

Pseudopotential approach to impurity-ion collisions with atomic and molecular targets

Alisher Kadyrov

Department of Physics and Astronomy, Curtin University, Perth, Australia

a.kadyrov@curtin.edu.au

The two-centre wave-packet convergent close-coupling (WP-CCC) approach developed in our group is capable of providing benchmark data on the integrated and differential cross sections for various processes taking place when fully stripped ions collide with atomic and molecular targets. The approach is based on expansion of the total scattering wave function using a two-centre pseudostate basis. This allows one to take into account all underlying processes, namely, direct scattering and ionisation, and electron capture into bound and continuum states of the projectile. The normalized wave packets constructed from the radial Coulomb wave functions are used to discretise the continuous spectrum of the target and projectile atoms. The generated orthonormal wave-packet bases are used in the two-centre expansion of the total scattering wave function. The utility of the method is demonstrated in our previous works on examples of proton and multiply-charged ion collisions with atomic hydrogen. The integrated, fully differential, as well as various doubly and singly differential cross sections for ionisation of hydrogen were calculated and a comprehensive set of highly accurate benchmark results obtained. Recently we have also developed a pseudopotential method to treat collisions involving multielectron targets [Phys. Rev. A **104**, 042820 (2021)]. The method allows one to reduce the multi-electron target to an effectively single-electron one and then use the standard WP-CCC approach. A competitive advantage of the method is that it does not rely on the independent-event model to model. The method has been used to calculate charge-exchange and ionization cross sections for proton collisions with alkalis. Obtained results are in very good agreement with experiment for charge exchange. We describe how this pseudopotential method can be used to model multi-electron injected impurity ion collisions with H. Preliminary results of calculations for the C^{Z+} ions, where $Z = 1 - 5$ is the charge of the dressed impurity ion, are discussed.