Effective collision strengths for Mg-like iron peak ions

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Abstract. Berrington et al [1] have calculated effective collision strengths for Fe XV using both the Breit-Pauli and Dirac R-matrix methods. The calculation was undertaken in the spirit of a case study to lay to rest assertions that the Dirac method is superior for such ions. They found good agreement between the two methods. Current development of the DARC program [2] is aimed at improving the quality of the target states. As a first step we have included the Breit interaction directly in the bound-bound continuum hamiltonians. DARC is based on the Dirac-Coulomb hamiltonian and in order to treat heavier systems correctly it is necessary to include the Breit interaction. We have also used Fe XV as a case study for this code development and in addition examined Cr XIII and Ni XVII. The effects on the effective collision strengths for the iron peak ions are as expected small. The work illustrates the extent to which the DARC program can be automated for isoelectronic series.

1. Introduction

The R-matrix method [3] is the tool of choice for the production of high quality collisional atomic data. Beginning with the publication [4] of the RMATRX code in 1974 a large number of FORTRAN programs have implemented this approach. These are used widely in producing data and also are continually being modified to incorporate new physics. An example of the latter is the use of target states built from relativistic gaussian-type-orbitals in a many-body perturbation theory framework [5]. This gives a fairly compact target representation of much higher accuracy. The effect of this modification on the calculational time is not apparent from the paper. A comparable level of accuracy can be achieved with the existent programs by using a large configuration interaction expansion. This requires considerable computational resources but the viability of such calculations is exemplified by a recent calculation for electron scattering by Fe V [6]. The large size of this calculation was not due to the configuration interaction expansion but rather to the number of low-lying and overlapping states in this ion. It should be possible to produce data of a high accuracy. Robust and reliable is how these programs are sometimes described, rarely are they described as easy to use.

‘Users’ of the atomic data, in for example astrophysical modelling, would ideally like the data to be of the highest quality. In conversation some admit that ‘anything would do’ and it seems in practice that medium quality data would suffice. Placing error bounds on the theoretical data is often difficult. R-matrix papers sometimes claim an accuracy of 10% for the data without much justification. As the target model increases in complexity there should be convergence in the atomic data and this will give some feel for the accuracy. The place of the high quality calculation is secure as a benchmark.
In principle with the free availability of the \( R \)-matrix programs [7] it should be possible for ‘users’ to generate their own atomic data. This study was undertaken in part to assess how feasible that would be. There is a benchmark calculation for Mg-like Fe XV [1]. This paper mainly demonstrates the expected near equivalence of the Breit-Pauli and Dirac hamiltonians for a system with this atomic number. In addition it has useful comments on the pitfalls of such a calculation. We have carried out simpler calculations for the ions Cr XIII, Fe XV and Ni XVII. The only essential change in the input data for the three ions was the atomic number. Our main purpose is obtain a overview of the complete calculation from target generation through to effective collision strength for a case of moderate size.

As part of code development to improve the target representation we have examined the inclusion of the Breit interaction in the bound-bound part of the continuum hamiltonian. This is only a partial introduction of the Breit interaction as it is not included in any radial integrals involving the continuum function. This is expected to be important for heavier systems.

2. Calculations
The configurations 3s\(^2\), 3s3p, 3p\(^2\), 3s3d, 3p3d and 3d\(^2\) were included in the target. This gives rise to 35 fine-structure levels. The target energies and orbitals were calculated using grasp0 [8]. The EAL (extended average level) MCDF (multi-configurational Dirac Fock) method was employed. We have not here included higher order radiative corrections because these corrections cannot be treated consistently in the present scattering calculation. The accuracy is at the 1 to 2\% when compared to NIST data. So it is not at the highest accuracy but we are not seeking that here.

The \( R \)-matrix calculations used DARC (Dirac Atomic \( R \)-matrix Code) [2] interfaced with the UK APAP asymptotic and utility codes [7].

Limitations in these calculations are the target representation (missing \( n = 4 \) orbitals and resultant configuration interaction) and a modest energy range for resolution of the resonance structure.

Results are shown in Figure 1 for transitions between the ground-state and the first 4 excited levels. For Fe XV a comparison is made with results taken from [1].

Some observations:
- Figure 1(c) shows a failure to resolve the resonance structure for Fe XV. The low energy contribution is not showing.
- Figure 1(d) shows a failure at the high energy for Fe XV. This is an allowed transition (3s\(^2\) \( ^1S_0 \) — 3s3p \( ^1P_1 \)) and there may be an inconsistency in the contribution from high partial waves (top-up).

Overall there is reasonable agreement given the limitations. The behaviour of the other ions looks consistent. The discrepancies point us towards how we can improve the data within the context of maintaining moderate accuracy.

Figure 2 shows the effect for Fe XV of including the Breit interaction in the bound-bound part of the continuum hamiltonian. The effect here is to modify the thresholds and move the resonance structure. As the change in the energies for this ion is small we only see corresponding small effects in the low energy effective collision strengths. For the allowed transition for which the resonance structure is not dominant the two calculations are nearly identical.

3. Conclusions
The calculation of the effective collision strengths involved the following sequence of FORTRAN programs

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\text{grasp0 } \rightarrow \text{darc0 } \rightarrow \text{darc1a } \rightarrow \text{darc1b } \rightarrow \text{darc2 } \rightarrow \text{dto3 } \rightarrow \text{stg3r } \rightarrow \text{stgf } \rightarrow \text{omadd } \rightarrow \text{adasexj}
\]
Figure 1. Effective collision strengths from $3s^2 \, ^1S_0$ to (a) $3s3p \, ^3P_0$; (b) $3s3p \, ^3P_1$; (c) $3s3p \, ^3P_2$; (d) $3s3p \, ^1P_1$. □ denotes the Fe XV data of [1].

The proliferation of programs is historic and in part due to computational limitations as the size of the problems increased. There are too many programs, each with its own input data and pitfalls, some of which we fell into. While it is true that each program can be run in a near default mode, there are hidden options and parameters. These parameters are sometimes solutions to numerical problems that have been discussed in the literature. Alternatively they may be adding new physics. Either way they reflect the long-time development of these programs. Supplied documentation is sparse.

The programs can be grouped into

- target: grasp0 $\rightarrow$ darc0
- R-matrix: darc1a $\rightarrow$ darc1b $\rightarrow$ darc2 $\rightarrow$ dto3 $\rightarrow$ stgf
- collision strength: stgf
- rate coefficient: omadd $\rightarrow$ adasexj

and this would make it more manageable. If we wish these programs to be a tool for ‘users’ to generate their own atomic data then we need such a merger together with a more consistent interface and documentation.
Figure 2. Effective collision strengths from $3s^2 \, ^1S_0$ to (a) $3s3p \, ^3P_0$ and $3s3p \, ^3P_1$, (b) $3s3p \, ^3P_2$ and $3s3p \, ^1P_1$, in Fe XV.

A more detailed account of these calculations will be made available at the website www.am.qub.ac.uk/apa.

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