Multi-electron effects in collisions of swift ions and atoms

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Synopsis State-to-state charge exchange cross sections are presented for ion-atom collision systems involving several active electrons. Focused in the intermediate and high impact energy regions, the results stem from a semiclassical close-coupling treatment taking into account dynamically several electrons and are compared with monoelectronic approximations.

Semiclassical close-coupling approaches within the molecular and asymptotic representations have been widely used with great success for one- or quasi-one-active electron ion-atom collisions [1]. For multielectronic systems and for the intermediate energy domain the situation is more complex and a majority of investigations have been performed using the independent electron, independent event approximations and/or frozen core approximation [2]. Much less non perturbative calculations taking into account the dynamics of several electrons have been done in the past due to the important computer resources they require. They often presented a limited control of convergence with respect to the number of states included in the basis sets employed.

In the symposium a recently developped approach based on a semiclassical multi-electron close coupling treatment will be presented. The solution of the time dependent Schrödinger equation is performed within a full configuration interaction (CI) approach by expanding the scattering wavefunction on a basis of mutielectronic states centred on target, projectile and both. These states are augmented by electron translational factors to ensure Galilean invariance of the results and to remove spurious dipolar coupling terms in the final equations to be solved [1]. The states are obtained by using a set of Gaussian type orbitals and their products, keeping all possible spin states for the different (charged) species involved in the collision, for a given, conserved, total spin.

We shall present cross sections from this approach, showing, its limits and also its advantages by comparison with results based on similar close coupling treatments but taking into account a single active electron and using independent electrons or frozen core approximations.

References

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