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Abstract: *The report reviews scientific task completion for project months 43-48.*

Contents

Chapter 1

Overview

The scientific activities of the final period of ADAS-EU have been principally committed to strengthening and exploiting the molecular theme, generalised-collisional-radiative (GCR) supplementary workpackages and the beam stopping/emission theme. The primary work for the molecular theme over ADAS-EU has been the H_2 collisional-radiative model and the database of electron and ion impact cross-sections upon which it depends. This last period has seen extended comparative testing of the codes by Dr. Guzman, assisted by Prof. K. Behringer. Full exploitation of the model does require the prediction of photon emissivities, photon efficiencies and the additional variants of the latter, such as dissociations per photon, appropriate to the molecular scene. These additions have been put in place (see module 3 of the dissemination report DISSEM4). Also Professor Summers and Prof. Behringer worked together to bring Prof. Behringer's Visual Basic H_2 spectral analysis tools into ADAS. The Behringer cabability spanned the Fulcher and Lyman bands of H_2, with highest precision for the isotopomers H_2, HD and D_2 and lower precision, at this time, for the others. For completness, Prof. Summers brought into play earlier spectral prediction for heteronuclear diatomics, including BeH isotopomers, in the same ADAS computational structure (see section 2.4.3 for details).

The progession of the high-grade modelling of the ionisation state of elements in plasma (the GCR activities) into the intermediate weight elements has continued. The main objectives in this period were to give attention to optimising the modelling for the neutral and near neutral atoms and to fill in the supplementary process computations, especially dielectronic recombination and electron impact ionisation. Details are in sections 2.1.1, 2.4.1 and 2.4.2. The exploitation of the GCR work (see, for example, section 2.1.2) was good, but there were some surprising and pleasing aspects which brought to bear and connected with fusion the solar astrophysical knowledge base of two of our ADAS-EU team (Giunta and Summers). A hard check was possible on oxygen line ratio modelling in the solar case (Giunta *et al.* . [1]) and a cross-exploration of dynamic ionisation (Doyle *et al.* [2]). It is interesting that the sophisticated spatially resolved spectral analysis of the oxygen line emission in the LHD stellarator of the National Institute for Fusion Science in Japan uses this ADAS work also successfully. The last, exciting development is the common ground for differential emisison measure analysis (see section 2.1.2) in fusion and astrophysics. This particular aspect is a key path for exploitation in our long term planning.

The continued development of the advanced hydrogen beam modelling, led by Dr. Menchero, has been a main objective. The complex computations have been extended to more excited states of the beam atoms in strong motional Stark fields. The work is designed for the ITER era with high energy negative ion source heating beams. From a mathematical and computational point-of-view, the first-order perturbative approach is invalid and the zeroth order solution with the full Hamiltonian is required (see Menchero *et al.* [3]). This solution provides the new basis for accurate Stark population modelling with other magnetic and electric field perturbations. The development is timely, as beam emission analysis for ITER will move away from single component polarimetry to whole Stark manifold intensity analysis. The additional computational infrastructure is now nearly assembled. This work is also a key path into the future with a new research student assigned to work with Dr. Menchero and Prof. Summers on the exploitation.

The fourth ADAS-EU course was presented on 26 September-4 October 2012 at C.E.A. Cadarache, France. Details are given in report DISSEM3. The ADAS workshop took place ADAS workshop on 23-25 September 2012 at C.E.A. Cadarache, France. This was a large meeting with around fifty participants, from as far afield as the USA, Korea, China and India. It included presentations from senior astrophysicists from the USA who promoted an absorbing

intercomparison of atomic physics applications in fusion and astrophysics.

The work package task 26-1-8 comprises the completion of this report.

Chapter 2

Individual contributions

2.1 Alessandra Giunta: GCR studies

This six month period included the developments of two main projects. The first task is closely related to the work on fundamental data production, carried out by Professor Hugh Summers. The second work concerns the use of fundamental and derived atomic data for the application to the Differential Emission Measure diagnostic technique, the improvement of the ADAS routines related to such a method and the results obtained when theory and measurements are compared. Furthermore, an appropriate use of the most updated GCR helium data has been applied in support of a work in progress on simulation of an helium jet in a non-stationary regime (time dependent collisional radiative model), performed by Dr. Tony Lefevre (CEA-Cadarache).

