An overview of recent R-matrix developments with a focus on heavy neutron-star merger and magnetically-confined fusion elements

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Talk Overview

- Recap of basic R-matrix ideas and terminology

- LS/Breit-Pauli R-matrix (split codes) codes : excitation
  : ionization

- GRASP0/DARC (Dirac Atomic R-matrix Codes) :excitation
  :ionization

(see Franck Delahaye's talk for use of the DARC photoionisation codes)

- GPU (Graphical Processing Unit) acceleration

(Test cases below)

- Magnetically confined fusion Tungsten (W I, WII) : excitation
  : ionization

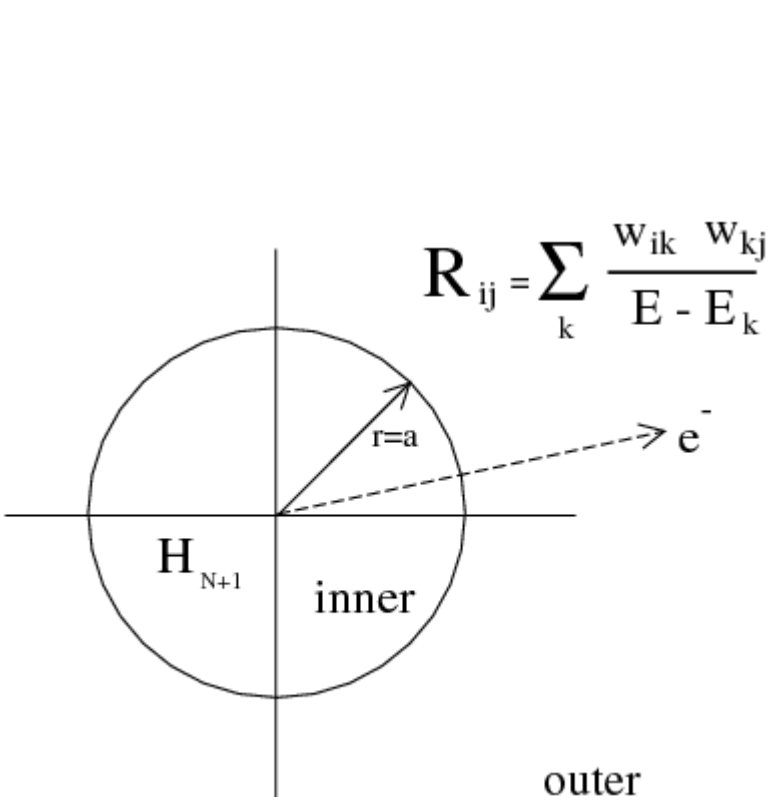
→ the difficulties of excited state ionisation

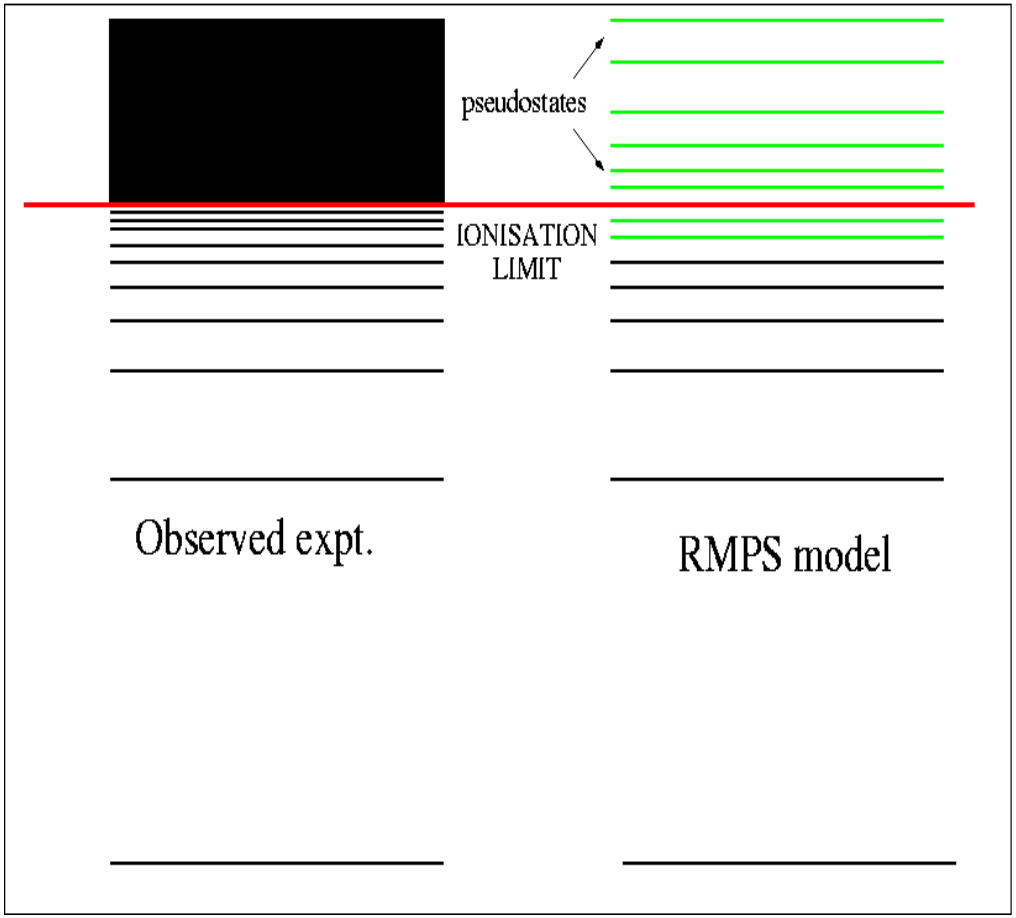
- Neutron star merger elements : Gold (Au I, Au II and Au III) : Excitation

→ the difficulties of open-f shell excitation and ionisation

(Complimentary talks : Dr Adam Foster (uncertainty quantification)
: Dr Martin O'Mullane (magnetically confined fusion)

R-matrix/RMPS (recap of terminology)





$$\Psi_k(x_1 \ldots x_{N+1}) = A \sum_{ij} c_{ijk} \bar{\Phi}_i(x_1 \ldots x_N, \hat{r}_{N+1}\sigma_{N+1}) u_{ij}(r_{N+1}) + \sum_j d_{jk} \phi_j(x_1 \ldots x_{N+1})$$

LS/Breit-Pauli/ICFT R-matrix codes

- **Terminolgy : [LS] LS coupling description of target and scattering**

[Breit-Pauli] = transformation of LS Hamiltonians into JK Hamiltonians which include first order relativistic effects such mass-velocity, Darwin and spin-orbit.

[ICFT] = Intermediate Coupling Frame Transformation

the transformation of LS resolved scattering K-matrices, into level-level resolved K-matrices. (benefits from diagonalizing only smaller LS resolved Hamiltonians.

What are the benefits of revision?

->New hardware capabilities , plus multi-level parallelization enable an order of magnitude increase in the target description and subsequent scattering calculation)

(hundreds of TERMS/LEVELS → thousands of TERMS/LEVELS)

This allows us to attempt non-perturbative close-coupling excitation /ionization of open-(p,d) shell systems for the ground and excited states.

