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Scientific progress report 7

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Abstract: *The report reviews scientific task completion for project months 37-42*

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Chapter 1

Overview

Good progress was made on scientific development of the main ADAS-EU themes in this period and also there was excellent engagement with fusion laboratory experiments. In reviewing the latter, in the context of the initially anticipated interactions specified in the work packages, the ADAS-EU team has reacted to changing focus and needs. By assigning some of these new activities to work packages, we have implicitly extended the original briefs. Main developments are summarised in the following paragraphs. More particulars of the scientific advances are given in the individual contributions of Giunta, Menchero and Summers below (but see ADAS-EU PUBL4, PUBL5 and PUBL6 for full description).

An important part of the infrastructure for generalised-collisional-radiative population and coefficient modelling for medium-weight species has been put in place by Dr. Giunta. This is automatic creation of metastable resolved ionisation coefficients build on manipulation of configuration-average-distorted-wave(*CADW*) cross-section calculations. It links directly to the metastable prescriptions put in place for medium weight species in ADAS *adf00* at *ls* and *ic* resolutions. This combines with the high level *nl*-bundled population modelling codes brought into play in this period by Prof. Summers (see section 2.4). The large scale ADAS *adf04* production in the distorted wave approximation (scripts and production will be finalised and reported in SCIENCE8) and *BBGP* approximation for recombination completes the picture.

Dr Menchero has now solved remaining computational issues for the exact solution of the full Hamiltonian for the motional Stark electric field experienced by fast hydrogen beam atoms. This original work provides, inter alia, field ionisation rates. First results are reported here and extension and integration steps will follow in the next half-year report (SCIENCE8).

The third ADAS-EU course was presented on 26-30 March 2012 at Consorzio RFX, Padua, Italy. This was a very successful meeting with twelve enthusiastic participants from as far afield as the USA, Korea, China and India. Dr Antidormi of the European Commission in Brussels visited during the meeting and gave an overview presentation. Details are given in report DISSEM3. ADAS-EU staff presenting the course materials, tutorials and discussions were Prof. Summers, Dr. O'Mullane, Dr. Guzman, Dr. Menchero and Dr. Giunta.

Dr. O'Mullane's engagement with ITER and diagnotics teams from the Domestic Agencies was very strong in the current conceptual design phase of the diagnostics. Details are not given here (see the separate report ITER2 for the full description). Likewise Prof. Badnell has continued his key work on electron collision processes, but again the details are not give here (see the separate report ECPW2 for the full description).

The work package task 26-1-7 comprises the completion of this report.

Chapter 2

Individual contributions

2.1 Alessandra Giunta: GCR studies

This report concerns the developments of the research projects carried out during this six month period. Three main aspects are expoited, as summarised in the following subsections. The first one is related to the extension and automation of GCR modelling to medium and heavy species. The second and third tasks are the application of a transient ionisation model to solar flare plasma, in collaboration with Professor Gerry Doyle (Armagh Observatory), and to data from MAST, provided by Dr. Hendrik Meyer and Dr. James Harrison. Analysis of transient feature spectrosocpy is an important issue for ADAS-EU interaction with fusion experiments - especially MAST at this time. It is viewed as an appropriate reactive extension of the experiment application briefs of work packages 2-3 and 16-3. Publications in this period include Doyle *et al.* [1].

2.1.1 GCR development: ionisation rates and metastable fractionation (work package 28-1)

Electron impact ionisation rate coefficients from ordinary excited states in GCR modelling adopt the Exchange Classical Impact Parameter (ECIP) procedure of Burgess & Summers [2]. This technique applies to any Rydberg level and is used in both *bn* and *bnl* methods. Concerning ionisation from ground and metastables states, there have been many studies from the early sixties (Lotz [3], [4]), up to present times (Dere [5]), which have examined experimental cross sections and compared them with relatively simple empirical or semi-empirical expressions. The intention has been to use these expressions universally. There has been no one fully theoretical approach which has been of sufficient precision or computability to be used universally. However the Configuration Average Distorted Wave (CADW) method including proper Auger branching of excitation-autoionisation channels now comes close to fulfilling these requirements. This method is used as baseline for ground to ground state ionisation calculation within ADAS. For GCR studies, ionisation resolved into ground and metastable initial and final states is required and semi-empirical formulae must be used to assist this. The semi-empirical method adopted here comes from the work of Burgess et al.[6] as extended to a greater range of ions by Burgess & Chidichimo [7] and to metastable resolution by Summers & Hooper [8]. The ionisation cross section computation performed by CADW are collected in the *adf23* ADAS data file for each ion. They include direct ionisation and excitation/autoionisation cross sections. The *adf07* collection, made from the *adf23* files, contains the ground to ground ionisation rate coefficients.

