Atomic Data: Calculation, evaluation and integration

R-matrix calculations of Mo I and W I

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(Queen's University of Belfast)

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Overview

- Capabilities of the R-matrix collision group at Queen's Belfast

- Calculations of varying degrees of complexity (Serial Code ---> Highly parallel codes)

- Evaluation of produced data, error uncertainty

- Integration of results within ADAS (open-adas) database and modelling suite

- Test cases: Mo I (excitation and ionisation) : W I (excitation)
R-matrix/R-matrix with Pseudostates (RMPS) review

\[ R_{ij} = \sum_k \frac{w_{ik} w_{kj}}{E - E_k} \]

\[ \Psi_k(x_1 \ldots x_{N+1}) = A \sum_{ij} c_{ijk} \Phi_i(x_1 \ldots x_N, \hat{r}_{N+1} \sigma_{N+1}) u_{ij}(r_{N+1}) \]

+ \sum_j d_{jk} \phi_j(x_1 \ldots x_{N+1})

Observed expt.

RMPS model

IONISATION LIMIT

pseudostates
Capabilities

- Most first order electron-impact driven processes
  - Electron-impact excitation
  - Electron-impact ionisation
  - Electron-impact recombination (DR/radiative)

- The codes should cover most of the periodic table, and there are LS coupling (non-relativistic), Breit-Pauli (semi-relativistic) and Dirac R-matrix suites of codes

- Photoionisation is also possible within the codebase, and is currently being used to update stellar opacities (CLOUDY, XSTAR)
High performance computing + scripting = comprehensive data sets

i.e. total photoionisation of every Fe XVII level

\[ 2p^6, 2p^5 \text{nl}(5), 2s2p^6 \text{nl}(5) \text{ total photoionisation} \]
Electron-impact excitation and ionization of $W^{3+}$ for the determination of tungsten influx in a fusion plasma

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Abstract

Tungsten will be employed as a plasma facing material in the ITER fusion reactor under construction in Cadarache, France; therefore, there is a significant need for accurate electron-impact excitation and ionization data for the ions of tungsten. We report on the results of extensive calculations of ionization and excitation for $W^{3+}$ that are intended to provide the atomic data needed for the determination of impurity influx diagnostics of tungsten in several existing tokamak reactors. The electron-impact excitation rate coefficients for this study were determined using the relativistic $R$-matrix method. The contribution to direct electron-impact ionization was determined using the distorted-wave approximation, the accuracy of which was verified by an $R$-matrix with pseudo states calculation. Contributions to total ionization from excitation autoionization were also generated from the relativistic $R$-matrix method. These results were then employed to calculate values of ionization per emitted photon, or SXB ratios, for four carefully selected spectral lines; these data will allow the determination of impurity influx from tungsten facing surfaces. For the range of densities of importance in the edge region of a tokamak reactor, these SXB ratios are found to be nearly independent of electron density but vary significantly with electron temperature.

Accurate Atomic Structure

+ Electron-impact excitation

+ Ground & metastable Ionisation

= spectral diagnostics + impurity influx predictions
The atomic data has been integrated into many astrophysical databases such as CLOUDY, XSTAR and AtomDB.

Conversion codes exist to convert ADAS formats into the required files needed for above astrophysical modelling codes.

Abstract

We present extensive calculations of radiative transition rates and electron impact collision strengths for Fe II. The data sets involve 52 levels from the 3d7, 3d54s, and 3d54s2 configurations. Computations of A-values are carried out with a combination of state-of-the-art multiconfiguration approaches, namely the relativistic Hartree–Fock, Thomas–Fermi–Dirac potential, and Dirac–Fock methods, while the R-matrix plus intermediate coupling frame transformation, Breit–Pauli R-matrix, and Dirac R-matrix packages are used to obtain collision strengths. We examine the advantages and shortcomings of each of these methods, and estimate rate uncertainties from the resulting data dispersion. We proceed to construct excitation balance spectral models, and compare the predictions from each data set with observed spectra from various astronomical objects. We are thus able to establish benchmarks in the spectral modeling of [Fe II] emission in the IR and optical regions as well as in the UV Fe II absorption spectra. Finally, we provide diagnostic line ratios and line emissivities for emission spectroscopy as well as column densities for absorption spectroscopy. All atomic data and models are available online and through the AtomPy atomic data curation environment.
Our goal is to produce, high quality atomic data in a timely fashion, so that it may be employed in current, ongoing experimental campaigns.

