An R-matrix approach for plasma modelling and the interpretation of astrophysical observation

C P Ballance, S D Loch, T Lee and M S Pindzola
Deptment of Physics, 206 Allison Labs, Department of Physics, Auburn University, AL 36849 , USA

B M McLaughlin
Centre for Theoretical Atomic, Molecular and Optical Physics, School of Mathematics and Physics, The David Bates Building, 7 College Park, Queen’s University Belfast, Belfast BT7 1NN, UK
E-mail: ballance@physics.auburn.edu

Abstract. Over the last decade an Auburn-Rollins-Strathclyde consortium has developed several suites of parallel R-matrix codes [1, 2, 3] that can meet the fundamental data needs required for the interpretation of astrophysical observation and/or plasma experiments. Traditionally our collisional work on light fusion-related atoms has been focused towards spectroscopy and impurity transport for magnetically confined fusion devices. Our approach has been to provide a comprehensive data set for the excitation/ionization for every ion stage of a particular element. As we progress towards a burning fusion plasma, there is a demand for the collisional processes involving tungsten, which has required a revitalization of the relativistic R-matrix approach. The implementation of these codes on massively parallel supercomputers has facilitated the progression to models involving thousands of levels in the close-coupling expansion required by the open d and f sub-shell systems of mid Z tungsten. This work also complements the electron-impact excitation of Fe-Peak elements required by astrophysics, in particular the near neutral species, which offer similar atomic structure challenges. Although electron-impact excitation work is our primary focus in terms of fusion application, the single photon photoionisation codes are also being developed in tandem, and benefit greatly from this ongoing work.

1. Introduction

We have been continually developing a suite of R-matrix codes to systematically address the fundamental data needs of fusion plasma. Beyond the studies of isolated systems in relation to experimental measurements, a more comprehensive approach along an entire iso-electronic sequence of a particular atom is also required for which all electron-impact collisional processes are calculated, from electron-impact excitation/ionization to dielectronic recombination. We employ a three stage process, in which this collation of the derived fundamental collisional rates as a function of electron temperature is the first step. Subsequently, a second stage effective collision database containing generalized ionization, recombination, photon emissivity, and
radiative power loss coefficients is generated, which are functions of both electron temperature and density. For atomic species we make use of the Atomic Data and Analysis Structure (ADAS) package\cite{4} to solve the collisional-radiative equations for the generalized coefficients. The contraction from the large all-excited-levels of stage one to the relatively small ground and metastable levels database of stage two greatly minimizes the computational effort needed at the third stage, namely the modelling of plasma transport and spectral line emission.

However, it is the accuracy of fundamental collisional rates that underpins diagnostic capability. The rest of the paper shall discuss present and future directions of the R-matrix approach to first order collisional processes such as electron-impact excitation and ionization, as well as photoionisation.

2. Electron-impact Excitation

2.1. Non-relativistic/semi-relativistic R-matrix

Comprehensive datasets now exist for all the ion stages of the first five elements of the periodic table, and have been processed into generalised coefficients\cite{5}. In terms of the other light fusion related species (Z ≤ 10) the electron-impact excitation cross sections are still required for some of the near-neutral ion stages of nitrogen and oxygen, and these remain challenging.

In terms of mid-Z atoms, currently significantly modified parallel versions of R-matrix I codes in conjunction with the ICFT (Intermediate Coupling Frame Transformation)\cite{6} are the main workhorses generating both iso-electronic and iso-nuclear electron-impact excitation rates\cite{7, 8, 9}. The iso-electronic sequence ICFT calculations introduce a further level of confidence in the results, as A-values and collision strengths are now available for a range of effective charge, with post-processing tools available to highlight any unexpected deviations along a particular Z sequence. The accuracy of the ICFT method is essentially comparable to the Breit-Pauli R-matrix method which includes the first order mass-velocity, spin-orbit and Darwin terms. However the overwhelming strength of the ICFT method over more direct approaches is that the majority of the computation is carried out within a LS coupling framework. Therefore, for example, the R-matrix inner region only involves the diagonalisation of smaller LS resolved Hamiltonians and the subsequent outer region calculation is also predominantly in LS coupling. Only at the last stage are the LS-coupled unphysical K-matrices transformed, first transformed to jK coupling and then into full intermediate-coupling physical K-matrices, from which level-to-level collisions strengths are extracted. Recent improvements in the LS Hamiltonian formation and the efficiency of the matrix diagonalisation have ensured that 3-5 thousand close-coupled channels are becoming routine, with the implication that ICFT calculations at the level of 10-20 thousand close-coupled channels will soon be possible.

