Peer-reviewed version available at Galaxies 2018, 6, 91; doi:10.3390/galaxies6030091

Article

Towards the Provision of Accurate Atomic Data for Neutral Iron

A T Conroy [1]*, C A Ramsbottom [1], C P Ballance [1] and F P Keenan [2]

[1] Centre for Theoretical Atomic, Molecular and Optical Physics, Queen's University Belfast, University Road, Belfast, BT7 1NN, United Kingdom.
[2] Astrophysics Research Centre, Queen's University Belfast, University Road, Belfast, BT7 1NN, United Kingdom.
* Correspondence: aconroy03@qub.ac.uk

Abstract: The rich emission and absorption line spectra of Fe I may be used to extract crucial information on astrophysical plasmas, such as stellar metallicities. There is currently a lack, in quality and quantity, of accurate level-resolved effective electron-impact collision strengths and oscillator strengths for radiative transitions. Here, we discuss the challenges in obtaining a sufficiently good structure for neutral iron and compare our theoretical fine-structure energy levels with observation for several increasingly large models. Radiative data is presented for several transitions for which the atomic data is accurately known.

Keywords: atomic data

1. Introduction

The extraction of information about plasmas from their spectra is made possible by accurate collisional-radiative modelling. This relies on the availability of accurate atomic data such as radiative transition rates and electron-impact excitation cross-sections. When considering astrophysical plasmas, we pay particular attention to the iron-peak species, whose abundance is owed to their nuclear stability. Moreover, open d-shell species present in such plasmas will produce rich spectra due to the number of ways in which the electronic angular momenta can couple to form different fine-structure levels. At the intersection of the iron-peak and open d-shell species lies neutral iron. In this work, we seek a description of the structure of the neutral iron atom and accurate values for the oscillator strengths for radiative transitions, with the aim of calculating accurate Maxwell-averaged electron-impact collision strengths (effective collision strengths) among the fine-structure levels of Fe I.

Despite its rich spectrum, complete and comprehensive atomic data for Fe I are lacking. For example, NIST provides accurate (A-rated) oscillator strengths for only 149 fine-structure transitions [1]. These include the 524.71 nm and 525.02 nm lines, whose ratio has been used in magnetic field and temperature diagnostics [2]. In terms of collisional data, the first and only set of **R**-matrix electron-impact excitation collision strengths was published in 2017 [3], albeit term-resolved rather than level-resolved. This lack of radiative and collisional data for fine-structure transitions prevents us from fully exploiting the Fe I spectrum. The absence of theoretical results is due to the difficulty of obtaining a sufficiently good structure of the atom. For neutral systems, the non-central correlation interaction between electrons is comparable to the central Coulomb interaction between electrons and the nucleus, and a large configuration interaction (CI) basis is required to accurately describe the structure. Conversely, the computational expense of a Dirac **R**-matrix calculation to obtain collisional data limits the size of CI basis we may use. The challenge we face is to describe the structure of the atom using a sufficiently small CI basis.

As a consequence of the presence of numerous absorption lines in the spectra of late-type stars, neutral iron provides chemical abundance diagnostics, with the ratio of the Fe I content to the hydrogen content, [Fe/H], sometimes being used to describe the metallicity of a star [4]. The extraction of

information from spectra on the abundance of neutral iron relies on the accurate population modelling of as many of its fine-structure levels as possible and, in particular, the availability of highly reliable oscillator strengths for many transitions.

In this paper, we discuss the difficulties in obtaining a sufficiently good structure for the iron atom. We present theoretical energy levels in section 2 and oscillator strengths in section 3, obtained from different structure calculations for neutral iron. These are compared to experimental data, paying particular attention to the final model presented which is currently being used to generate a set of level-resolved collisional data for this species.

2. Atomic structure

To obtain oscillator strengths for radiative transitions and collision strengths for electron-impact (de-)excitations, we required a suitable description of the neutral iron atom. This was obtained using the fully relativistic atomic structure package GRASP^0 [5], which finds the approximate eigenstates of the Dirac-Coulomb Hamiltonian, $\hat{H}$, given by (in atomic units):

$$\hat{H} = \sum_{m=1}^{N} \left(-ic\boldsymbol{\alpha} \cdot \boldsymbol{\nabla}_m + (\beta - I_4)c^2 - \frac{Z}{r_m} \right) + \sum_{m>n} \frac{1}{|\mathbf{r}_m - \mathbf{r}_n|}, \tag{1}$$

where $N = Z = 26$ for Fe I. Eigenstates of this Hamiltonian may be grouped together into $J\pi$-symmetry blocks, where J is the total angular momentum of the state and π its parity. This problem is solved using an extensive basis set of configuration state functions (CSFs) obtained using the multi-configurational Dirac-Fock method (MCDF). Extended average level (EAL) calculations were performed on different configuration sets, where a set of variational one-electron orbitals are found such that the weighted trace (with each $J\pi$ level assigned weight $2J + 1$, the degeneracy of the level) of the Dirac-Coulomb Hamiltonian is minimised.

