Protons in collision with hydrogen atoms: Influence of unitarity and multiple scattering

E. O. Alt[a], A. S. Kadyrov[b], and A. M. Mukhamedzhanov[c]

[a]Institut für Physik, Universität Mainz, D55099 Mainz, Germany

[b]Electronic Structure of Materials Centre, The Flinders University of South Australia, GPO Box 2100, Adelaide 5001, Australia

[c]Cyclotron Institute, Texas A&M University, College Station, TX 77843, USA

We present results of an application of three-body integral equations to energetic proton-hydrogen collisions. We emphasize in particular the important rôle played by unitarity and by Coulombic multiple scattering within each pair of particles, in leading to a very satisfactory explanation, not only of total electron exchange cross sections but simultaneously also of differential cross sections for both elastic scattering and electron exchange.

1. INTRODUCTION

Three-body integral equations when applied to collisions of protons with hydrogen atoms yield the amplitudes for direct scattering and electron exchange which automatically satisfy two-body and (if solved exactly also) three-body unitarity. As a consequence, differential cross sections (DCS) for both reactions are calculated on equal footing, and the total exchange cross section (TCS) results from the corresponding DCS. This is to be contrasted with standard models used in atomic physics which either are of the (Distorted-Wave)Born type (to be applied at higher energies), or solve the Schrödinger equation by expanding the wave function in a basis (close-coupling method which has problems especially for rearrangement processes). Hence, at higher energies in general separate models have to be developed to describe the DCS for either direct scattering or electron exchange, and frequently also for the TCS. For instance, the most sophisticated traditional models which provide a very good reproduction of the TCS data are the continuum distorted wave [1] and the boundary corrected first Born model [2]. Both, however, fail to describe differential cross sections which represent a much more stringent test.

On the other hand, three-body integral equations suffer from the principal defect that their kernels are not compact when particles with charges of different sign are involved, as it happens in applications to atomic reactions (references can be traced from [3]). The consequence is that naive application of standard solution methods of integral equations theory would not be justified. Additional, practical difficulties arise from the complicated singularity structure of the off-shell two-particle Coulomb T-matrix which is the basic dynamical ingredient. As is well known, the latter develops nasty singularities in the on-shell limit and, in case of attraction, has in addition an infinite number of poles.

Both types of problems have been dealt with successfully in our recent investigations. The non-compactness problem has been avoided by (i) going over to the effective-two-body formulation of the AGS three-body theory [4], (ii) taking resort to a K-matrix (on-shell) approximation, and (iii) by transformation to impact parameter space reducing the resulting 2-dimensional integral equations to algebraic ones (IPFA [5], with the later additional development into the three-body eikonal approach (TBEA) [6]). For more details see [7]. The problems arising from the singularity structure of the off-shell Coulomb T-matrix have been resolved by developing techniques to *exactly* include the latter in the first order direct and exchange contributions to the effective potentials [8,9] (see below).

2. RESULTS

General results for TCS and elastic and exchange DCS for scattering of protons off hydrogen atoms in the ground state have already been published [7]. Here, we work out two specific aspects. Firstly, instead of using only the separate Born (= driving) terms for the direct and the exchange reaction a set of coupled integral equations is solved. This provides the unitarisation of the former and at the same time introduces the coupling between the channels. Secondly, in the driving terms the exact off-shell Coulomb T-matrix T^C is taken into account. As compared to approximating the latter by the Coulomb potential V^C this takes care of multiple scattering within each pair of particles and improves upon three-body unitarity. Presently we restrict ourselves to considering only the $1s$ state of hydrogen in the intermediate and the final state.

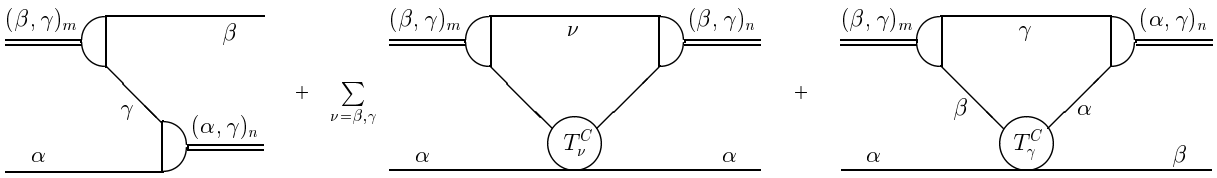

Figure 1. Diagrammatic representation of the driving terms used in the integral equation. Semicircles denotes hydrogenic bound state wave functions.