2.1.1 GCR developments: verification and re-process of AUTOSTRUCTURE PWB and DW calculations (work package 27-2)

The improvement of the ADAS *baseline* database for intermediate weight species, up to zinc, has been established by a set of PERL scripts, implemented by Professor Hugh Summers (see report SCIENCE6 section 2.2). The automatic mass production of *adf04* ADAS data files has been verified by a systematic re-running of all PWB and DW, in *ls* and *ic* resolutions, calculations using the JAC machines at JET. The driver files *adf27* have been produced from the templates written for each iso-electronic sequence, with suitable adjustments for the near-neutral and neutral cases, especially for species such as clorine and argon. This last issue has been addressed by Professor Nigel Badnell and Professor Hugh Summers, with the objective to make up an automatic procedure to be applied to arbitrary complex systems. The full set of *adf04* files of type 1 and 5 and their conversion to type 3 are ready to be released in the upcoming ADAS distribution.

2.1.2 Differential Emission Measure (DEM) in fusion and astrophysics (work package 2-3, 16-3)

In both astrophysics and fusion domains, the analysis of plasmas using observations of their spectra is one of the most precise and informative route of study and the atomic population models provide the link to interpret such spectra in terms of the source from which they are emitted. The derivation of the emission measure (and its further refinement, called Differential Emission Measure, DEM) from the measured spectra is a powerful method to obtain the properties of the plasma source. The DEM describes the temperature and density structure of the emitting plasma and allows the reconstruction of the observed emission in terms of theory. Such diagnostic technique is currently used in the astrophysical environment to give information about the distibution of electron temperature and electron density of the source and to compare theoretical and observed spectral line intensities. The need of accurate atomic data and models is essential to provide reliable results. Within ADAS this technique is implemented through the Glasgow code, which adoptes the *data adaptive smoothing approach* of Thompson [4], and automated by the routine ADAS601. The

input data are archived in the directory */adas/adas/arch601/*, which contains the observed intensities and the atomic data in the form of a set of contribution functions (i.e. the product of the excited population densities and he ionisation fractional abundances). The contribution functions, also called G-functions, are built up under the assumption of constant electron density or constant electron pressure and are given as a function of electron temperature in the *adf20* ADAS data format. The procedure to provide the G-function sets is implemented in a semi-automatic manner through the routines ADAS412 and ADAS506. The DEM technique has been used, during the six month period, to refine the helium enhancement work, described in section ... . The results are collected in a paper, almost ready for the submission. Although this method is less familiar in spectroscopic studies of fusion plasma, it can be applied to determine impurity concentration, impurity variation in time and impurity influx in fusion (e.g. Von Hellerman & Summers, 1992). This can be done because, in the fusion case, the electron temperature and electron density values and their spatial variations are often known from indepentent measurement. On the other hand, given the impurity concentration, the DEM analysis can be an alternative way to estimate elentron temperature and electron density variations, along a specific line of sight, in the plasma edge of a tokamak where T_e and N_e measurements are more uncertain (e.g. Stangeby & McCracken [5] and reference therein). Hence, this project lies in a more general perspective with application addressed to both astrophysical and fusion plasmas.

2.1.3 Use of atomic data for the simulation of the helium jet in a non-stationary regime (work packages 2-3, 16-3)

The purpose of this task is to provide atomic data in an appropriate format for a simulation of the helium jet in a non stationary regime in a tokamak. This work supports the project carried out by Dr. Tony Lefevre (CEA - Cadarache). The basis of this work comes from the hybrid time dependent/independent modelling developed for TEXTOR by Munoz et al. [6]. They derived a diagnostic method which allows simultaneous measurements of electron temperature and electron density, by evaluating ratios of selected He I line emission profiles from the singlet and triplet helium spin systems. Their model overcomes the issue of long relaxation times for metastable based population (e.g. the ^3S terms for neutral helium), by the implementation of an analytical solution for the time dependent problem. The atomic data provided for neutral helium include in the model the first 29 energy terms up to $5p\,^1P$. Energy levels come from the NIST database. The radiative transition probability for the transition $1s^2\,^1S - 1s2p\,^3P$ has been taken from Lach & Pachucki [7]. For the configurations up to $1s4f$ recently assessed data are already available in the ADAS database. These data were assembled by Paton [8]), including earlier surveys of De Heer et al. [9] and R-matrix calculation of Ballance (2003 - private communication) [10]. Plane Wave Born calculations, using the Cowan code through the ADAS801 routine, have been performed to add transitions which involve $n = 5$ configurations and then merged with the more accurate R-matrix calculations. The ionisation and recombination data are also provided, following the full GCR approach.

