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ELECTRON-IMPACT EXCITATION OF FE^{2+}: A COMPARISON OF INTERMEDIATE COUPLING FRAME TRANSFORMATION, BREIT-PAULI AND DIRAC R-MATRIX CALCULATIONS

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ABSTRACT

Modeling the spectral emission of low-charge iron group ions enables the diagnostic determination of the local physical conditions of many cool plasma environments such as those found in H II regions, planetary nebulae, active galactic nuclei etc. Electron-impact excitation drives the population of the emitting levels and, hence, their emissivities. By carrying-out Breit-Pauli and intermediate coupling frame transformation (ICFT) R-matrix calculations for the electron-impact excitation of Fe^{2+} which both use the exact same atomic structure and the same close-coupling expansion, we demonstrate the validity of the application of the powerful ICFT method to low-charge iron group ions. This is in contradiction to the finding of Bautista et al. [ApJ, 718, L189, (2010)] who carried-out ICFT and Dirac R-matrix calculations for the same ion. We discuss possible reasons.

Keywords: atomic data — atomic processes — plasmas

1. INTRODUCTION

The electron-impact excitation of low-charge ion group ions is an important process in many cool astrophysical plasmas. The subsequent spectral emission can be used to diagnose the physical conditions of H II regions, planetary nebulae, active galactic nuclei and many stars — see for example Johansson et al. (2000); Vestergaard & Wilkes (2001); Esteban et al. (2004); Mesa-Delgado et al. (2009); Mehner et al. (2010); Madura et al. (2012); Zhang et al. (2012); McClelland et al. (2013).

In order to have confidence in the temperatures, densities, and chemical compositions deduced from modeling such emission it is important that the uncertainties in the atomic data be well understood and their effects modeled. Energy levels can be compared with observed. Radiative data can usually be computed with increasingly large configuration interaction expansions to demonstrate convergence to a sufficient degree. The case of electron-impact excitation is more problematic. The complexity of the open $3d$-subshell leads to a large number of low-lying target levels which should be coupled together in a scattering calculation (Burke et al. 1994). The R-matrix method is paramount here. It has been advantageous to introduce some approximations into the scattering problem which leads to the highly efficient and widely used intermediate coupling frame transformation (ICFT) R-matrix method (Griffin et al. 1998).

Bautista et al. (2010) recently modeled Fe III line intensities from the Orion nebulae which had been observed by Mesa-Delgado et al. (2009). They found much better accord between theory and observation when they used excitation data which they calculated with the Dirac Atomic R-matrix code (DARC) methodology (Ait-Tahar et al. 1996; Norrington 2004) than that they calculated with the ICFT method. Their ICFT Maxwellian-averaged collision strengths for transitions from the ground level to all other levels of the $3d^6$ configuration differed by up to a factor 3 (both larger and smaller) from their DARC ones at 10^4 K. They attributed this difference "to the limited treatment of spin-orbit effects in near-threshold resonances" by the ICFT method. This surprising finding has implications not just for the validity and use of the ICFT method but also the R-matrix II (Burke et al. 1994) FINE method (Burke 2010) with which it shares some similarities.

There are a number of issues which can be raised about the comparison made by Bautista et al. (2010). It has long been known that to be able to deduce anything meaningful about two scattering methods from a comparison of collision data it is necessary that the differences in the atomic structure be kept to an absolute minimum. Bautista et al. (2010) used a much larger configuration interaction (36 configurations) for their ICFT atomic structure compared to that for their DARC one (8 configurations). They also used a number of pseudo orbitals in their ICFT target description while the DARC ones were purely spectroscopic — pseudo-orbitals lead to pseudo-resonances. They retained 283 levels in their ICFT close-coupling expansion but 322 levels in their DARC one.

We report-on the results of parallel ICFT and BPRM R-matrix calculations for Fe^{2+} that use the exact same atomic structure (an 8 configuration interaction expansion) and the same close-coupling expansion (322 levels). We find excellent agreement between the two ($< 5\%$ where Bautista et al. (2010) found factors of 3). We also find excellent agreement with a similar DARC calculation which we have carried out. Many of the differences found by Bautista et al. (2010) disappear once we correctly label their DARC transitions. Some differences remain with their ICFT results and for which the source is likely one of the possible causes listed in the preceding paragraph.

