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Atomic and Molecular Collision Data for Plasma Science[1]

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Accurate data for electron and heavy-particle collisions with atoms, ions, and molecules are required for many modelling applications in plasma science. Depending on the particular application and the electron or ion temperature in the plasma, the energy range of the projectile may cover a very large range, from a few meV to many MeV.

Since it is virtually impossible to measure all the data needed for state-of-the-art collisional radiative models (CRMs), much of the responsibility for generating sufficiently comprehensive datasets has been put on theory. There is a vast variety of methods available to generate the data, ranging from classical to semi-classical to fully quantal approaches, with the latter based on the first- and sometimes second-order plane-wave or distorted-wave Born approximation as well as non-perturbative close-coupling methods that can be systematically driven to convergence for relatively simple collision problems. For complex targets, such as large molecules, often only comparatively simple methods are available, but then the total (integrated over all scattering angles) cross sections or even rate coefficients (integrated over the collision energies with some prescribed weight function) are usually required. Clearly, estimating the uncertainty in such calculations is essential, as discussed in detail in Ref. [1]. It is worth noting that experimental data, too, have uncertainties. Especially when it comes to absolute cross sections, these uncertainties may be difficult to quantify, certainly more difficult than, for example, the relative energy or angular dependence of a particular cross section.

For some of these methods, computer codes of vastly varying complexity are publicly available. In all but the simplest cases, running these codes is far from trivial for non-experts. Hence, many databases exist around the world, in which the original data (energy levels, oscillator strengths, cross sections) are stored and utility codes are provided to extract the data and perform calculations of the parameters of interest for the modeler. One of many such databases is LXCat [2], which is widely used for modelling electron collisions in low-temperature plasmas.

In this contribution, I will give a (necessarily incomplete) overview of what is currently available, both regarding the methods and the resulting data. Recently, the idea of machine-learning to generate new data from and/or assess the accuracy of existing datasets has been put forward. Time permitting, I may discuss some of these ideas.

[1] H.K. Chung *et al.*, Journal of Physics D **49** (2016) 363002. [2] https://us.lxcat.net/home/

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