Abstract Submitted
for the GEC16 Meeting of
The American Physical Society

A non-iterative treatment of the non-local exchange terms in the Complex Optical Potential method ALLAN STAUFFER, York University, ROBERT MCEACHRAN, Australian National University — Non-local exchange terms in atomic scattering equations are usually treated iteratively. This method normally works well but there can be problems with convergence, either requiring a large number of iterations or converging to a spurious value. It has long been known [1] that these terms can be treated non-iteratively but at the cost of expanding the number of equations needed to be solved. With the vastly increased memory and speed of modern computers, this approach is now feasible even for heavier targets. We have decided to implement this method in our calculations of electron elastic scattering from atoms using the Complex Optical Potential (COP) method [2] which is based on the relativistic Dirac equations. This method accounts for incident flux lost to the elastic channels through inelastic processes (excitation and ionization) via the imaginary part of the optical potential and also provides a value for the total cross section for these processes. The basis for the method will be given along with sample calculations where the iterative method fails. [1] Marriott R, Proc. Phys. Soc. A **70** 288 (1957), **72** 121 (1958) Marriott R 1958 Proc. Phys. Soc. A 72 [2] Chen S, McEachran R P and Stauffer A D, J. Phys. B: At. Mol. Opt. Phys. **41** 025201 (2008)

Allan Stauffer
York University

Date submitted: 13 Jun 2016 Electronic form version 1.4