The difference for simpler targets (closed-shell→ 2 electrons outside a core) reveals neutral to doubly ionized targets differences of up to 30% in excitation

LS/Breit-Pauli/ICFT R-matrix codes

- **LS/Breit-Pauli RMPS calculations grow computationally expensive with the complexity of the target**

  i.e. Hydrogen : 1s-5s spectroscopic orbitals , n=6-19, l=0-9 pseudo
  = approximately 120 terms in close-coupling expansion

  Helium : 1s^2,1snl((Singlet/Triplet) (n=2-5 spectroscopic)
  n=6-19,l=0-8
  = approximately several hundred terms in close coupling expansion

  …. however by, Neutral Tungsten

- **e + W I (5d^4 6s^2) → WII (5d^4 6s + e +e)**
  → WII (5d^36s^2 + e +e)
  → WII(5p^55d^46s^2 + e + e)

This requires 5d^46s nl, 5d^36s^2 nl and 5p^55d^46s^2 pseudostate expansions , which amounts to thousands of terms in the close coupling expansion

LS/Breit-Pauli/ICFT R-matrix codes

- **Solution : Multi-level parallelism (in this case fortran 90 + mpi)**

  Each partial wave is carried out concurrently (embarrassingly parallel) but there is now also the parallel construction of each Hamiltonian as well.

  (1) All unique N-electron target terms S L Pi are gathered together (typically between 24-70 depending on target complexity and the orbitals of the pseudostate expansion)

  (single variable change to R-matrix input deck : ntarsym)

  (2) the interaction of each symmetry subblock with each other is carried out concurrently.

- **Some targets do not couple in the current partial wave symmetry and hence are very quick. Some target symmetries couple to multiple angular momentum for a particular symmetry and are slower**

- **Code modified to reduce DIRECT access usage, minimum usage of integer*8 to construct large Hamiltonians.**

- **Result : Hamiltonians large : YES! But reduced to the time for one H_cc block**

LS/Breit-Pauli/ICFT R-matrix codes

Case Study : W III ionization (experimental results of Stenke et al)

Target description (using AUTOSTRUCTURE) : groundstate 5d^4, 5p^45d^6
: 5d^3 *nl* , 5d^26s *nl*
: n=1s-6s (spectroscopic), n=7-12(pseudo)

→ 5803 TERMS, with 62 unique TERMS (singlets, triplets, quintets L=0-10)

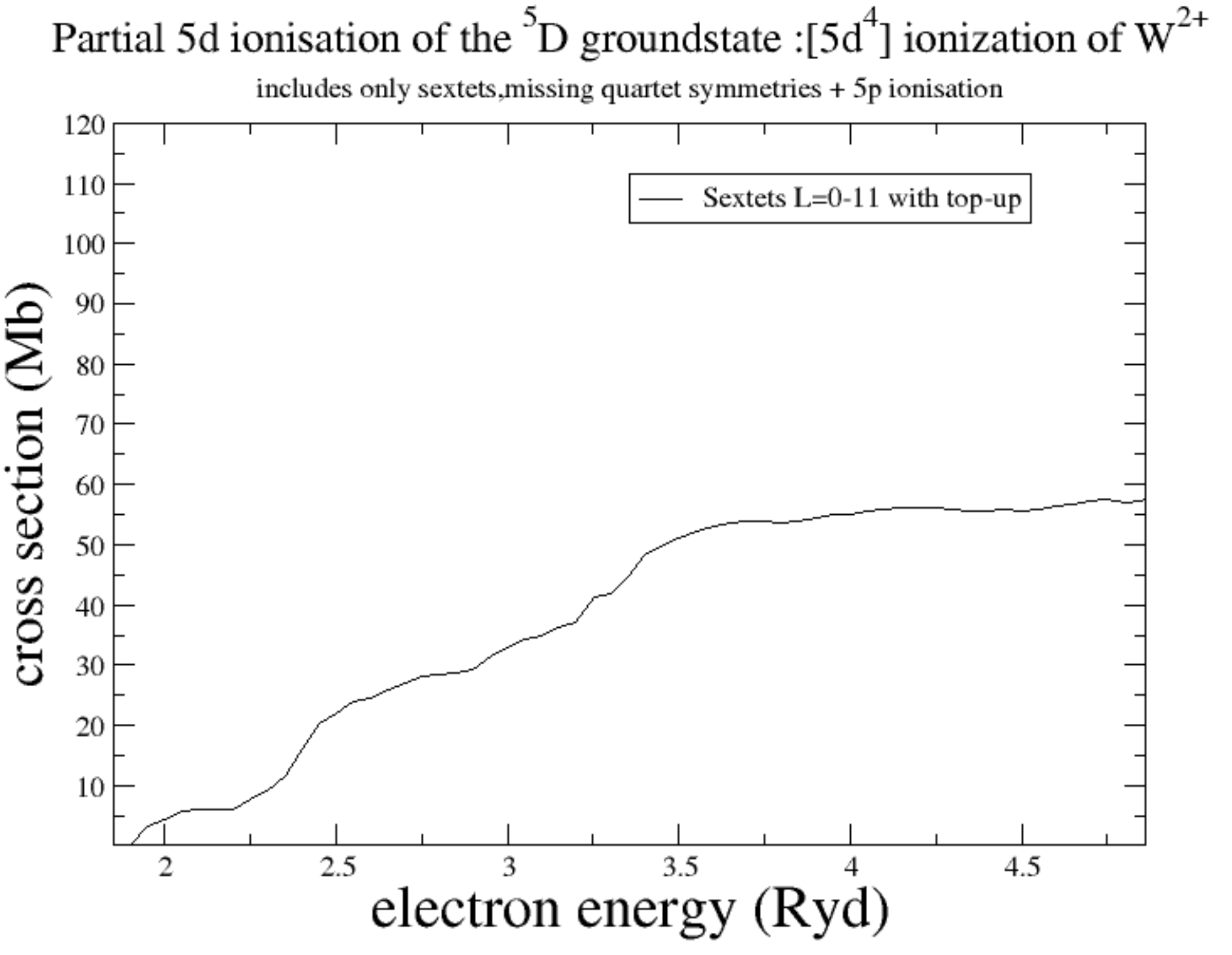
Therefore, NTRSYM=62

```
39M       STG2HCC000000
88M       STG2HCC000001
624M      STG2HCC001000
278M      STG2HCC001001
6.0G      STG2HCC002000
3.4G      STG2HCC002001
...
329M      STG2HCC061001
4.4G      STG2HBB000000
4.1G      STG2HBB000001
65G       STG2HBC000000
61G       STG2HBC000001
```

STG2HCC(ntarsym identifier)(pw identifer)

Time is the longest H_cc block !!!

```
---------
 NCHAN = 8175 NCONHP = 212550 MNP1 = 237220     4     2     0
 NCHAN = 8496 NCONHP = 220896 MNP1 = 246482     4     2     1
```


Partial 5d ionisation of the ^{5}D groundstate :[5d^4] ionization of W^{2+}
includes only sextets,missing quartet symmetries + 5p ionisation
Sextets L=0-11 with top-up
cross section (Mb)
120
110
100
90
80
70
60
50
40
30
20
10
2
2.5
3
3.5
4
4.5
electron energy (Ryd)

LS/Breit-Pauli/ICFT R-matrix codes

Question : Capability there, but what plasma issue does ground and excited state ionization address ?