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

26 Sep.-5 Oct. 2012 ADAS-EU course, CEA Cadarache, France: participated in the ADAS course lectures and tutorials.

2.2 Francisco Guzman

The main objectives and achievements in this closing period of the ADAS-EU Project have been the continuing consolidation, verification and useful extensions of the primary work carried out in the earlier periods. This has included ion impact cross-sections which excite beam atoms and are complementary to charge exchange cross-sections, extension to the molecular hydrogen cross-section database and the linking of H_2 molecular collisional-radiative modelling more closely to observational spectroscopy. Additional activity has been in dissemination; the communication of latest results of the modelling and ensuring the inclusion of the latest derived data in plasma models - especially those at FZ-Juelich which were a stepping-off point at the beginning of ADAS-EU.

2.2.1 Consolidation of charge exchange spectroscopy analysis (work package 9-3)

In the completion of the tasks of the charge exchange spectroscopy theme in previous work periods, it has been pointed out that the complementary excitation cross-sections of the hydrogen beam atoms should be obtained consistently with the charge exchange cross-sections in the one calculation. An ADAS-EU visit was made by Dr. Guzman to the University Autonoma in Madrid in 2010 to this end. Dr. Guzman and Dr. Suarez have worked togther to complete this task. These data have now been put together for the ions Li^{+3}, Ne^{+10} and Ar^{+18} in collision with H(1s) and cross-sections recommended [11]. The results do suggest that a universal approximate fit, of the form created by Summers for the state-selective charge exchange cross-sections (see ADAS315), is possible. This aspect is on-going, continuing the valuable connection of the ADAS-EU/ADAS teams with he University Autonoma team.

2.2.2 Molecular database additions and extensions (work package 17-1)

New recommended cross sections on excitation by proton impact were put into ADAS *mdf02* format (*fg13_h2#i.dat*) paralleling the electron impact data (*fg13_h2#e.dat*). Extraction of these data into the population codes was enabled. A recall visit to the JET Facility was made from 8-10 Oct 2012 to test the datasets and ensure matching of the developmental codes with the final versions for ADAS release. This included the primary *mdf02* interrogation code ADAS901 which was refined and cross-checked with Dr. O'Mullane.

2.2.3 H_2 collisional-radiative model extension and validation (work package 18-3, 18-4, 19-1)

Improvement has been made in the ADAS904 program to output conveniently the ordinary states population for emissivity prediction and to generate photon emissivities, ionisations per photon and similar quantities required for the molecular case (see PUBL6). Also the ADAS9XX subroutines were adjusted to handle correctly charge exchange processes. A second and final recall visit was made to the JET Facility from 2-14 Dec 2012 to coincide with a visit by Prof. Kurt Behringer. The purpose was to conduct a series of tests on ADAS904 under the supervision of Prof. Behringer to ensure detailed vibronic population behaviour was as expected and consistent with other (mostly lower resolution) calculations. Prof. Behringer brought special expertise through his instigation and overseeing of the earlier IPP Garching work of Fantz and Fantz & Wunderlich. A number of bugs were found and corrected. Guzman also worked with Dr. O'Mullane during this visit on finalizing the ADAS design of the vibronic population code ADAS904 for release. The last purpose of the recall visit was to align vibronic population output from ADAS904 for input to the rovibrational spectral analysis tools for diatomic spectra concurrently being developed by Prof. Behringer and Prof. Summers. The latter work, based on Boltzmann vibrational populations and upward projection to excited states, can be put on an abolsute basis by this linkage. The rovibrational spectral modelling and fitting developments are described by Prof. Summers in section 2.4.4. A first publication has been made ('ADAS Tools for Collisional-Radiative Model for Molecules' - F. Guzman, M. O' Mullane & H.P. Summers [12]) and a second ('Collisional-radiative effective coefficients for homonuclear diatomic molecules' - F. Guzman, H.P. Summers & M. O'Mullane) is in draft form.

