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Hybrid approach to calculating proton stopping power in hydrogen

J J Bailey¹, A S Kadyrov, I B Abdurakhmanov, I Bray

Curtin Institute for Computation and Department of Physics, Astronomy and Medical Radiation Sciences, Curtin University, GPO Box U1987, Perth 6845, Australia

E-mail: jackson.bailey@postgrad.curtin.edu.au

Abstract. Proton stopping power in hydrogen is calculated using a hybrid method. A two-centre convergent close-coupling method is used for calculations involving the proton fraction of the beam, while the Born approximation is used for the hydrogen fraction. For proton-hydrogen collisions rearrangement processes are explicitly included via a two-centre expansion. Hydrogen-hydrogen collisions are calculated including one- and two-electron processes. Despite using the first-order approximation in the hydrogen-hydrogen channel, overall reasonably good agreement with experiment is seen above 100 keV.

1. Introduction

Detailed knowledge of proton beam interactions with atoms and molecules provides a basis for accurate simulations using the low-energy models of Geant4 [1]. The first study of proton stopping in hydrogen was performed by Dalgarno and Griffing [2]. They applied the first Born approximation (FBA) to calculate the proton-hydrogen (p-H) and hydrogen-hydrogen (H-H) stopping powers and combined the results by weighting each contribution by its charge-state fraction. Rearrangement processes in the case of p-H scattering and two-electron processes in the case of H-H scattering were included and agreement with proton-H₂ experiment above 120 keV was obtained. Their calculations underestimated experiment at low energies. This discrepancy was attributed to the failure of the Bragg summation rule since the proton fraction of the beam should be higher for H₂ than for H. Schiwietz [3] performed single-centre coupled-channel atomic-orbital (AO) calculations for the proton fraction of the beam. They used FBA calculations for the hydrogen fraction (including single excitation and single ionisation processes only) and experimental charge-state fractions of Allison [4] to obtain the total stopping power. Agreement with experiment within 5% was obtained at low and high energies however results underestimated the experiment by 10-15% at intermediate energies. It was suggested that the deterioration was due to an inaccurate ionisation cross section in H-H collisions as electron-electron correlations were neglected. Schiwietz and Grande [5] later built on this work by replacing single-centre AO results below 30 keV with two-centre (AO+) ones. They included partial excitation, electron capture, and total ionisation cross sections. Additionally, a hydrogen-like screened potential was used to perform AO calculations for H+H collisions. Continuing to use the experimental H₂ charge-state fractions, these authors achieved 5% agreement with the H₂ stopping-power experiments over the whole energy range. Fainstein *et al.* [6] used the continuum-distorted-wave eikonal-initial-state (CDW-EIS) model to calculate the stopping power of protons impinging on atomic hydrogen. When combined with the FBA H-H results of Dalgarno

¹ To whom any correspondence should be addressed.



and Griffing [2] good agreement with experiment was obtained above 70 keV. Disagreement with the experiment below 70 keV was attributed to the usage of the FBA in the H-H channel.

The convergent close-coupling (CCC) method has recently been applied to calculate stopping powers of antiprotons in atomic [7] and molecular [8] targets. The CCC method is based on expansion of the scattering wave function using a large basis of specially-generated negative- and positive-energy pseudostates. Here we present our first results for the proton stopping power in hydrogen including electron-capture channels.

2. Theory

The stopping power, the energy loss per unit path length, is defined as a product of the stopping cross section S and the number of target atoms per unit volume. Since the proton-hydrogen collision system involves rearrangement processes it is necessary to take into account the charge state of the projectile. The total stopping cross section for the proton-hydrogen system at a given incident energy of the projectile is given by

$$S = f^{\text{H}^+} S^{\text{H}^+} + f^{\text{H}^0} S^{\text{H}^0}, \quad (1)$$

where f^{H^+} (f^{H^0}) is the positive (neutral) charge-state fraction of the beam and S^{H^+} (S^{H^0}) is the stopping cross section for the case of the beam consisting entirely of positively-charged (neutral) projectiles. We neglect the negative charge state as the probability of H^- formation is insignificant. The charge-state fractions can be calculated from the electron-capture and electron-loss cross sections in p-H and H-H collisions. They are given by $f^{\text{H}^+} = \sigma_1 / (\sigma_c + \sigma_1)$ and $f^{\text{H}^0} = \sigma_c / (\sigma_c + \sigma_1)$, where σ_c (σ_1) is the electron-capture (electron-loss) cross section. This highlights the importance of full two-centre calculations.

