

Charge exchange cross sections in nitrogen ions and hydrogen collisions

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During the talk, we first discussed the motivation of this project, and in particular why we will focus on nitrogen ions and hydrogen collisions. The workplan, in terms of systems, schedule and employed theoretical approaches, was then presented. After this introduction, we shortly described the straight-line impact parameter method (IPM) which will be used to compute cross sections for electronic processes in ion-atom collisions in the collision energy range going from 1 keV/u to 100 keV/u. In the IPM, one assumes that the relative motion of the projectile and target is described by a classical trajectory defined as $\vec{R}(t) = \vec{b} + \vec{v}t$ (see figure). In the collision energy range of interest this assumption is valid since the impact energy largely exceeds the energy loss from the inelastic electronic processes and the scattering diffusion angle is small. The IPM leads to the Time-Dependent Schrödinger Equation (TDSE) for the electron(s) in the moving field of the nuclei.

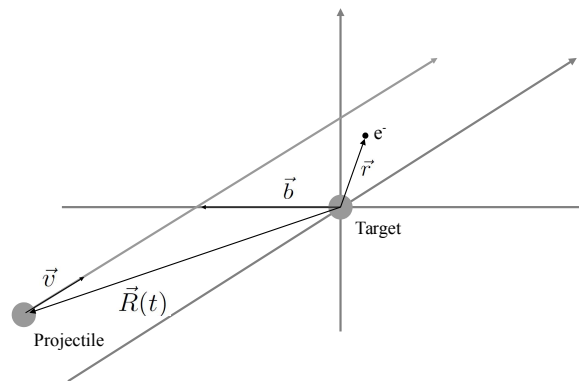


Fig. 1 Collision geometry. The impact parameter \vec{b} and the projectile velocity \vec{v} define the collision plane. The position of the electron with respect to the target center is denoted \vec{r} .

After introducing the IPM, our implementation was presented in details. In order to solve the TDSE, the total electronic wavefunction is expanded in the basis of the eigenstates of the isolated target and projectile states. One is then left with solving a set of first order differential equations for the time-dependent coefficients of the expansion. In our implementation, the eigenstates of the collision partners are described as linear combinations of multi-centered Cartesian Gaussian Type Orbitals (GTO). The advantages of GTO were discussed and the choice of the sets of GTO to be employed was reported. Some other details of the implementation were described.