The work related to ionisation concerns two main developments. The first update is related to the production of these basic ionisation rates using CADW. The second advance is the automation of the metastable splitting using the semi-empirical formula of Burgess & Chidichimo [7] and adjusting the results to the CADW calculation for the ground. The metastable fractionation was perfomed as *ad hoc* hand manipulation of a spreadsheed, but now this step has been automated in order to provide the metastable resolved *adf07* for all ions from hydrogen to iron. The programs for this semi-automatic creation, collected in */adas/idl/adaslib/proc_adf/*, are the following:

1. pathways_adf07.pro

2. fractionate_adf07.pro
3. split_adf07.pro

The first two routines create automatically the spreadsheets containing the metastable fractionation parameters and formulae for each element, while the last program converts the spreadsheet into the resolved *adf07*. The *ls* resolution is adopted for the production of the *adf07* ionisation rate collection, using the metastable fractionation procedure. However, the following step will be the extension to *ic* resolution, as it is more appropriate for medium weight and heavy species. This is also required as a consequence of the extensive mass production of *ls* and *ic* DW *adf04* data files, set up by Professor Hugh Summers (see SCIENCE8).

2.1.2 Diagnostic analysis undergoing transient ionisation (work packages 2-3, 16-3)

This task is the development of the project, in collaboration with the Armagh observatory, concerning the investigation of the role of transient ionisation during the impulsive phase of solar flares (observed with instruments on-board during the Solar Maximum Mission). The results obtained for the enhancement of the O V 1372 Å line emission during a solar flare, occurred on 2 November 1980 (Poland et al., 1984) and its correlation with the hard X-ray emission are used as diagnostic potential of high temporal resolution UV spectral data when transient ionisation is considered. The technique is described and tested in a particular flare event in the paper *The Diagnostic Potential of Transition Region Lines Undergoing Transient Ionization in Dynamic Events* by Doyle *et al.* [1]. This work can be used as analysis tool for the study of the electron temperature and density of impulsive events which will be observed by the forthcoming Interface Region Imaging Spectrograph, IRIS (satellite launch estimated for April 2013). The atomic physics and modelling underlying this project make the connection between the astrophysical and fusion plasmas and give the basis for the task described in the next section.

2.1.3 Time-dependent helium modelling (work packages 2-3, 16-3)

The previous transient study has been applied to the interpretation of measurements from MAST, which have been provided by Dr. Hendrik Meyer and Dr. James Harrison. The analysis is concentrated on the He II 4685.7 Å emission line, observed by a poloidal and a toroidal lines of sight. The purpose is to reconstruct and interpret the measured emission in order to yield the density gradient profile for He II. The integrated photon counts from He II are used in conjunction with the electron temperaure, T_e, and electron density, N_e, profiles from Thompson scattering. Furthermore, the D_α signal as a function of time is used to identify the ELM phases. Three MAST shots (#28191,#28330 and #28179) have been selected and analysed using the CELESTE diagnostic. As starting point, a time sample has been selected. This allowed the analysis of the He II emission where the values of T_e and N_e were known from scattering Thompson dianostic. Firstly, the impurity transport was ignored and the local emissivity of He II 4685.7 Å has been evaluated combining the coefficients collected in *adf11* and *adf15* ADAS data files. This work is still in progress and requires a larger grid of T_e and N_e values as a function of time. The final goal will be to provide the He velocity, assuming that helium is in equilibrium with the other species observed (e.g. deuterium, carbon). In principle, this would allow one to derive the velocity of the plasma.

