Two-centre convergent-close coupling approach to ion-atom collisions

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Synopsis We report on recent progress in applications of the two-centre convergent close-coupling approach to ion-atom collisions. This includes a development of a wave-packet continuum-discretisation approach to the description of the target structure and applications to antiproton, proton and multiply-charged ion collisions with hydrogen and helium.

Ion-atom collisions are important in astrophysics, radiobiology and fusion energy. We have developed two distinct versions of the one- and two-centre convergent close-coupling (CCC) approaches to address this challenge. In one the relative motion of the heavy particles is treated fully quantum-mechanically (QM-CCC) [1, 2], the other classically (SC-CCC) [3, 4]. Depending on the properties of the collision system we tackle the problem using either one- or two-centre model. In the one-centre treatment the total scattering wave function is expanded in terms of only target pseudostates. This model is ideal for collisions where the likelihood of rearrangement is negligibly small, e.g. for collisions with antiproton projectiles at sufficiently large energies. Two-centre treatment is applied to collisions where the projectile can capture the target electron. In this case two separate expansions utilising projectile and target-centred states are used to form the scattering wave function. The two-centre CCC approach allows addressing the target electron loss in a way where we can exactly tell which part is due to ionisation and which is due to electron capture.

Successful implementation of the CCC approach relies on the accurate description of the target structure. Previously the CCC approach relied on the target continuum discretisation using the basis of orthogonal Laguerre pseudostates. There the Laguerre pseudostates are produced with energies distributed only in a certain way which cannot be changed arbitrarily. Also, distributions of pseudostates for different angular momenta are not aligned, which makes calculations of differential ionisation cross sections more complicated. Recently we have developed an alternative approach, where the continuous spectrum of the target is discretised using the wave packets (WP) constructed from the Coulomb wave functions. Unlike the Coulomb functions the generated wave packets are normalisable and suitable for scattering calculations. Due to the flexibility in choosing state energies, WP-CCC approach is ideal for differential ionisation studies. These wave packets have been incorporated into both one- and two-centre CCC approaches.

For antiproton-impact ionisation of hydrogen [3] a comprehensive set of benchmark results from integrated to fully differential cross sections has been obtained. Implementation of the wave packets to proton-hydrogen collisions produced accurate cross sections for all undergoing processes including ionisation and excitation of the target and electron capture to the projectile's bound and continuum states. In addition, this allowed to investigate various differential ionisation cross sections where the accurate calculations of the breakup amplitudes corresponding to direct ionisation and electron capture to the continuum is important. For helium single ionisation by energetic protons, the WP-CCC gives excellent agreement with recent experiment [5].

We have also 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. A comprehensive test of the CCC computer code has been performed. We have also reproduced small-basis coupled-channel calculations, reported by other authors, reasonably well. 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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