The rest of this paper is structured as follows: in Section 2 we describe the key differences between the different R-matrix methods we use; in Section 3 we give details of both the atomic structure and atomic collision calculations; in Section 4 we present our results and discuss their agreement with and differences from the results of

Table 1
Lowest 17 energy levels (Ryd) of the $3d^6$ ground configuration of Fe^{2+}.

Term/Level	Observed[a]	AS[b]	GRASP0[b]	GRASP0[c]
$^5D_4$	0.0	0.0	0.0	0.0
$^5D_3$	0.003975	0.004001	0.003408	0.003613
$^5D_2$	0.006733	0.006803	0.005823	0.006162
$^5D_1$	0.008497	0.008602	0.007381	0.007803
$^5D_0$	0.009361	0.009483	0.008147	0.008608
$^3P2_2$	0.176830	0.18434	0.19477	0.19564
$^3P2_1$	0.188527	0.19636	0.20543	0.20690
$^3P2_0$	0.193266	0.20122	0.20994	0.21161
$^3H_6$	0.182719	0.20976	0.22119	0.22244
$^3H_5$	0.184995	0.21173	0.22282	0.22416
$^3H_4$	0.186645	0.21370	0.22444	0.22588
$^3F2_4$	0.195578	0.21026	0.22199	0.22313
$^3F2_3$	0.197744	0.21313	0.22439	0.22571
$^3F2_2$	0.199177	0.21468	0.22572	0.22712
$^3G_5$	0.223796	0.24873	0.26285	0.26437
$^3G_4$	0.227278	0.25202	0.26558	0.26729
$^3G_3$	0.229114	0.25367	0.26700	0.26878

[a]NIST (2013)
[b]Present work.
[c]From Bautista et al. (2010)

Bautista et al. (2010); and in Section 5 we draw some key conclusions.

2. THEORY

Relativistic effects can be expected to be important in general for the iron group — just compare energies and radiative data calculated with and without such an allowance. The case for their inclusion in the description of electron-impact excitation at low stages of ionization is less clear. The Iron Project argued (Hummer et al. 1993) that algebraic recoupling of LS-coupling scattering matrices alone was sufficient to determine level-resolved collision data and adopted such an approach. Essentially this is because electron-impact excitation is mediated by a two-body operator while the dominant fine-structure operator is one-body. Only more recently (Ramsbottom et al. 2007) has it become practical to carry-out similarly sized R-matrix calculations which include relativistic interactions explicitly. Large differences with the earlier Iron Project results have been noted (Ramsbottom et al. 2007; Bautista et al. 2010) but it is difficult to separate out the difference due to the choice of the collision representation from the difference due to the differing atomic structure representations adopted. Obtaining a sufficiently accurate atomic structure is itself a non-trivial exercise for these ions.

Relativistic interactions can be included using either the Breit-Pauli (BPRM) or Dirac Atomic (DARC) R-matrix codes. A full Dirac treatment is not necessary here ($Z \leq 30$) but the DARC suite of codes has lent itself more readily to large-scale parallelization. Level-resolved R-matrix inner-region codes lead to the need to diagonalize large Hamiltonians (e.g. rank $> 10^5$) and to solve a large set of coupled equations (e.g. ~ 10000) in the R-matrix outer region.

The BPRM method lends itself to useful approximation because the scattering problem is set-up initially in term-resolved LS-coupling and subsequently transformed to level-resolved jK-coupling upon the addition of fine-structure relativistic operators (e.g. spin-orbit). If the relativistic operators are not too large then they can be treated perturbatively. The R-matrix II approach (Burke et al. 1994) diagonalizes the LS-coupling scattering Hamiltonian and then transforms the resulting eigen-vectors (surface amplitudes) to jK-coupling. It allows for relativistic effects through a further transformation which makes use of term coupling coefficients (Jones 1975). The outer region problem is then solved as in the original BPRM method. This reduces the computational time (for the diagonalization) by an order of magnitude or allows a much larger scattering expansion to be used instead.