Obtaining a good structure for this neutral, open d-shell system is difficult. In the MCDF equations used to obtain the orbitals, correlation interactions are spherically averaged. The non-central component of this interaction is accounted for by using an extensive basis of CSFs with which to diagonalise the Hamiltonian matrix. For a neutral system, the correlation interaction is comparable to the central Coulomb interaction between electrons and the nucleus, and a small (in terms of the CSF basis size used) model of the atom cannot be expected to yield an accurate structure. However, the computational expense of any Dirac **R**-matrix calculation to obtain scattering data prohibits the use of very large models. To this end, the configuration set employed in a model must be carefully chosen so that correlation effects are reasonably well-described, while avoiding excessively large CSF bases. As we will see, if we limit the number of basis functions used, some states are more accurately described than others.

Another major problem we may encounter is the failure of the MCDF equations to converge for an orbital. In some cases, we may achieve convergence by using a different trial function for this orbital. In our work, one of the obstacles encountered was extending the orbital set beyond 4p by introducing a 4d orbital, which often resulted in convergence problems for both the 4d and 3d orbitals.

Presently, our working model of the Fe I atom consists of 21 non-relativistic configurations, giving rise to 5955 relativistic configurations and fine-structure levels, which we call Model 6. However, Models 1 to 5 are also discussed here, to illustrate the difficulties in obtaining a sufficiently good structure. Table 1 shows the configurations included in each model. Note that all configurations listed have a closed core, all orbitals are spectroscopic and each model includes the configurations from the previous model as well as those listed in the relevant column of the table.

In Model 1 (6 configurations and 995 levels), we included the ground configuration ($3p^6 3d^6 4s^2$), expanding this into a 6-configuration model by moving electrons between the 3d, 4s and 4p orbitals. For Model 2 (8 configurations and 1162 levels), we allowed double excitations from the 3p orbital

Table 1. Six models of the iron atom, described by their configuration sets.

Model 1	Model 2	Model 3	Model 4	Model 5	Model 6
$3p^63d^64s^2$	$3p^43d^84s^2$	$3p^63d^84d^6$	$3p^63d^64s5s$	$3p^63d^75p$	$3p^43d^94p$
$3p^63d^64s4p$	$3p^43d^94s$	$3p^63d^74d$	$3p^63d^75s$	$3p^63d^65p^2$	$3p^43d^94d$
$3p^63d^74s$		$3p^63d^64s4d$	$3p^63d^65s^2$		$3p^43d^95s$
$3p^63d^74p$		$3p^63d^64p4d$			$3p^43d^85s^2$
$3p^63d^8$					
$3p^63d^64p^2$					

to the 3d orbital for two even configurations to generate more even parity states, with the hope of lowering the energy eigenvalues of the even levels. In Model 3 (12 configurations and 4644 levels), we expanded the orbital set to include a 4d orbital. The $3d^64d^8$ configuration was included to allow for the convergence of the 3d and 4d orbitals in the MCDF calculation. Models 4 (15 configurations and 4842 levels) and 5 (17 configurations and 5396 levels) introduced a 5s and 5p orbital, respectively. In Model 6 (21 configurations), we allowed excitations from the 3p orbital to the 3d orbital for four configurations.

Table 2 shows the NIST values of the fine-structure energy levels [1], relative to the ground state, alongside the percentage differences with those obtained in these calculations. By careful choice of configuration state basis, we have achieved an average percentage discrepancy from NIST of 7.2% over 300 fine-structure levels. One of the clear achievements of Model 6, compared to Model 1, is the improvement in energy of the low-lying ^{5}F, ^{3}F and ^{5}P terms. The most marked change in these energies occurs in Model 4, when the 4d orbital was introduced. This demonstrates the effect of configuration mixing and correlation effects in neutral iron, and illustrates why obtaining a good structure is difficult; the addition of configurations to the model can result in large changes in the fine-structure energies relative to the ground state. In Model 6, over the first 30 levels, discrepancies differ from term to term, varying from around -3% for the ^{7}D^o term to around +25% for ^{3}H. Although we expect the energies to converge to the observed values as the CSF basis size increases, we cannot afford to describe all levels equally accurately. This is shown in the decreasing accuracy of the excited levels of the ground term, ^{5}D, as the number of configurations increases.