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

26 Sep.-5 Oct. 2012	ADAS-EU course, CEA Cadarache, France: participated in the ADAS course lectures, and tutorials and made special presentations on molecular modelling
24-26 Sept. 2012	ADAS Workshop, CEA Cadarache, France: presented talk 'A New Molecular Collisional-Radiative Model in ADAS'.

2.3 Luis Menchero

2.3.1 Study of neutral hydrogen atom under a constant electric field (work packages 11-1, 11-2)

Prior to Jul. 2012, the complex coordinate rotation method was developed to get the resonances of a neutral hydrogen atom under a constant electric field. We used a basis set of Laguerre-mesh polynomials, and we tested the implementation for a small basis set of size $N = 16$, which corresponds to $N^2 = 256$ basis functions. We got acceptable results for energies, widths and wave functions of the shells $n = 1, 2, 3$ of hydrogen.

From Jul. - Dec. 2012, we focused in increasing the size of the basis set to get results for higher excited shells. We found a problem when increasing the set up to $N > 20$ the diagonalisation routine crashed and no eigenvalues and eigenvectors were outputed. The problem was localised in a loss of precision of the Laguerre-mesh polynomials for high degrees, and it was necessary to change its way to be calculated in the routine *starkinteg* to go to higher orders. We split the calculation in two regions: near the avoidable singularity x_k (see report for January to July 2012) $x_{k-1} < x < x_{k+1}$, and wide the singularity otherwise, for the extremes we took $x_0 = 0$ and $x_{N+1} = 2x_N - x_{N-1}$. Then we calculated the Laguerre-mesh polynomials and its derivatives as the direct quotient of the Laguerre polynomial $\Lambda_{Nk}(x) = \frac{L_N(x)}{x-x_k}$ wide the singularity and as its Taylor expansion near the singularity. This method gives a very good stability and accuracy to the Laguerre-mesh polynomials respect the error in the calculation of the roots x_k. We obtained good results for a basis set of $N = 25$, a good description for the shells $n \leq 4$ of hydrogen and all its wave functions. Nevertheless and as it was expected, the computation time of the diagonalisation routine *starkccr* increases considerably. Our last attempt is to put a basis set dimension $N = 30$, which it has been tested it will get good results for the shells $n \leq 5$. A paper was published in the first months of 2013 [13] along with an Max Planck Institute for Plasma Physics, EURATOM Association report with extended figures [3].

Results

In the following figures we show the obtained results for a basis set with $N = 25$, we obtain good accurate results for energies (Fig 2.1) and widths (Fig 2.2) for the shells up to $n = 4$ of hydrogen. In figures (2.3) to (2.7) we show the wave functions, modulus to the square versus the two variables ξ and η and partially integrated ψ_ξ and ψ_η to identify the approximated quantum numbers.