The intermediate coupling frame transformation (ICFT) R-matrix method (Griffin et al. 1998) goes a step further. It solves the outer region coupled channel problem in LS-coupling as well. It then transforms (asymptotically) the scattering or reactance matrices to jK-coupling and again uses term coupling coefficients. The ICFT method is an order of magnitude more efficient in the outer region as well. It does require that it is sufficiently accurate to delay the treatment of fine-structure relativistic effects until reaching asymptopia[1]. The original comparisons (Griffin et al. 1998, 1999; Badnell & Griffin 1999) between the results of ICFT and BPRM calculations demonstrated agreement between the Maxwellian-averaged collision strengths to within a few percent. This is well within the uncertainties for complex ions which are introduced by truncating both the target configuration interaction expansion and the close-coupling scattering expansion.

[1] All BPRM/ICFT methods treat the one-body non-fine-structure operators without further approximation — they are included in the scattering Hamiltonian to be diagonalized.

Table 2
Maxwellian effective collision strengths for Fe^{2+} at 10^4 K
from the $^5D_4$ ground-level to the next 16 levels as listed in Table 1.

Term/Level	LS(jK)J[a]	ICFT(Obs.)[a]	ICFT[a]	BPRM[a]	DARC[a]	DARC[b]	ICFT[b]
$^5D_3$	3.19(+0)	3.09(+0)[c]	3.11(+0)	3.03(+0)	2.73(+0)	2.54(+0)	4.57(+0)
$^5D_2$	1.45(+0)	1.45(+0)	1.45(+0)	1.41(+0)	1.22(+0)	1.11(+0)	1.94(+0)
$^5D_1$	6.79(−1)	7.14(−1)	6.85(−1)	6.65(−1)	5.91(−1)	5.33(−1)	8.79(−1)
$^5D_0$	1.99(−1)	2.14(−1)	2.01(−1)	1.97(−1)	1.74(−1)	1.60(−1)	2.51(−1)
$^3P2_2$	6.99(−1)	7.13(−1)	7.94(−1)	8.06(−1)	7.00(−1)	7.14(−1)	7.14(−1)
$^3P2_1$	2.16(−1)	1.79(−1)	2.22(−1)	2.20(−1)	1.80(−1)	1.96(−1)	1.84(−1)
$^3P2_0$	3.39(−2)	3.07(−2)	4.35(−2)	3.79(−2)	3.05(−2)	3.25(−2)	3.83(−2)
$^3H_6$	1.41(+0)	1.45(+0)	1.43(+0)	1.44(+0)	1.30(+0)	1.21(+0)	2.66(+0)
$^3H_5$	5.05(−1)	6.44(−1)	6.38(−1)	6.62(−1)	5.50(−1)	5.33(−1)	1.10(+0)
$^3H_4$	9.45(−2)	2.48(−1)	2.16(−1)	2.20(−1)	2.11(−1)	1.91(−1)	2.41(−1)
$^3F2_4$	1.10(+0)	1.16(+0)	1.12(+0)	1.13(+0)	9.96(−1)	9.84(−1)	1.47(+0)
$^3F2_3$	4.51(−1)	5.43(−1)	5.15(−1)	5.26(−1)	4.52(−1)	4.54(−1)	6.42(−1)
$^3F2_2$	1.60(−1)	1.99(−1)	1.88(−1)	1.95(−1)	1.66(−1)	1.73(−1)	2.11(−1)
$^3G_5$	1.34(+0)	1.27(+0)	1.31(+0)	1.32(+0)	1.07(+0)	1.11(+0)	1.11(+0)
$^3G_4$	5.29(−1)	4.90(−1)	5.36(−1)	5.51(−1)	4.15(−1)	4.21(−1)	1.24(+0)
$^3G_3$	1.28(−1)	1.40(−1)	1.62(−1)	1.67(−1)	1.21(−1)	1.35(−1)	4.52(−1)

[a]Present work.
[b]Bautista et al. (2010) (but DARC order corrected.)
[c](m) denotes $\times 10^m$.

3. CALCULATIONAL DETAILS

3.1. *Structure*

We used the same 8 configuration interaction target expansion for our ICFT, BPRM and DARC calculations: $3s^23p^63d^6$, $3s^23p^63d^54s$, $3s^23p^63d^54p$, $3s^23p^53d^7$, $3s^23p^43d^8$, $3s^23p^43d^74s$, $3s^23p^43d^74p$, and $3p^63d^8$. This is the same target expansion that was used by Bautista et al. (2010) in their DARC calculation. It gives rise to 994 terms and 2578 levels. All orbitals are taken to be physical ones.

