Dirac R-matrix and Breit-Pauli distorted wave calculations of the electron impact excitation of W^{44+}

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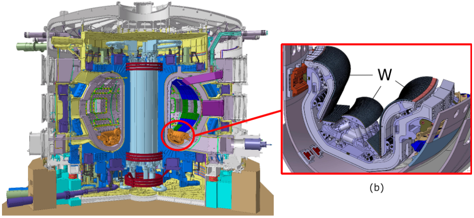
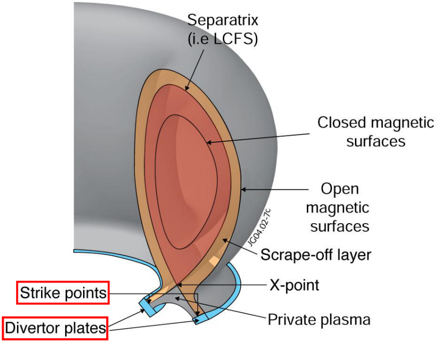
Context: The Divertor and Impurity Species



(a)

(b)

[1] [2]

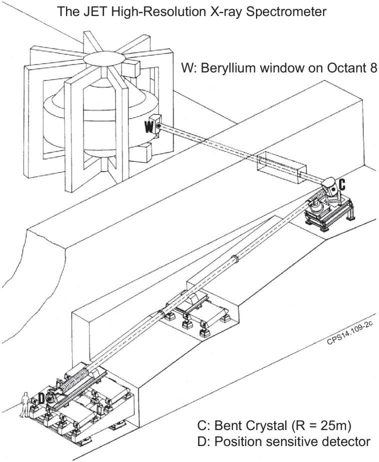


[3]

- Research question: how can we quantify W's impact as an impurity species once it has infiltrated via interations at the divertor targets?
- Many facets to the impurity problem: transport of impurities, impact on transport properties of the plasma (via Z_{eff}), dilution of fuel, radiation losses

Perspective: Spectroscopy and Diagnostics

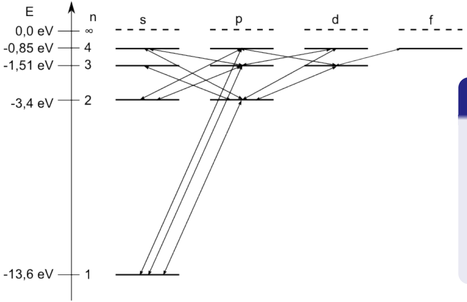
- The radiative rate, A_{ji}, between the excited atomic state, j, and lower state, i, scales as Z^4, so high Z species are much more likely to radiate $\rightarrow$ cause of radiation losses
- For detection of impurities in the plasma during operation, we must rely on spectroscopic diagnostics
- Interpreting the emission lines detected requires the application of atomic physics theory



KX1: JET high resolution X-Ray crystal spectrometer

Atomic Population Modelling

- A large A_{ji} value does not guarantee that the emission from this particular transition will be seen in a diagnostic
- First, one must consider the abundance of the ion under consideration, then the "population" of the levels for a group of these ions
- Both are determined by the statistical balance of the "web" of excitation and de-excitation process rates, connecting all of the considered levels
- collisional-radiative theory used to construct the web



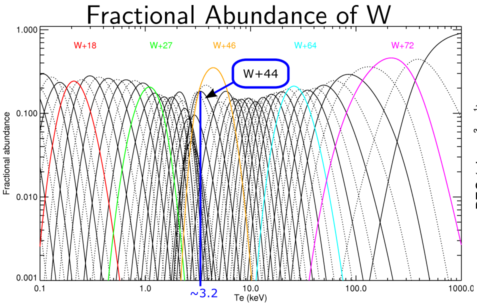
Grotrian diagram for Hydrogen

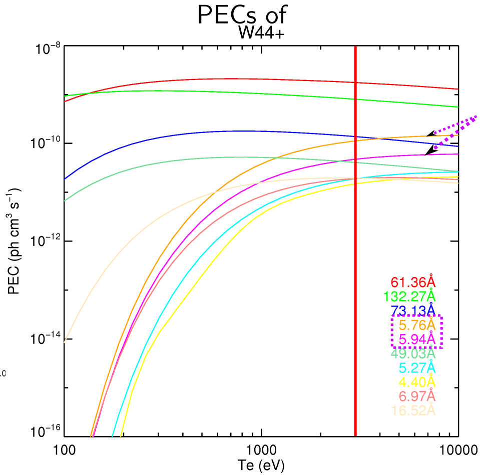
Photon Emissivity Coefficient ($\mathcal{PEC}$)