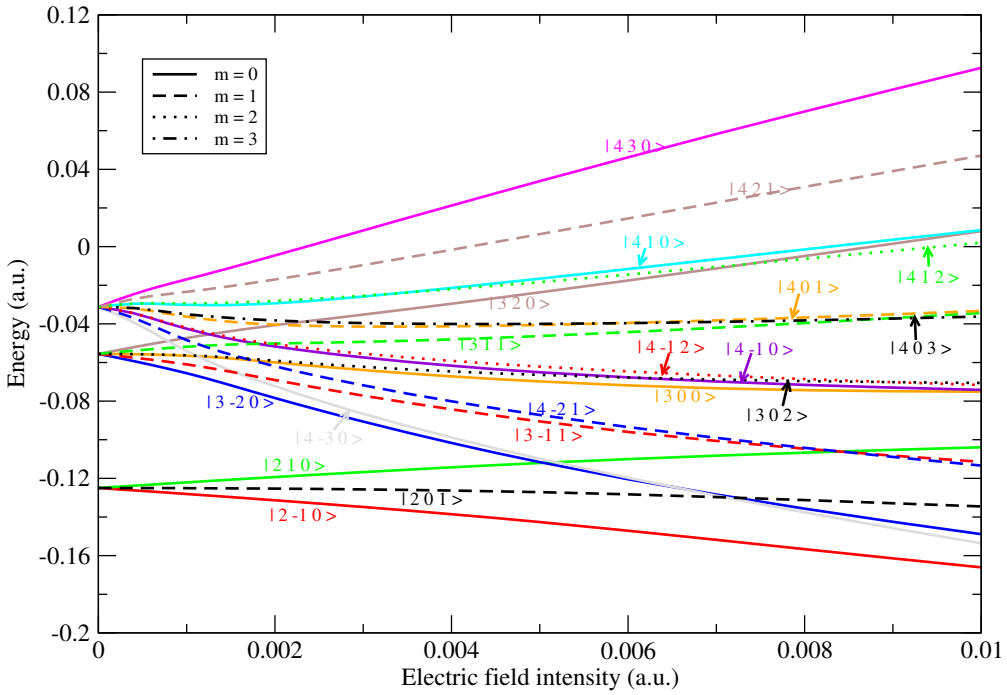


Figure 2.1: Calculated energies for the $n = 2, 3, 4$ shells of the hydrogen atom versus the field intensity.

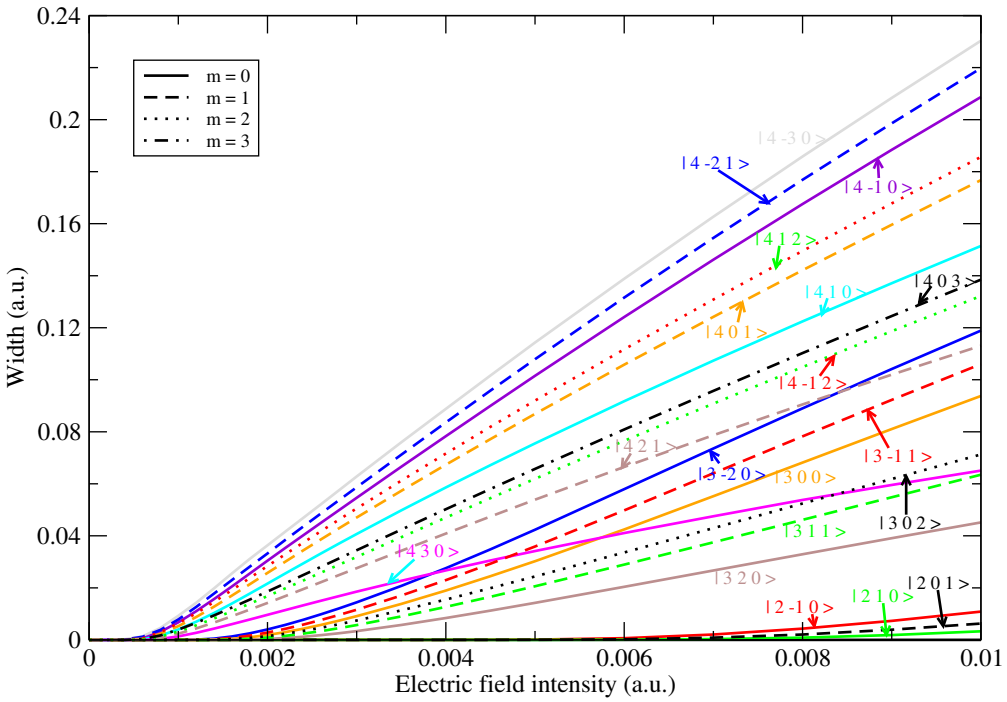
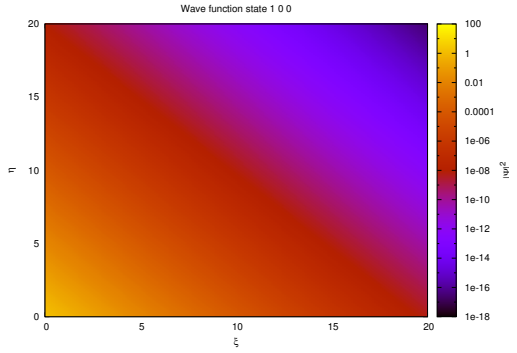
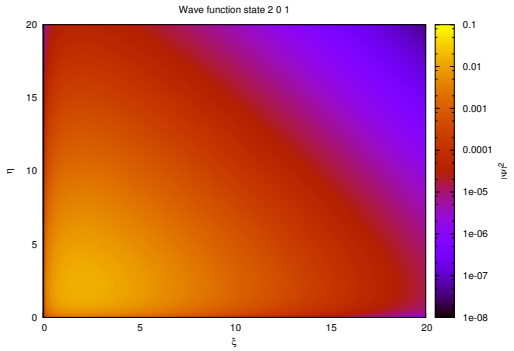


