Multielectron description of ion-atom collisions by a semiclassical non perturbative method

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Synopsis We present the semiclassical non perturbative approach that we have developed and implemented on computers to describe electronic processes in ion-atom (and ion-molecule) collisions. We focuse on the description of single or multielectronic processes in multielectronic collision systems. We illustrate this approach by presenting results for electron transfer and excitation in various systems in a wide impact energy domain, ranging from 0.1 to 1500 keV/u.

The modelling of electronic processes in numerous multielectronic collision systems is a major challenge for non perturbative approaches, while its counterpart for (quasi-) monoelectronic systems is generally well mastered, e.g. [1-3]. It is now important to take up this challenge to produce reliable cross sections to be used for modeling macroscopic systems such as plasmas, e.g. for astrophysics and fusion sciences and also in chemistry, with cold plasma reactor [4]. The difficulties that arise when studying multielectronic atomic and molecular collisions are of different kinds:

(i) the spectra of the isolated target and projectile get very rich, the number of states of importance (e.g. within a specific energy domain) in the scattering increasing very much, nearly as the power of the number of electrons,

(ii) even when neglecting spin-orbit effects, the electron spin has to be taken into account with care. Indeed although the total spin of the system is conserved, it is not the case for the spins of the target and projectile centers, when isola-ted, i.e. before and after the collision,

(iii) the electron-electron interactions has to be included and implies the calculations of a very large number of different two-electron repulsion integrals involving orbitals/states located around the same center or around the two centers, i.e. traveling relative to each other,

(iv) when molecules are considered, these three difficulties are further amplified by the multicentric nature of the species under consideration, even without taking into account the breakdown of the sudden approximation (frozen nuclei in molecules).

In the symposium, we shall present our approach and illustrate its use and the difficulties encountered in different ion-atom systems, for monoelectronic and bielectronic processes. We shall consider carbon and oxygen ions impacting helium atoms and processes populating low lying states at intermediate impact energies (keV/u for these light elements) and doubly-excited states in the high (MeV/u) energy domain, e.g. [5-7].

References

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