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Fully quantum-mechanical treatment of proton-hydrogen scattering

I. B. Abdurakhmanov[1], **A. S. Kadyrov, S. K. Avazbaev, and I. Bray**

Department of Physics, Astronomy and Medical Radiation Sciences, Curtin University,

GPO Box U1987, Perth, WA 6845, Australia

Synopsis A fully quantum-mechanical convergent close-coupling approach to proton collisions with atomic hydrogen has been developed. Cross sections for target ionisation and electron capture by the projectile have been calculated in the energy range from 20 keV to 1 MeV. Calculated electron capture cross sections are in good agreement with the experiment, however for ionisation discrepancies between theory and experiment at intermediate energies still remain.

Accurate knowledge of charge exchange, excitation and ionisation processes occurring during collisions between positive ions and various atomic and molecular targets is important in a number of fields including astrophysics, plasma physics, atmospheric modelling and hadron therapy. Proton-hydrogen scattering is the simplest prototype of such collisions. Even for this simplest three-body system there is no agreement between theory and experiment when ionisation is concerned.

A new fully quantum-mechanical convergent close-coupling approach has been developed and applied to the proton-hydrogen scattering problem. It is based on the solution of Lippmann-Schwinger (LS) integral equations emerging from the two-center expansion of the total scattering wave function. For the first time, the integral over the off-shell momentum in the LS equations has been evaluated analytically. This procedure allowed to greatly reduce the computational time and memory requirements for solving the scattering problem.

Here we present the results of our fully symmetric calculations which include s, p and d states both for the target and projectile. In figure 1 we show our calculated total ionisation (TICS) and electron capture (TECCS) cross sections in comparison with the experiment and other calculations for p-H collisions. As one can see, the present results for electron capture are in very good agreement with the experiment at all energies. For ionisation the discrepancies with the experiment at intermediate energies seen in the other semiclassical calculations [8–10] still remain. The present results are convergent in terms of the included s, p and d states. Results with larger angular momentum states will be reported later.

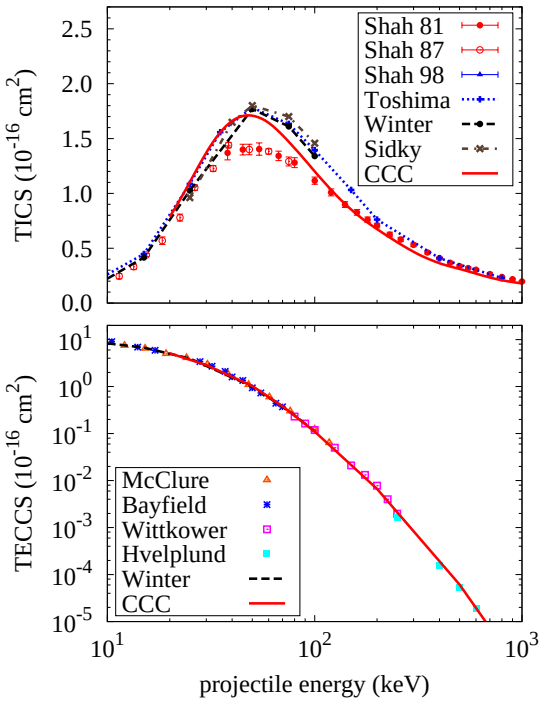

Figure 1. Total ionisation and electron capture cross sections for p-H collisions. The present CCC results are compared with the experimental data [1–7] and two-centre close-coupling calculations of Toshima [8], Winter [9], and Sidky and Lin [10].

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[1]E-mail: Ilkhom.Abdurakhmanov@curtin.edu.au