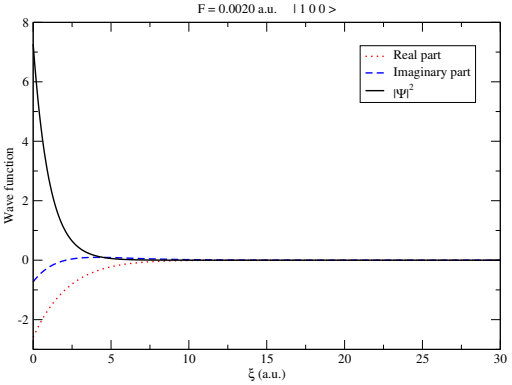
Figure 2.2: Calculated widths for the $n = 2, 3, 4$ shells of the hydrogen atom versus the field intensity.



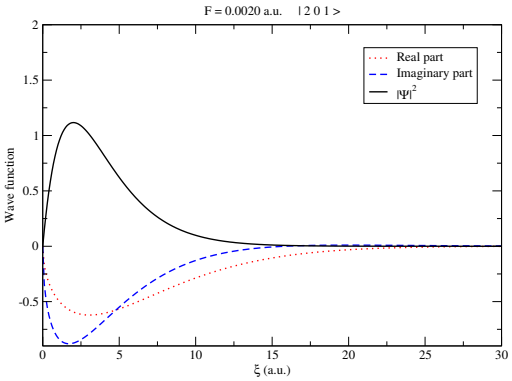
(a) $|\psi_{100}|^2(\xi,\eta)$



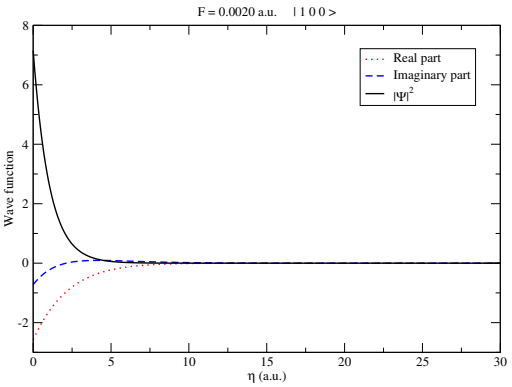
(d) $|\psi_{201}|^2(\xi,\eta)$



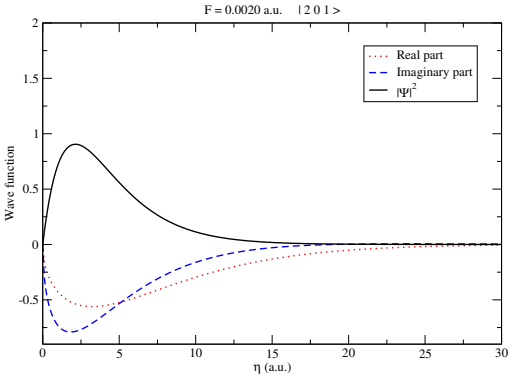
(b) $\psi_{\xi 100}(\xi)$



(e) $\psi_{\xi 201}(\xi)$

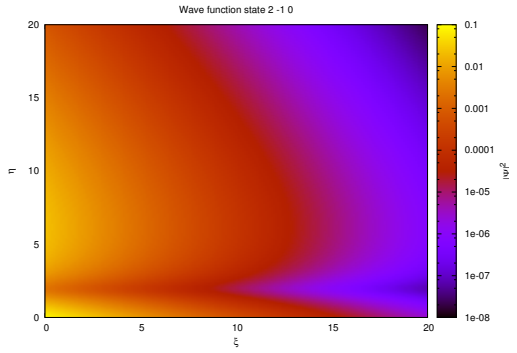


(c) $\psi_{\eta 100}(\eta)$

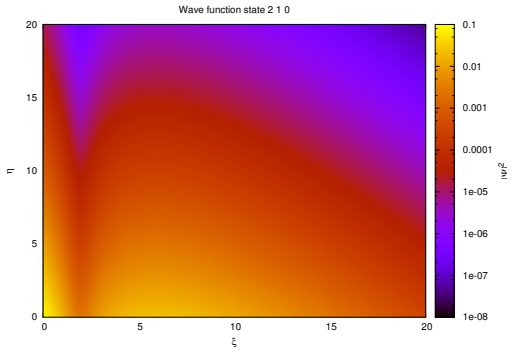


(f) $\psi_{\eta 201}(\eta)$

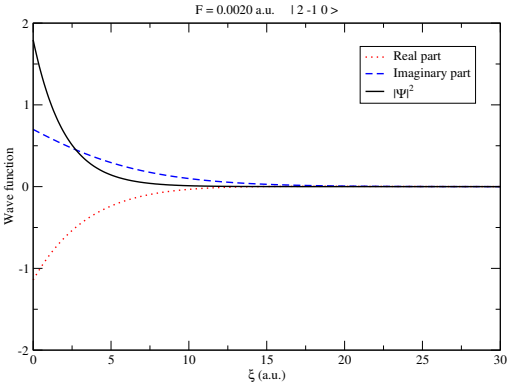
Figure 2.3: (Colour on line) Wave function of the Stark states $|\,1\,0\,0\,\rangle$ and $|\,2\,0\,1\,\rangle$ for a field intensity of $F = 0.0020$ a.u..