Answer : Impurity influx diagnostics using SXB coefficients

The intensity of a spectral line can be related to its influx rate [Behringer PPCF 31 2059 (1989)]

. However it must be corrected for the fact that some of the impurity has already ionized

- **The number of 'ionizations per photon' (or SXB) is directly proportional to the impurity influx (Γ).**

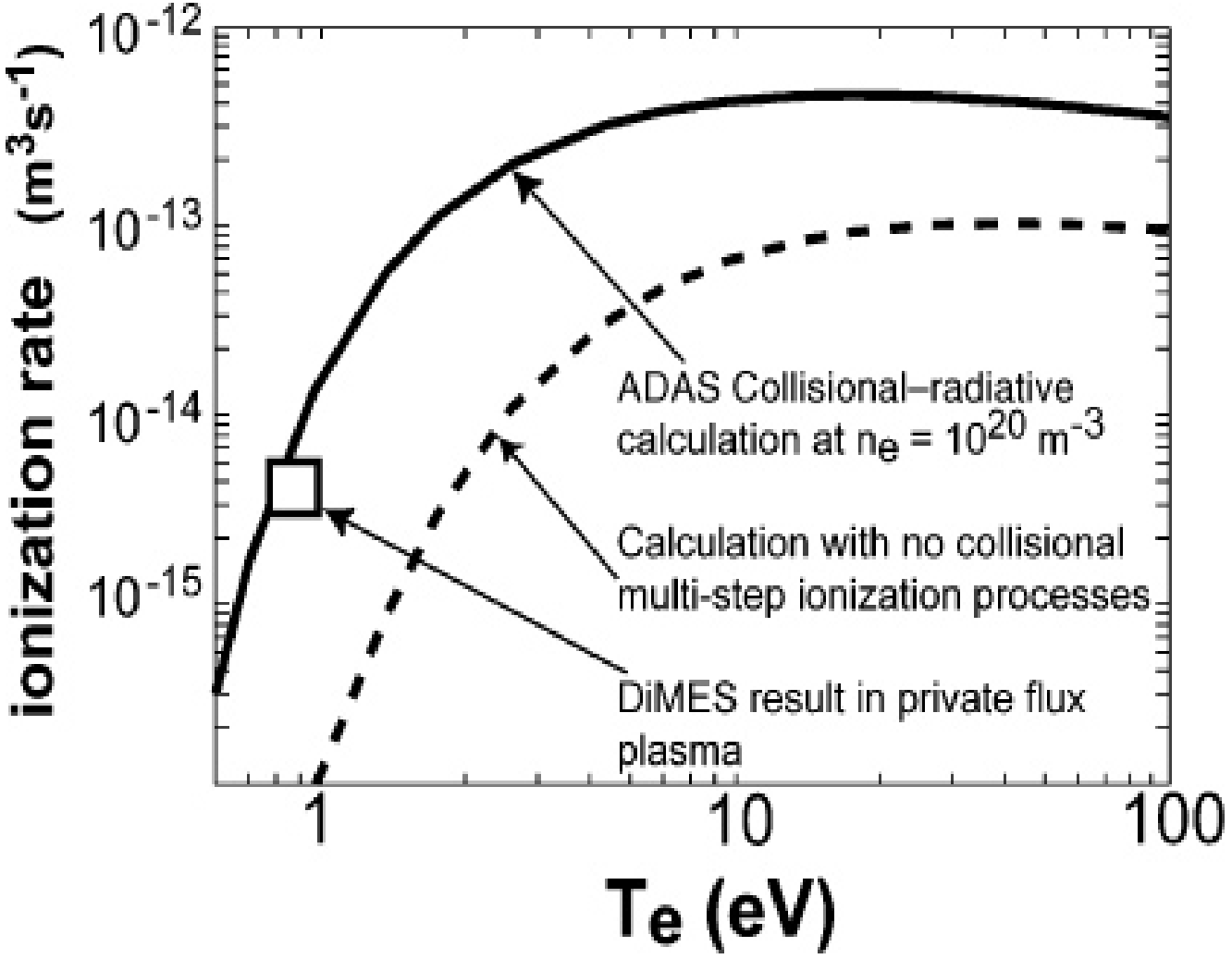
$$\Gamma = \int_0^\infty N_e S^{z \to z+1} N^z \, dx$$

$$\Gamma = \int_0^\infty N_e \frac{S^{z \to z+1}}{A_{i \to j} \frac{N_i}{N^z}} \left(A_{i \to j} \frac{N_i}{N^z} \right) N^z \, dx = \int_0^\infty N_e SXB^z_{i \to j} \left(A_{i \to j} \frac{N_i}{N^z} \right) N^z \, dx$$

$$SXB^z_{i-j} = \frac{S^{z \to z+1}(Ne, Te)}{A_{i \to j} \frac{N_i}{N_z}(Ne, Te)}$$

Effective ionization rate =weighted sum of ground and excited state ionization

As with simpler lithium systems studied before, it is the case with tungsten that the majority of the contribution to the effective ionization rate comes from excited state ionization



And is there a relativistic equivalent to the RMPS codes ?

(but as TERMS become LEVELS, and we transition from LS coupling to jj coupling, the problem becomes an order of magnitude more difficult.)

However, the approach is similar, build N+1 electron Hamiltonians in parallel, Hcc, Hbc, Hbb parts.

Improvements : (1) a dry-run to calculate dimensions [Ready]

(2) angular algebra calculated first [Steady]

(3) Hamiltonian construction and all partial waves carried out concurrently[Go]

Needless, to say mpi, modern fortran and arbitrary precision implemented throughout.

We want to extend the DRMPS (Dirac R-Matrix with PseudoStates) method to enable ionisation from the groundstate and metastables of near-neutral Tungsten. If we want SXBs we need this!

Prof Badnell pioneered the method for neutral hydrogen

Jarod Gouldie/Connor Ballance have extended the method to light systems such as Carbon.

Journal of Physics B: Atomic, Molecular and Optical Physics

Dirac *R*-matrix with pseudo-states

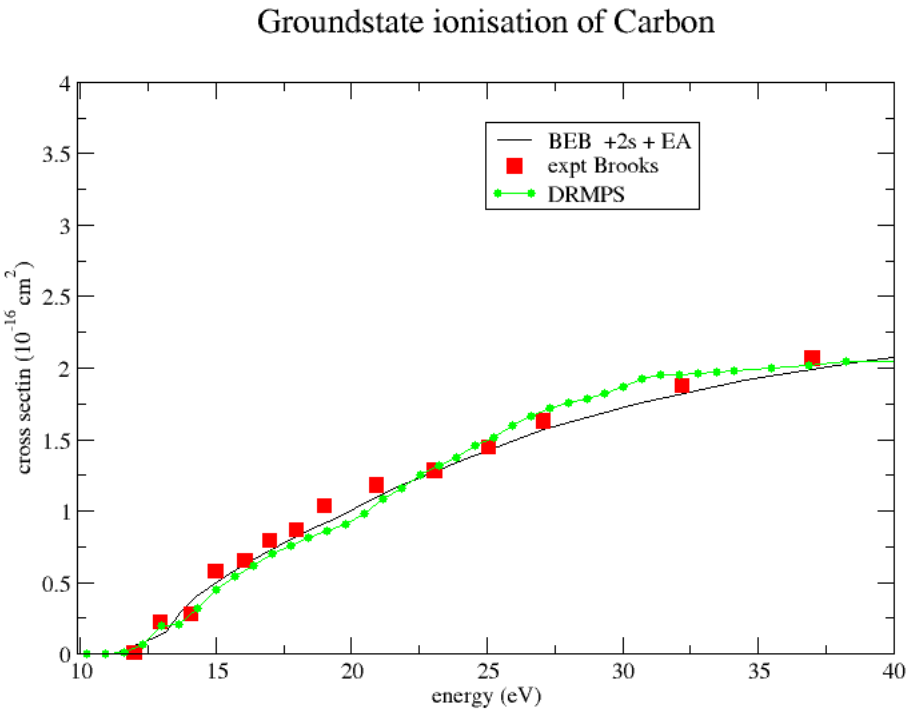
N R Badnell[1]

