Relativistic calculations for electron-impact excitation and other things

ADAS Workshop 2009

Connor Ballance

John Ludlow, Stuart Loch

Auburn University, US

Nigel Badnell

Strathclyde University, UK

Progress towards larger scale calculations and (interactive production runs) for mid scale calculations.

Code development has essentially reduced the time for electron-impact scattering to the time required to calculate a single partial wave.

Concurrent parallel diagonalisation has been implemented in the in the R-matrix codes for all coupling schemes.

-----> process Terabytes instead of Gigabytes of angular algebra and Hamiltonian matrix elements in a matter of hrs

------> slow,steady progress towards the open d-shell systems of W Fe, and Ni.

-------> Downside: Needs thousands of processors rather than hundreds

Electron-impact excitation along the entire Argon sequence (John Ludlow -submitted J Phys B)

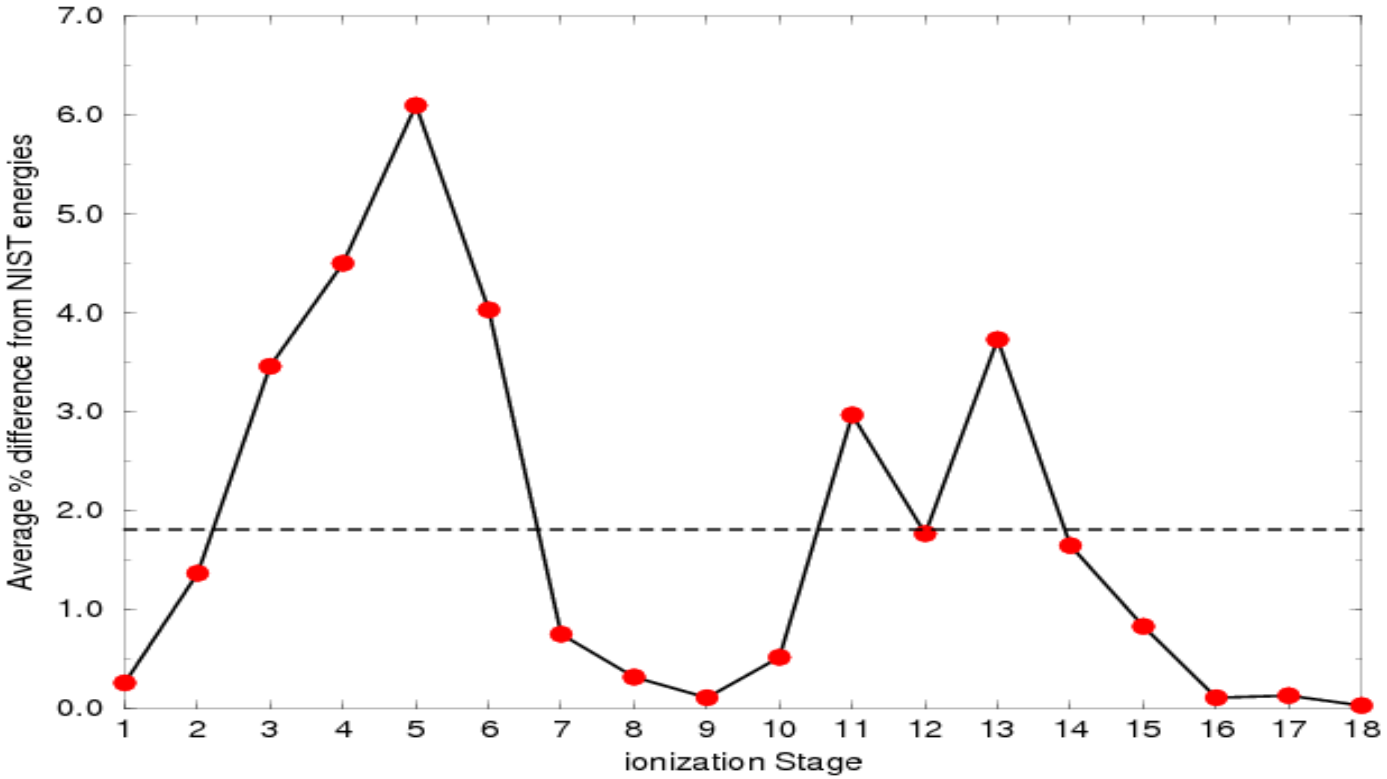
* Complements ongoing sequence work of Guiyan Liang, Mike Witthoeft and Allan Whiteford

