"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

The Breit-Pauli R-matrix code and magnetic interactions

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The Belfast R-matrix code[1] has been the workhorse for computing electron impact excitation and photoionization of atoms and positive ions in two ambitious international collaborations: the Opacity Project and the Iron Project[2], each in its wake triggering a big development push since the first codings four decades ago. This report focuses on two recent developments, both associated with the magnetic moment of the electron.

(1) High lying correlation states of the target can give rise to a sizable number of channels one must retain merely for the sake of completeness. Otherwise term coupling, which is due to spin-orbit effects, spoils inelastic transition amplitudes with spurious contributions from monopole terms in elastic reactance matrix elements, in particular for high ℓ partial waves in weak transitions. However for computational economy one may yet truncate the sets of coupled channels if the contracted matrices of term coupling coefficients are variationally re-orthonormalized (in routine `BOUNDJ` of the Breit-Pauli R-matrix stage `recupd` employing program `VA04A`).

(2) In a major coding effort Chen Guo-xin[3] and W. Eissner have been extending the collision code to include *all* magnetic interactions among target and (partial wave) collisional electrons — known in structure codes as mutual spin-orbit, spin-other-orbit and spin-spin interaction. Among the Breit terms of Pauli order the standard code retains only the one-body contributions (which are of order $(Z\alpha)^2(Z^2\,\mathrm{Ry})$), though in the Iron Project version one step beyond: an *effective* spin-orbit parameter introduced by Blume and Watson[4] accounts for closed-shell magnetic interactions on valence and collisional electrons. Now all two-body magnetic effects between valence and collisional electrons (hence of relative order $1/Z$) are also considered, closing a gap in the Breit-Pauli R-matrix code. Two-body finestructure terms play no great role for valence shell excitation of very highly ionized atoms because of overwhelming second order ordinary spin-orbit contributions. But the picture changes for low to medium ionization and even more when exciting inner shells, the K-shell in particular, when Blume-Watson screening can in no way be applied.

[1] P G Burke and K A Berrington: *Atomic and Molecular Processes: an R-matrix Approach,* IoP Publishing London 1993

[2] K A Berrington, W Eissner and P H Norrington: R-matrix code, *Comput. Phys. Commun.* **92** (1995) 290–420

[3] G X Chen and W Eissner: On the Development of a Full Breit-Pauli R-Matrix Code, for *J. Phys. B* in preparation

[4] M Blume and R E Watson, *Proc. R. Soc.* A **270** (1962) 127–143.