2.1.4 ADAS-EU visits, travel and conference presentations (work packages 20)

26-30 Mar. 2012	ADAS course Consorzio RFX, Padua, Italy: participated in the ADAS course lectures and tutorials

2.2 Francisco Guzman

2.2.1 Science progress (work packages 18-1, 6-4, 8-1, 8-2, 9-1)

Code ADAS904, performing collisional-radiative calculations from mdf04 files, was programmed during the last month of 2011 and the first three months of 2012. At the same time mdf11 formats were defined in their final form and pre-dissociation and auto-ionization data were recorded on mdf38 format files. The programming of ADAS904 routines implied a revision and improvement of ADAS903 that also was checked in order to fix bugs and other errors. First results were obtained during end of March and beginning of April and were presented oat the Aachen PSI 2012 Conference (May 21st - 25th). The proceedings for the PSI conference was submitted during the first days of May before the conference deadline and it is now published [9].

At the same time, preparatory work for quality assessment experiments on Ar CX spectroscopy was carried out. The initial plans was set up by video-conference meeting on March with the participation of Rmy Guirlet, Marco Sertoli, Rachael McDermot, Luis Fernandez and Francisco Guzmn. It was agreed that F. Guzmn would be the experiment leader and that the experiment would be carried either in April or after the PSI conference. Finally it was decided to make it on the week of June 25th - 29th. I went a week before to discuss the experiment shots preparation and learn about the use of CHICA CX analysis code. Experiments were performed with good results and there were discussed in a talk given by F. Guzmn (attached) on a Garching Monday meeting on July 16th.

A third activity was the preparations for an external paper on excitation from the ADAS-EU report made on 2010 titled ‘Excitation cross sections from classical and semiclassical methods in a wide energy range for the reactions (Li^{+3}, Ne^{+10}, Ar^{+18}) + H(1s) -¿ (Li^{+3}, Ne^{+10}, Ar^{+18}) + H(n)’ was carried out in coordination with coauthors Jaime Surez and Luis Errea in Universidad Autnoma de Madrid (UAM) and B. Pons in Bordeaux University. It was agreed that a trip was going to be made on the week of July 16th - 20th to UAM in order to finalize the paper during the second half of 2012 (see SCIENCE8).

2.2.2 ADAS-EU visits, travel and conference presentations (work packages 20, 21)

13-17 Feb. 2012	JET Coordination meeting: Discussions with ADAS staff on key points of molecular collisional-radiative model programming; Linkage with central ADAS.
26-30 Mar. 2012	Padua ADAS-EU course: Organiser, teaching and contact person.
16 Apr. 2012:	CEA Cadarache Scientific and technical meeting: Presentation ’Molecular Collisional-Radiative Model for ADAS’
20-25 May 2012	PSI-Aachen: Presentation of poster ’Adas Tools for Collisional-Radiative Model for Molecules’
29 May 2012	FZ-Julich: Discussions on molecular collisional-radiative model and first results with Julich collaborators D. Reiter and R. Janev.
16 Jun.2012:	IPP Garching Monday meetings: Presentation on ’Ar CX data quality assesment experiment on 26/06/2012’
25-29 Jun. 2012	IPP Garching: Preparation and execution experiments on Ar CXS quality assessment as experiment leader and proposer.

2.3 Luis Menchero

2.3.1 Study of neutral hydrogen atom under a constant electric field (work packages 11-1)

Theory

At this point it had been checked reviewing the works of S. Henderson shown in the Publication 4, that perturbation theory does not reproduces proper results for high field intensities and high excited states. One possible solution proposed was to go to higher orders in perturbation theory and include the continuum states in the perturbation series to obtain the state widths, nevertheless, the required effort to go on with such implementation was even higher than using an *ab initio* method beyond perturbation theory.