* Every ion stage < 250 levels is carried-out in 3-5 hrs of computation

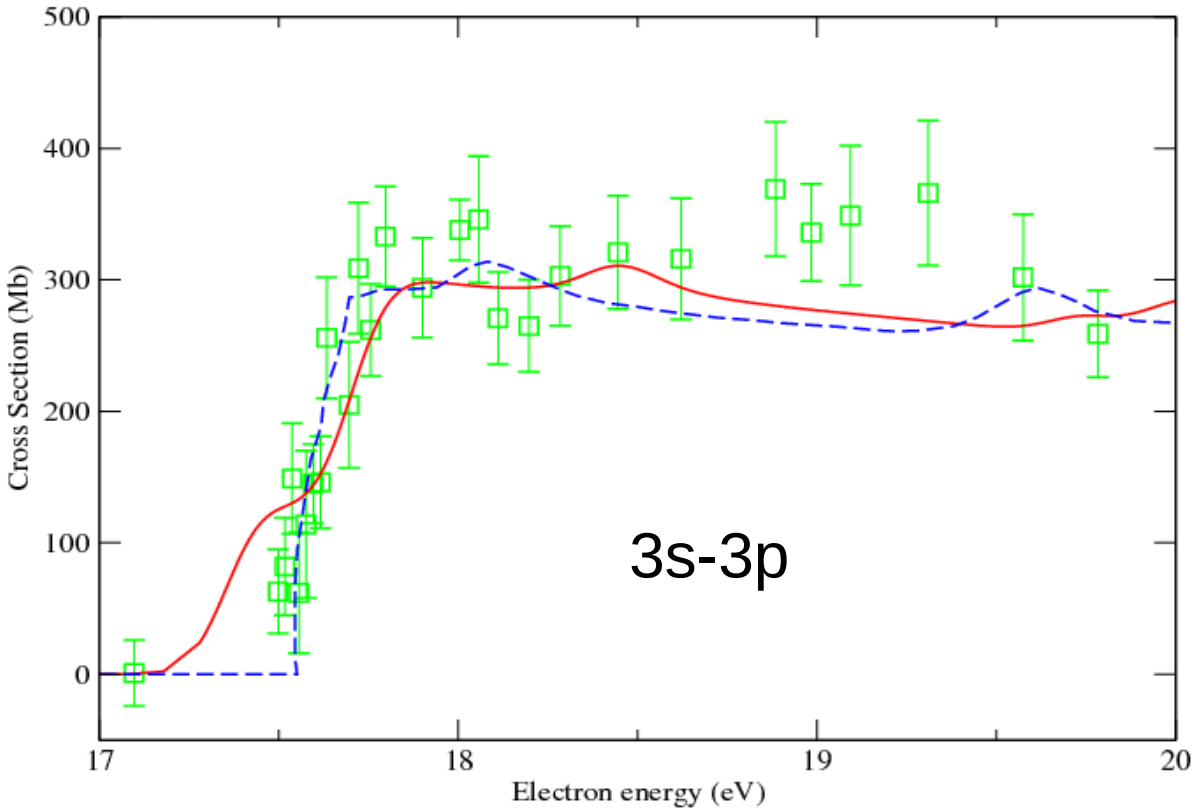
TABLE I. Configurations included in the scattering calculations

