Dirac R-matrix calculations  
(electron-impact excitation/ionisation)  
in support of tungsten plasma diagnostics

Connor Ballance  
(Queen's University of Belfast )

Collaborators: Nicole Dunleavy, Ryan Smyth, Stuart Loch, Curtis Johnson,  
David Ennis and M O’Mullane

Queen's University of Belfast / Auburn University/ Strathclyde University

IAEA Technical meeting April 2021

Funded in part by the UK STFC consolidated astrophysics grant to Queen's Belfast
Overview

• Motivation: Provide the atomic structure, electron-impact excitation/ionisation rates used for temperature and density diagnostics (+ impurity influx) for W I and W II


• W I, W II (NEW): excitation

• W I: ionisation (ground and excited state)

• Conclusions, uncertainty, future directions
High Z materials are leading candidates for first wall materials, especially divertor region

- **Allowable impurity concentration lower for high-Z materials**
  - High-Z materials radiate much more than previously used materials
  - Radiation significant enough to denigrate plasma performance
    - Concentration needs to be less than ~1E-4 (Putterich)
  - Need to accurately quantify and minimize erosion of wall
R-matrix/RMPS in a nutshell

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

\[ H_{N+1} \]

inner

outer

\[ \Psi_k(x_1 \ldots x_{N+1}) = A \sum_{ij} c_{ijk} \Phi_i(x_1 \ldots x_N, \hat{r}_{N+1}\sigma_{N+1})u_{ij}(r_{N+1}) + \sum_j d_{jk} \phi_j(x_1 \ldots x_{N+1}) \]
Dirac $R$-matrix calculations for the electron-impact excitation of neutral tungsten providing noninvasive diagnostics for magnetic confinement fusion

Phys. Rev. A 97, 052705 – Published 7 May 2018

ABSTRACT

Neutral tungsten is the primary candidate as a wall material in the divertor region of the International Thermonuclear Experimental Reactor (ITER). The efficient operation of ITER depends heavily on precise atomic physics calculations for the determination of reliable erosion diagnostics, helping to characterize the influx of tungsten impurities into the core plasma. The following paper presents detailed calculations of the atomic structure of neutral tungsten using the multiconfigurational Dirac-Fock method, drawing comparisons with experimental measurements where available, and includes a critical assessment of existing atomic structure data. We investigate the electron-impact excitation of neutral tungsten using the Dirac $R$-matrix method, and by employing collisional-radiative models, we benchmark our results with recent Compact Toroidal Hybrid measurements. The resulting comparisons highlight alternative diagnostic lines to the widely used 400.88-nm line.
Snapshot of W I

Groundstate: \(4f^{14} 5d^{4} 6s^{2}\)

Method: GRASP0 structure groundstate
+ 24 excited state configurations
(\(\sim 7500\) levels)

: Dirac R-matrix calculation
keeps 250 levels in the
close-coupling expansion

(a) Known (NIST/literature) even levels

(b) Known (NIST/literature) odd levels

(c) & (d) unknown or at least only partially
designated even and odd levels
We must exploit High Performance Computing resources

- Electron-impact calculations involves hundreds of level-resolved target states and thousands of close-coupled channels $\rightarrow$ large Hamiltonian matrices.
- Huge effort goes into the parallel construction of hundreds of Hamiltonians, which require diagonalisation (now employing GPU accel.)
C has been very useful for tungsten studies.

- The emission was indeed strongest in the UV!
- We identified 30 new tungsten spectral emission lines.
- Results in Johnson et al., Plasma Physics and Controlled Fusion, Volume 61, 095006 (2019).

Compact Toroidal Hybrid (CTH) has been an invaluable test of the electron-impact excitation dataset.
Temperature derived from lines within R Smyth W I adf04 file and those measured with a Langmuir probe on the Auburn CTH experiment.
To assure spectroscopic wavelengths, pre-diagonalisation of Hamiltonian, energy levels are shifted to experimental values. Easy for low levels, not so for excited states.
W II calculation (NEW), currently being tested against CTH spectra at 30 eV and a density of $1\times10^{12}\,\text{cm}^{-3}$.
W II calculation (NEW), currently being tested against CTH spectra at 30 eV and a density of $10^{12}$ cm$^{-3}$. 
W II calculation (NEW), currently being tested against CTH spectra at 30 eV and a density of $1e+12$ cm$^{-3}$, but at higher wavelengths.
Excitation Summary

- W I (published, Ryan Smyth et al 2018)
  
  adf04 (Maxwellian averaged collision strength)
  
  10.1103/PhysRevA.97.052705

- W II (work completed, Nicole Dunleavy
  
  adf04 under testing)

- W III (To be done!)

