Electron correlation in simultaneous electron transfer and excitation: results of new 2eAOCC calculations and comparison to experiment in 50-500 keV He + + H/H 2 collisions

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A Dubois[1*] and T J M Zouros[2†]

[1] Sorbonne Université, CNRS, Laboratoire de Chimie Physique-Matière et Rayonnement, Paris, France
[2] Department of Physics, University of Crete, P.O. Box 2208, GR 71003 Heraklion, Greece

Synopsis New two-electron semiclassical atomic orbital coupled channel calculations (2eAOCC) are compared to experiment and to older coupled channel calculations. Progress in these type of calculations is assessed in an effort to investigate the effect of electron correlations in this fundamental collision system.

The study of multi-electron processes occurring in ion-atom collisions is still a theoretical challenge due to the importance of static and dynamic correlation in these transitions. It is therefore interesting to investiage the dynamics of true two-electron systems, where the transfer of an electron and the excitation of another is likely. From this point of view, He^+- H collisions, inducing transfer-excitation (TE) processes to autoionizing states of He, can be considered as a benchmark system.

Here, we present cross sections for such TE processes, especially

$$He^+ + H \rightarrow He(2l2l' \ ^1L) + H^+$$

for impact energies ranging from 50 to 500 keV. Results are obtained with a full configuration interaction (CI) close coupling semiclassical approach [1]: the two electrons are taken into account and the time-dependent Schrödinger equation is solved with an unprecedented large basis set to allow for convergence of the non perturbative scheme. These results are compared with three-decade old theoretical results [2], as well as with experimental data obtained with zero-degree Auger projectile spectroscopy for dihydrogen molecular target [3].

The discussion and interpretation of the results in terms of one- and two-step mechanisms, so called resonant (correlated) transfer-excitation (RTE) [4] and non resonant transfer-excitation (NTE) [5], respectively, are particularly interesting when comparing with converged two-electron ab initio calculations, in which all mechanisms are described coherently. We shall present cross sections for production of $2p^2\ ^1D$ (see Fig. 1), $2p^2\ ^1S$ and $2s2p\ ^1P$ autoionising states.

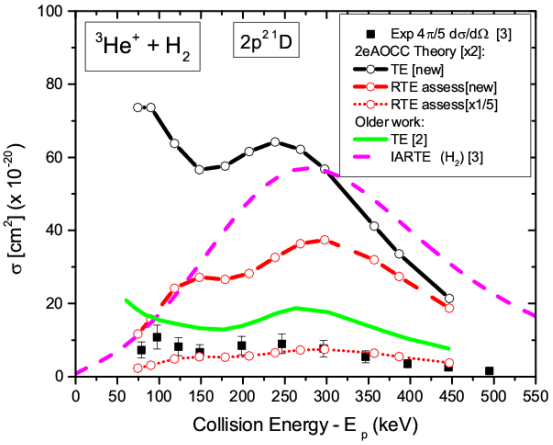

Figure 1. Comparison of cross sections for the production of the $He(2p^2\ ^1D)$ state in collisions with hydrogen. Theory: He^+ + H, 2eTE cross sections multiplied by two to account for H_2 target in experiment (squares) [3]. Impulse Approximation RTE (IARTE) (long dashes violet).

References

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* E-mail: alain.dubois@sorbonne-universite.fr
† E-mail: tzouros@physics.uoc.gr