3. Radiative data

Oscillator strengths for fine-structure transitions were calculated using the OSCL package in GRASP^0. In Table 3, we present electric dipole (E1) oscillator strengths for Models 4, 5 and 6, in length form, for a selection of transitions among the first 30 fine-structure levels with accurately known radiative data [1]. In Model 6, we see that the addition of new configurations makes little difference to the oscillator strengths obtained. Discrepancies with NIST for the oscillator strengths from Model 6 vary, with the 23-2 transition 6.5% above the NIST value, whereas the 23-2 transition is almost 6 times greater. However, for five of these eight transitions, agreement with NIST is within 20%.

4. Conclusions and outlook

In this paper, we have contrasted the amount of information contained in neutral iron spectra with the lack of appropriate, high quality atomic data for this species, and discussed the challenges in obtaining a sufficiently good structure for the neutral iron atom with which to obtain theoretical results, keeping in mind that future Dirac **R**-matrix calculations prohibit excessively large structures. We have compared the atomic data obtained from structure calculations on six increasingly large models.

Our present working model is currently being used to calculate electron-impact collision strengths for Fe I, using the Dirac **R**-matrix method, with 300 target levels. In future, additional structures will also be used to generate level-resolved collisional data. This is important due to the lack of

Table 2. Percentage differences of the energy levels from different GRASP^0 structures with the NIST values.

No.	Level	NIST	GRASP^0					
			Model 1	Model 2	Model 3	Model 4	Model 5	Model 6
1	$3d^64s^2\ ^5D_4$	0.00000	-	-	-	-	-	-
2	$3d^64s^2\ ^5D_3$	0.00379	0.8	1.0	-9.9	-9.6	-9. 0	-7.2
3	$3d^64s^2\ ^5D_2$	0.00642	1.7	1.4	-9.1	-8.8	-8.3	-6.6
4	$3d^64s^2\ ^5D_1$	0.00809	2.4	1.7	-8.6	-8.3	-7.7	-6.1
5	$3d^64s^2\ ^5D_0$	0.00891	2.6	1.9	-8.4	-8.1	-7.5	-5.9
6	$3d^74s\ ^5F_5$	0.06314	489.2	522.4	-77.5	-67.5	-53.2	-10.8
7	$3d^74s\ ^5F_4$	0.06722	457.9	489.0	-72.9	-63.7	-50.1	-10.1
8	$3d^74s\ ^5F_3$	0.07042	435.4	465.5	-69.7	-60.9	-47.9	-9.7
9	$3d^74s\ ^5F_2$	0.07277	420.8	449.6	-67.6	-58.9	-46.4	-9.4
10	$3d^74s\ ^5F_1$	0.07431	411.4	439.8	-66.2	-57.7	-45.5	-9.2
11	$3d^74s\ ^3F_4$	0.10914	294.9	313.5	-27.9	-27.0	-17.8	6.3
12	$3d^74s\ ^3F_3$	0.11446	279.8	297.7	-28.1	-25.9	-17.3	5.9
13	$3d^74s\ ^3F_2$	0.11818	270.6	287.6	-30.3	-25.2	-16.7	5.7
14	$3d^74s\ ^5P_3$	0.15993	225.6	231.0	-31.6	-27.7	-21.8	-5.6
15	$3d^74s\ ^5P_2$	0.16154	223.1	228.5	-31.2	-27.3	-21.4	-5.4
16	$3d^74s\ ^5P_1$	0.16337	220.2	225.5	-21.2	-27.0	-21.3	-5.4
17	$3d^64s^2\ ^3P_2$	0.16747	27.6	11.8	29.6	24.7	2.29	9.0
18	$3d^64s4p\ ^7D^o_5$	0.17634	-23.6	-8.0	-6.4	-6.5	-4.2	-3.3
19	$3d^64s^2\ ^3H_6$	0.17670	10.9	18.3	63.3	30.0	24.9	24.3
20	$3d^64s^2\ ^3P_1$	0.17818	26.6.	11.8	26.3	51.3	13.8	7.4
21	$3d^64s4p\ ^7D^o_4$	0.17827	-23.1	-7.9	-6.5	-6.5	-4.3	-3.4
22	$3d^64s^2\ ^3H_5$	0.17880	10.7	17.9	29.0	29.5	24.2	23.8
23	$3d^64s4p\ ^7D^o_3$	0.18004	-22.9	-7.8	-6.5	-6.5	-4.3	-3.4
24	$3d^64s^2\ ^3H_4$	0.18031	10.5	17.1	28.8	28.4	24.4	23.1
25	$3d^64s4p\ ^7D^o_2$	0.18146	-22.6	-7.7	-6.5	-6.5	-4.3	-3.4
26	$3d^64s4p\ ^7D^o_1$	0.18243	-22.5	-7.6	-6.5	-7.5	-4.3	-3.4
27	$3d^64s^2\ ^3P_0$	0.18260	26.3	11.8	25.6	26.3	27.8	6.9
28	$3d^64s^2\ ^3F_4$	0.18810	19.2	13.5	21.8	21.6	20.6	19.0
29	$3d^64s^2\ ^3F_3$	0.19022	19.0	12.9	21.5	21.3	20.3	18.3
30	$3d^64s^2\ ^3F_2$	0.19172	18.9	12.8	21.2	21.0	20.0	18.3