We chose a complex coordinate rotation method [10] to get the resonances of the Stark Hamiltonian, making a direct integration in parabolic coordinates, so the Hamiltonian is written as

$$H(\vartheta) = -\frac{2\,\mathrm{e}^{-2i\vartheta}}{\xi+\eta}\frac{\partial}{\partial\xi}\left(\xi\frac{\partial}{\partial\xi}\right) - \frac{2\,\mathrm{e}^{-2i\vartheta}}{\xi+\eta}\frac{\partial}{\partial\eta}\left(\eta\frac{\partial}{\partial\eta}\right) - \frac{\mathrm{e}^{-2i\vartheta}}{2\xi\eta}\frac{\partial^2}{\partial\phi^2} - \frac{2\,\mathrm{e}^{-i\vartheta}}{\xi+\eta} + \frac{\mathrm{e}^{i\vartheta}}{2}F(\xi-\eta), \tag{2.1}$$

where ϑ is the complex coordinate rotation angle. The wave function is expanded in a basis set as

$$\psi(\xi,\eta,\phi) = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{im\phi}\sum_{k=1}^{N}\sum_{l=1}^{N}c_{klm}\,(\xi\eta)^{\frac{|m|}{2}}\,f_k(\xi)\,f_l(\eta). \tag{2.2}$$

So we obtain the matrixes for the Hamiltonian

$$\begin{aligned} H_{klk'l'm}(\vartheta) = \int_0^\infty \mathrm{d}\xi \int_0^\infty \mathrm{d}\eta\,\xi^{|m|}\,\eta^{|m|}\,f_k^*(\xi)\,f_l^*(\eta)\left[-\frac{\mathrm{e}^{-2i\vartheta}}{2}\left(\xi\frac{\mathrm{d}^2 f_{k'}(\xi)}{\mathrm{d}\xi^2}f_{l'}(\eta) + \eta\,f_{k'}(\xi)\frac{\mathrm{d}^2 f_{l'}(\eta)}{\mathrm{d}\eta^2}\right.\right.\\ \left. + (|m|+1)\frac{\mathrm{d}f_{k'}(\xi)}{\mathrm{d}\xi}f_{l'}(\eta) + (|m|+1)\,f_{k'}(\xi)\frac{\mathrm{d}f_{l'}(\eta)}{\mathrm{d}\eta}\right)\\ \left. + \left(-\frac{\mathrm{e}^{-i\vartheta}}{2} + \frac{\mathrm{e}^{i\vartheta}}{8}F(\xi^2-\eta^2)\right)f_{k'}(\xi)\,f_{l'}(\eta)\right] \end{aligned} \tag{2.3}$$

and the overlaps

$$S_{klk'l'm} = \int_0^\infty \mathrm{d}\xi \int_0^\infty \mathrm{d}\eta\,\frac{1}{4}(\xi+\eta)\,\xi^{|m|}\,\eta^{|m|}\,f_k^*(\xi)\,f_l^*(\eta)\,f_{k'}(\xi)\,f_{l'}(\eta). \tag{2.4}$$

So we just have to solve the secular equation to obtain the roots:

$$(\mathbf{H} - \mathbf{E}\,\mathbf{S})\,\mathbf{C} = 0. \tag{2.5}$$

Several basis sets were tried for the problem, namely, Lagrange-Laguerre-mesh polynomials, Laguerre polynomials, B-Splines and Airy functions. Finally we checked that the best stability for our problems were the Laguerre-mesh polynomials $\{\Lambda_{Nk}\}_{k=1}^{N}$, defined as:

$$\Lambda_{Nk}(x) = (-1)^k\,\sqrt{x_k}\,\frac{\mathrm{L}_N(x)}{x-x_k}, \tag{2.6}$$

where $\mathrm{L}_N(x)$ is the Laguerre polynomial of grad N, and x_k is its k-th zero. The used basis set was the Laguerre-mesh polynomial times an exponential decay

$$f_k(x) = \Lambda_{Nk}(x)\,\mathrm{e}^{-\frac{x}{2}}. \tag{2.7}$$

This basis set is orthonormal and it has very good stability properties.

Implementation

The programing code to solve the Stark effect in neutral hydrogen was implemented in two parts, the first one to calculate the matrix elements of **H** and **S** making the integrals (2.3) and (2.4), and a second module to make the diagonalisation.

