of the relevant potentials. The method involves the solution of a large set of coupled Lippmann-Schwinger equations, which are obtained by taking the multichannel expansion of the total wave function. All of the negative and positive target states are square integrable, and so may be included in the close-coupling formalism. Upon solution of the coupled equations, the total cross section is formed by summing the individual cross sections of all states, with positive and negative energies, or may also be obtained via the optical theorem. This cross section is divided into two parts. The first is the cross section where the electron remains bound to the nucleus, and is found by summing the cross sections for states with negative energies multiplied by the projection of this state onto the true discrete subspace [2]. It consists of the elastic plus the excitation cross sections, and we refer to it as the nonbreakup cross section. In our model for positron energies below 13.6 eV this cross section is equal to the total cross section, and below 10.2 eV it is just the elastic cross section. The second part is the breakup cross section, which is formed by subtracting the nonbreakup cross section from the total cross section. For energies where the Ps cross section is not negligible, this corresponds to an approximation of the total ionization plus Ps formation cross section. We are unable to separate these individually. The quality of this approximation is energy dependent. In the projectile energy region where the Ps cross section dominates the breakup cross section, this approximation may be quite poor. For example, between the Ps-formation threshold of 6.8 eV and the ionization threshold of 13.6 eV, the model yields the incorrect value of identically zero for the breakup cross section. For the higher energies, where the breakup cross section is dominated by the ionization cross section, the model result becomes more accurate.

In order to be confident of stability in our results we repeat our calculations at each energy with an ever increasing number of basis states until convergence, to a desired accuracy, is obtained. In Fig. 1 we present our CCC and Born results for the total breakup cross section from the

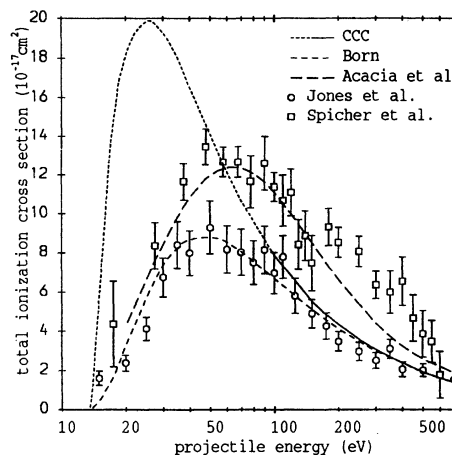


FIG. 1. Total ionization cross section for positron scattering on atomic hydrogen. The CCC results yield this cross section above 100 eV (solid line) where the Ps-formation cross section is negligible. Below 100 eV (dashed line) they give an approximation to the total breakup, positronium-formation plus ionization cross section. See text for more details. The calculations are due to Acacia *et al.* [10], Jones *et al.* [8], and Spicher *et al.* [9].

ionization threshold to 700 eV. Above 100 eV this is just the total ionization cross section. Convergence in our results, to an accuracy of a few percent, was achieved by treating  $10s$ ,  $9p$ ,  $8d$ , and  $7f$  states via the close-coupling formalism. The Born result was obtained using the same set of target states, with the  $T$  matrix being set to only the first-order term rather than solving the coupled equations. Note that in this case the total cross section may not be obtained by the optical theorem, as the imaginary part of the forward elastic scattering amplitude is zero, and so is calculated by simply summing the individual Born cross sections. We see that the CCC results, at this energy range, are in excellent agreement with the measurements of Jones *et al.* and the Born approximation, and so disagree with the measurements of Spicher *et al.* and the calculations of Acacia *et al.* Below 100 eV our results include contributions from the Ps cross section and so are characteristically higher than the total ionization cross-section measurements. For comparison of the measurements with a number of other theories, most of which favor the latest measurements, see Refs. [8–10], and references therein.

In Fig. 2 we look at the CCC total cross-section results, and compare them with the two sets of measurements of Zhou *et al.* [12]. The label denoting each set corresponds to the amount of atomic hydrogen assumed to be mixed with molecular hydrogen in the interaction region, giving an upper and a lower bound for the true result. There is good agreement with the measurements down to 30 eV. As discussed above, this is a consequence of the fact that the model must give correct results above 100 eV, but incorrect results around 13.6 eV. It is very pleasing to find that the method does not fail immediately below 100 eV, but extends down to 30 eV where, by comparison with experiment in Fig. 1 we see that the Ps cross section gives around 25% of the contribution to the total cross

section. Note that the CCC method yields correct results below 6.8 eV, where we used the same set of states as described in Ref. [6].

Agreement with the total cross-section measurements at the higher energies further increases our confidence in the resolution of the discrepancy between the total ionization cross-section measurements. In Fig. 2 we also presented the elastic, excitation, and breakup contributions to the total cross section. We find that the excitation cross section is the largest contribution to the total cross section above 100 eV. At 200 eV the total cross section is measured and calculated to be around  $12 \times 10^{-17} \text{ cm}^2$ . The total ionization measurements of Jones *et al.* are in good agreement with the theoretical prediction of  $4 \times 10^{-17} \text{ cm}^2$  at this energy, but the measurements of Spicher *et al.* yield around  $9 \times 10^{-17} \text{ cm}^2$ , which is an unlikely 75% of the total cross section.

In conclusion, we have presented total and total ionization cross-section results for positron impact of atomic hydrogen accurate to a few percent at energies above 100 eV. We base this belief on the fact that the CCC method is able to obtain quantitative agreement with the total ionization cross section for electron impact of atomic hydrogen [2], and that the model to which CCC has been employed is valid whenever the Ps formation cross section is negligible [6], which has been found to be the case above 100 eV by Sperber *et al.* [7]. We therefore conclude that in this energy range the recent measurements of Jones *et al.* [8] are likely to be the most accurate. Agreement with the total cross-section measurements down to 30 eV indicates that the model does not immediately break down once the Ps formation cross section is no longer negligible. Finally we emphasize that the results presented are a fully convergent set obtained using the CCC method for the model discussed and as such may be of wider interest in that they provide a benchmark to test other methods of solution.

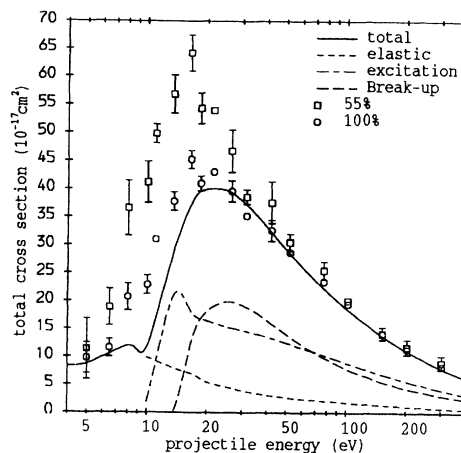


FIG. 2. Total cross section for positrons scattering on atomic hydrogen calculated using the CCC method. For this system this method is only strictly valid below 6.8 eV and above 100 eV. See text for more details. The elastic, excitation, and breakup contributions to the total cross section are also presented. The measurements are due to Zhou *et al.* [12] and are labeled by the percentage of atomic hydrogen assumed to be in the interaction region, giving an upper and a lower bound for the true result.

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