Electron-Impact Excitation of Fe-peak Ions for Astrophysical Applications

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Abstract. This paper discusses one of the major outstanding problems in atomic collision physics, namely the accurate theoretical treatment of electron scattering from open d-shell systems, and explores how this issue has been addressed over recent years with the development of the new parallel $R$-matrix suite of codes. It focuses on one code in particular - the new parallel $R$-matrix package PRMAT, which has recently been extended to account for relativistic fine-structure effects. This program facilitates the determination of accurate electron-impact excitation rates for complex open 3d-shell systems including the astrophysically important Fe-peak ions such as Ni II, Fe II and Fe III. Results are presented for collision strengths and Maxwellian averaged effective collision strengths for the optically forbidden fine-structure transitions of Ni II. To our knowledge this is the most extensive calculation completed to date for this ion.

1. Introduction

There has been profound progress in the theoretical treatment of electron collision processes in recent years, most notably in the development of robust computer codes which have proved highly successful in both aiding our understanding of the scattering process and in acting as predictive tools for providing much needed atomic data. However, one of the major outstanding problems in atomic collision physics has been the accurate treatment of electron scattering from open d-shell systems. Many such systems have important applications, for example, ions of the Fe-peak elements, which have important astrophysical applications, have an open 3d-shell. This complex open d-shell structure results in a number of difficulties. It gives rise to hundreds of target state energy levels and typically thousands of closely coupled channels which need to be accurately incorporated into the model. These target states require large configuration interaction expansions for their accurate representation. Further complications arise from the infinite number of Rydberg resonances, converging onto each target state threshold, which are found to dominate the low energy electron scattering region. Calculations have to be carried out over a very fine mesh of incident electron energies, typically involving thousands of energy points, in order to properly resolve these complex resonance structures.

The consequence of these complications is a highly intensive computational challenge which has prompted the development of the new parallel $R$-matrix suite of codes. Over recent years Queen’s University Belfast and Daresbury Laboratory (UK) have embarked upon an intensive programme of research to develop a new parallel $R$-matrix package, PRMAT [1], which allows for a more complete treatment of correlation effects. This program has been most recently
extended to allow for the inclusion of relativistic effects, enabling the computation of converged collision strengths and effective collision strengths between fine-structure levels. These codes are currently exploiting the rapidly increasing power and availability of high performance parallel computing facilities. This new generation of parallel codes now make the aforementioned formidable calculations computationally viable, yielding high quality atomic data for Fe-peak ions.

2. PRMAT - A new generation of parallel codes

The essential principle of R-matrix theory is the partitioning of configuration space into two main regions, namely the internal region and the external region. In the internal region, electron exchange and correlation effects between the scattered electron and target are crucial. Consequently, it is necessary to expand the collision complex using a configuration interaction approach similar to that utilised in bound state calculations:

$$\psi_k(x_1 \ldots x_{N+1}) = \mathcal{A} \sum_{ij} c_{ijk} \Phi_i(x_1 \ldots x_N; \hat{r}_{N+1} \sigma_{N+1}) u_{ij}(r_{N+1}) + \sum_j d_{ijk} \chi_j (x_1 \ldots x_{N+1}).$$

(1)

In this equation, $\mathcal{A}$ is the customary antisymmetrisation operator, $\Phi_i$ are the channel functions representing the target eigenstates $\Phi_i$ and $\chi_i$ represents the quadratically integrable functions which are included for completeness and vanish at the surface of the internal region. The continuum orbitals, $u_{ij}$, represent the motion of the colliding electron and are the only terms in equation (1) which are non-zero on the internal region boundary. Finally, the coefficients $c_{ijk}$ and $d_{ijk}$ are obtained by diagonalising the the $(N+1)$-electron Hamiltonian, $H^{N+1}$, in this finite space

$$(\psi_k | H^{N+1} | \psi_{k'}) = E_k \delta_{kk'},$$

(2)

where the round brackets indicate the finite range of integration.