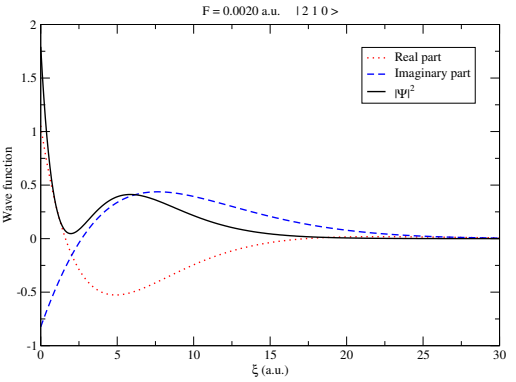
(a) $|\psi_{2-10}|^2(\xi,\eta)$



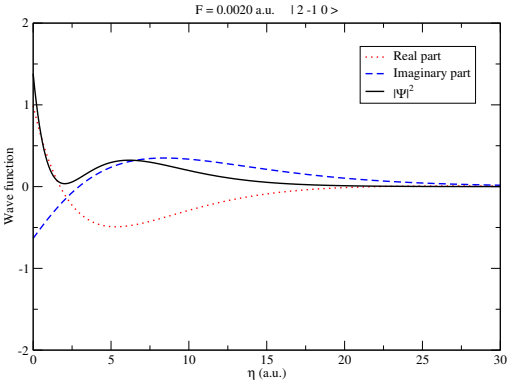
(d) $|\psi_{210}|^2(\xi,\eta)$



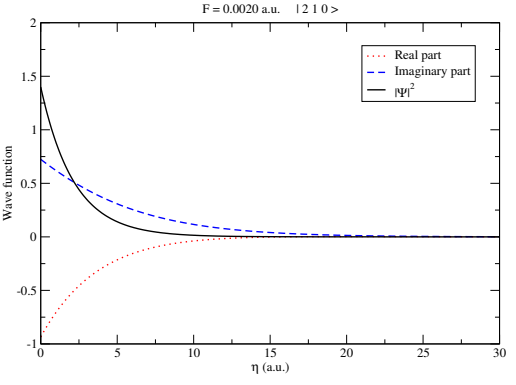
(b) $\psi_{\xi 2-10}(\xi)$



(e) $\psi_{\xi 210}(\xi)$