2.2. Relativistic electron-impact R-matrix

However, relativistic corrections can play an increasingly significant role for atoms with charge Z ≥ 18\cite{10}. As mentioned previously, semi-relativistic Breit-Pauli and ICFT calculations has been successfully applied to atomic ions below Z=30 for numerous atomic systems by scientists across the world\cite{11}. For atomic ions with Z > 30, a Dirac-Coulomb approach to the atomic structure and scattering can be important, with relativistic effects required in accurately modelling these systems. Our approach is analogous to the non-relativistic codes, starting with the distributive generation of the millions of integrals, the subsequent formation of
every \( J\) wave and finally concurrent diagonalisation of each Hamiltonian matrix, which currently permits calculations at three to four thousand coupled channel level.

Computationally, the increased number of relativistic orbitals over the corresponding non-relativistic orbitals can cause a dramatic increase both in the number of integrals required and in the complexity of the angular algebra. For example, we note that in a recent work for the electron-impact excitation of \( \text{Fe}^{4+} \) [12] and \( \text{Fe}^{5+} \) [13] hundreds of millions of Racah coefficients were calculated for the relativistic treatment of this open-d shell system.

To address the future challenge of electron scattering in which thousands of levels and tens of thousand of scattering channels are to be considered an efficient parallel version [2] of the DARC [14] suite of codes continues to be developed.

In Figure 1, we consider the electron-impact excitation of \( \text{Fe}^{2+} \) from \( ^5D_4 \) to \( ^5D_3 \) level within the 34 level 3d\(^6\) groundstate complex. Both the ICFT and DARC calculation give comparable collision strengths in an atomic system where both approaches should be valid. The oscillator strengths between the 3d\(^6\) groundstate level and the excited state 3d\(^5\)4s, 4p levels are greatly improved by allowing for a double promotion of 3p electrons in to the 3d shell. However, a simultaneous half open p shell and d shell configuration quickly gives rise to several hundred levels that we are only now able to include within the close coupling expansion. We note that we are not claiming to present a ‘definitive’ structure calculation for \( \text{Fe}^{2+} \) but would argue that we are able to perform calculations at sufficiently accurate level to provide theoretical line intensities that compare well with observational measurement [15].

3. Electron-impact Ionization

Accurate electron-impact ionization cross sections involving the ground and excited states of neutral atoms and low-charged atomic ions are needed for the collisional-radiative modelling of the moderately dense plasmas found in magnetic fusion energy experiments[16]. At low densities, only ionization cross sections from the ground and metastable states are needed. For moderately dense plasmas, ionization from excited states becomes important due to the increased overall frequency of electron-atom collisions. Along an iso-nuclear sequence the neutral atom and low-charged atomic ions are most sensitive to excited state ionization since the collision frequency for these ions can easily become higher than the radiative decay frequencies. Generally, for light elements of charge \( q \geq 3 \) in moderately dense plasmas environments, it is the ground and metastable state ionization cross sections that dominate the effective ionization rate coefficient, therefore the excited state ionization cross sections are not so important. However, for near neutral light atomic species the effective ionization rate coefficient can often be dominated by ionization from excited states. For example, in neutral lithium at an electron density of \( 1 \times 10^{14} \) cm\(^{-3}\) the effective ionization rate coefficient was calculated to be about an order of magnitude larger than the ground state ionization rate coefficient only. This was confirmed experimentally by lithium experiments at the DIII-D tokamak[17]. Thus, accurate atomic data for excited state ionization cross sections, often from very high n-shells, are needed for near neutral species.