In the external region, electron exchange between the two bodies can be neglected, thereby simplifying the problem considerably. The total collision wavefunction is expanded as follows

$$\Psi(x_1 \ldots x_{N+1}) = \sum_i \hat{\Phi}_i(x_1 \ldots x_N; \hat{r}_{N+1} \sigma_{N+1}) F_i(r_{N+1}),$$

(3)

where the $\hat{\Phi}_i$ are the same channel functions as in expansion (1), but no antisymmetrisation is required in this region. Substituting equation (3) into the time-independent Schrödinger equation and projecting onto the channel functions results in a set of coupled second-order differential equations satisfied by the reduced radial wavefunctions $F_i$.

This theory, though very simplified here, is implemented in the PRMAT program. These codes have been described in detail by Sunderland et al. [1], hence we follow with only a brief overview.

2.1. Internal region calculations

Having established an ideal target model representation and orbital parameters using an atomic structure program (usually CIV3 [2]), we proceed to running the internal region program which comprises of three main stages - RAD computes the radial integrals, ANG computes the angular integrals and these are combined in HAM to form the Hamiltonian matrix elements. It is also possible to diagonalise the Hamiltonian matrix within HAM, however if the size of the
Hamiltonian matrix becomes too large another parallel diagonalisation code can be utilised. From this point, we turn our attention to the FINE code and the inclusion of relativistic fine-structure effects. For atoms or ions with $Z < 30$ we can transform the $R$-matrix in $LS$-coupling at energy $E$, $R^{LS\pi}(E)$, to an $R$-matrix in pair coupling, $R^{J\pi}(E)$. This is carried out on the $R$-matrix boundary between the internal and external regions. However, instead of carrying out this transformation at each energy, we can transform the energy independent surface amplitudes. Hence the recoupling is performed only once for each $LS\pi$ and $J\pi$ symmetry rather than for each scattering energy $E$. This is performed by the new program FINE [3]. To take account of term splitting in the target, the $R^{J\pi}$ can be further transformed by term coupling coefficients which are the mixing coefficients for the individual $L_iS_i\pi_i$ states forming a $J_i\pi_i$ state.

This particular transformation method has a number of advantages. Firstly, using $LS$-coupling in the internal region allows for the inclusion of sophisticated CI wavefunctions for both the target and scattering complex. Secondly, transforming the $R$-matrix on the $R$-matrix boundary, as opposed to the asymptotic boundary, allows fine-structure channels to be included in the external region.

2.2. External and asymptotic region calculations
A number of powerful parallel codes exist which can be used in conjunction with these internal region codes. These include PFARM - based on an earlier serial program FARM [4] - and PSTGF [5]. Our tests have shown that the same results are obtained using either.

3. Application - Electron Collisions with Ni II
Reliable and extensive atomic data for the highly abundant Fe-peak elements is of crucial importance in astrophysics. In particular, electron-impact collision strengths and effective collision strengths are needed to facilitate the interpretation of astronomical spectra, since lines from the Fe-peak elements in low ionisation stages are observed from a wide variety of stellar objects. For example, major Fe II and Ni II contributions have been detected in the spectra of gaseous nebulae, supernovae and various stars. There is therefore an overwhelming need for high quality atomic data for these important Fe-peak elements so that these spectral lines can be properly understood and meticulously modelled.

As an illustration of an ongoing application of PRMAT, we describe the current scattering calculation in which collision strengths and effective collision strengths for the electron-impact excitation of Ni II have been computed for all of the optically forbidden fine-structure transitions. Nickel is the second most abundant Fe-peak element after iron itself. However, despite the importance of Ni II in astrophysics, there is comparatively little data currently available for this ion, particularly data for collision strengths between fine-structure levels. Indeed, the current demand for electron excitation data for this particular ion has been further fuelled by the recent observation of Ni II emission lines within the circumstellar nebula of the symbiotic star $\eta$ Carinae [6], a luminous blue variable (LBV).

