

"High Accuracy Atomic Physics in Astronomy", IP/ITAMP workshop, August 7-9, 2006, The Harvard-Smithsonian Center for Astrophysics, Cambridge, MA, in honor of Prof. Micheal J. Seaton

AN OVERVIEW OF A PARALLEL SUITE OF NON-RELATIVISTIC, SEMI-RELATIVISTIC AND FULLY-RELATIVISTIC R-MATRIX CODES FOR ELECTRON-IMPACT EXCITATION AND PHOTOIONISATION OF ATOMIC SYSTEMS.

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From the late nineties onward, a Rollins/Strathclyde/Auburn collaboration began to develop a fully parallel set of non-relativistic, semi-relativistic and fully relativistic electron-impact excitation codes. Our aim was to overcome computational bottlenecks that restricted calculations performed using the serial programs to $(N + 1)$ -electron Hamiltonian matrices of order 10-20 K and several hundred scattering channels. We now able to routinely handle cases with Hamiltonian matrices of order 30,000 to 50,000 with the largest matrix to date being of order 100,000.

Recently, the efficient production of bound-free dipole matrix elements has been incorporated into the aforementioned electron-scattering codes, for the inclusion of resonance radiation damping effects in highly ionised relativistic species. Of course, this development has also enhanced photoionisation and photo-excitation capabilities for all the various coupling schemes.

I will present an overview of the suite of codes, illustrating the current electron-impact excitation/ionisation and photoionisation capabilities in the context of current/forthcoming experiments.