Update on light-ion calculations

David R. Schultz
Department of Physics
University of North Texas

Planned CRP scope (CFADC):
• Elastic and transport processes extending recent light ion/atom work
• Charge transfer for light ions colliding with hydrogen
• Proton-hydrogen excitation to support BES, MSE diagnostics

Revised CRP scope (UNT):
• Stopped work on elastic and transport processes
• Charge transfer for light ions colliding with H, H₂, He
• H⁺, He²⁺, Be⁴⁺, C⁶⁺+H excitation to support BES, MSE diagnostics

US DOE closure of the Controlled Fusion Atomic Data Center
Elastic and transport related data

- All hydrogen isotopic variants if \((H^+, H) + (H, H_2, He)\)
- Needed to model plasma charge, momentum, energy, and particle transport – DEGAS 2 → Center for Plasma Edge Simulation
- Fully quantal calculations of differential and integral elastic cross sections and transport moments
  - Fitting formulae
  - Scaling laws
  - IAEA “Greenbook” Vol. 8
- Raw data on web
- 250 integral, 3000 differential cross sections

Elastic scattering database c. 1998
<table>
<thead>
<tr>
<th>Reaction</th>
<th>Refs.</th>
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<tbody>
<tr>
<td>((\text{H}^+,\text{D}^+,\text{T}^+)) + ((\text{H},\text{D},\text{T}))</td>
<td>Refs. 12-19</td>
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<tr>
<td>((\text{H},\text{D},\text{T})) + ((\text{H},\text{D},\text{T}))</td>
<td>Refs. 12-14, 19, 20</td>
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<tr>
<td>((\text{H}^+,\text{D}^+,\text{T}^+)) + ((\text{H}_2,\text{D}_2,\text{T}_2,\text{HD},\text{HT},\text{DT}))</td>
<td>Refs. 13-14, 21</td>
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<td>((\text{H},\text{D},\text{T})) + ((\text{H}_2,\text{D}_2,\text{T}_2,\text{HD},\text{HT},\text{DT}))</td>
<td>Refs. 13, 22, 23</td>
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<tr>
<td>(\text{H} + \text{H}_2^+)</td>
<td>Ref. 21</td>
</tr>
<tr>
<td>((\text{H}^+,\text{D}^+,\text{T}^+)) + (\text{He})</td>
<td>Refs. 13, 19, 24, 25</td>
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<tr>
<td>((\text{H}^+,\text{D}^+,\text{T}^+)) + (\text{(Li, Be, B)})</td>
<td>Refs. 32, 33</td>
</tr>
<tr>
<td>((\text{H},\text{D},\text{T})) + (\text{(Li}^+, \text{Be}^+, \text{B}^+))</td>
<td>Refs. 32, 33</td>
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<tr>
<td>((\text{H},\text{D},\text{T})) + (\text{Li})</td>
<td>Refs. 32, 33</td>
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<tr>
<td>((\text{H}^+,\text{D}^+,\text{T}^+)) + (\text{C})</td>
<td>Refs. 24, 26</td>
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<tr>
<td>((\text{H}^+,\text{D}^+,\text{T}^+)) + (\text{Ne})</td>
<td>Refs. 24, 25</td>
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<tr>
<td>((\text{H}^+,\text{D}^+,\text{T}^+)) + (\text{Ar})</td>
<td>Refs. 24, 25, 27</td>
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<tr>
<td>((\text{H}^+,\text{D}^+,\text{T}^+)) + (\text{Kr})</td>
<td>Ref. 24</td>
</tr>
<tr>
<td>((\text{H}^+,\text{D}^+,\text{T}^+)) + (\text{Xe})</td>
<td>Ref. 24</td>
</tr>
<tr>
<td>((\text{H},\text{H}^+,\text{H}_2,\text{H}_3^+)) + (\text{H}_2)</td>
<td>Compilation of other work in Ref. 12</td>
</tr>
<tr>
<td>((\text{H},\text{D})) + (\text{He})</td>
<td>Compilation of other work in Ref. 12</td>
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</tbody>
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Work continued over the years to treat other systems requested by the fusion community: the CRP would have extended this to include \(\text{H}^+ + \text{O}, \text{O}^+ + \text{H}, \text{H}^+ + \text{N}, \text{N}^+ + \text{H}, \text{H}^+ + \text{O}_2, \text{H}^+ + \text{N}_2\)

Krstic and Schultz, PoP 16, 053503 (2009)
Latest work: Extend recent calculations to include O and N to complete data set for H up to Ne
Charge transfer diagnostics and modeling

- Accurate data for charge transfer involving impurity ions is important for modeling and diagnosing fusion plasmas (both total and state-selective cross sections are needed).
- Ongoing experiments for total cross sections for C, N, and O ions at ORNL motivates new theoretical calculations.