Ion	configurations	Levels	Transitions
Ar^{3+}	$3s^23p^3$,$3s^23p^23d$-$3s^23p^25s$,$3s3p^4$,$3s^23p3d^2$	181	16290
Ar^{4+}	$3s^23p^2$,$3s^23p3d$-$3s^23p5s$,$3s3p^3$,$3s3p^23d$,$3p^4$,$3s3p3d^2$	220	24090
Ar^{5+}	$3s^23p$,$3s^23d$-$3s^25s$,$3s3p^2$,$3s3p3d$-$3s3p5s$,$3p^3$,$3p^23d$	155	11935
Ar^{7+}	$2p^63s$-$2p^65g$,$2p^53s^2$,$2p^53s3p$,$2p^53p^2$	62	1891
Ar^{8+}	$2p^6$,$2p^53s$-$2p^55g$	115	6555
Ar^{10+}	$2s^22p^4$,$2s^22p^33s$-$2s^22p^35s$,$2s2p^5$,$2s2p^43s$,$2p^6$	228	25878
Ar^{11+}	$2s^22p^3$,$2s^22p^23s$-$2s^22p^25s$,$2s2p^4$-$2s2p^33s$,$2p^5$	186	17205
Ar^{12+}	$2s^22p^2$,$2s^22p3s$-$2s^22p4f$,$2s2p^3$,$2s2p^23s$-$2s2p^23d$,$2p^4$	198	19503
Ar^{13+}	$2s^22p$-$2s^25g$,$2s2p^2$,$2p^3$	36	630
Ar^{14+}	$2s^2$,$2s2p$-$2s5g$,$2p^2$,$3s^2$	53	1378
Ar^{17+}	1s-5g	25	300

Average energy difference of theoretical results with NIST energy values. Though shifted to NIST values in final adf04 files.



Comparions with experimental cross sections are made where available



Red solid
(present BP R-matrix)

Green squares
(Guo et al, Phys Rev A R9 47 (1993))

Electron-impact ionisation of highly excited states of fusion related species

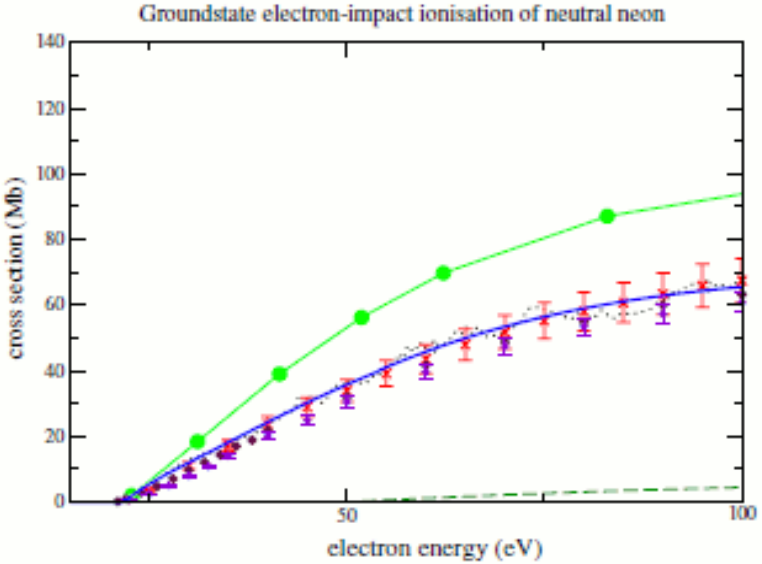


Figure 1. Electron-impact ionization of the neutral neon ground state. The dotted black curve corresponds to the raw RMPS theoretical values and the solid blue curve a Rost/Younger fit to those values. The red crosses correspond to the experimental measurement of Krishnakumar and Srivastava (1988), the diamonds correspond to the measurement of Wetzel *et al* (1987) and maroon circles correspond to the experimental measurements of Rejoub *et al* (2002). The connected green circles correspond to a CADW direct 2p ionization. The green dashed line corresponds to the associated contribution of the 2s ionization to the total ionization from 50 eV onwards calculated within the CADW approximation.