We used the program AUTOSTRUCTURE (Badnell 2011) to generate our common ICFT/BPRM target. The scaling parameters associated with the Thomas-Fermi-Dirac-Amaldi model potentials were determined by an iterative variational scheme. They are given by $\lambda_{1s-3p} = 1.110$, $\lambda_{3d} = 1.024$, $\lambda_{4s} = 1.002$, and $\lambda_{4p} = 1.180$.

Our DARC target was generated using GRASP0 (Parpia et al. 1996; Norrington 2004) by varying all orbitals simultaneously. The GRASP0 (and subsequent DARC) calculations were 'repeated' because it was initially thought that the original detailed results (e.g. collision strengths) were lost. They were recovered subsequently. We do not have access to the level energies for the structure which Bautista et al. (2010) used for their ICFT collision calculation.

We compare our AUTOSTRUCTURE energies (AS) for the lowest 17 levels with those from GRASP0 in Table 1. The two sets of GRASP0 energies differ slightly. The original orbitals were optimized slightly differently it seems. This provides us with an opportunity to look at the sensitivity of the subsequent DARC collision strengths to such target differences. We compare our calculated energies with those obtained from NIST (2013) as well. They lie 10–15% above the observed ones for levels belonging to excited terms. Those from AUTOSTRUCTURE are slightly closer to observed. The AUTOSTRUCTURE/GRASP0 energies lie above/below the observed for levels of the ground term. The AUTOSTRUCTURE ones are markedly closer ($\sim 1\%$) to observed than the GRASP0s' ($10 - 15\%$).

3.2. *Scattering*

We used the same 3 configuration close-coupling target expansion for our ICFT, BPRM and DARC calculations: $3s^23p^63d^6$, $3s^23p^63d^54s$, and $3s^23p^63d^54p$. It gives rise to 136 terms and 322 levels. There is nearly a 2 Ryd gap to the next (configuration interaction) level (323). We included all partial waves explicitly up to $2J = 59$. The contribution from higher-J was 'topped-up' following the procedures of Burgess (1974) for dipole transitions and Badnell & Griffin (2001) for non-dipole allowed. The ICFT/BPRM calculations explicitly dropped electron exchange above $2J = 19$ for efficiency. We used 11 continuum basis orbitals and our scattering energy extended to 4 Ryd. We used an energy step of $5 \times 10^{-5} z^2$ ($z = 2$) Ryd in the resonance region leading to 10000 energies. We used a step of $10^{-3} z^2$ Ryd elsewise. The Maxwellian convolution of the ordinary collision strengths utilized their infinite energy Born and Bethe limit points (Burgess & Tully 1992) to interpolate values at higher energies as they were needed.

4. COLLISION RESULTS

In Table 2 we present and compare effective collision strengths at 10^4 K for transitions from the Fe^{2+} $^5D_4$ ground level to the next 16 levels. The most immediate and important observation is the very close agreement between our present ICFT and BPRM results ($< 5\%$). Only the relatively weak excitation of the $^3P2_0$ level differs by more (13%). We note next that the agreement between BPRM and the present DARC results is typically 20%. This can only be attributable to differences in

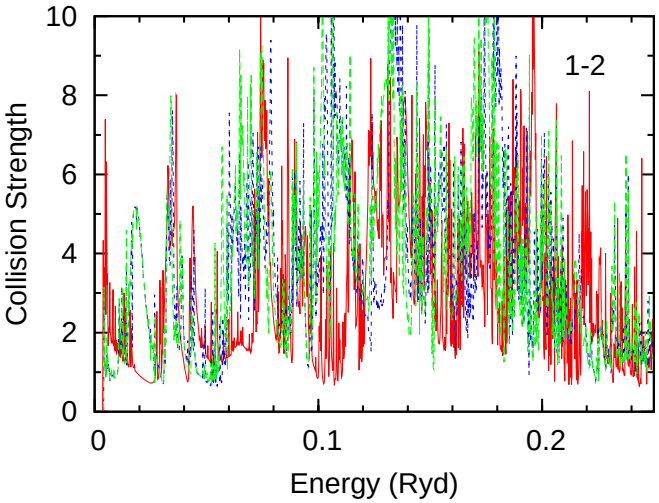

Figure 1. Collision strengths for the $3d^6\ ^5D_4 - ^5D_3$ transition in Fe^{2+}: ICFT (green long-dashed curve) and Breit-Pauli (blue short-dashed curve) R-matrix from the present work; Dirac R-matrix (red solid curve) due to Bautista et al. (2010).

