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Computational Methods for Electron-Atom Collisions[1]

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In recent years, much progress has been achieved in calculating reliable cross-section data for electron scattering from atoms and ions, in particular quasi-one and quasi-two electron systems such as H, He, the alkalis, and the alkaline-earth metals. Until recently, however, accurate calculations of electron collisions with more complex targets, such as the heavy noble gases Ne−Xe, have remained a significant challenge to theory. We will give an overview of the computational methods presently used for *ab initio* electron-atom collision calculations, with particular emphasis on their strengths and weaknesses, range of applicability, and expected accuracy. In particular, we will illustrate with a few examples how the B-spline R-matrix (BSR) method with non-orthogonal orbitals [1-3] has been able to dramatically improve the quality of theoretical datasets for oscillator strengths [4] and in particular for electron collisions with the heavy noble gases [5].

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