Journal of Physics: Conference Series **488** (2014) 092004 doi:10.1088/1742-6596/488/9/092004

Interference effects in double electron capture in H^+-H^- collisions at low and intermediate impact energies

Gabriel Labaigt[1], **Nicolas Sisourat**[2] **and Alain Dubois**[3]

Laboratoire de Chimie Physique - Matière et Rayonnement,
Université Pierre et Marie Curie, 75005 Paris, France

Synopsis Double electron transfer in H^+-H^- collisions is investigated using a semiclassical coupled-channel approach in which the scattering wavefunction is developed onto a two-center/two-electron atomic basis. Cross sections are presented in a wide energy domain, from 50 eV to 30 keV and exhibit a strong oscillatory behavior, in agreement with earlier measurements. Using a semi-classical model based on the relevant molecular energy curves we demonstrate that these oscillations are the signatures of interferences between direct and sequential channels leading to double capture.

It is well known that the differential cross sections for electron transfer present an oscillatory nature in symmetric ion-atom collisions at low impact energies. Resonant capture in H^+-H system is the benchmark process to observe such behavior which is readily explained and quantitatively described by a simple two-state model involving the phase differences between the two relevant molecular energy curves [1]. These oscillations are averaged in the integration over trajectories so that they do not survive in total cross sections when plotted as function of impact energy or velocity. However several collision systems show an oscillatory nature in integral cross sections, see for example [2] for He-Ne collisions. One of the most challenging one is H^+-H^- where the resonant process is the double capture (DC) channel: it presents the advantages to be a genuine two-electron system and to possess an unique double transfer channel but it experiences the strongest possible static and dynamical effects of electronic repulsion and a complex interplay between ionic and neutral channels (i.e. single and double capture). For the last three decades this system has been studied theoretically [3-6] and experimentally at low [3,7] and intermediate (up to 25 keV) [4] energies. These different investigations showed oscillatory DC cross sections but the theoretical ones were not consistent with experimental data, neither in the period of the oscillations nor in the magnitude of the cross sections. In [5] a diabatic approach within a two-state model was proposed: the results, depending upon an arbitrary parameter, show an oscillatory behavior in a wide energy region but overestimate the cross sections by more than one order of magnitude. No clear agreement between data has therefore ever been reached, keeping the understanding of this benchmark system a real challenge.

During the conference we shall present DC cross sections obtained from a semiclassical treatment where the electronic wavefunction is developed over spin-symmetrized (singlet) products of Gaussian-type orbitals centered on target and projectile and augmented by electron translation factor [1]. The time-dependent Schrödinger equation is then solved non perturbatively, allowing a very large number of channels to be populated. The results for DC show an oscillatory behavior that is for the first time coherently predicted for energies ranging from 50 eV to 25 keV. We also present a model derived from our coupled channel computations which shows that the oscillations stem from the interferences between direct DC and various sequential processes, involving transfer-excitation and single transfer processes.

References

[1] B.H. Bransden and M.R.C. McDowell 1992 *Charge Exchange and the Theory of Ion-Atom Collisions* Oxford University Press
[2] W. G. Planje, W. B. Westerveld and A. Niehaus 2000 *Phys. Rev. Lett.* **85** 2713
[3] F. Brouillard *et al.* 1979 *J. Phys. B* **12** 1253
[4] H. Bräuning *et al.* 2007 *Phys. Rev. Lett.* **99** 173202
[5] R. Shingal and B. Bransden 1990 *J. Phys. B* **23** 120
[6] J. Wang, J. P. Hansen and A. Dubois 2000 *J. Phys. B* **33** 241
[7] B. Peart and R.A. Forrest 1979 *J. Phys. B* **12** L23

[1] E-mail: gabriel.labaigt@upmc.fr
[2] E-mail: nicolas.sisourat@upmc.fr
[3] E-mail: alain.dubois@upmc.fr