level-resolved collision strengths for this species. Several sets of collisional data will allow a meaningful error analysis of the atomic data calculated in this investigation.

Acknowledgments: This work is supported by a Special Research Studentship at Queen's University Belfast and funding from the UKRI Science and Technology Facilities Council. All calculations were undertaken on a computer cluster at Queen's University Belfast.

Author Contributions: Conceptualization, Catherine Ramsbottom, Connor Ballance and Francis Keenan; Investigation, Andrew Conroy; Supervision, Catherine Ramsbottom, Connor Ballance and Francis Keenan; Writing – original draft, Andrew Conroy; Writing – review & editing, Catherine Ramsbottom, Connor Ballance and Francis Keenan.

Conflicts of Interest: The authors declare no conflict of interest.

1. Kramida, A..; Ralchenko, Yu..; Reader, J..; NIST ASD Team. NIST Atomic Spectra Database (version 5.5.6). https://physics.nist.gov/asd, 2018. Accessed: 2018-06-19.
2. Holzreuter, R..; Solanki, S. K.. Three-dimensional non-LTE radiative transfer effects in Fe lines - I. Flux sheet and flux tube geometries. *A&A* **2012**, *547*, A46.
3. Bautista, Manuel A..; Lind, Karin.; Bergemann, Maria. Photoionization and electron impact excitation cross sections for Fe. *A&A* **2017**, *606*, A127.

Table 3. E1 oscillator strengths from various models compared with the accurate NIST values

Wavelength / nm	Transition ($j - i$)	Oscillator strength			
		NIST	Model 4	Model 5	Model 6
525.50	25 - 4	5.74×10^{-6}	5.03×10^{-6}	6.56×10^{-6}	6.38×10^{-6}
525.02	26 - 5	1.15×10^{-5}	7.09×10^{-6}	1.02×10^{-5}	1.03×10^{-5}
524.71	23 - 3	2.26×10^{-6}	3.19×10^{-6}	3.68×10^{-6}	3.37×10^{-6}
522.55	26 - 4	5.42×10^{-6}	2.45×10^{-6}	3.88×10^{-6}	4.02×10^{-6}
520.46	25 - 3	9.31×10^{-6}	5.63×10^{-6}	8.37×10^{-6}	8.55×10^{-6}
516.89	23 - 2	1.53×10^{-5}	1.13×10^{-5}	1.62×10^{-5}	1.63×10^{-5}
512.77	25 - 2	1.07×10^{-7}	7.01×10^{-7}	7.53×10^{-7}	7.04×10^{-7}
511.04	21 - 1	1.93×10^{-5}	1.61×10^{-5}	2.24×10^{-5}	2.23×10^{-5}

4. Bergemann, Maria.; Lind, K..; Collet, R..; Magic, Z..; Asplund, M.. Non-LTE line formation of Fe in late-type stars I. Standard stars with 1D and 3D model atmospheres. *Monthly Notices of the Royal Astronomical Society* **2012**, *427*, 27–49.
5. Dyall, K. P..; Grant, I. P..; Johnson, C. T..; Parpia, F. A..; Plummer, E. P.. GRASP: a general-purpose relativistic atomic stucture program. *Comp. Phys. Comm.* **1996**, *94*, 249.