Two-centre convergent close-coupling approach to scattering of multiply-charged ions on atomic hydrogen

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Synopsis Two-centre convergent close-coupling approach is applied to collisions of various multiply-charged ions with atomic hydrogen. Convergence of the ionisation and electron-transfer cross sections is investigated.

The two-centre convergent close-coupling (CCC) approach is a general-purpose formalism applicable to a wide range of atomic collision processes. It was originally developed for positron scattering on atomic hydrogen including positronium formation [1]. Later, it was extended to direct scattering and ionisation in ion-atom and ion-molecule collisions using the impact-parameter representation (see [2] and references therein). Recently, we have generalised the CCC approach for heavy projectiles to include electron-transfer channels. We have developed two distinct versions of the two-centre CCC approach to ion-atom collisions. The quantum-mechanical convergent close-coupling (QM-CCC) approach [3] is based on the exact fully quantum-mechanical three-body Schrödinger equation for the total scattering wave function and leads to a set of coupled Lippmann-Schwinger integral equations for the transition amplitudes. The relative motion of the heavy particles is treated fully quantum-mechanically. The total scattering wave function is expanded using a two-centre pseudostate basis. This allows one to take into account all underlying processes, namely, direct scattering and ionisation, electron capture into bound and continuum states of the projectile. The off-shell integration in the coupled-channel Lippmann-Schwinger integral equations is taken analytically which greatly reduces computational effort and memory requirements. The semiclassical convergent close-coupling (SC-CCC) approach [4] is based on the semiclassical time-dependent Schrödinger equation for the electronic part of the scattering wave function and leads to a system of coupled differential equations for the transition probability amplitudes. Both methods have been applied to antiproton collisions with various atomic and simple molecular targets in the energy range from 1 keV to 1 MeV [2]. The methods have also been applied to proton collisions including rearrangement channels. In particular, the SC-CCC approach has been used to calculate the integral alignment parameter for polarisation of Lyman-α emission and the cross sections for excitation and electron capture into the lowest excited states [4]. The QM-CCC approach has been used to investigate ionisation including electron capture into the continuum of the projectile [3].

Recently we have further developed the SC-CCC approach using an alternative continuum-discretisation procedure. In this so-called wave-packet convergent close-coupling (WP-CCC) method [5] the continuous spectrum of the target and projectile atoms is discretised using stationary wave packets constructed from the Coulomb wave functions, the eigenstates of the target and projectile atom Hamiltonian, respectively. Wave-packet continuum discretisation allows one to generate pseudostates with arbitrary energies and distribution. This feature is ideal for detailed differential ionisation studies.

We have been applying the various implementations of the CCC method to collisions of multiply-charged ions (in particular, He^{2+} and C^{6+}) with atomic hydrogen and hydrogen-like targets. A comprehensive test of the CCC computer code has been performed. When the channels are decoupled we reproduce the first Born cross sections for ionisation and electron capture, tabulated in the literature. We have also reproduced small-basis coupled-channel calculations, reported by other authors, reasonably well. Having validated our code, presently, we are performing full-scale convergence studies for excitation, ionisation and electron-capture cross sections. The results will be reported at the conference.

References

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