Numerical calculation of charge exchange and excitation cross sections for plasma diagnostics*

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Cross sections for charge exchange in ion-H collisions are the basic data required in charge exchange diagnostics of tokamak plasmas [1]. However, these data are in general not accessible experimentally and they are commonly obtained theoretically. The precision of the calculations depends on the collision energy and is in general unknown. In the present work we present a method to solve numerically the time dependent Schrödinger equation [2], which is based on the package GridTDSE [3]. In the calculation of charge exchange cross sections the wave function, which is initially an atomic travelling orbital, is evaluated in the points of a 3D Cartesian grid centered on the projectile nucleus and propagated by solving numerically the corresponding first order differential equation. The projections of the final wave function on the different bound states yield the charge exchange probabilities and cross sections. This technique can be employed in a wide energy range, and, given that the computational procedures are completely different, the comparison with the results of other methods (close coupling, classical trajectory Monte Carlo) provides an estimate of the uncertainties of the data. We have employed the grid numerical method to evaluate charge exchange n-resolved cross sections for collisions of Be^{4+} and B^{5+} with H(1s) at collision energies between 1 and 500 keV/u.

In this work we also show that the method can be applied to describe excitation and electron loss of atoms in ion-atom collisions, which are relevant in determining the density of diagnostics beams [4] and in the stopping of heating neutral beams. In this work we present calculations for excitation and electron loss in Be^{4+} + H(1s) collisions and we estimate the uncertainties of these data by comparison with once center atomic orbital expansions [5].

*Acknowledgments This work has been partially supported by project ENE2014-52432-R (Ministerio de Economía y Competitividad, Spain).

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