Uncertainty Quantification of theoretical atomic and molecular collisional data

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Synopsis There is a growing interest in quantifying uncertainties of fundamental data such as atomic and molecular data as they propagate through to the global uncertainty of an integrated modeling of fusion applications. Uncertainties associated with calculated atomic and molecular structure and collisional data are discussed.

An integrated modeling of fusion research often requires a wide range of atomic and molecular data, and generally calculated data are used to meet the needs of fusion community [1]. While uncertainty quantification of global uncertainties of integrated fusion modeling warrants uncertainties of input atomic and molecular data, accuracies of calculated data are rarely quantitatively defined. The mission of the Atomic and Molecular (A+M) Data Unit at IAEA is to provide evaluated and recommended atomic and molecular data in support of nuclear fusion and other plasma applications and has encouraged work to develop guidelines for critically assessing theoretical atomic and molecular structure and collision data in the last few years.

The provision of uncertainty estimates for calculated atomic and molecular data is of rather recent interest and procedures for uncertainty quantification are much less developed for atomic and molecular data than they are for nuclear data. For most of atomic and molecular physics a well-defined governing (Schrödinger) equation exists and one strives to solve for an appropriate many-body quantum system with known (Coulombic) interactions. On the other hand, the nuclear data field does not have such a fundamental equation, but builds a model based on nuclear model input parameters, which are calibrated with experimental data. The calibration procedures based on the Bayesian theorem yield uncertainty distributions of calculated nuclear data derived from uncertainties of the nuclear model input parameters and experimental data [2].

With an editorial standard of Physical Review A requiring uncertainty information for certain classes of atomic data [3], there is a growing interest in developing methods for uncertainty quantification of calculated data. A joint ITAMP-IAEA workshop was organized in 2014 to discuss sources of uncertainty in the physical models and computational methods employed for studying atomic and molecular processes. The discussion led to the publication of an extensive review of uncertainty estimates for theoretical atomic and molecular data [4], which is presented here.

References

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