Close-coupling CI-approach of atomic and molecular collisions: new perspectives on inner-shell processes in H^+ - Li

G. Labaigt[1,2] and A. Dubois[1,2]

[1] *Sorbonne Universités, UPMC Univ Paris 06, UMR 7614, Laboratoire de Chimie Physique-Matière et Rayonnement, F-75231 Paris Cedex 05, France*
[2] *CNRS, UMR 7614, LCPMR, 75005 Paris, France*

Presenting Author: gabriel.labaigt@upmc.fr

We present a novel approach to describe multi-electronic processes (electron transfer, excitation and ionization) occurring in ion-atom and ion-molecule collisions in the intermediate keV energy range. The treatment is based on the so called impact parameter semiclassical approximation [1,2] in which the electronic time-dependent Schrödinger equation is solved non perturbatively, taking into account all the electrons of the system with static and dynamic correlations.

The equation is solved using a CI approach where the scattering wave function carries all information about spatial symmetry and spin multiplicity for the total system and for the isolated partners of the collision. For that purpose we use the permutation group theory together with Young diagram formalism instead of a Slater determinant approach [3].

We apply this model to a genuine, benchmark, three-electron system, H^+ - Li, for which we present results for exchange processes from valence and inner-shell compared with experimental results [4] when available. In the conference we shall give a peculiar insight on new features brought by this full multi-electronic treatment compared to the quasi one-electron model commonly used. We shall focus our attention on the couplings between valence and inner shell processes that can lead to two types of inner-shell capture mechanisms : direct or two-steps. Differences will be highlighted by the analysis of the inner-electron density temporal profile, as shown in the figure below.

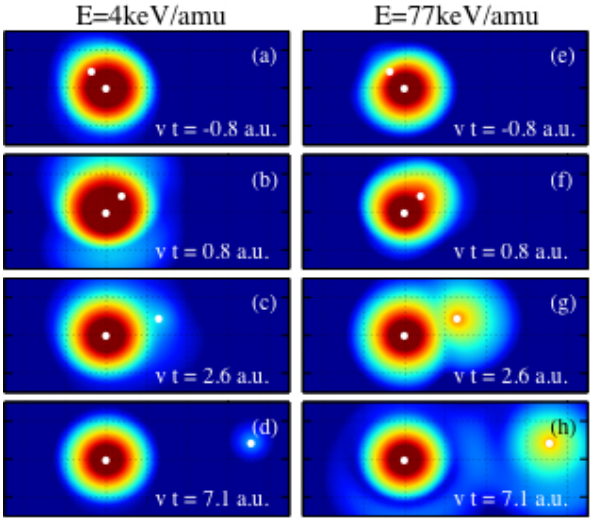

Figure 1: *Inner-electron density in the x,z plane calculated for two different collision energies at four different times. The spatial grid interval is 2 a.u. The color palette extends over 4 orders of magnitude.*

References

[1] W. Fritsch and C. Lin, Phys. Rep. **202**, 1 (1991)
[2] J. Caillat *et al.* Phys. Rev. A **70** 032715 (2004)
[3] F. A. Matsen, J. Phys. Chem. **68** 3282 (1964)
[4] D. Wutte *et al.* Atom. Data and Nucl. Data **65** 155 (1997) and references therein.