ATOMIC-ORBITAL CLOSE-COUPLING CALCULATIONS FOR COLLISIONS OF HIGHLY CHARGED IONS WITH ATOMIC HYDROGEN

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The use of charge exchange recombination spectroscopy (CXRS) [1] in nuclear fusion research has renewed the interest in fundamental ion-atom collisions, since high precision atomic data for these collisions is crucial for the analysis of experimental data from CXRS. The de-excitation lines following a charge exchange (CX) into high lying n-levels in the ion spectra can be used to make predications about the plasma ion temperature and density as well as (by utilizing the Doppler shift) the direction of the plasma flow [1].

The atomic-orbital close-coupling (AOCC) method in its impact parameter formulation is used to calculate CX and ionization (ION) cross sections. This technique has already been used successfully in the past [2,3]. In this method, the wavefunction of the active electron is expanded in terms of atomic orbitals (including pseudostates to model ionization) as basis states. The number of basis states used in the expansion limits the method's accuracy. For lighter ions with $q \leq 8$ as little as 46 AO states [3] are enough to accurately describe the collision system. However, visible spectral lines suitable for CXRS originate from higher n-shells, which makes it necessary to enlarge the basis set. Additionally also n-shells above those responsible for the visible lines should be included in order to account for cascade effects. A full and accurate AOCC calculation can therefore require several hundred basis states even for lighter ions [4,5].

When describing heavier ions such as Ne^{q+} or Ar^{q+}, the basis sets have to include up to and more than a thousand states. This type of calculation exceeds by far the computational limits of ordinary AOCC implementations and new computational techniques (e.g. parallelization) in combination with higher computational power (i.e. clusters) have to be used. Furthermore, numerical precision and stability become major issues to be considered during such calculations.

In our contribution, we will present our continuing efforts in the optimization of previously existing numerical implementations [6] as far as numerical precision and stability are concerned. Furthermore we will present CX and ION cross-sections for selected collision systems and show their application in nuclear fusion research.

References:
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