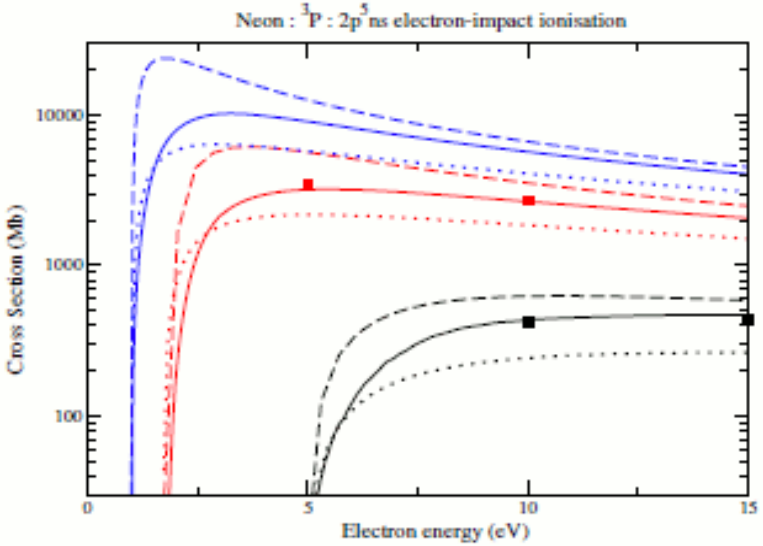


Figure 2. Electron-impact ionization of the excited $2p^5ns$ terms of neon. The black solid, dashed and dotted lines correspond to the direct ionization of the $^3P : 3s$ term by the RMPS, CADW and ECIP methods, respectively. The red solid, dashed and dotted lines correspond to the direct ionization of the $^3P : 4s$ term by the RMPS, CADW and ECIP methods, respectively. The blue solid, dashed and dotted lines correspond to the direct ionization of the $^3P : 5s$ term by the RMPS, CADW and ECIP methods, respectively. The black solid squares refer to the TDCC direct ionization of the 3s and the solid red squares refer to the TDCC direct ionization of the 4s.

Current state of ongoing boron and carbon calculations for ADAS

All calculations, both electron-impact excitation and ionisation for boron have been completed. However, in light of the neon excited state ionisation results higher n shell have now been Calculated.

For carbon, only the ionisation/excitation of the neutral and singly ionised cases remain. Ionisation shall be calculated this autumn. Unsual 2s2p^3 ionisation must be considered.

Developement of a magnetic sublevel collision strength code. With the possibility of CR modelling at the magnetic sub level (Inal and Dubau – J Phys B 20 4221 (1987)

The inelastic electron-ion scattering amplitude for an atom or ion is given by:

$$f_{if}(\theta,\phi)=\frac{i\sqrt{\pi}}{\sqrt{k_i k_f}}\sum_{\substack{\ell_i\ell_f J_i J_f J\\ m_{\ell_f} m_{j_i} m_{j_f} M}} i^{(\ell_i-\ell_f)}\sqrt{2\ell_i+1}\; e^{i(\sigma_{\ell_i}+\sigma_{\ell_f})}\; C^{\ell_i s_i j_i}_{0 m_{s_i} m_{j_i}} C^{\ell_f s_f j_f}_{m_{\ell_f} m_{s_f} m_{j_f}} C^{J_i j_i J}_{M_i m_{j_i} M} C^{J_f j_f J}_{M_f m_{j_f} M} \tag{1}$$

$$T^{J\pi}_{\ell_i j_i \ell_f j_f}(\beta_i J_i \to \beta_f J_f) Y_{\ell_f m_{\ell_f}}(\theta,\phi)\,,$$

where σ_ℓ is the Coulomb phase shift for an ion of charge q = Z - N. Here, it is assumed that the incident electron is along the z-axis and the T-matrix is in the j-j coupled representation with initial and final states: $\beta_i J_i k_i \ell_i j_i JM$ and $\beta_f J_f k_f \ell_f j_f JM$, respectively. Of course, the T-matrix is independent of the value of M. Now for unpolarized electrons, we can average over the initial spins and sum over the final spins to determine the inelastic differential cross section in units of a_0^2/sr for the transition $J_i M_i \to J_f M_f$:

$$\frac{d\sigma_{J_i M_i \to J_f M_f}}{d\Omega}=\frac{1}{2}\frac{k_f}{k_i}\sum_{m_{s_i} m_{s_f}}\left|f_{if}(\theta,\phi)\right|^2, \tag{2}$$