For example, level resolved Argon Breit-Pauli R-matrix data was used at DIII-D.
Ideally, in some situations the highest accuracy is required, and months of effort are given to the atomic structure and scattering calculation.

but in other cases, comprehensive coverage along iso-electronic sequences is more important, and hence a R-matrix script (in perl) was created for this purpose and also for the novice user.

This script is employed to produce data in a format immediately accepted by ADAS (adf04). This well-prescribed format can (and has) been converted to other database formats such as CLOUDY.
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ADAS adf04 : helike_cb12#o6.dat
Excitation generation : ICFT script

This is a perl script, that runs the R-matrix suite of codes from the atomic structure through to a Maxwellian averaged collision strengths (adf04) file without further user input.

(Dr Whiteford, Dr Witthoeft, Dr Loch and myself)

It does allow for various optimisations both in terms of the atomic structure and the collisional calculation, but minimally only requires the user to provide a list of configurations.

This allows for the efficient calculation along iso-electronic sequences, and been carried out for F-like, Neon-like, B-like sequences by Dr Liang and others.

The script is also the foundation of our Monte Carlo error sensitivity, which I will discuss later.
ICFT script: Acquisition and installation

Acquire

Install
ICFT script: Use (example)
R-matrix/RMPS : ionisation

We have the capability to calculate electron-impact ionisation (ground & metastable) for light to mid-Z elements. With the availability of Prof Badnell's DRMPS (Dirac R-matrix with Pseudo-States) code, the heavier elements are now feasible.

It is the accuracy of the excited states that can prove problematic.
Ultimately, the electron-impact excitation and ionisation are both required if we to produce Generalised Collisional Radiative (GCR) coefficients that are both temperature and density dependent.

**Generalized collisional-radiative (GCR) coefficients**

- **Effective ionization rates**
  \[
  S_{CD,\sigma \rightarrow \nu} = \mathcal{R}_{\nu \sigma} - \sum_{j=1}^{\nu} \mathcal{R}_{\nu j} \sum_{i=1}^{\sigma} c_{ji}^{-1} c_{i \sigma}
  \]

- **Effective recombination rates**
  \[
  R_{CD,\nu \rightarrow \sigma} = \mathcal{R}_{\nu \sigma} + \sum_{j=1}^{\nu} \mathcal{R}_{\nu j} \sum_{i=1}^{\sigma} c_{ji}^{-1} \mathcal{R}_{i \nu}
  \]

- **Total Line Power Loss**
  \[
  P_{LT,\sigma} = \sum_{k,j} \Delta E_{kj} A_{j \rightarrow k} F_{j \sigma}^{exc}
  \]

  - j→k transition energy
  - excitation rates
  - spontaneous emission rates
  - RR and DR rates
  - CR matrix elements
  - Ionization rates
  - A^{q+}
  - A^{(q+1)+}
  - \nu
Effective ionization rate coefficient vs density and electron temperature

- Density dependence comes in through the role of ionization from excited states.

Loch et al., ADNDT, 92 813 (2006)

IAEA A+M Data, Nov 18-20, 2009
Uncertainty in Theoretical Calculations

Baseline Studies
- Uncertainty is quantified as the difference between different theoretical approaches
- Representative of differences in the literature
- Quickly provides a generous uncertainty on an atomic dataset, while providing the correct temperature and density trends of more elaborate calculations.
- May not reflect the tighter constrained uncertainties derived from more elaborate calculations.
- Fundamental atomic structure and collisional rates remain uncorrelated.