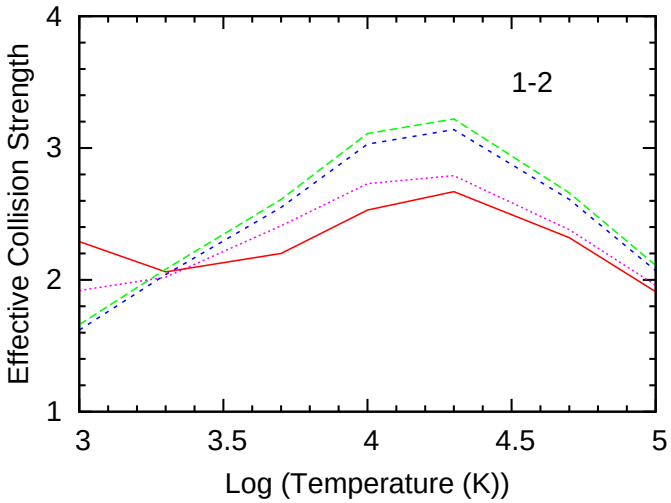

Figure 2. Effective collision strengths for the $3d^6\ ^5D_4 - ^5D_3$ transition in Fe^{2+}: ICFT (green long-dashed curve), Breit-Pauli (blue short-dashed curve) and Dirac (purple dotted curve) R-matrix from the present work; Dirac R-matrix (red solid curve) due to Bautista et al. (2010).

the atomic structure and is quite reasonable for this system — Bautista et al. (2010) discuss the wide variation found in the literature.

Where does that leave us with respect to the findings of Bautista et al. (2010)? If we compare our present DARC results with those that they give in their Table 1 we find complete disagreement from the $^3H_5$ level on upwards and by factors that are comparable with the differences they observed from their ICFT results. Investigation of their original detailed collision strengths reveals that the Maxwellian effective collision strengths which they list in their Table 1 are in their DARC energy order. If we look at the energies in our Table 1 we see that the level ordering in their Table 1 (which we repeat in our Table 2) does not correspond to energy order. Indeed, the result which they attribute to $3d^6\ \ ^3G_5$ actually belongs to their $3d^54s^7S_3$ level. We present their correctly ordered/labeled DARC results in our Table 2. They all agree with our present DARC results to within 10%. This is consistent with the degree of agreement of the target level energies from the two GRASP0 calculations which is much closer than with those from AUTOSTRUCTURE.

We turn next to the ICFT results of Bautista et al. (2010) and which we show in our Table 2. Most of the large factor differences from DARC (and ICFT & BPRM) have now disappeared except for the last two levels which appear 'reversed'. We do not have access to their original ICFT results to check whether the labeling is correct or not. Remaining transitions for which the original ICFT results are on the large side also show the present ICFT/BPRM results to be 20–30% larger than the original DARC ones. Nevertheless, several largish differences remain with the $^3H_6$ one approaching a factor of 2. We can only attribute this to their use of pseudo orbitals. Our present ICFT and BPRM results differ by less than 1% for this excitation.

Bautista et al. (2010) noted good agreement between their ICFT and DARC background collision strengths and attributed the cause of the difference in the effective collision strengths to be due to the ICFT resonance structure being shifted to slightly lower energies — see for example their Figure 2 for the $3d^6\ ^5D_4 - ^5D_3$ transition. By subsequent use of both sets of effective collision strengths to predict line intensities measured in the Orion Nebula Bautista et al. (2010) concluded that the DARC ones were to be favored.