Published 26 August 2008 • 2008 IOP Publishing Ltd
Journal of Physics B: Atomic, Molecular and Optical Physics, Volume 41, Number 17
Citation N R Badnell 2008 *J. Phys. B: At. Mol. Opt. Phys.* **41** 175202

+ Article information

Abstract

We describe the development of the Dirac *R*-matrix with pseudo-states (DRMPS) method for electron and photon collisions with arbitrary atoms and ions. An *N*-electron atom is represented by an anti-symmetrized product of single-particle spinors comprising the usual four-component Dirac spinors as well as paired two-component Laguerre spinors (L-spinors). The convergent L-spinor basis forms a discretization of the electron and positron continua. This representation has been implemented quite generally within the general relativistic atomic structure package (grasp) specifically grasp^0. An (N + 1)th 'scattering' electron is represented by the exact same L-spinor basis plus the usual *R*-matrix box-state spinors which are chosen so as to form a combined complete finite linearly independent orthogonal basis. The (non-diagonal) Buttle correction is determined consistently. This representation has been implemented quite generally within the Dirac atomic *R*-matrix code (DARC). Results of some simple model problems are presented which demonstrate the correctness of the implementation.



A very high degree of efficiency must be obtained when building the Hamiltonians representing the partial waves in parallel.

A useful tool is gprof, that analyzes where the time is spent.

```
Flat profile:

Each sample counts as 0.01 seconds.
  %   cumulative   self              self     total
 time   seconds   seconds    calls  Ks/call  Ks/call  name
 75.00   1496.82  1496.82        1     1.50     1.96  cmat_
 11.43   1724.91   228.09 3259716476     0.00     0.00  cmatx_
 11.31   1950.67   225.77 397564189     0.00     0.00  fincc_
  0.50   1960.70    10.03        1     0.01     0.01  aij2_
  0.35   1967.72     7.02        1     0.01     0.01  aijz_
  0.32   1974.11     6.39  7544513     0.00     0.00  clrx_
  0.25   1979.16     5.05 386841601     0.00     0.00  loccc_
  0.15   1982.10     2.94 413576727     0.00     0.00  place_
  0.10   1984.16     2.06        1     0.00     0.00  mcpinc_
  0.09   1985.98     1.82  7881612     0.00     0.00  setup_
  0.09   1987.76     1.79        1     0.00     0.00  bmatx_
