DAMOP07-2007-000148

Abstract for an Invited Paper
for the DAMOP07 Meeting of
the American Physical Society

High-Precision Calculations for Electron-Impact Excitation and Ionization of Complex Atoms[1]

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While electron collisions with the valence electrons of light (quasi-)one- and (quasi-)two-electron atoms, such as H, He, the alkalis, and the alkali-earth elements, can now be handled very accurately by various theoretical methods (convergent close-coupling, R-matrix with pseudo-states, exterior complex scaling, or time-dependent close-coupling), the situation is much less satisfactory for complex open-shell targets such as Mo or Fe, or for collisions involving excitation or ionization of inner shells in the heavy noble gases. In recent years, our group has further developed an alternative version of the R-matrix (close-coupling) method, using a B-spline basis with non-orthogonal sets of term-dependent orbitals [1-3]. This method allows us to generate target descriptions of unprecedented accuracy in collision calculations, which turn out to be of critical importance for accurate results, particularly for resonances in the near-threshold region. In addition, a hybrid method, combining a second-order distorted-wave method for a fast ionizing projectile with a convergent R-matrix with pseudo-states approach for the initial bound state and the ejected electron [4], has been very successful in treating ionization of heavy noble gases [5] and simultaneous ionization-excitation of He [6]. Examples will be presented at the conference.

[1] O. Zatsarinny and C. Froese Fischer, J. Phys. B **33** (2000) 313. [2] O. Zatsarinny and K. Bartschat, J. Phys. B **37** (2004) 2173. [3] O. Zatsarinny, Comp. Phys. Commun. **174** (2006) 273. [4] Y. Fang and K. Bartschat, J. Phys. B **34** (2001) L19. [5] K. Bartschat and O. Vorov, Phys. Rev. A **72** (2005) 022708. [6] S. Bellm, J. Lower, and K. Bartschat, Phys. Rev. Lett. **96** (2006) 223201.

[1]Major contributions to the work presented in this talk were made by Oleg Zatsarinny. This work is supported by the United States National Science Foundation under grants PHY-0244470 and PHY-0555226.