We compare our ICFT and BPRM collision strengths with the DARC ones of Bautista et al. (2010) for this $(3d^6\ ^5D_4 - ^5\ D_3)$ transition in Figure 1. We focus on the energy range $0 - 0.25$ Ryd since this covers the main resonance structure and 10^4 K corresponds to 0.06 Ryd. There is no discernible shift in the position of the ICFT and BPRM resonance structures and they are in good overall agreement. The DARC collision strengths of Bautista et al. (2010) show a little weaker resonance structure compared to the ICFT/BPRM ones, in so much as one can isolate it from the background. They are also somewhat different qualitatively. The present DARC results (not shown) are qualitatively very similar to the original DARC ones of Bautista et al. (2010), but with a somewhat stronger resonance structure. These agreements and differences reflect those observed in row one of Table 2 for said methods.

In Figure 2 we compare effective collision strengths for the $3d^6\ ^5D_4 - ^5D_3$ transition over the temperature range $10^3 - 10^5$ K. We see that 10^4 K is representative of the largest differences. Our ICFT and BPRM effective collision strengths track each other over the entire temperature range. Our present DARC ones are consistently closer to them than the original DARC ones of Bautista et al. (2010). The peak effective collision strength at 2×10^4 K reflects the maximal contribution of the strong resonance structure spread over $0 - 0.25$ Ryd.

We have investigated further the sensitivity of the effective collision strengths to 'small' changes in resonance positions due to shifts in the threshold to which they are attached. We repeated our ICFT R-matrix calculation utilizing observed energies for the lowest 127 levels (NIST 2013). This includes all levels of the ground $(3s^23p^63d^6)$

and first excited ($3s^2 3p^6 3d^5 4s$) configurations as well as those levels of the $3s^2 3p^6 3d^5 4p$ configuration which overlap them. Three levels within this range are not observed apparently ($3d^6\ ^1D_2$, $^1S_0$ and $3d^5 4s^1 S_0$). We shift them by amounts comparable to those used for similar observed levels.

The largest changes to the effective collision strengths at 10^4 K are typically $\pm 15\%$ but most differences with our unshifted ICFT results are less than $\pm 10\%$. The one exception again is the $^3P2_0$ for which the shifted ICFT result is 30% smaller than the unshifted. We recall that the unshifted ICFT result was 13% larger than the BPRM. There is no particular systematic increase and/or decrease between the shifted and unshifted ICFT results. The differences of the GRASP0 energies from observed are larger than our AUTOSTRUCTURE ones and so one might expect somewhat larger changes/uncertainties in the DARC effective collision strengths as a result.

We close with the observation that if we neglect fine-structure relativistic effects completely then our resulting pure algebraic $LS(jK)J$ recoupling effective collision strengths agree with our ICFT ones to within 20% except for excitation of the $^3H_4$ level for which the difference is a factor of 2. They are also in good accord with similar algebraic recoupling results of Zhang (1996) including for the $^3H_4$ now (not shown). There is no need for us to use such an approach because we have never reached the stage of having carried-out the $LS(jK)J$ recoupling and not been able to carry-out the final term coupling transformation to take account of fine-structure effects. We note that the Iron Project also concluded that algebraic recoupling sufficed for low-charge iron-group ions in most instances (Hummer et al. 1993). With but a little extra effort we can effectively replace a full Breit-Pauli R-matrix calculation by an LS-coupling one.

5. CONCLUSIONS

We have carried-out ICFT and Breit-Pauli[2] R-matrix calculations for the electron-impact excitation of Fe^{2+} which use the exact same atomic structure and the same close-coupling level expansion. The results demonstrate that the ICFT R-matrix method can be expected to provide accurate effective collision strengths for near neutral iron group ions which are well within the uncertainties which exist due to the accuracy of the representation of their atomic structure.

The advantage of the ICFT approach over the Breit-Pauli and Dirac R-matrix approaches is that calculations which require the resources of massively parallel supercomputer centers can typically be carried-out on small local clusters. This facilitates the study of near neutral iron group ions which are omnipresent in cool astrophysical plasmas and which shine a light on their physical conditions.

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[2] A full Breit-Pauli dataset for all 322 levels (energies, radiative transition probabilities and effective collision strengths) is available in electronic form from the APAP website (www.apapnetwork.org).