  0.07   1989.19     1.43        1     0.00     0.02  cont_
  0.07   1990.51     1.32   979591     0.00     0.00  da1_
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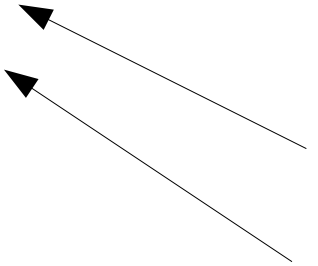


Hamiltonian continuum-continuum

This completely consumes the time, especially as the size of the calculations increase. Parallelism helps to mitigate the problem But the code needs refactorization to increase effiecency.

i.e. 2*10^2 secs / (3*10^9 calls) => < 10^-7 sec per call

We are taking 2 approaches to ground and metastable ionisation of W I-III

(Andrew White/Stuart Loch; Auburn)

*** Extend the standard LS RMPS code to handle to handle > 2 electrons In open f and g shells.**

*** Strength : much easier and smaller ionisation calculations than level resolved models**

*** Weakness : must be statistically split to merge with level-resolved electron-impact excitation For collisional-radiative modelling**

Coupling-scheme may not be appropriate, fespecially for inner shell ionisation.

To test, collectively does this matter?

(Connor Ballance/Nigel Badnell)

*** Implement DRMPS (ie Dirac RMPS)**

***Strength : very little compromise In terms of physics.**

Merges very well with electron-impact excitation work. Both level resolved.

***Weakness : very, very computationally demanding**

Electron-impact Excitation of Heavy Elements using the DARC codes.

→ employs a light weight version of GRASP that runs very efficiently (in terms of Memory) and can handle up to 1-2 hundred non-relativistic configurations but Would not compete with GRSP2018/GRASP2K versions!

But has the angular algebra precalculated, adaptive memory and calculates The Lspinors (the relativistic version of the Laguerre pseudo-orbitals used In RMPS) for ionisation

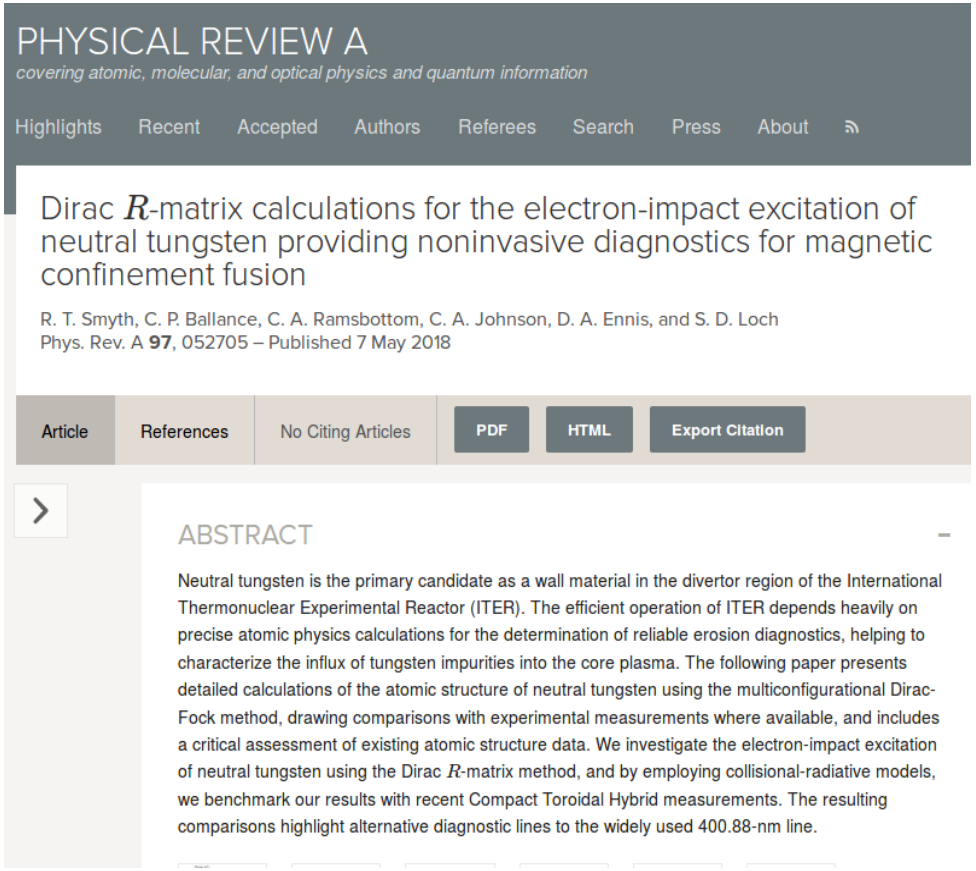
→ Not all calculations need to be DRMPS (certaily reduces workload)

→ The excitation codes benefit from all the changes made for ionization

→ All lot of the work developed for Tungsten carries over into many of the elements required for binary neutron star merger work (Gold, Platinum and Lead)

Tungsten electron-impact excitation is in good shape but the ionization, and more particularly excited state ionization requires work.

W I



PHYSICAL REVIEW A

covering atomic, molecular, and optical physics and quantum information