Integrals

A basis set size N (2.6) leads to a total of N^2-variable two basis functions, so to matrixes $\mathbf{H}$ and $\mathbf{S}$ size $N^2 \times N^2$. Nevertheless it is not necessary to calculate the hole $2N^4$ two-variable integrals as the equations (2.3) and (2.4) can be split in products of one-variable integrals defining the $N \times N$ matrixes

$$\begin{aligned}
\mathcal{T}_{kk'} &= \int_0^\infty \mathrm{d}x\, x^{|m|}\, \mathrm{e}^{-x}\, \Lambda_{Nk}(x) \left[x\, \frac{\mathrm{d}^2 \Lambda_{Nk'}(x)}{\mathrm{d}x^2} + (|m| + 1 - x)\, \frac{\mathrm{d}\Lambda_{Nk'}(x)}{\mathrm{d}x} \right. \\
&\quad \left. + \left(\frac{1}{4} x - \frac{1}{2} |m| - \frac{1}{2} \right) \Lambda_{Nk'}(x) \right] \\
\mathcal{I}_{kk'} &= \int_0^\infty \mathrm{d}x\, x^{|m|}\, \mathrm{e}^{-x}\, \Lambda_{Nk}(x)\, \Lambda_{Nk'}(x) \\
\mathcal{F}_{kk'} &= \int_0^\infty \mathrm{d}x\, x^{|m|+2}\, \mathrm{e}^{-x}\, \Lambda_{Nk}(x)\, \Lambda_{Nk'}(x) \\
\mathcal{S}_{kk'} &= \int_0^\infty \mathrm{d}x\, x^{|m|+1}\, \mathrm{e}^{-x}\, \Lambda_{Nk}(x)\, \Lambda_{Nk'}(x) \,.
\end{aligned} \tag{2.8}$$

Then the Hamiltonian and overlap matrixes can be written as:

$$H_{klk'l'm}(\vartheta) = -\frac{\mathrm{e}^{-2i\vartheta}}{2} \left(\mathcal{T}_{kk'}\, \mathcal{I}_{ll'} + \mathcal{I}_{kk'}\, \mathcal{T}_{ll'} \right) - \frac{\mathrm{e}^{-i\vartheta}}{2}\, \mathcal{I}_{kk'}\, \mathcal{I}_{ll'} + \frac{\mathrm{e}^{i\vartheta}}{8}\, F \left(\mathcal{F}_{kk'}\, \mathcal{I}_{ll'} + \mathcal{I}_{kk'}\, \mathcal{F}_{ll'} \right) \tag{2.9}$$

$$S_{klk'l'm} = \frac{1}{4} \left(\mathcal{S}_{kk'}\, \mathcal{I}_{ll'} + \mathcal{I}_{kk'}\, \mathcal{S}_{ll'} \right) . \tag{2.10}$$

As a first attempt we used the Gauss quadrature formula [11] as the Laguerre-mesh polynomials fulfil the quadrature conditions, but we appreciated that for high values of the magnetic quantum number m the integrands of (2.8) become more unstable and the Gauss quadrature formula looses accuracy. In the other hand, integrals (2.8) do not depend neither the field intensity F nor the complex rotation angle ϑ, so they should be calculated just once for each value of m, stored in a file and then used in the next module, so it does not matter if the integration calculation takes a long computation time, it will not affect in the main module. So we chose a variable step Simpson formula to calculate the integrals $\mathcal{T}$, $\mathcal{I}$, $\mathcal{F}$ and $\mathcal{S}$ and they were stored in a binary file to be transferred to the diagonalisation routine.

During the integration we dealt a new problem, the Laguerre-mesh polynomial Λ_{Nk}, resulting from the extraction of the k-th root to the Laguerre polynomial of degree N L_N has an avoidable singularity in the point $x = x_k$, and it is a polynomial of degree $N - 1$ in the hole complex plane. Computationally this takes numerical instabilities in the neighbourhood of the singularity, which get larger with the error of the calculation of the Laguerre polynomial root, and they even are amplified for the derivatives of Λ_{Nk}. To solve this we used a technique to avoid the singularity making a Taylor expansion of the Laguerre polynomial centered in the singularity, using the derivation properties of the Laguerre polynomials, the Laguerre-mesh polynomial can be written as

$$\Lambda_{Nk}(x) = (-1)^k \sqrt{x_k} \sum_{j=0}^{N-1} \frac{(-1)^{j+1}}{(j+1)!}\, \mathrm{L}^{j+1}_{N-j-1}(x_k)\, (x - x_k)^j \,, \tag{2.11}$$

where the singularity has been avoided and there are no more numerical instabilities. The routine which makes the one-variable integrals is called *starkinteg*.