For the positive charge-state contribution we use the two-centre CCC method [9, 10]. Both bound and continuum spectra are modelled via a pseudostate expansion on the projectile and target centres. This type of expansion allows us to accurately calculate rearrangement processes. Since the continuum is discretised we may write the positive charge-state electronic stopping power as

$$S_e^{\text{H}^+} = \sum_f (\varepsilon_f - \varepsilon_i) \sigma_{fi} + \sum_k (\varepsilon_k - \varepsilon_i + v^2/2) \sigma_{ki}. \quad (2)$$

The first summation represents direct transitions and goes over all the target pseudostates. The second term represents capture processes, both to bound and continuum states depending on whether ε_k is negative or positive. The $v^2/2$ term represents the kinetic energy of an electron travelling with the speed of the incident proton after being captured.

For the neutral charge-state contribution we apply the Born approximation. With this method we are able to model both single-electron (single excitation and single ionisation) and two-electron (double excitation, double ionisation and ionisation with excitation) processes. For bound states we use the known hydrogen wave functions and for the continuum we use a two-body Coulomb wave function assuming that the ejected electron moves in the field of its parent nucleus only. The neutral charge-state stopping cross section is then given by

$$\begin{aligned} S_e^{\text{H}^0} = & 2 \sum_f (\varepsilon_f - \varepsilon_i) \sigma_{fi} + 2 \int_0^{E_0 + \varepsilon_i} (\varepsilon - \varepsilon_i) \frac{d\sigma}{d\varepsilon} d\varepsilon + \sum_{f \neq i} \sum_{k \neq i} (\varepsilon_f - \varepsilon_i + \varepsilon_k - \varepsilon_i) \sigma_{f,ki} \\ & + \int_0^{E_0 + \varepsilon_i} \int_0^{E_0 + \varepsilon_i} (\varepsilon - \varepsilon_i + \varepsilon' - \varepsilon_i) \frac{d\sigma}{d\varepsilon d\varepsilon'} d\varepsilon d\varepsilon' + 2 \sum_{f \neq i} \int_0^{E_0 + \varepsilon_i} (\varepsilon_f - \varepsilon_i + \varepsilon - \varepsilon_i) \frac{d\sigma_{fi}}{d\varepsilon} d\varepsilon, \end{aligned} \quad (3)$$

where the individual terms represent the contribution to the stopping cross section from single excitation, single ionisation, double excitation, double ionisation, and ionisation with excitation, respectively.

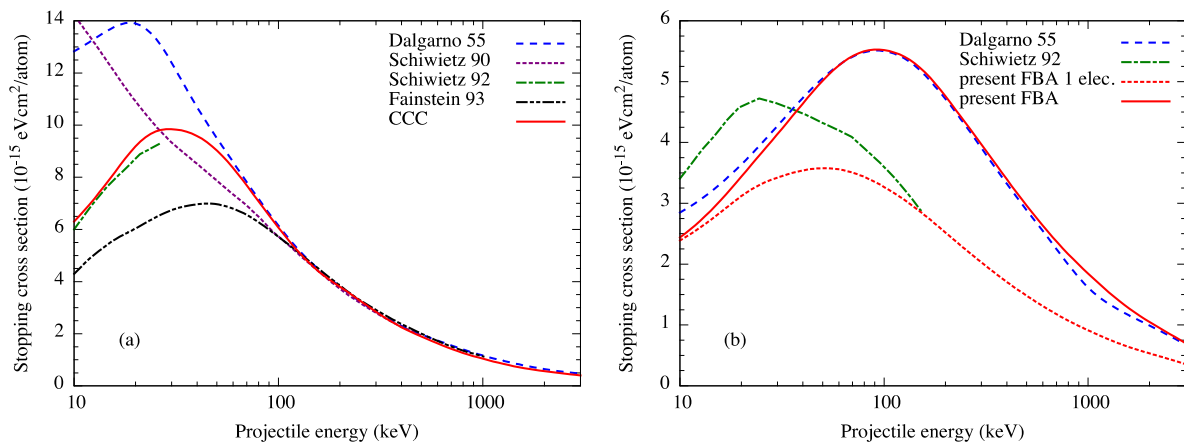


Figure 1. The stopping cross section for a beam of protons (a) and hydrogen atoms (b) passing through hydrogen. The present results for protons and hydrogen atoms are obtained using the CCC method and FBA, respectively. The theoretical calculations by Dalgarno and Griffing [2], Schiwietz [3], Schiwietz and Grande [5], and Fainstein *et al.* [6] are also shown.

