Differential study of ionisation in p+H_2 collisions

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Synopsis Accurate description of experimental data on energy and angular distributions of electrons emitted in intermediate-energy p+H_2 collisions has remained a long-standing challenge. We have developed a coupled-channel method that provides an accurate solution to this problem. Calculations of the singly and doubly differential cross sections for ionisation demonstrate excellent agreement with available experimental data.

Accurate calculation of the energy and angular distribution of electrons emitted in proton collisions with H_2 is a significant challenge. Experimental data for the singly differential cross section (SDCS) and doubly differential cross section (DDCS) for ionisation differential in the energy and angle of the electron have been available for many decades. However, theoretical results, currently available for selected electron energies and angles, show inconsistent agreement with the data.

We have developed a wave-packet convergent close-coupling (WP-CCC) method to calculate all types of the molecular orientation-averaged SDCS [1] and DDCS [2] for single ionisation in p+H_2 collisions. The approach expands the total scattering wave function in terms of both target and projectile-centred basis states. Substituting this expansion into the Schrödinger equation for the scattering system leads to a set of coupled differential equations to solve for the unknown expansion coefficients. The latter are then used to calculate the differential cross sections. The two-centre expansion allows us to determine direct ionisation and electron capture into the continuum of the projectile. Both components contribute significantly to the ionisation process at intermediate energies.

Figure 1 shows our results for the orientation-averaged DDCS as a function of the projectile scattering angle and electron energy for 75 keV protons incident on H_2. The WP-CCC calculations agree very well with the experimental data, within experimental uncertainty, and provide the first non-perturbative calculations of this cross section for H_2.

The WP-CCC approach to differential ionisation is the first theoretical method capable of accurately describing the DDCS across the entire kinematic regime of the emitted electron in p+H_2 collisions, which currently available perturbative methods are unable to accurately reproduce [2].

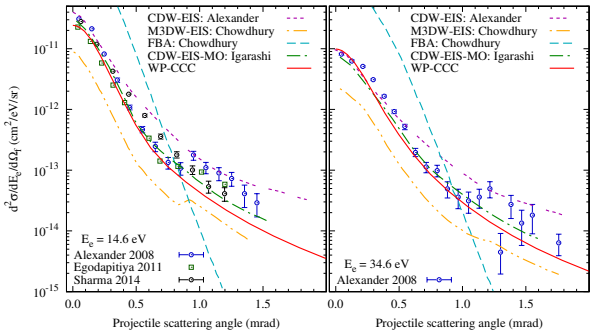

Figure 1. DDCS for ionisation as a function of projectile scattering angle and energy of the ejected electron in 75 keV proton collisions with H_2. Experimental data are by Alexander *et al.* [3], Egodapitiya *et al.* [4] and Sharma *et al.* [5]. Theoretical results are: present WP-CCC method, CDW-EIS [3], M3DW-EIS [6], FBA [6], and CDW-EIS-MO [7] methods.

References

[1] Plowman C T *et al.* 2022 *Eur. Phys. J. D* **76** 129
[2] Plowman C T *et al.* 2023 *Phys. Rev. A* **107** 032824
[3] Alexander J S *et al.* 2008 *Phys. Rev. A* **78** 060701
[4] Egodapitiya *et al.* 2011 *Phys. Rev. Lett.* **106** 153202
[5] Sharma S *et al.* 2014 *Phys. Rev. A* **89** 052703
[6] Chowdhury U *et al.* 2011 *Phys. Rev. A* **83** 032712
[7] Igarashi A *et al.* 2018 *J. Phys. B* **51** 035201

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