Of course, apart from the \( R \)-matrix with pseudo-states (RMPS)[18, 19], it has been shown that other non-perturbative methods including the convergent close-coupling (CCC)[20], the exterior complex scaling (ECS)[21], and the time-dependent close-coupling (TDCC)[22] methods give comparable results, but usually at a large computational cost beyond hydrogenic systems. Perturbative methods, including those calculated with the distorted-wave method, exhibit differing trends in relation to their non-perturbative counterparts. The first trend is the well known fact that the agreement between close-coupling and distorted-wave calculations for the direct ionization cross section of the ground state along an iso-nuclear sequence becomes progressively better as the charge on the atomic ion increases. As the three-body interaction between the
Figure 1. Electron-impact excitation within the groundstate complex of Fe\(^{2+}\) using both the parallel ICFT/BPRM and DARC codes. The log of the collision strength is plotted against the energy in Rydbergs relative to the excited state.

Outgoing electrons and the remaining target core becomes dominated by the stronger residual target charge, a perturbative approximation becomes better. The second trend is that for electron-impact ionization from high n shell, for neutral and singly ionized atomic systems the distorted-wave method becomes progressively worse with increasing n shell. However, we note in contrast, that a recent study on three times ionized carbon, revealed the 5s distorted wave ionization to be comparable once more with the non-perturbative result.

Our current philosophy, accepting that under certain circumstances the effective ionization from a particular ion stage may be dominated by the very high n shells, is to use the highest non-perturbative RMPS result to scale the classical result achieved through formulas, such as the Burgess-Vriens:

\[
\sigma_{\text{single}} = \frac{4\pi R^2}{E + 2I_n} \left( \frac{5}{3I_n} - \frac{1}{E} - \frac{2I_n}{3E^2} \right),
\]

where the ionization potential for the n shell is given by:

\[
I_n = \frac{R(Q + 1)^2}{n^2},
\]
$Q$ is the charge on the atomic ion, $E$ is the energy of the incident electron in eV, and $R = 13.6$ eV. In the following figure, we show the ionization from the bundled $n$ shell of B, B$^+$ and B$^{2+}$ (top-bottom) and compare the ionization from the bundled $n=4,4$ and 5 RMPS results respectively (solid black line), with a scaled Burgess Vriens (dashed line). We observe that as the charge of the atom increases, this scaling factor becomes closer to unity. The major perturbation to employing this scaling technique are the presence of large excitation-autoionisation peaks superimposed upon the ionization cross section. These may actually dominate over the direct ionization, and therefore we must persist with explicit RMPS calculations for every term of an $n$ shell, to high enough $n$ that the direct ionization dominates once more over excitation-autoionisation.

![Figure 2](image_url)

**Figure 2.**

Using non-perturbative RMPS calculations to scale semi-empirical Burgess-Vriens to higher $n$-shell. The last bundled $n$ for the explicitly calculated term-resolved RMPS calculation for B, B$^+$ and B$^{2+}$ was 4, 4 and 5 respectively. The Burgess-Vriens result was scaled to this value.

### 4. Photoionisation

The tandem development of a parallel dipole suite of R-matrix codes ensures that as well as the calculation of photoionisation cross sections which can be used in the determination of metastable fractions of ongoing experiments, the same bound-free dipole matrix elements can also be employed in radiatively-damped electron-impact excitation cross sections or for dielectronic recombination cross sections [29]. The majority of the parallel DARC dipole code development has gone into the distributing the formation of these dipole matrix elements across...
a sufficient number of processors, as the calculation involves all the eigenvectors of a dipole allowed pair of symmetries, each of which can currently exceed 20 Gb in size. As a result we are now able to carry out complete photoionization calculations in the low energy region and reproduce the large majority of features observed in the experimental measurement. We are able to reproduce these features in such fine detail, due to our capacity to calculate at a photon energy mesh of $10^{-7} - 8$ Rydbergs with 6-30 million energy points, spreading the calculation over 1-10 thousand processor cores.