3. Results

In Fig. 1a we show our present results of the stopping cross section for a beam consisting entirely of protons. As mentioned above these calculations were performed using the two-centre CCC method, which explicitly includes rearrangement processes. We included a basis of 20 *s*-states, 19 *p*-states, and 18 *d*-states on both projectile and target centres. We obtain good agreement with other theories above 100 keV. We also see reasonably good agreement with the AO+ results of Schiwietz and Grande [5]. In Fig. 1b we show our FBA results of the stopping cross section for a beam consisting entirely of hydrogen atoms. These calculations take into account single and double excitation and single and double ionisation as well as simultaneous excitation with ionisation. For excitation processes transitions up to the $n = 3$ shell were included. As expected our Born calculations are in good agreement with the similar calculations of Dalgarno and Griffing [2]. Schiwietz [3] used a static AO method to calculate the stopping cross section including only single-electron transitions. These calculations show a significant increase over the FBA calculation involving one-electron processes below 100 keV.

In order to calculate the total stopping cross section the present results shown in Fig. 1 need to be combined appropriately as detailed earlier. To this end we need to calculate the charge-state fractions. This in turn requires the knowledge of the electron-capture cross section in proton-H collisions and the electron-loss cross section in H-H collisions. The electron-capture cross section is the sum of transitions to all negative-energy projectile states, while the electron-loss cross section is the sum of the cross sections for single and double ionisation, and ionisation with excitation. The calculated charge-state fractions are presented in Fig. 2a. The experimental results of Allison [4] obtained using a H_2 target are also shown. In Fig. 2b we show our results for the total stopping cross section, which is the combination of two-centre CCC calculations and present FBA calculations. Despite the first-order approximation being used in the hydrogen-hydrogen channel, overall we obtain good agreement with experiment above 100 keV. However, at intermediate energies our results slightly overestimate experiment and at low energies they significantly underestimate experiment. Work is underway to eliminate approximations used in the hydrogen-hydrogen channel.

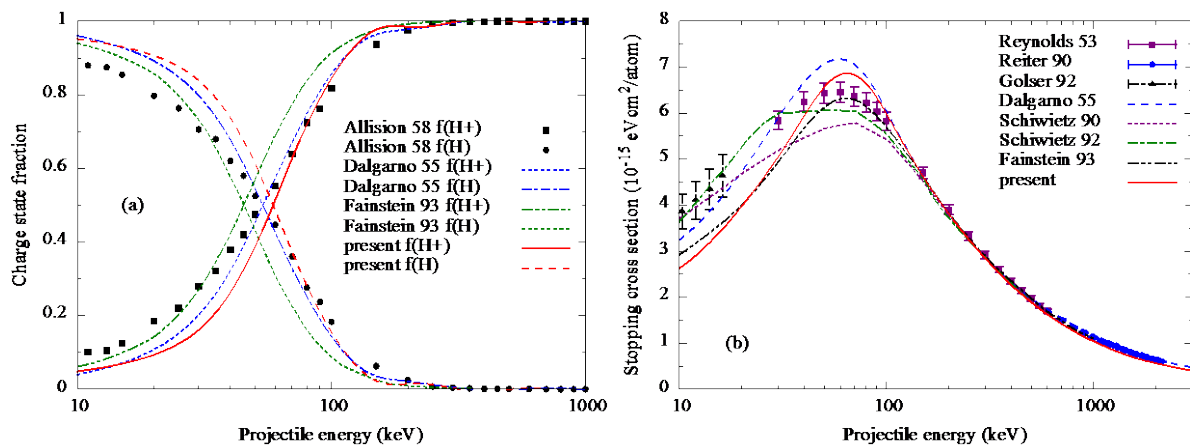


Figure 2. Charge-state fractions (a) and the total stopping cross section (b) for the proton-hydrogen collision system. The present results are obtained using a combination of the CCC method and FBA. Experimental measurements of the charge-state fractions have been performed by Allison [4]. The total stopping cross section have been measured by Reynolds *et al.* [11], Reiter *et al.* [12], and Golser and Semrad [13]. The theoretical calculations by Dalgarno and Griffing [2], Schiwietz [3], Schiwietz and Grande [5] and Fainstein *et al.* [6] are also shown.

4. Conclusion

In conclusion, we have presented a hybrid approach to calculating proton stopping in hydrogen. The stopping cross section is calculated using the two-centre CCC method for positive charge-state fraction and the Born approximation for the neutral charge-state fraction. Overall good agreement with experiment is obtained, however more theoretical work is required for complete solution of the problem at low energies.

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