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Dirac R-matrix calculations for the electron-impact excitation of neutral tungsten providing noninvasive diagnostics for magnetic confinement fusion

R. T. Smyth, C. P. Ballance, C. A. Ramsbottom, C. A. Johnson, D. A. Ennis, and S. D. Loch
Phys. Rev. A **97**, 052705 – Published 7 May 2018

Article References No Citing Articles PDF HTML Export Citation

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.

W II

A Dirac *R*-matrix calculation for the electron-impact excitation of W^+

N L Dunleavy[3,1], C P Ballance[1], C A Ramsbottom[1], C A Johnson[2], S D Loch[2] and D A Ennis[2]

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Citation N L Dunleavy *et al* 2022 *J. Phys. B: At. Mol. Opt. Phys.* **55** 175002
DOI 10.1088/1361-6455/ac8089

Article PDF

Figures References Open science

+ Article and author information

Abstract

Aims: tungsten has been chosen for use as a plasma facing component in the divertor for the ITER experiment, and is currently being used on existing tokamaks such as JET. W^+ plays an integral role in assessing the impurity influx from plasma facing component of tokamaks and subsequent redeposition. Together with previously calculated a neutral tungsten electron-impact dataset this study allows us to determine neighbouring spectral lines in the same wavelength window of the spectrometer, and detect if there is strong blending of overlapping lines between these two ion stages as well as providing ionisation per photon ratios for both species. The new data is to be used for tungsten erosion/redeposition diagnostics. *Methods*: a significantly modified version of the GRASP0 atomic structure code in conjunction with DARC (Dirac Atomic *R*-matrix Code) are used to calculate the Einstein *A* coefficients and collisional rates used to generate a synthetic W II spectrum. The W II spectrum is compared against tungsten spectral emission experiments. *Results*: this study is used to model the spectrum of W II, providing the predictive capability of identifying spectral lines from recent experiments. These results provide an integral part of impurity influx and redeposition determination, as the ionisation rates may be used to calculate S/XB ratios.

Snapshot of W I

Groundstate : 4f^14 5d^4 6s^2

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

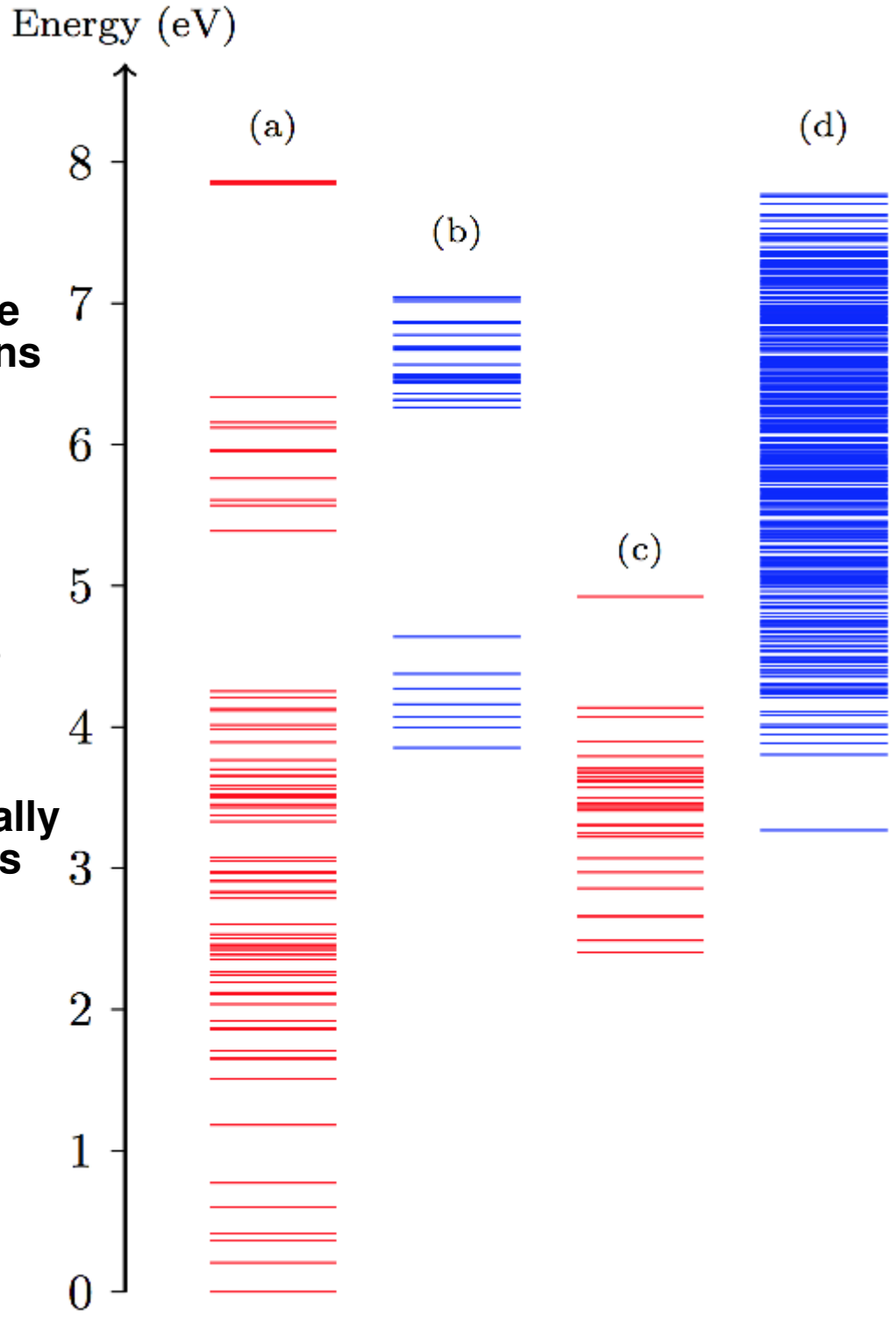
: Dirac R-matrix calculation
keeps 300 levels in the
close-coupling expansion