The radiative rate for a particular transition having considered the effect of atomic level populations; dependent on temperature and density; the desired end result

Abundance Curves and PECs

W^{44+} has been identified as a potentially important species for diagnostics motivated by previous calculations (below); the transitions of interest are $3d^{10}4s^2\ {}^1S_0 \leftrightarrows 3d^9 4s^2 4f\ L_i S_i J_i \pi_i$





Link to Atomic Structure and Collision Data

- $\mathcal{PEC}$s and abundance curves require excitation mechanisms and their cross sections $\rightarrow$ fundamental atomic data
- In fusion plasmas, electron impact excitation (EIE) dominates:

$$\underbrace{\mathcal{A}^{z+}(i)}_{\text{initial atomic state}} + \underbrace{e^{-}(kl)}_{\text{initial free electron}} \rightarrow \underbrace{\mathcal{A}^{z+}(f)}_{\text{final atomic state}} + \underbrace{e^{-}(k'l')}_{\text{final free electron}}$$

- We initially calculate a collision strength, $\Omega(i,j)$, which is trivially related to the cross-section, $\sigma(i \rightarrow j)$:

$$\sigma(i \rightarrow j) = \frac{\pi a_0^2 I_{\mathrm{H}}}{g_i k^2} \Omega(i,j) \tag{1}$$

- For modelling purposes we need rates, so a thermal average of $\Omega(i,j)$ is conducted to obtain the effective collision strength, Υ_{ij}:

$$\Upsilon_{ij} = \int_0^{\infty} \Omega(i,j) e^{\left(\frac{-\epsilon_j}{kT_e}\right)} \mathrm{d}\left(\frac{\epsilon_j}{kT_e}\right) \tag{2}$$

Atomic Structure: The Dirac Equation

- The quantum scattering problem builds directly upon the atomic structure of the target, and the high energy behaviour of collision strengths is determined by the Born limits, which come from the radiative rates of the structure
- Analysis of the non-relativistic Schrödinger Hamiltonian shows that the first order relativistic correction terms are $O(\alpha^2 Z^2)$
- As $\alpha Z \to 1$ (*i.e.* $Z \to 137$) these terms become important
- The single electron Dirac Hamiltonian in atomic units is [4]:

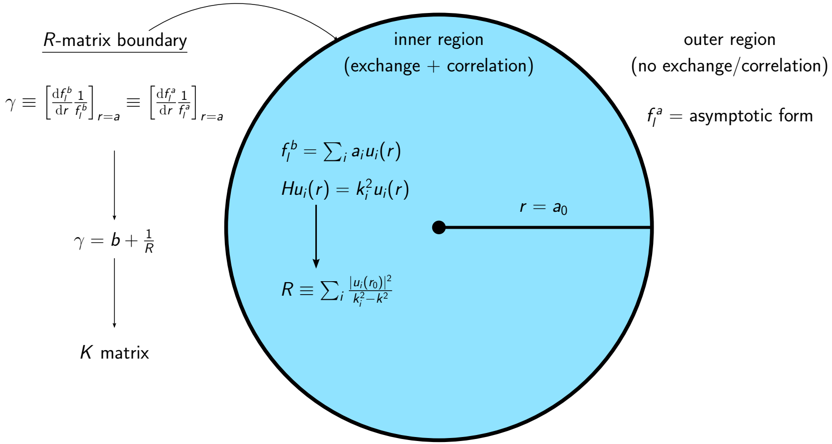
$$H_D = c\boldsymbol{\alpha} \cdot \mathbf{p} + c^2\boldsymbol{\beta} + V(\mathbf{r}) \tag{3}$$

- Solutions ("orbitals") are of the form:

$$\psi_{nkm}(\mathbf{r}) = \frac{1}{r}\begin{bmatrix} P_{nk}(r)\chi_{k,m}(\theta,\phi) \\ iQ_{nk}(r)\chi_{-k,m}(\theta,\phi) \end{bmatrix} \tag{4}$$

- Appropriately coupled Slater determinants of these orbitals form the quantization basis of our structure and collision calculations