In terms of astrophysical plasmas, the photoionization of atomic ions is an important process in determining the ionization balance and hence the abundances of elements in photoionized astrophysical nebulae. Recently it has become possible to detect neutron(n)-capture elements (atomic number $Z > 30$, e.g. Se, Kr, Br, Xe, Rb, Ba and Pb) in a large number of ionized nebulae [24, 25, 26]. These elements are produced by slow or rapid n-capture nucleosynthesis (the “s-process” and “r-process,” respectively) [25, 27]. Measuring the abundances of these elements helps to reveal their dominant production sites in the Universe, as well as details of stellar structure, mixing and nucleosynthesis [23]. These astrophysical observations provide an impetus to determine the photoionization and recombination properties of n-capture elements.

As a representative sample of our work, the photoionization of Xe$^+$ has been studied recently by Bizau and co-workers [30] at an experimental photon energy spread of 25 meV. Here we report on Xe$^+$ photoionization cross-section measurements that were performed at even lower photon energy spreads down to only 4 meV. The experiments were carried out at the Advanced Light Source synchrotron radiation facility in Berkeley, California. The Xe$^+$ ions were produced from a 10-GHz ECR ion source. The experimental photon energy range from threshold to approximately 30 eV covered the valence-shell energy region of this ion. In the following figure, a medium-scale 326 level DARC calculation was able to reproduce the experimental spectrum, and also concur with the experimental quantum defect for the $5s^25p^4 \left(^1D_2\right)nd$ sequence.

Ongoing photoionisation calculations for the other neutron(n)-capture elements mentioned above and their ions are underway, with the same degree of agreement with experiment expected. Development into an automated approach to photoionisation of more complex systems where there are 10 to 100s of metastable levels will also need to be addressed in the coming years.

5. Conclusions

In summary, we have shown that our suite of R-matrix codes provides systematic coverage for a wide range of collisional processes required for plasma modelling. For atomic systems $Z \leq 30$, several sequences are already in the literature [7, 8, 9], with others ongoing. The remaining future challenges include the continued development of the electron-impact excitation DARC codes $Z > 30$ focusing more on the open-shell p, d and f systems of W, and in particular utilising the recently developed DRMPS (Dirac R-matrix with PseudoStates)[31] for the electron-impact excitation/ionisation of the near-neutral stages of W.

Acknowledgments

This work was supported in part by grants from the US Department of Energy, the US National Science Foundation, and the UN International Atomic Energy Agency. Computational work was carried out at the National Energy Research Scientific Computing Center in Oakland, California and at the National Institute for Computational Science in Oak Ridge, Tennessee, USA.
Figure 3. Total photoionisation of Xe\(^+\). The experimental data (green circles) are given in the photon energy range 21.84–22.08 eV at a photon energy resolution of 4 meV and compared with the theoretical results (red full line) from a 326-level Dirac-Coulomb R-matrix calculation convoluted with a Gaussian of 4 meV FWHM and statistically averaged over the ground and metastable states to simulate the measurements. The bars mark the energies of [5s\(^2\)5p\(^4\) (\(^3\)P\(_1\)) nd] resonances determined to have a quantum defect of 0.16.

