Abstract Submitted for the GEC08 Meeting of The American Physical Society

A Fully Relativistic B-Spline R-Matrix Method for Electron and Photon Collisions with Atoms and Ions¹ OLEG ZATSARINNY, KLAUS BARTSCHAT, Drake University — We have extended our B-spline R-matrix (closecoupling) method [1] to fully account for relativistic effects in a Dirac-Coulomb formulation. Our numerical implementation of the close-coupling method enables us to construct term-dependent, non-orthogonal sets of one-electron orbitals for the bound and continuum electrons. This is a critical aspect for complex targets, where individually optimized one-electron orbitals can significantly reduce the size of the multiconfiguration expansions needed for an accurate target description. Core-valence correlation effets are treated fully *ab initio*, rather than through semi-empirical model potentials. The method is described in detail and will be illustrated by comparing our theoretical predictions for e-Cs collisions [2] with benchmark experiments for angle-integrated and angle-differential cross sections [3], various spin-dependent scattering asymmetries [4], and Stokes parameters measured in superelastic collisions with laser-excited atoms [5]. [1] O. Zatsarinny, Comp. Phys. Commun. 174, 273 (2006). [2] O. Zatsarinny and K. Bartschat, Phys. Rev. A 77, 062701 (2008). [3] W. Gehenn and E. Reichert, J. Phys. B 10, 3105 (1977). [4] G. Baum et al., Phys. Rev. A 66, 022705 (2002) and 70, 012707 (2004). [5] D.S. Slaughter et al., Phys. Rev. A 75, 062717 (2007).

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