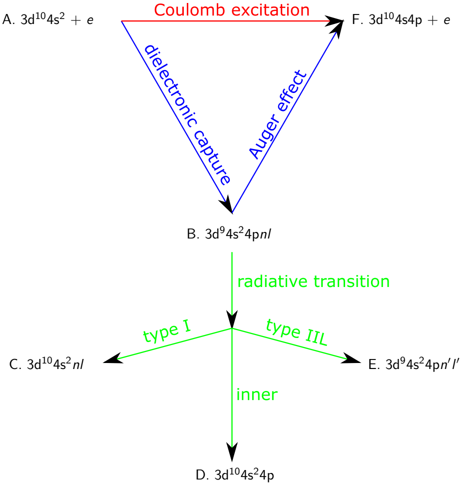
Scattering Problem: The *R*-matrix Method [5]



Resonances: poles of the R-matrix occur at $k = k_i$, leading to large values for Ω (or σ); $k \to k_i$ when $f_l^b \to u_i$, which is only possible when $E_N + k^2 = E_N' - \frac{Z^2}{n^2} = E_{N+1}$

Radiation Damping

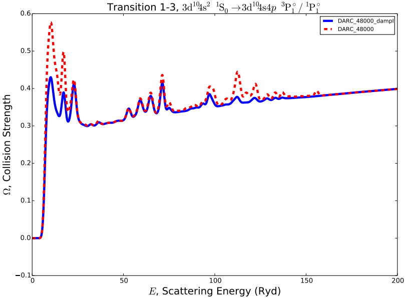
Radiative transitions from intermediate resonances reduces the overall cross-section; should be considered for high Z



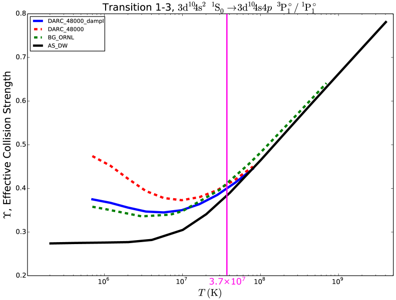
Methodology

- Structure codes
  - AUTOSTRUCTURE: LSJ-coupled basis; Breit-Pauli Hamiltonian
  - GRASP0 (General-purpose Relativistic Atomic Structure Package): *jjJ*-coupled basis; relativistic Dirac-Hamiltonian
- Collision codes
  - AUTOSTRUCTURE Distorted Wave (DW): uncoupled radial equations for scattering electron
  - Dirac Atomic *R*-matrix Codes (DARC): *R*-matrix with Dirac-Fock spinors
- Key parameters
  - Configuration interaction (CI): $[1s^2 2s^2 2p^6 3s^2 3p^6]$ $3d^{10}4s^2$, $3d^{10}4s4p$, $3d^{10}4s4d$, $3d^{10}4s4f$, $3d^{10}4p^2$, $3d^{10}4p4d$, $3d^{10}4p4f$, $3d^{10}4d^2$, $3d^{10}4d4f$, $3d^9 4s^2 4p$, $3d^9 4s^2 4d$, $3d^9 4s^2 4f$, $3d^9 4s4p4d$
  - Asymptotic code resonance region energy mesh: 48 000 points
  - only type I damping included
- Previous calculations
  - Ballance and Griffin (2007) [6]; henceforth BG
  - fully damped DARC calculations
  - crucially, do not open up the 3*d* shell, so no $3d^{10}4s^2\ ^1S_0 \leftrightarrows 3d^9 4s^2 4f\ L_i S_i J_i \pi_i$

Results I

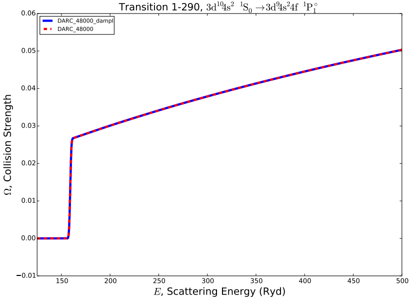


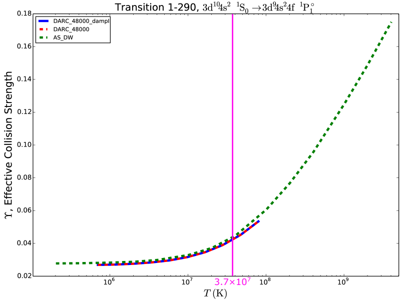
Convoluted collision strengths for our DARC EIE damped (blue) and undamped (red) calculations



Effective collision strengths for AS DW (black), BG DARC damped (green), our DARC damped (blue) and undamped (red)