The ORNL merged beams apparatus

Representative data, for ions of charge state 4
Status of charge transfer calculations

- Total cross sections calculated to compare, in particular, to experiment, and state-selective results calculated for use in diagnostics

- Multiple theoretical methods used, each valid in overlapping collision energy regimes, allowing for inter-comparison to check accuracy and to provide recommended results over a wide range of energies

- Published (or presently being submitted) since start of the CRP


Status of charge transfer calculations

- Calculations made using the molecular orbital close coupling (MOCC; research groups of Phillip Stancil and Robert Buenker), atomic orbital close coupling (AOCC; DRS) and classical trajectory Monte Carlo (CTMC; DRS) methods

- Completed other light ion species since start of the CRP, yet to be published
  - $C^{5+}, C^{6+}, O^{7+}, O^{8+} + \text{He}$ (AOCC, CTMC complete, MOCC in progress), relevant for helium plasmas, further tests of theory and experiment
  - $C^{6+} + H, H_2, \text{He}, \text{Kr}$ (CTMC, AOCC, other theory from the literature, experiment complete), X-ray emission following charge transfer experiments provide important test of theory
Status of charge transfer calculations: $\text{N}^6+ + \text{H}$

Large scale calculation of potential energy curves, couplings, and MOCC cross sections
Status of charge transfer calculations: $\text{N}^{6+} + \text{H}$

Comparison of results in the region of overlapping applicability allows state-selective cross sections to be recommended over a wide collision energy range, CTMC extends results to higher $n$-levels.
Status of charge transfer calculations: $O^{6+} + H$

Theoretical investigation of total and state-dependent charge exchange in $O^{6+}$ collisions with atomic hydrogen

Y Wu$^{1,2}$, P C Stancil$^1$, D R Schultz$^{3,4}$, Y Hui$^4$, H P Liebermann$^5$ and R J Buenker$^5$

Good agreement of present and independent AOCC calculations with measurements by Dijkkamp
Status of charge transfer calculations: $C^{5+} + H$

Final-state-resolved charge exchange in $C^{5+}$ collisions with H

J L Nolte, P C Stancil, H P Liebermann, R J Buenker, Y Hui, and D R Schultz

Good agreement of AOCC with measurements

MOCC, AOCC, and CTMC combine to provide recommended state-selective results
Excitation calculations to support diagnostics

Diagnostics such as charge exchange recombination spectroscopy, beam emission spectroscopy, and motional Stark effect spectroscopy depend on atomic data for charge transfer and excitation.

Plasma parameters such as field strength, temperature, density, and magnetic field orientation can be determined from these diagnostics.

Data needed includes that for excitation of neutral hydrogen by plasma protons, fusion alphas, and ions of primary impurities beryllium and carbon.

Collisional-radiative models need not only cross sections for excitation to specific states, but also density matrix elements.
Excitation calculations to support diagnostics

Comprehensive new AOCC calculations for $H^+ + H$ were made at the beginning of the CRP over a very wide range of collisions energies, with a fine energy spacing, and with a series of basis sets designed to overcome certain numerical and pathological difficulties of the method.

New calculations were needed not only to fill the whole, relevant collision energy range, and to seek improvement over existing data in the literature, but because the collisional-radiative model required the density matrix elements.

Results of collisional-radiative modeling based on these calculations and those for higher n-levels in the Glauber approximation were published.

Excitation calculations to support diagnostics

Example of the diagonal density matrix elements, otherwise known as the cross sections, shows good agreement with other state of the art calculations, but reveals the need for more independent results to definitively confirm details.
Excitation calculations to support diagnostics

AOCC results have been completed, and collisional-radiative modeling is being developed, for He\textsuperscript{2+}, Be\textsuperscript{4+}, C\textsuperscript{6+} + H excitation to support diagnostics.

Cross sections have been compared with existing data, density matrix elements computed for the C-R model, and topped up by collaborators using the Glauber approximation.

Present results agree in magnitude with existing recommended cross sections, but differ in the positions and existence of oscillations.

Physical origin of the oscillations uncovered in the late 1990’s

The way to improve these and other heavy particle data ...

Contemporary computers and computational techniques enable improved fidelity, particularly when coupled with close comparison to analogously improving measurements.

The time-dependent Schrödinger equation (TDSE) may be solved iteratively in time on a multidimensional lattice (LTDSE) using discrete mathematics techniques, avoiding certain approximations and difficulties of other approaches.

I. The electronic wf is discretized on a multidimensional grid

II. The wf is propagated in time, observables and other quantities are analyzed
The way to improve these and other heavy particle data ...

LTDSE has previous improved knowledge of $H^+ + H$ excitation cross sections, and could be used to compute the required density matrix elements. It has also provided accurate results for charge transfer for higher charge states, i.e., $He^{2+}$, $Be^{4+} + H$.

- $H^+ + H$ excitation
- $He^{2+} + H$ charge transfer
- $Be^{4+} + H$ charge transfer
LTDSE - Experiments: Ionization in slow ion-atom collisions and the newly discovered role of vortices

- Pioneering imaging experiments: 1996
- Sigma/π model: 1998
- LTDSE solution: 2002
- Vortices: 2009
- RLTDSE solution: 2007
- 2-electrons: 2013

Role in angular momentum transfer

Hydrodynamic interpretation

Ubiquity: electron, photon interactions
Update on light-ion calculations

- Charge transfer for light ions colliding with H, H₂, He
- H⁺, He²⁺, Be⁴⁺, C⁶⁺ + H excitation to support BES, MSE diagnostics
- Future work to improve all calculations and consider other systems of interest