Diagonalisation

The routine which calculates the eigenvalues and eigenvectors of the secular equation (2.5) is called *starkccr*. Firstly the routine reads the output file coming from *starkinteg* containing the one-variable integrals $\mathcal{T}$, $\mathcal{I}$, $\mathcal{F}$ and $\mathcal{S}$. Then it makes the products (2.9) and (2.10) to get the Hamiltonian and overlap matrixes. At last step it solves the secular equation using the routine *zggev* from the Linear Algebra PACKage (LAPACK) library, which solves a general secular equation and gets the eigenvalues and eigenvectors of a general complex non-Hermitian matrix.

Then we get the complex eigenvalues of the Hamiltonian and the coefficients of the expansion (2.2). Then applying the complex coordinate theorem we can map the eigenvalues λ in the complex plane versus the rotation angle ϑ and

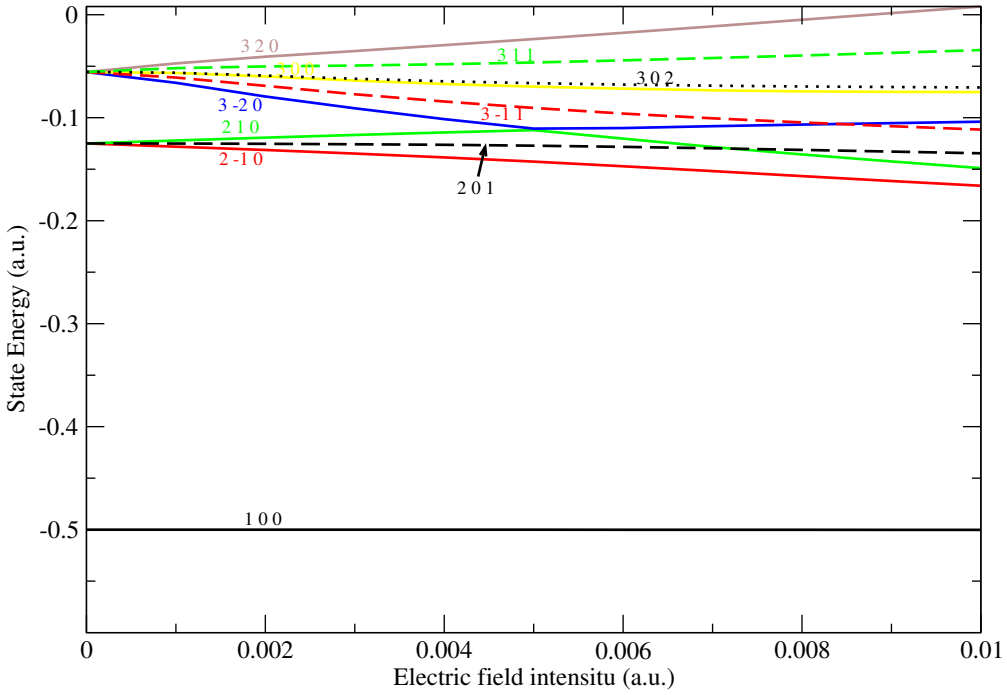

Figure 2.1: Calculated energies for the $n = 1, 2, 3$ shells of the hydrogen atom versus the field intensity.

then we can identify the energies E and widths Γ in terms of the real and imaginary part of the eigenvalue when it becomes independent of the rotation angle.

