Wave-packet continuum-discretization approach to ion-atom scattering

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Synopsis Current progress in applications of the two-centre wave-packet convergent close-coupling approach to scattering of various fully-stripped ions on one- and two-electron atoms is presented.

The wave-packet convergent close-coupling approach is based on solving the full three-body Schrödinger equation using a two-center expansion of the total scattering wave function. The wave function is expanded in orthonormal basis sets built from eigenstates, and wave-packet pseudostates representing the continuum, of both the target atom and the atom formed by the projectile after capturing the electron. With a sufficiently large basis, due to the strong coupling between channels, the method produces converged cross sections for all underlying processes.

The approach is used to study C^{6+} collisions with hydrogen at projectile energies from 1 keV/amu to 10 MeV/amu [1]. While there is excellent agreement with experiment for the total electron-capture cross section over the entire energy range, the total ionization cross section slightly overestimates the only available measured point. The singly and doubly differential ionization cross sections at 1 and 2.5 MeV/amu are in good agreement with experiment. At 100 keV/amu the present singly differential cross section in the ejected angle of the electron shows a pronounced peak in the forward direction. It is concluded that at low energies electron capture into the continuum strongly enhances electron ejection in the forward direction.

The approach is also used to calculate excitation, ionization and electron-capture cross sections for proton collisions with $n = 2$ states of hydrogen, where n is the principal quantum number. The cross sections for scattering on the metastable $2s$ state are compared with other theoretical results. Considerable disagreement with previous calculations is found for some transitions at various incident energies [2].

Balmer emission in proton-hydrogen scattering is studied at energies from 5 keV to 1 MeV [3]. This requires the cross sections for target excitation into the final states with $n = 3$ and 4. A substantial variation in the cross sections for population of magnetic sublevels obtained in different theoretical approaches is found. The cross section for excitation of the $n = 3$ shell as a whole does not agree with experiment, but supports earlier calculations. At the same time, the individual cross section for excitation of the $3p$ state displays excellent agreement with available experiment. The results for polarisation fraction of the Balmer emission significantly disagree with experimental measurements at high energies.

Recently, the approach has been extended to proton collisions with helium [4]. The target is treated as a three-body system, where correlations between the electrons are taken into account. A frozen-core approximation is used, assuming one of the electrons always remains in the He^+ $1s$ orbital. Electron-capture and single- and double-ionization cross sections are calculated in the projectile energy range from 15 keV to 1 MeV. The results are in good agreement with available experimental data and other calculations, except for double ionization.

References

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