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Close-coupling approach to antiproton-impact ionisation of H_2 with analytical spherical averaging

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Synopsis Integrated cross section for single ionisation of molecular hydrogen by antiproton impact has been calculated in a wide range of impact energies from 1 keV up to 2 MeV using a close-coupling approach. For the first time all possible orientations of the molecular target have been accounted for using an *ab initio* analytical spherical averaging technique. Obtained results are in good agreement with experiment.

We investigate single ionisation of the hydrogen molecule by antiprotons in the incident energy range from 1 keV to 2 MeV. The orientation of the molecular axis with respect to the direction of the incident antiproton plays a key role in the reaction dynamics. Presently available theories calculate experimentally measured observables by averaging the results for only three orthogonal orientations of the internuclear axis [1, 2].

We have developed a time-dependent convergent close-coupling (CCC) approach capable of taking into account all possible orientations of the H_2 target. The approach is based on analytic orientation averaging and requires solving only one set of coupled equations independent of molecular orientation. In addition, we fully account for the electron exchange effects by using the target pseudostates obtained from diagonalizion of the target Hamiltonian. For this we use a set of antisymmetrized two-electron configurations, built from one-electron Laguerre orbitals, for each target symmetry characterized by the projection of the total orbital angular momentum, parity, and spin.

In Fig.1 we compare our results for the total ionisation cross section with the measurements [4, 5, 6], and theoretical results of Lee *et al* [1] and Lühr *et al* [2, 3]. At high impact energies present results and calculations by Lühr *et al* [2, 3] agree very well with the measured data. Below 20 keV results of Lühr *et al* obtained from averaging three orthogonal molecular orientations overestimate the experiment. Results of Lee *et al* [1] which are also obtained from three orthogonal molecular orientations are closer to the experiment at lowest calculated energies. However, the disagreement with experiment gets stronger as energy increases. As one can see the present results which include contributions from all molecular orientations are in good agreement with all measured data available except in a small energy region from 20 keV to 90 keV where the experimental points exhibit somewhat sharper maximum.

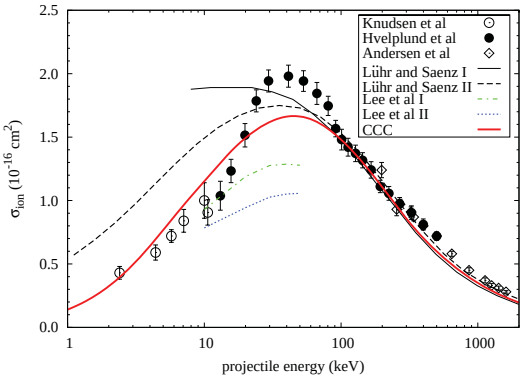

Figure 1. The total cross section for single ionisation of H_2 by antiprotons. Present CCC results are compared with the experimental data [4, 5, 6], and theoretical calculations of Lee *et al.* [1] with (I) and without (II) allowance for excited H_2^+ states, and Lühr and Saenz with one-active-electron (I) [3] and full four-particle (II) [2] treatment of the target.

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