(a) Known (NIST/literature) even levels

(b) Known (NIST/literature) odd levels

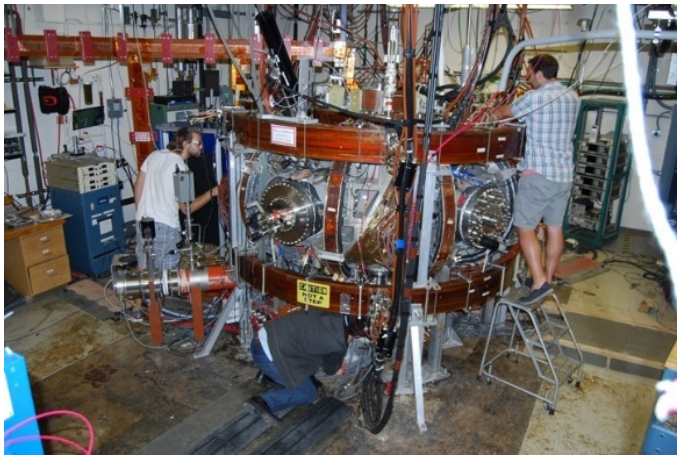
(c) & (d) unknown or at least only partially designated even and odd levels

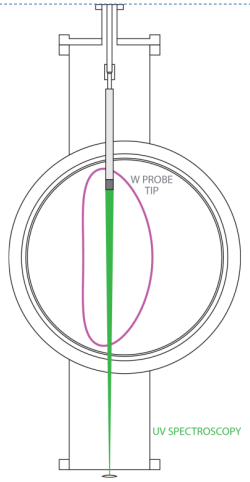
(might be slightly out of date in terms Of completeness)



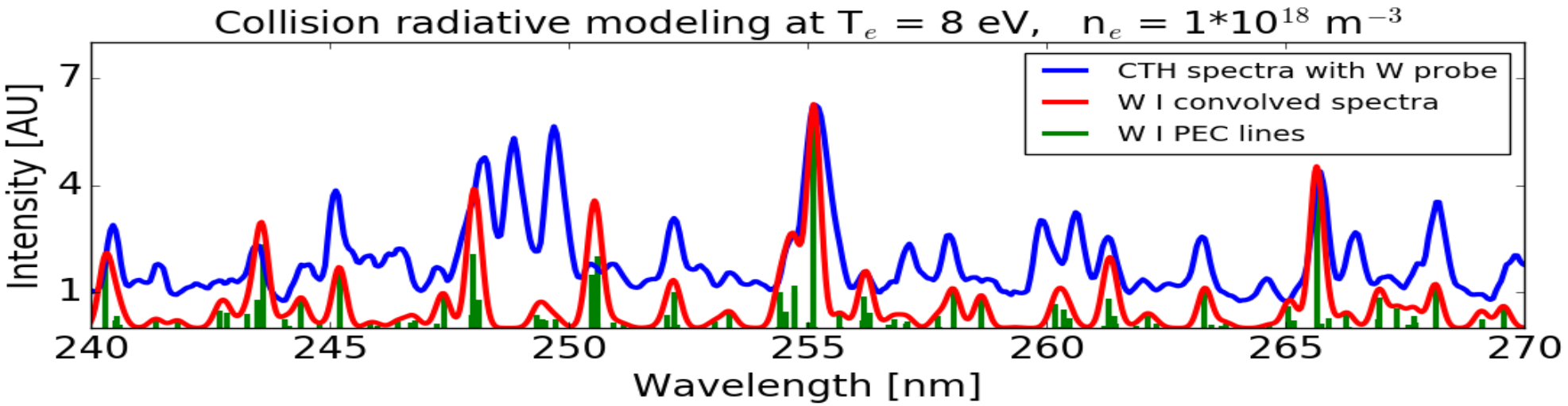
Compact Toroidal Hybrid (CTH) has been an invaluable test of the electron-impact excitation dataset

- 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).

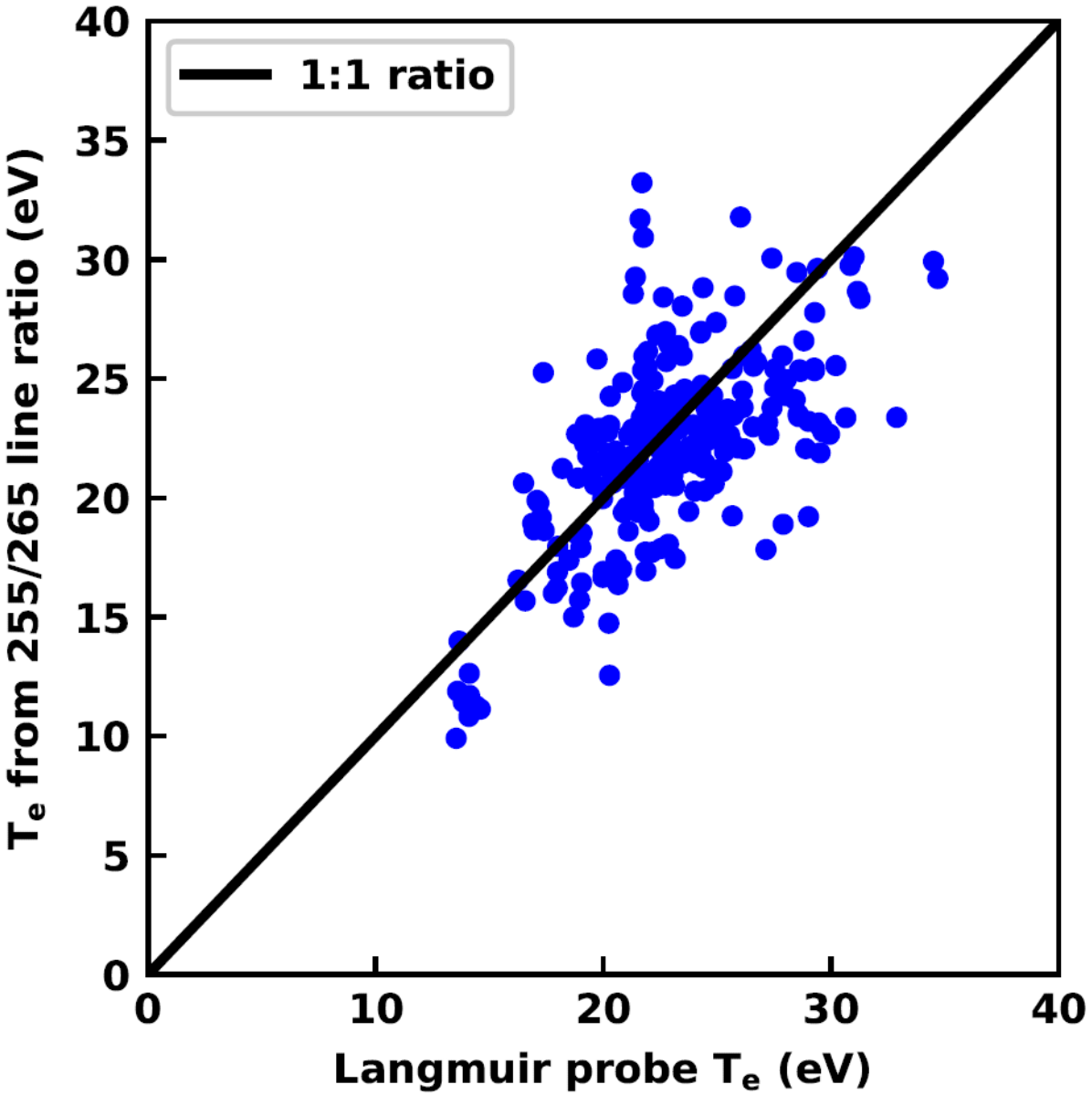




CTH cross section with probe and UV spectrometer line of sight



Temperature derived from lines within R Smyth W I adf04 file and those measured with a Langmuir probe on the Auburn CTH experiment.



Neutron-star merger atomic structure employs the GRASP0 code, but the low temperature ~1eV of the merger and only moderate density suggests that the focus should be on the lowest 20-30 levels. Perhaps, large structure but to optimize the oscillator strengths of the lowest levels.

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https://doi.org/10.1093/mnras/stab3285

Atomic data calculations for Au I–Au III and exploration in the application of collisional-radiative theory to laboratory and neutron star merger plasmas

FAC (atomic structure/Distorted- wave)

Vrs

GRASP + DARC (R-matrix)

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ABSTRACT

Neutron binary star mergers have long been proposed as sufficiently neutron rich environments that could support the synthesis of rapid neutron capture elements (r-process elements) such as gold. However, the literature reveals that beyond neutral and singly ionized systems, there is an incompleteness of atomic data for the remaining ion stages of importance for mergers. In this work, we report on relativistic atomic structure calculations for Au I–Au III using the GRASP^0 codes. Comparisons to calculations using the Flexible Atomic Code suggest uncertainties on average of 9.2 per cent, 5.7 per cent, and 3.8 per cent for Au I–Au III level energies. Agreement around ~50 per cent is achieved between our computed *A*-values and those in the literature, where available. Using the GRASP^0 structure of Au I, we calculated electron-impact excitation rate coefficients and use a collisional-radiative model to explore the excitation dynamics and line ratio diagnostics possible