

Production of cross sections for atomic collisions with Asymptotic Orbital Semiclassical Coupled Channel calculations

Tuesday, 30 March 2021 14:35 (30 minutes)

Cross sections for bound-bound (excitation, capture) and bound-free (ionisation) transitions occurring in ion-atom and ion-molecule collisions are required for diagnostic and modelling of plasmas. These collisions involve low-Z atoms naturally present in the plasmas but not only (impurities, elements from the vessels, ...), all in various oxidation degrees but also in ground and excited states, prior to the collisions.

The present contribution will present our approach and code implementation to produce cross sections for these processes and collisions, for impact energies ranging from below keV/u to MeV/u. It is based on the semiclassical approximation, with a classical description of the relative motion between target and projectile, while the electron dynamics is described by solving non perturbatively the time-dependent Schrödinger equation (TDSE). This kind of treatment is required for the impact energy domain of interest but can be declined in different approaches. We use an approach where the TDSE is solve using a scattering wavefunction expanded on asymptotic atomic or molecular states, i.e. on states describing isolated target and projectile, and for which up to 4 active electrons are taken into account. All coupling are then taken into account, as well as the total spin state but also the individual target and projectile spin states, when required. In the presentation we shall illustrate the use of our approach and code for several collision systems of interest.

Primary authors: Mr DUBOIS, Alain (Sorbonne Universite); Dr GAO, Junwen (Sichuan University); Dr SISOURAT, Nicolas (Sorbonne Universite)

Presenter: Mr DUBOIS, Alain (Sorbonne Universite)

Session Classification: MOD/2 A+M Data