Preliminary results

The routines *starkinteg* and *starkccr* were tested for a small basis set with $N = 16$. Then we get good accurate results for the first shells of hydrogen of main quantum number $n = 1, 2, 3$, we got acceptable results for the energies and widths for a value of the field up to 0.01 a.u. and magnetic quantum number $m = 0, 1, 2$, we got also the wave functions for all the states of these shells and a value for the Stark splitting of Balmer α line which agrees with the experimental measures.

The approximate quantum numbers $\tilde{n}_1$ and $\tilde{n}_2$ are identified as the number of quasi-nodes of the partially integrated wave functions

$$\begin{aligned} \psi_\xi(\xi) &= \int_0^\infty \mathrm{d}\eta\, \psi(\xi, \eta) \\ \psi_\eta(\eta) &= \int_0^\infty \mathrm{d}\xi\, \psi(\xi, \eta)\,, \end{aligned} \tag{2.12}$$

for its similar shape as the zero field case, when the nodes are real and the quantum numbers become exact. The states are labelled in its parabolic approximate quantum numbers $|\tilde{n}\tilde{k}m\rangle$, being $\tilde{n} = \tilde{n}_1 + \tilde{n}_2 + |m| + 1$ and $\tilde{k} = \tilde{n}_1 - \tilde{n}_2$.

The preliminary results were shown in ADAS workshop 2012.

Further work

After checking the method works for a small basis set, our next step is to increase it to get results for more excited shells and better accurate wave functions. This will be reported on in the next period (see SCIENCE8).

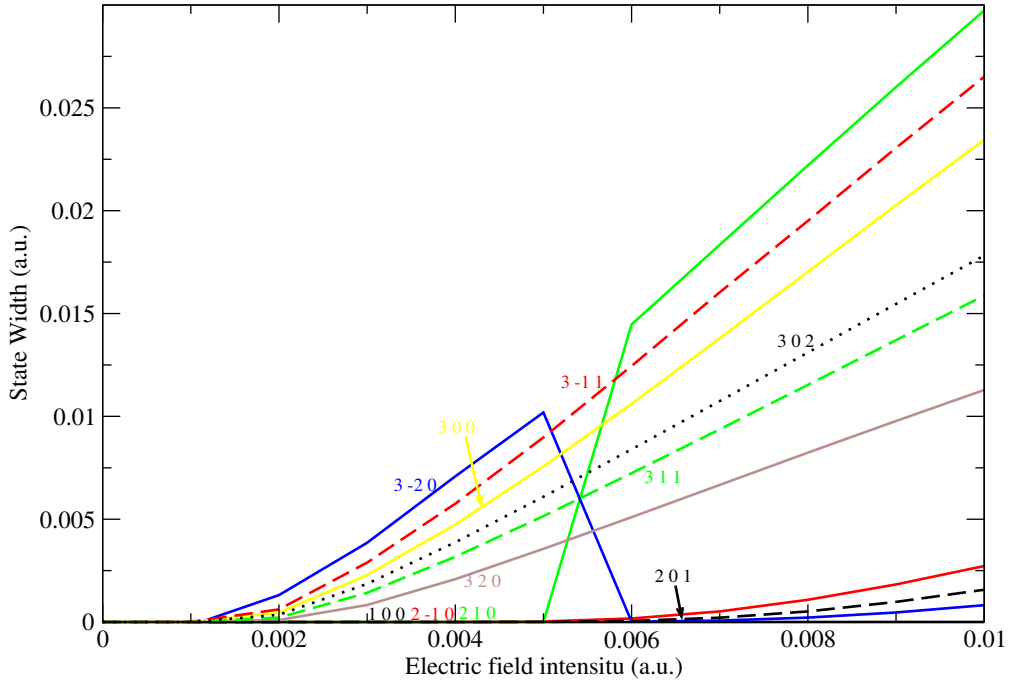

Figure 2.2: Calculated state widths for the $n = 1, 2, 3$ shells of the hydrogen atom versus the field intensity.

2.3.2 Other activities

Determination of impurity concentration through Charge Exchange Spectroscopy (work package 6-4)

The following was in collaboration with Rachael Mc Dermott, Thomas Pütterich and Ralph Dux, from Max Plank Institut für Plasmaphysik in Garching.