Results II

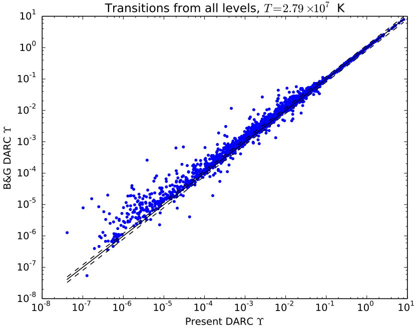


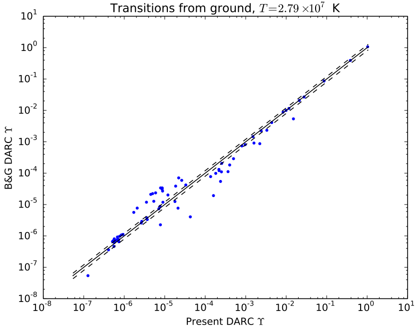


Convoluted collision strengths for our DARC EIE damped (blue) and undamped (red) calculations

Effective collision strengths for AS DW (green), our DARC damped (blue) and undamped (red)

Results III





Linear comparison plots of effective collision strength values. The ground transitions (right) do not show any systematic diferences, and 40% = (28 / 70) * 100 lie within the 20% error region. Comparing all matching transitions (left) tends to show a trend to lower Υ values for our present calculations; however, 63% = (1568 / 2483) * 100 lie within the 20% error region.

Concluding Remarks

- Successful generation of electron impact excitation data for W^{44+} using DARC and AS DW
- There is a fair amount of agreement between our results and B&G overall, although notable differences are present for a slight majority of the ground transitions
    - More investigation into the ground transitions that lie outside the 20% error region is necessary (e.g. Are these predominantly spin-changing/forbidden transitions?)
    - As there is no systematic trend, it does not appear that these differences are due to our neglect of the other forms of radiation damping
    - In general, it is mostly lower magnitude Υ's that tend to disagree (as should be expected); from a population modelling perspective, how much should we worry about this impacting our results?
- Next steps:
    - use collision data (R-matrix and DW) in atomic population modelling to fully investigate the soft x-ray transitions of interest via PECs, and compare to previous results
    - then, compare these results with experiment

References I

[1] ITER Organization. The ITER Tokamak, 2013.

[2] ITER Organization. Cross section of the ITER divertor, 2013.

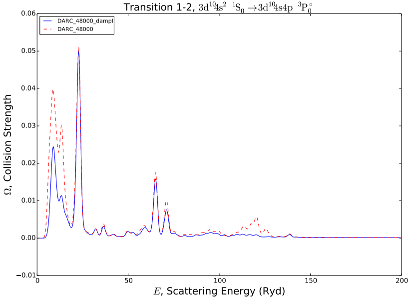
[3] EFDA. Geometry of a toroidal magnetic field with a divertor.

[4] I.P. Grant. *Relativistic Quantum Theory of Atoms and Molecules: Theory and Computation*. Springer, 2007.

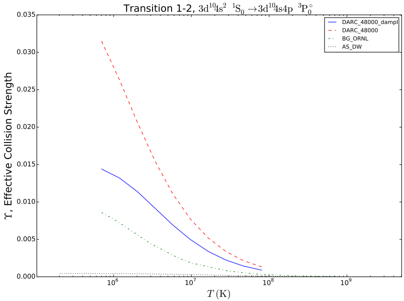
[5] Philip G. Burke. *R-Matrix Theory of Atomic Collisions*. Springer, 2011.

[6] C P Ballance and D C Griffin. Electron-impact excitation of W 44+ and W 45+. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 40(2):247–258, January 2007.

Backup



Convoluted collision strengths for our DARC EIE damped (blue) and undamped (red) calculations



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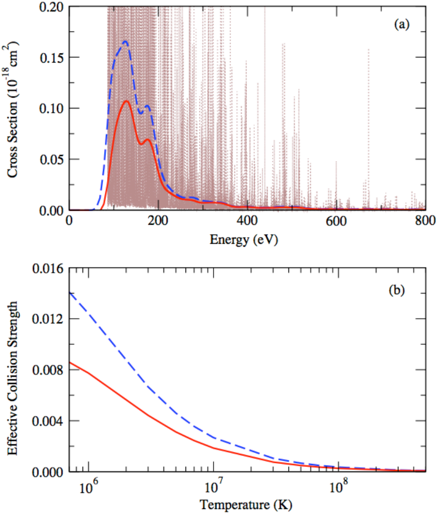

Figure 1. Electron-impact excitation of W^{44+} from the ground state to the $4s4p(1/2, 1/2)_0$ metastable level (level 2). (a) The dotted curve is the damped cross section, the dashed curve is