in neutron star merger environments. We find that proper accounting of metastable populations is critical for extracting useful information from ultraviolet–visible line ratio diagnostics of Au I. As a test of our data, we applied our electron-impact data to study a gold hollow cathode spectrum in the literature and diagnosed the plasma conditions as $T_e = 3.1 \pm 1.2$ eV and $n_e = 2.7^{+1.3}_{-0.9} \times 10^{13}$ cm^{-3}.

Key words: atomic data – neutron star mergers – line: identification – plasmas – scattering – techniques: spectroscopic.

It seems that under the current plasma conditions, neutral gold (Au I) is not in local thermal equilibrium and hence requires an electron-impact excitation and perhaps ionization calculation as well

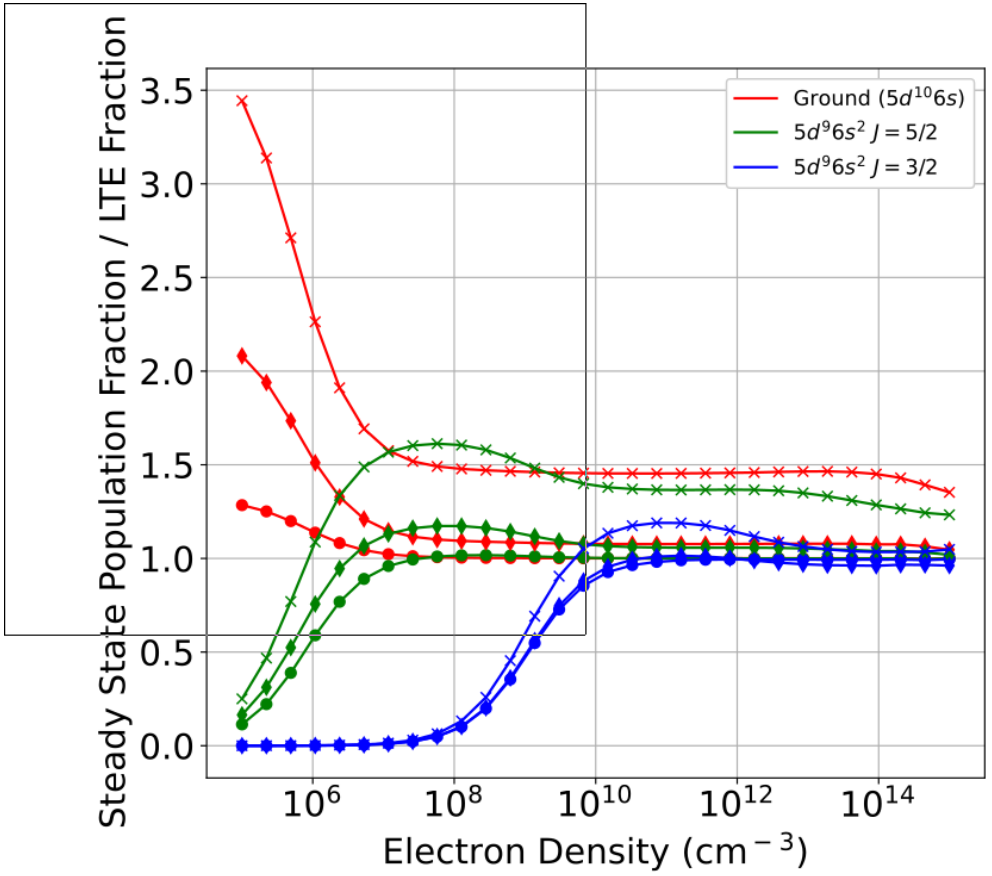


Figure 7. Steady-state population fractions for the ground and metastable levels of Au I divided by their temperature-dependent LTE population fraction at temperatures of 0.5 (°), 1 (◇), and 1.5 eV (×). For each temperature, the populations are normalized so that the total population of the CR and LTE models is each set to 1.

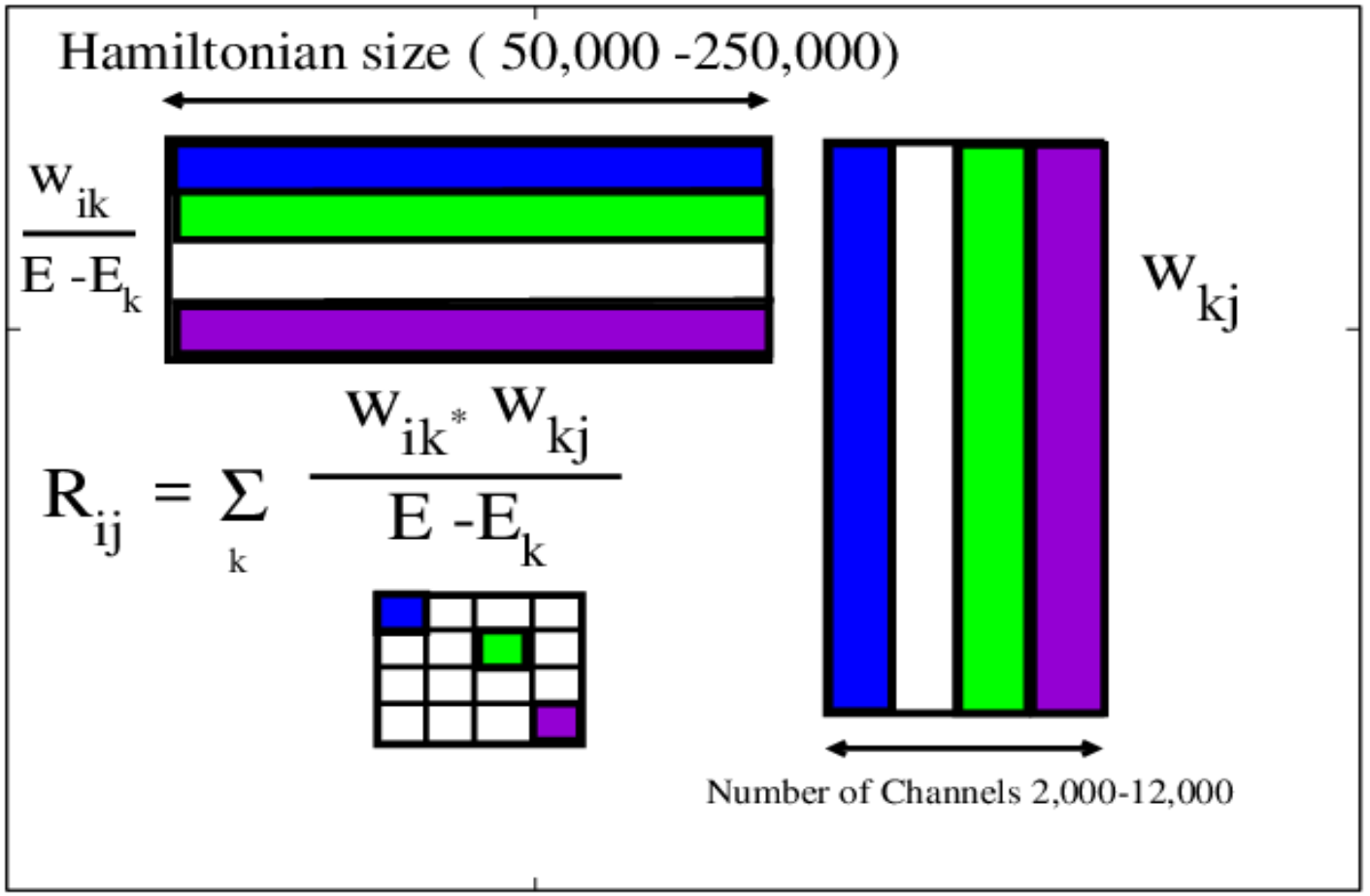
Current and future directions of R-matrix codes

- With GPU(Graphical Processing Units) here to stay in the near future, the dense linear algebra. (ie.matrix-multiply/diagonalisation)
- With local machines having 128 cores with 4 GPUs per node and large national supercomputer resources such as NERSC (perlmutter) having at least 1 GPU per node it may be the time to develop.
- Nvidia compiler (portland compiler) has pre-existing lapack and blas libraries which are highly optmised
- User needs only decide how to move data to GPU and carry out calculation and return result to CPU
- I recommend cublas libraries ...

Example : R-matrix formation

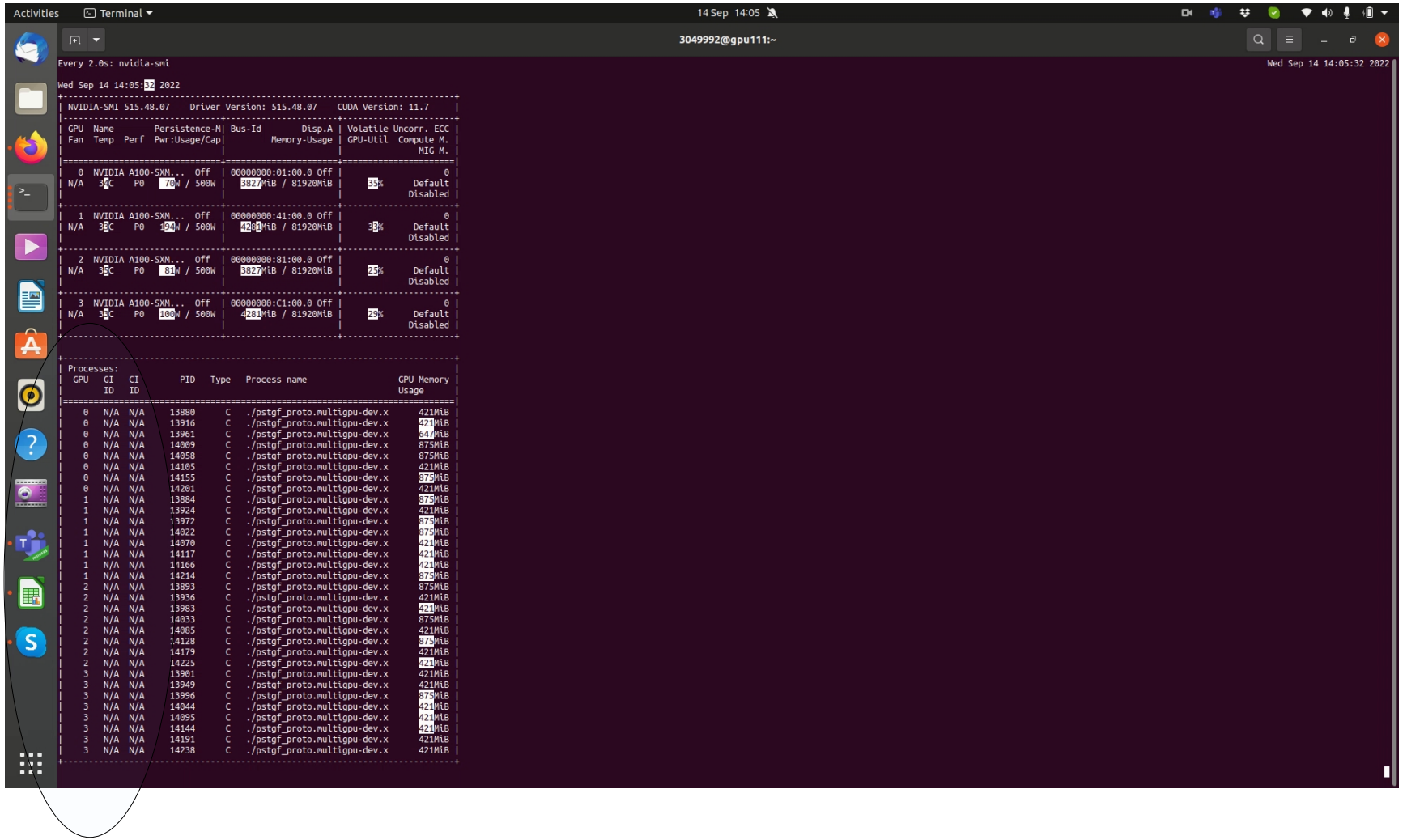
The R-matrix must be formed for every energy point and partial wave, and is And intensive matrix multiply. For 10,000 channels + matrices exceeding 100K by 100 K

→ 10,000*10,000*100,000= 10^13 operations ….. and modern CPUs only are of the order 10^9 operations per sec. Do you wait an hour per energy point ?



Example : R-matrix formation

128 CPUs matched one of four GPUS



All R-matrix asymptotic packages : stgb (bound state), pstgf(electron-impact), pstgbf0 (photoionisation) are GPU enabled.

Thank-you for your attention: questions?