To begin with consider the charge transfer reaction $H^+ + H(1s) \to H(1s) + H^+$. The corresponding Born term is given by the Chen-Kramer (CK) model [10] which combines the elementary electron exchange with the first rescattering contribution (first and last diagram in Fig. 1). Thus, comparison of our results with CK illustrates the importance of unitarisation and inclusion of the coupling to the elastic channel. Moreover, a solution of the integral equation but with T^C approximated by V^C in the driving terms (Fig. 1) has been achieved in TBEA [6]. Thus, comparison of the present results with TBEA demonstrates the influence of multiple scattering and improved three-body unitarity.

The TCS is shown in Fig. 2. Inspection reveals that CK very nicely reproduces the data at higher energies but, not surprisingly, begins to fail as the energy decreases. This deficiency of CK is removed by unitarisation and cross-channel coupling which is seen

to be highly effective in reproducing the data also at lower energies (TBEA and present results). An additional improvement over TBEA, in particular at the higher energies, is achieved by the use of the full Coulomb T-matrix T^C which is instrumental in finally leading to a very good agreement with data over the whole energy region considered.

DCS for the electron exchange reaction at 60 and 125 keV are presented in Figs. 3 and 4, respectively. Again, CK reproduces the pronounced forward-scattering peak rather well, which is not so surprising in view of the TCS results, but clearly fails for non-forward angles. Unitarisation and cross-channel coupling improves CK for larger scattering angles, but overshoots if only the single-scattering contribution (TBEA) is introduced. In these figures we include for comparison the IPFA results [5] which follow from the integral equation but with only the elementary electron exchange (first diagram of Fig. 1) included as driving term. It is obvious that the first rescattering contributions (second and third diagram of Fig. 1) are very important in reducing the DCS to their experimental values.

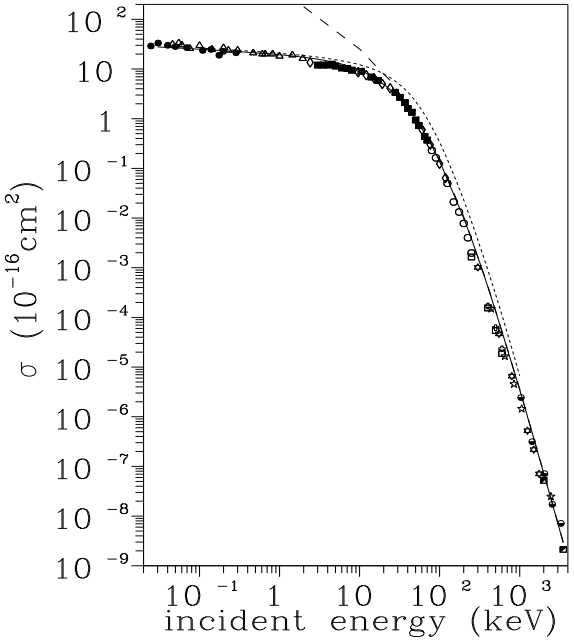

Figure 2. TCS for $H^+ + H(1s) \rightarrow H(1s) + H^+$: solid line, present results; dotted line, TBEA [6]; dashed line, CK [10]. Data are from different sources (see [7]).

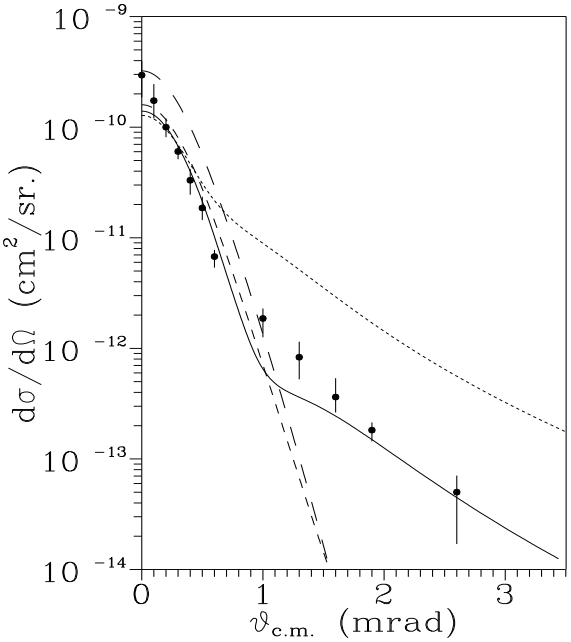

Figure 3. DCS for $H^+ + H(1s) \rightarrow H(1s) + H^+$ at 60 keV: solid line, present results; long-dashed line, IPFA [5]; dotted line, TBEA [6]; short-dashed line, CK [10]. Data are from [11].

Our coupled integral equations yield at the same time also the elastic scattering amplitudes. The corresponding DCS at 60 keV is shown in Fig. 5. Using only the Born terms (FBA) (second diagram of Fig. 1) overshoots the data while both IPFA and TBEA underestimate the cross section. Clearly, only the full theory including multiple scattering and channel coupling is able to describe the experimental data.

