The integrated propagation of atomic structure and collisional uncertainties through to plasma diagnostics

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Although the atomic and molecular collisional communities have invested considerable effort in developing various highly accurate approaches to electron-impact excitation, ionization and dielectronic-recombination, systematic studies of the uncertainty for each process has not been given the same amount of attention.

Furthermore we are finding that uncertainty in plasma diagnostics is not simply the sum of these isolated collisional rates, but are often the product of multiple interacting processes that are a function of electron density and temperature. For example, an effective ionization rate [1] for a particular ion stage is a weighted summation over the groundstate and meta-stable ionization cross-sections. The contribution from the excited state ionization to the effective ionization rate depends directly on the population of the excited states relative to the groundstate, therefore sampling the variation in a wide variety of radiative and electron-impact excitation transitions.

Therefore, although associating a meaningful uncertainty in each fundamental collisional process is the first step, the propagation of these variations into plasma diagnostics requires an uncertainty grid which is a function of electron density and temperature and is the longer term goal. We outline in [2] a method by which these uncertainty contributions can be propagated through to plasma diagnostics.

In order to provide one aspect of these uncertainties, a perl-script front-end to an R-Matrix with Pseudo-States (RMPS) package has been written, through which a Monte-Carlo approach varies the underlying atomic structure behind these collisional calculations many, many times. The subsequent excitation, ionization and di-electronic recombination results from these calculations will provide more realistic variation in the uncertainty from an atomic structure foundation upwards. We intend not only to provide an uncertainty file for each of the fundamental collisional processes, but also on the secondary derived parameters such as effective recombination/ionization rates.

References

1. http://www.adas.ac.uk/manual.php
2. C. P. Ballance, S. D. Loch, A. R. Foster, R. K. Smith, M. C. Witthoeft, T. R. Kallman
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