where:

$$\sum_{m_{s_i} m_{s_f}}\left|f_{if}(\theta,\phi)\right|^2=\frac{\pi}{k_i k_f}\sum_{m_{s_i} m_{s_f}}\sum_{\substack{\ell_i\ell_i'\ell_f\ell_f' m_{\ell_f} m_{\ell_f}'\\ j_i j_i' J_f J_f' m_{j_i} m_{j_i}' m_{j_f} m_{j_f}'\\ JJ' MM'}} i^{(\ell_i-\ell_f)} i^{(\ell_f'-\ell_i')}\sqrt{(2\ell_i+1)(2\ell_i'+1)}\; e^{i(\sigma_{\ell_i}-\sigma_{\ell_i'}+\sigma_{\ell_f}-\sigma_{\ell_f'})}$$

$$C^{\ell_i \frac{1}{2} j_i}_{0 m_{s_i} m_{j_i}} C^{\ell_i' \frac{1}{2} j_i'}_{0 m_{s_i} m_{j_i}'} C^{\ell_f \frac{1}{2} j_f}_{m_{\ell_f} m_{s_f} m_{j_f}} C^{\ell_f' \frac{1}{2} j_f'}_{m_{\ell_f}' m_{s_f} m_{j_f}'} C^{J_i j_i J}_{M_i m_{j_i} M} C^{J_i j_i' J'}_{M_i m_{j_i}' M'} C^{J_f j_f J}_{M_f m_{j_f} M} C^{J_f j_f' J'}_{M_f m_{j_f}' M'} \tag{3}$$

$$\left[T^{J\pi'}_{\ell_i' j_i' \ell_f' j_f'}(\beta_i J_i \to \beta_f J_f)\right]^* T^{J\pi}_{\ell_i j_i \ell_f j_f}(\beta_i J_i \to \beta_f J_f) Y^*_{\ell_f' m_{\ell_f}'}(\theta,\phi) Y_{\ell_f m_{\ell_f}}(\theta,\phi)\,.$$

The total cross section for the transition $J_i M_i \to J_f M_f$ is given by

$$\sigma_{J_i M_i \to J_f M_f}=\int_0^{2\pi}\int_0^{\pi}\frac{d\sigma_{J_i M_i \to J_f M_f}}{d\Omega}\sin\theta\, d\theta\, d\phi\,. \tag{4}$$

the total cross section for the transition $J_i M_i \rightarrow J_f M_f$ is given by:

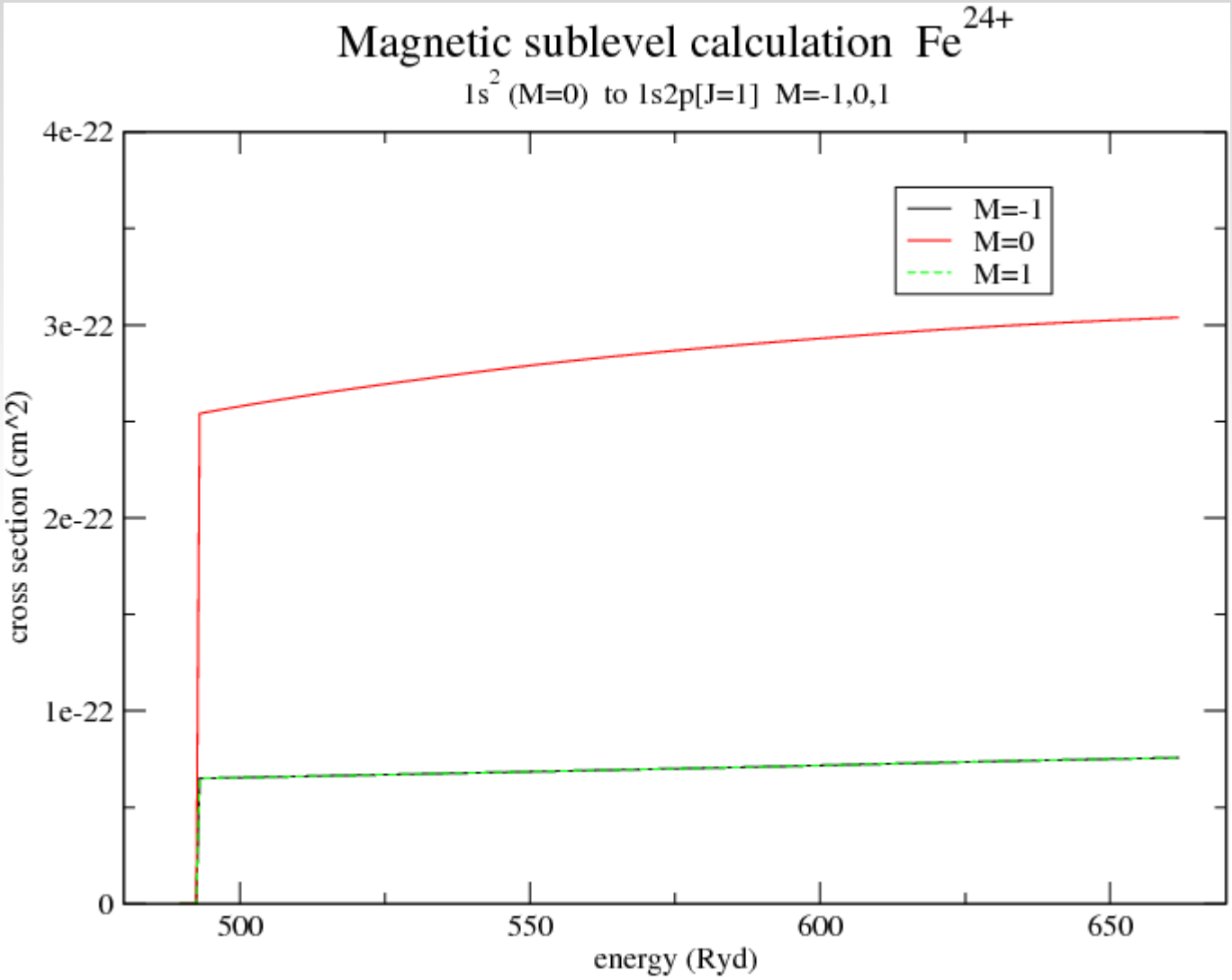
$$\sigma_{J_i M_i \rightarrow J_f M_f} = \frac{\pi}{2k_i^2} \sum_{\substack{\ell_i j_i \ell_i' j_i' \ell_f j_f \\ m_{s_i} m_{j_f} J J' M}} i^{(\ell_i - \ell_i')} \sqrt{(2\ell_i + 1)(2\ell_i' + 1)}\, e^{i(\sigma_{\ell_i} - \sigma_{\ell_i'})} C^{\ell_i \frac{1}{2} j_i}_{0 m_{s_i} m_{s_i}} C^{\ell_i' \frac{1}{2} j_i'}_{0 m_{s_i} m_{s_i}} C^{J_i j_i J}_{M_i m_{s_i} M}$$

$$C^{J_i j_i' J'}_{M_i m_{s_i} M} C^{J_f j_f J}_{M_f m_{j_f} M} C^{J_f j_f J'}_{M_f m_{j_f} M} \left[T^{J' \Pi'}_{\ell_i' j_i' \ell_f j_f} (\beta_i J_i \rightarrow \beta_f J_f) \right]^* T^{J \Pi}_{\ell_i j_i \ell_f j_f} (\beta_i J_i \rightarrow \beta_f J_f).$$

Whereas, the magnetic sublevel collision strengths are difficult to calculate, the J_iM_i → J_fM_f line strength is simply a Clebsch-Gordan Coeff ^2 * the J_i ->J_f line strength.

(… phew one less phase to think about!)

* This has been implemented in the relativistic structure code GRASP0 of Dr Patrick Norrington.


Magnetic sublevel calculation Fe24+
1s2 (M=0) to 1s2p[J=1] M=-1,0,1
4e-22
3e-22
2e-22
1e-22
0
cross section (cm^2)
500
550
600
650
energy (Ryd)
M=-1
M=0
M=1