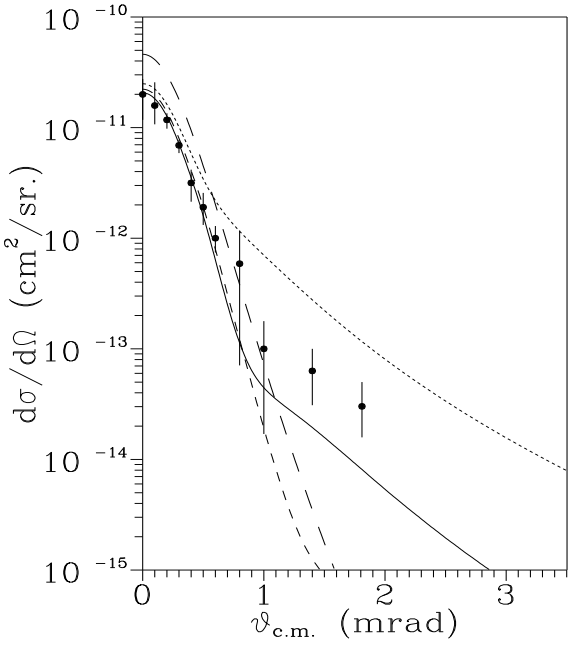

Figure 4. DCS for $H^+ + H(1s) \to H(1s) + H^+$ at 125 keV: solid line, present results; long-dashed line, IPFA [5]; dotted line, TBEA [6]; short-dashed line, CK [10]. Data are from [11].

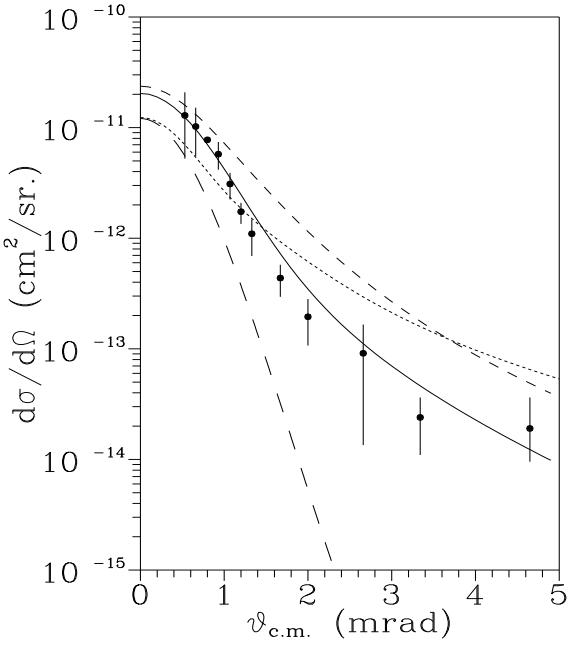

Figure 5. DCS for $H^+ + H(1s) \to H^+ + H(1s)$ at 60 keV: solid line, present results; long-dashed line, the lowest order IPFA [5]; dotted line, TBEA [6]; short-dashed line, FBA. Data are from [12].

Concluding our investigations clearly demonstrate that, with sufficient care, the *ab-initio* three-body theory can successfully be applied to atomic reactions.

REFERENCES

1. Dž. Belkić et al., Phys. Rep. **56** (1979) 279.
2. Dž. Belkić et al., Phys. Rev. A **36** (1987) 1601.
3. A. M. Mukhamedzhanov et al., Phys. Rev. C **61** (2000) 064006.
4. E. O. Alt, P. Grassberger, and W. Sandhas, Nucl. Phys. **B2** (1967) 167.
5. G. V. Avakov et al., J. Phys. B: At. Mol. Opt. Phys. **23** (1990) 4151.
6. E. O. Alt et al., J. Phys. B: At. Mol. Opt. Phys. **B** 27 (1995) 4653.
7. E. O. Alt, A. S. Kadyrov, and A. M. Mukhamedzhanov, Phys. Rev. A **60** (1999) 314.
8. E. O. Alt et al., J. Phys. B: At. Mol. Opt. Phys. **B** 28 (1995) 5137.
9. E. O. Alt, A. S. Kadyrov, and A. M. Mukhamedzhanov, Phys. Rev. A **54** (1996) 4091.
10. J. C. Y. Chen and P. J. Kramer, Phys. Rev. A **5** (1972) 1207.
11. P. J. Martin et al., Phys. Rev. A**23**, 3357 (1981).
12. J. T. Park, in *Proceedings of XII ICPEAC, Gatlinburg, 1981*, edited by S. Datz (North-Holland, Amsterdam, 1982).