- W IV (Ballance et al, adf04 available, 2013)
  
  DOI: 10.1088/0953-4075/46/5/055202)
If we first consider the ground and meta-stable ionisation for the simpler cases of hydrogen and lithium, what uncertainties should we expect as a function of principal quantum number.

**RMPS : ionisation**

It is the accuracy of the excited states that can prove problematic.
Ionisation: Increase in complexity

- Unlike ‘one-electron’ systems the ground-state of W I: \(4f^{14} 5d^{4} 6s^{2}\) requires direct ionisation of 6s and 5d ionisation:
  - \(5d^{4} 6s^{n} n'l\) where \(n=7-14, l=0-6\)
  - \(5d^{3} 6s^{2} n'l'\) where \(n=7-14, l=0-6\)
which amounts to several hundred TERMS in a close coupling expansion and Hamiltonians in excess of 360,000 by 360,000.
The standard techniques, DW, Cowan HFR, configuration average TDCC, RMPS work for the groundstate .... but for excited states ....

Unfortunately, the effective ionisation rates is completely dominated by excited state ionisation!
Ultimately, the electron-impact excitation and ionisation rates 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**
  
  \[ S_{CD,\sigma \rightarrow \nu} = S_{v\sigma} - \sum_{j=1}^{Q} S_{v,j} \sum_{i=1}^{Q} \mathcal{C}_{ji}^{-1} \mathcal{C}_{i\sigma} \]

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

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

- **Ionization rates**
  
  \[ A^{(q+1)+} \]

- **CR matrix elements**
  
  \[ A^{q+} \]

- **Effective recombination rates**
  
  \[ S_{v,j} \]

- **Excitation rates**
  
  \[ S_{v,j} \]

- **Spontaneous emission rates**
  
  \[ S_{v,j} \]

- **Total Line Power Loss**
  
  \[ P_{LT,\sigma} \]

- **j→k transition energy**
  
  \[ \Delta E_{kj} \]

- **RR and DR rates**
  
  \[ \Delta E_{kj} A_{j \rightarrow k} F^{exc}_{j\sigma} \]
Effective ionization rate coefficient vs density and electron temperature

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

IAEA A+M Data, Nov 18-20, 2009
The intensity of a spectral line can be related to its influx rate [Behringer PPCF 31 2059 (1989)].

The number of ionizations per photon (S/XB) is directly proportional to the impurity influx,

\[ \Gamma = \int_0^\infty N_e N^x S^{z \rightarrow z+1} \, dx = \int_0^\infty N_e \frac{S^{z \rightarrow z+1}}{A_{i \rightarrow j} \frac{N_i}{N^x}} \left( A_{i \rightarrow j} \frac{N_j}{N^x} \right) N^x \, dx \]

\[ = \int_0^\infty N_e SXB_{i \rightarrow j}^z \left( A_{i \rightarrow j} \frac{N_j}{N^x} \right) N^x \, dx \]

where \( SXB_{i \rightarrow j}^z = \frac{S^{z \rightarrow z+1}(N_e, T_e)}{A_{i \rightarrow j} \frac{N_i}{N^x} (N_e, T_e)} \)

Note electron temperature and density dependence.
Conclusions/Future Directions

- Electron-Excitation: in reasonable shape, has predictive and diagnostic capability. Only W III remains for W I-IV to be complete.

- Electron-impact ionisation: Difficult to achieve a sufficiently accurate representation of excited states. This is the dominant contribution to effective ionisation rate.

- We hope to constrain the uncertainties in SXB ratios.
Future Directions: Uncertainty propagation through models

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.

Monte-Carlo Collisional Radiative Modeling

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.

Emissivities
Uncertainties
Monte-Carlo line ratio diagnostics

Monte-Carlo ionization balance
Uncertainties
Uncertainties on Te and Ne
Uncertainties on abundances and ionization age

Effective ionization and recombination
Uncertainties