GEC13-2013-000096

Abstract for an Invited Paper
for the GEC13 Meeting of
the American Physical Society

Large-scale B-spline R-matrix calculations of electron impact excitation and ionization processes in complex atoms[1]

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In recent years, the B-spline R-matrix (BSR) method [1] has been applied to the treatment of a large number of atomic structure and electron-atom collision problems. Characteristic features of the BSR approach include the use of B-splines as a universal basis to describe the projectile electron inside the R-matrix box and the employment of term-dependent, and hence non-orthogonal, orbitals to construct the target states. The latter flexibility has proven to be of crucial importance for complex targets with several partially filled subshells. The published computer code [2] has since been updated and extended to allow for a fully relativistic description at the level of the Dirac-Coulomb hamiltonian. Also, the systematic inclusion of a large number of pseudo-states in the close-coupling expansion has made it possible to extend the range of applicability from elastic and inelastic low-energy near-threshold phenomena to intermediate energies (up to several times the ionization threshold) and, in particular, to describe ionization processes as well. The basic ideas of the BSR approach will be reviewed, and its application will be illustrated for a variety of targets. Particular emphasis will be placed on systems of relevance for applications in gaseous electronics, such as the generation of complete datasets for electron collisions with the heavy noble gases Ne-Xe. Many of our data, which are needed for the description of transport processes in plasmas, are available through the LXCat database [3].

[1] O. Zatsarinny and K. Bartschat. J. Phys. B **46** (2013) 112001.
[2] O. Zatsarinny, Comp. Phys. Commun. **174** (2006) 273.
[3] http://www.lxcat.laplace.univ-tlse.fr/database.php

[1]This work was performed in collaboration with Klaus Bartschat. It is supported by the National Science Foundation under Grant No. PHY-1212450 and the XSEDE Allocation PHY-090031.