References

[1] C P Ballance and D C Griffin, J. Phys. B 37, 2943 (2004).
[2] C P Ballance and D C Griffin, J. Phys B 39, 3617 (2006).
[3] K A Berrington, W B Eissner, and P H Norrington Comput. Phys. Commun. 92, 290 (1995).
[4] H. P. Summers and M. G. O’Mullane in Nuclear Fusion Research, eds. R. E. H. Clark and D. H. Reiter, 399-413 (Springer Press 2005).
[5] S D Loch, M S Pindzola, C P Ballance, D C Griffin, J Colgan, N R Badnell, M G O’Mullane, and H P Summers, Atomb. Data and Nucl. Data Tab. 94, 257 (2008).
[6] Griffin D C, Badnell N G and Pindzola M S J. Phys. B: At. Mol. Opt. Phys. 31, 3713 (1998).
[7] M C Witthoeft, A D Whiteford and N R Badnell J. Phys. B: At. Mol. Opt. Phys. 40 (2007).
[8] G Y Liang and N R Badnell Astron. Astrophys. 518 A64 (2010).
[9] J A Ludlow, C P Ballance, S D Loch and M S Pindzola J. Phys. B: At. Mol. Opt. Phys. 43, 074029 (2010).
[10] I P Grant Quantum Theory of Atoms and Molecules: Theory and Computation (New York, USA: Springer) (2007).
[11] D G Hummer, K A Berrington, W Eissner, A K Pradhan, H E Saraph and J A Tully, Astron. Astrophys. 279, 298 (1993).
[12] C P Ballance, D C Griffin and B M McLaughlin J. Phys. B: At. Mol. Opt. Phys. 40 F327 (2007).
[13] C P Ballance and D C Griffin J. Phys. B: At. Mol. Opt. Phys. 41, 195205 (2008).
[14] P H Norrington and I P Grant I F P, J. Phys. B: At. Mol. Opt. Phys. 20, 4869 (1987).
[15] M A Bautista, C P Ballance and P Quinet Ap. J. Letters, 718 L189 (2010)
[16] H. P. Summers, W. J. Dickson, M. G. O'Mullane, N. R. Badnell, A. D. Whiteford, D. H. Brooks, J. Lang, S. D. Loch, and D. C. Griffin, Plasma Phys. Control. Fusion 48, 263 (2006).
[17] J P Allain, D G Whyte, and J N Brooks, Nucl. Fusion 44, 655 (2004).
[18] K. Bartschat, E. T. Hudson, M. P. Scott, P. G. Burke, and V. M. Burke, J. Phys. B 29, 115 (1996).
[19] Gorczyca T W and Badnell N R J. Phys. B 30, 3897 (1997)
[20] I. Bray, D. V. Fursa, A. S. Kheifets, and A. T. Stelbovics, J. Phys. B 35, R117 (2002).
[21] C. W. McCurdy, M. Baertschy, and T. N. Rescigno, J. Phys. B 37, R137 (2004).
[22] M. S. Pindzola, F. Robicheaux, S. D. Loch, J. C. Berengut, T. Topcu, J. Colgan, M. Foster, D. C. Griffin, C. P. Ballance, D. R. Schultz, T. Minami, N. R. Badnell, M. C. Witthoeft, D. R. Plante, D. M. Mitnik, J. A. Ludlow, and U. Kleiman, J. Phys. B 40, R39 (2007).
[23] N C Sterling, H L Dinerstein, S Hwang, S Redfield, A Aguilar, M C Witthoeft, D Esteves, A L D Kilcoyne, M Bautista, R A Phaneuf, R Bilodeau, C P Ballance, B M McLaughlin and P H Norrington Pub. Astron. Soc. Aust. (PASA) 26 339 (2009)
[24] N C Sterling, H L Dinerstein and T R Kallman, Astrophys. J. Suppl. Ser. 169 37 (2007)
[25] B Sharpee, Y Zhang, R Williams, E Pellegrini, K Cavagnolo, J A Baldwin, M Phillips and X W Liu Astrophys. J. 659 1265 (2007)
[26] N C Sterling and H L Dinerstein Astrophys. J. Suppl. Ser. 174 157 (2008)
[27] K Langanke and M Wiescher Rep. Prog. Phys.64 1657 (2001)
[28] V V Smith and D L Lambert Astrophys. J. Suppl. Ser. 72 387 (1990)
[29] C P Ballance, S D Loch, M S Pindzola and D C Griffin J. Phys. B: At. Mol. Opt. Phys. 43 205201 (2010)
[30] J. M. Bizau et. al. J. Phys. B 44 055205 (2011)
[31] N R Badnell J Phys B: At Mol Opt Phys 41 175202 (2008)