

Coupled-Channel Approach to Proton Scattering on Molecular Hydrogen Using an Effective One-Electron Model

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Proton scattering on molecular hydrogen receives considerable attention in the literature, see e.g. [1] and references therein. This is partly due to the demand for accurate cross sections needed for Monte Carlo simulations for proton therapy treatment planning [2]. H_2 is the simplest neutral molecular target and provides a useful starting point for developing theories to tackle collisions with more complex targets. However, developing accurate scattering theories for H_2 targets still represents a considerable theoretical challenge in itself. The two-electron target wave function is not known analytically and the multicentre nature of the target provides an additional challenge over scattering on atomic targets.

We have extended the two-centre wave-packet convergent close-coupling approach to ion-atom collisions to study $p + \text{H}_2$ collisions. To our knowledge this is the first time two-centre coupled-channel calculations have been performed for this collision system. This approach includes all strong coupling effects between interaction channels and the two-centre expansion of the total scattering wave function allows us to explicitly differentiate between pure ionisation and electron capture into the bound states of the projectile atom in the final channel.

We used a model potential to represent the molecular target as an effective one-electron spherically symmetric system. Despite the simplicity of the approach, we found that calculated total cross sections for electron capture, single ionisation, and excitation processes generally agree well with experimental data and other theoretical calculations where available [3]. However, the total electron capture cross section was found to overestimate the experimental data at low projectile energies where electron-electron correlations are expected to play an important role in the collision dynamics. Additionally, we calculated state-resolved cross sections for capture into the $1s$, 2ℓ , and 3ℓ states of the projectile atom where deviation between various previous calculations is substantial. Here our calculations lead to significant improvement between theory and experiment.

[1] D. Schultz, H. Gharibnejad, T.E. Cravens and S. Houston, *At. Data Nucl. Data Tables* **132**, 101307 (2020).

[2] I. Abril, R. Garcia-Molina, P. de Vera, I. Kyriakou and D. Emfietzoglou, *Adv. Quantum Chem.* **65**, 129 (2013).

[3] C.T. Plowman, I.B. Abdurakhmanov, I. Bray, and A.S. Kadyrov, *Eur. Phys. J. D* **76**, 31 (2022).