3.1. Target Data
To date, the best available fine-structure calculation for Ni II (Bautista [7]) has included 77 $jj$-levels corresponding to only the first four basis configurations - $3d^84s$, $3d^74s^2$ and $3d^84p$. Thirteen additional configuration functions were also included in this work as CI to properly represent the target state wavefunctions. The present work extends this calculation to include a further excited basis configuration - $3d^74s4p$, which gives rise to a total of 295 $jj$-levels as seen in Table 1, an increase of 218 target levels on the work of [7].

This enables us to examine not only all of the additional transitions that involve these levels, but also to obtain accurate collision strengths for the low-lying transitions at much higher energies than has been possible to date.
Table 1. The number of target states and coupled channels arising from the addition of each basis configuration.

| Ni II Target Configurations | No. of Target States (LS) | Max. No. of Channels (LS) | No. of Target States (jj) | No. of Channels (jj) |
|-----------------------------|---------------------------|---------------------------|--------------------------|----------------------|
| $3p^63d^2$                  | 1                         | 3                        | 2                        | 10                   |
| $3p^63d^84s$                | 8                         | 20                       | 18                       | 100                  |
| $3p^63d^74s^2$              | 16                        | 46                       | 37                       | 220                  |
| $3d^4p$                     | 35                        | 99                       | 82                       | 490                  |
| $3d^74s4p$                  | 113                       | 327                      | 295                      | 1930                 |

Before embarking on the formidable 295 $jj$-level, 1930 coupled channel scattering calculation however, precursory work involved the determination of accurate representations of the target state and collision wavefunctions. This initial work is carried out in $LS$-coupling. The 113 $LS$ target states are optimally represented by configuration interaction expansions in terms of nine orthogonal basis orbitals, eight spectroscopic - 1s, 2s, 2p, 3s, 3p, 3d, 4s, 4p - and one 4d pseudo orbital included to allow for additional correlation effects. Together with the five target configurations listed in Table 1, an additional nine correlation functions were included in the configuration interaction expansion of the complex Ni II target. These additional nine configurations are listed as: $3d^74p^2$, $3d^64s^24p$, $3d^64s4p^2$, $3d^64d$, $3d^74d^2$, $3d^74s4d$, $3d^74p4d$, $3d^64s^24d$, $3d^64s4d^2$.

3.2. Fine-structure collision strengths
The 14-configuration CI target model described above was adopted to compute converged total collision strengths, and Maxwellian averaged effective collision strengths obtained by averaging the finely resolved collision strengths over a Maxwellian distribution of electron velocities, for all of the fine-structure forbidden transitions in this study. The present 295 $jj$-level calculation was carried out for all singlet, triplet, quintet and septet $(N + 1)$ spin symmetries with both even and odd parities. All partial waves with angular momentum $J \leq 12$ were considered in this work. A very fine mesh of incident electron energies were used in the external region in order to properly resolve the characteristic Rydberg resonance structures which are found to occur as far as the highest target threshold. Approximately 12000 energy points were considered in this region. Above this, where there are no resonances, a much coarser mesh can be adopted. Approximately 200 points were considered above the highest lying target threshold to the final energy of interest at 10 Rydbergs.

In the course of this work we have noted dramatic differences in the complex resonance effects dominating the low energy electron scattering region. These structures were found to depend sensitively on the scale and sophistication of the target model employed in the scattering calculations. In order to emphasise this the contribution from the $J = 1$ partial wave to the collision strength of an important Ni II transition is presented, the collision strength having been computed for two models of varying complexity.