Sensitivity Studies
- Uncertainty is determined from the sensitivity of the calculation to key input parameters.
- Can produce fully correlated uncertainties.
- The objective choice of variation in the input parameters that reflects meaningful physical values remains difficult.
- Does not determine the absolute uncertainty between methods.
- More time and resource intensive.

Monte-Carlo Collisional Radiative Modeling

Emissivities
Uncertainties

Monte-Carlo line ratio diagnostics

Effective ionization and recombination

Uncertainties

Monte-Carlo ionization balance

Uncertainties on Te and Ne
Uncertainties on abundances and Ionization age
Current work for Molybdenum and Tungsten

Collaborators: Curtis Johnston, Stuart Loch, David Ennis (Auburn) : Steve Alan (DIIIID)

(i) Mo I/Mo II excitation and ionisation

(ii) W I excitation
Motivation

• Molybdenum/Tungsten employed in several fusion devices such as NSTX-U, DIII-D and EAST and CTH

• They have favourable physical properties such as high thermal conductivity
Overview of DIII-D parameters

- Magnetic Field $B < 2.2$ T
- Major radius $R \ 1.67$ m
- Minor radius $a \ 0.67$ m
- Plasma Current $< 3$ MA
- Pulse duration $< 7$ s
- Majority ions Deuterium
- Temperatures and densities depend on chosen operating mode
- During metal tiles campaign
- Heating power $< 26$ MW for these experiments
FIG. 1. Energy level spectrum of Mo I organised by electronic configuration. Each horizontal line designates a specific fine structure level listed in the NIST database.
We do have the experimental A-values From Whaling et al, and for such a complicated systems we have reasonable agreement between experiment and theory.

The lines below are categorized as strong diagnostic lines

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TABLE II. Table showing the radiative transition rates (in $s^{-1}$) obtained from the present model compared to experimental values given in [18]. The rates shown are obtained after shifting energies to experimental values.

(i) $z^5P^0_{1,2,3} \rightarrow a^5S_2$ (557.0 nm, 553.3 nm, 550.6 nm)
(ii) $z^7P^0_{2,3,4} \rightarrow a^7S_3$ (390.3 nm, 386.4 nm, 379.8 nm)
(iii) $y^7P^0_{2,3,4} \rightarrow a^7S_3$ (319.4 nm, 317.0 nm, 313.3 nm)
FIG. 6. Measured spectrum from the CTH plasma (solid blue line), compared with theoretical results. The solid black sticks show the PEC coefficients for the Mo I transitions, while the dashed red curve shows a theoretical spectrum based upon Gaussian convolved PEC data. A FWHM for the Gaussian convolution of 0.15 nm was used, based upon the instrument resolution, and the PECs are shown for an electron temperature of 6 eV and an electron density of $1 \times 10^{12} \text{ cm}^{-3}$. 
RMPS : Mo I/Mo II ionization

1) Required multiple levels of parallelisation (by partial wave, also by Hamiltonian)

2) At 11,216 terms in the close-coupling expansion, probably the largest electron-impact carried out.
Tungsten
Currently, two WI adf04 files

Cowan code, 3 configs in the scattering plane-wave Born calculation

GRASP + pDARC suite of R-matrix Codes (24 configurations)
Overview of CTH measurements for Tungsten

- W I 265.65 nm observed to be on the order of the widely used 400.89 line:
  - Atomic calculations using ADAS confirm that W I 265.65 nm is strong for divertor temperatures and densities $\sim 1\times10^{19} \text{ m}^3 \sim 10\text{eV}$
- Multiple W I lines in the region around 265.65 region:
  - High density of lines in this region motivates higher resolution spectrometer/instrument
Ongoing and future Goals

- Development and use of R-matrix suite of codes for electron-impact excitation, ionisation and photoionisation.
- Focus on the near neutral systems but with the use of the ICFT script for comprehensive coverage
- Use of the Monte-Carlo perl script to provide an error file for each process
- Integration of data within magnetically-confined plasma databases such as ADAS, with conversion codes to facilitate integration into other formats.
- Integrate PhD (3) and post-doc(1) students into the group to continue the passing of knowledge.