R. Mc Dermott developed during the last months the tool CHarge exchange tool for Impurity Concentration Analysis (CHICA). This tool takes the data of charge exchange effective emission coefficients *adf12* for the determination of the impurity concentration through the Charge Exchange Spectroscopy of the neutral beams with the impurities of the plasma. CHICA calculates four components of the beam emission: one corresponding to each energy component E, $E/2$ and $E/3$ of the positive preionised neutral beam injectors installed in ASDEX Upgrade tokamak, and a forth one from the halo. The halo component forms as follows: the deuterium ions of plasma can also capture an electron from the neutral beam as the impurities, then they form neutral deuterium in an excited state $n = 2, 3$, then this deuterium excited can produce thermal charge exchange with the impurities of the plasma, so thermal charge exchange radiation is also detected. This radiation of thermal charge exchange of the halo can sometimes be of the same order or even larger than the direct charge exchange with the beam [12]. The task of ADAS team in this collaboration was to determine these thermal charge exchange effective emission coefficients of hydrogen in an excited state with a fully stripped impurity and order it in a *adf12* format to be read for CHICA, changing the energy of the beam for the ion temperature in the *adf12* format. CHICA was used in the argon charge exchange experiment carried out in ASDEX Upgrade some months later, participating the ADAS team. The results from this experiment are waiting for publication.

Study of the evolution of the cloud during a Massive Gas Injection (work package 8-4)

The following was in collaboration with Kinga Gál and Gabriela Pautasso, from Max Plank Institut für Plasmaphysik in Garching.

Massive Gas Injection (MGI) is a commonly used technique to avoid disruptions in tokamaks. It is important to understand the evolution of the noble gas cloud in the inerhalb of the tokamak during the MGI and how it absorbs the

energy from the plasma [13]. K. Gal and G. Pautasso started a research for the evolution of a noble gas cloud during an MGI. In that topic it is important to know the transport coefficients, which are related to the atomic collision cross sections, and the absorption of energy from the plasma. For the problem it is necessary to know the cross sections including: Electron impact cross sections with the noble gas, excitation and ionisation; Proton impact cross sections, excitation and ionisation; Charge exchange of the noble gas with protons: Collisions with the noble gas with itself and its ions, excitation, ionisation and charge exchange.

2.3.3 Travel, visits and presentations (work package 20)

26-30 Mar. 2012 ADAS course Consorzio RFX, Padua, Italy: participated in the ADAS course tutorials; gave two talks, the first one about *interactive ADAS*, and the second about *New developments in beam models*, including progress in Stark effec and using the complex coordinate rotation method; assisted in one-to-one talks with attendees.

2.4 Hugh Summers (work packages 7-2, 1-2, 28-1)

2.4.1 Extensions for modelling charge exchange for highly ionised heavy ions

The delivery of *nl*- selective charge exchange data from ADAS-EU sub-contracts with the Madrid and Vienna groups for N^{+7}, Ar^{+18} and Kr^{+36} allows a revision of the ADAS Universal Charge Exchange fits of format *adf49* and generation of format *adf01* data for arbitrary heavy element ions. The shift ot the dominant capture at high Z to higher n-shells and the lowered z-scaled electron density, justifies the incorporation of a full bundl-*nl* collisional-radiative population model as an alternative to the simpler bundle-n model used by ADAS316. The planned code ADAS317 will require driver data sets of format *adf25/a25_p317*. The definition of *adf25/a25_p317* and the reading code *xxdata_25.for* has been modifuied for l-resolution parameters. Code ADAS317 must operate to very high n-shells merging smoothly at high n-shells, typically around $n \sim 30$, into *nl*-resolution. This requires special inverse cubic spline interpolation techniques between repreaentative *nl*- shells developed by Summers for astrophysics. This code is now running in its basic form valid to very low temperatures. This code also satifies the requirements for GCR population modelling of medium-weight species.

2.5 Martin O'Mullane

Activities of O'Mullane in this period relate the support of the ITER diagnostic system conceptual design phase (CDR) and are to be found in the document ITER2.

2.6 Nigel Badnell

Activities of Badnell relate to the Electron Collision Working Party (ECWP) and are to be found in the document ECWP2.

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