Figure 1 corresponds to a forbidden transition between the split ground state levels and displays the collision strength calculated using a primitive 4-configuration, 82 $jj$-level model.
together with the collision strength computed using a much more advanced 14-configuration, 295 $jj$-level model. Although the collision strengths were computed for energies up to 10 Rydbergs, attention is concentrated on the low energy scattering region, where the masses of Rydberg resonances converging onto each target state threshold are clearly evident. The differences between the collision strengths of the two models is considerable. The additional correlations and target levels of the 14-configuration model cause a significant shift of the collision strength. The difference in the positioning of the prominent resonance peak is striking. The basic 4-configuration model initially locates this feature at approximately 0.36 Rydbergs, whereas the more elaborate 14-configuration model causes a substantial shift of this large resonance structure and it is now predicted to occur at approximately 0.29 Rydbergs. This will undoubtedly affect our Maxwellian averaging when it comes to the calculation of effective collision strengths. This same trend was noted in all of the forbidden transitions considered.

Investigations have shown that both the additional correlation functions and target levels included within the 14-configuration model have contributed to these shifts in the collision strength. This highlights the huge importance of including each of these highly influential factors within scattering calculations. Today’s new generation of parallel computer codes are able to accommodate the inclusion of these factors without any difficulty, thereby ensuring that the Maxwellian averaging used to compute the effective collision strengths is of the desired highest level of accuracy.

We conclude the discussion of our Ni II scattering calculation by presenting a number of Maxwellian averaged effective collision strengths computed using the 14-configuration CI model. A total of 43365 transitions were considered at twenty-seven individual electron temperatures ranging from 30 - 100 000 K (the temperatures of astrophysical importance). Figure 2 presents the total effective collision strength as a function of log electron temperature in Kelvin for the 3d$^9$ 2D$_{5/2}$ - 3d$^9$ 2D$_{3/2}$ fine-structure transition. Comparisons are made between the present 295 level calculation (diamonds) and the 77 level calculation (stars) of Bautista [7]. At present these fine-structure effective collision strengths are the only fine-structure data available for comparison. The results of each are in good agreement, however effective collision strengths at much lower and higher temperatures have been obtained in the present calculation. Table 2 presents the numerical effective collision strengths for this transition, together with a number of others. Again, the agreement with the values of [7] is very satisfactory. We are confident that the present calculation provides the most extensive and accurate set of collisional data to date for Ni II.

We have come a long way in the last 30 years with electron-impact excitation calculations.
for Fe-peak elements, gradually increasing in sophistication alongside the development of more powerful codes. The rapidly increasing power and availability of the current generation of parallel codes and computing facilities enables the computation of converged effective collision strengths of the highest degree of accuracy attainable for electron collisions with open 3d-shell Fe-peak elements. We need to continue to push the boundaries on the scale of these calculations in order to determine the most accurate and comprehensive collisional data for these important ions of astrophysical interest. Together with Ni II, large scale calculations for a number of other ions have been carried out. Calculations for Fe II and Fe III have been completed, while calculations for Ni II, Ni V and Cr II are ongoing with further results soon to be published.

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Table 2. Comparison of effective collision strengths between fine-structure levels from the present calculation and those of Bautista (MB) [7].

| Transition       | 5000 K | 10000 K | 20000 K |
|------------------|--------|---------|---------|
|                  | Present | MB      | Present | MB      | Present | MB      |
| \(3d^9 2D_{3/2} - 3d^9 2D_{3/2} \) (1 - 2) | 2.10    | 2.19    | 2.02    | 1.95    | 1.81    | 1.73    |
| \(3d^9 2D_{5/2} - 3d^9 4s^2F_{5/2} \) (1 - 3) | 1.75    | 2.07    | 1.70    | 1.91    | 1.49    | 1.62    |
| \(3d^9 2D_{3/2} - 3d^9 4s^2F_{7/2} \) (2 - 7) | 0.536   | 0.420   | 0.477   | 0.407   | 0.403   | 0.423   |

Figure 2. Total effective collision strength as a function of log electron temperature in Kelvin for the \(3d^9 2D_{5/2} - 3d^9 2D_{3/2} \) fine-structure transition.