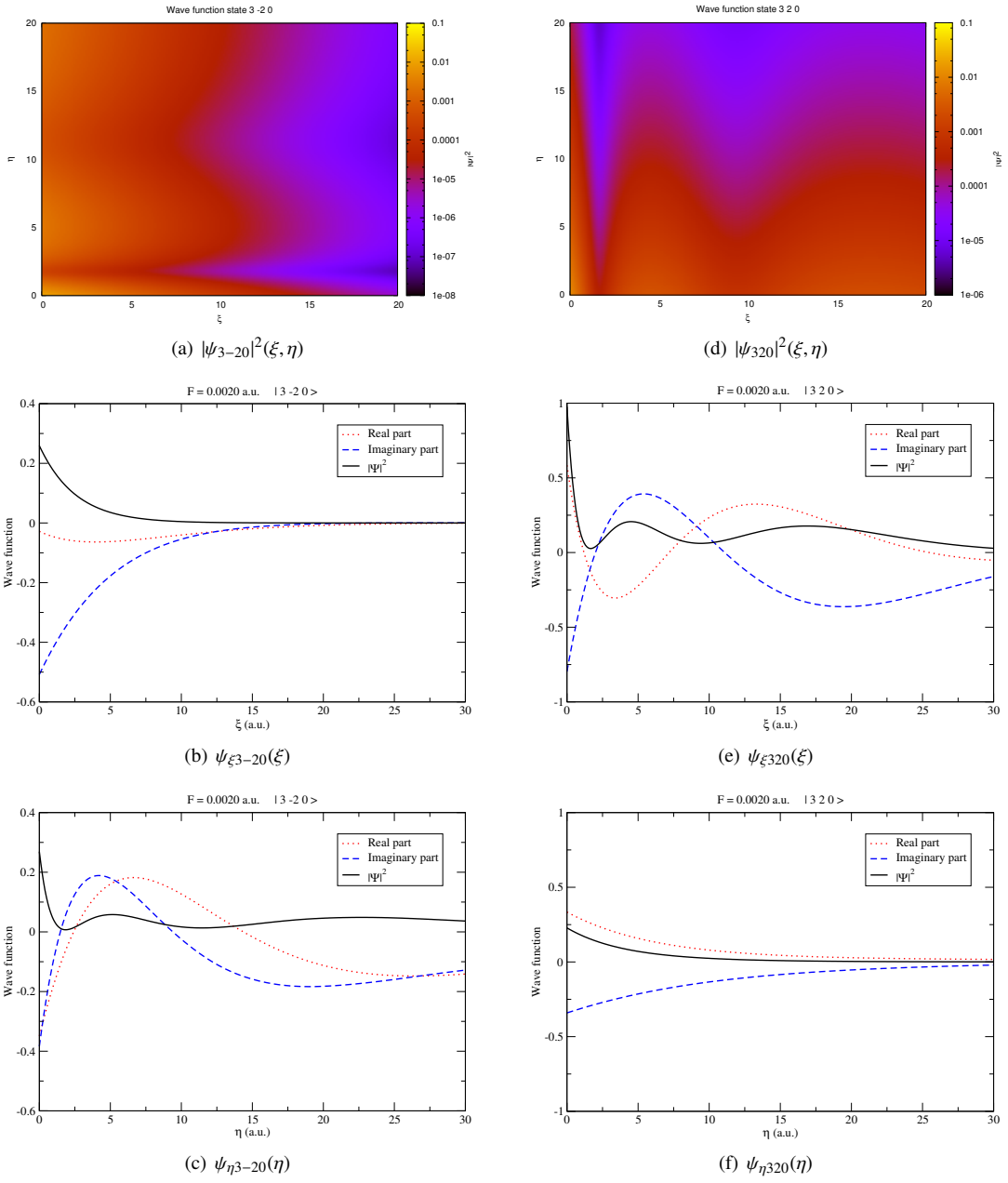


(c) $\psi_{\eta 2-10}(\eta)$



(f) $\psi_{\eta 210}(\eta)$

Figure 2.4: (Colour on line) Wave function of the Stark states $|2\ -1\,0\rangle$ and $|2\,1\,0\rangle$ for a field intensity of $F = 0.0020$ a.u..

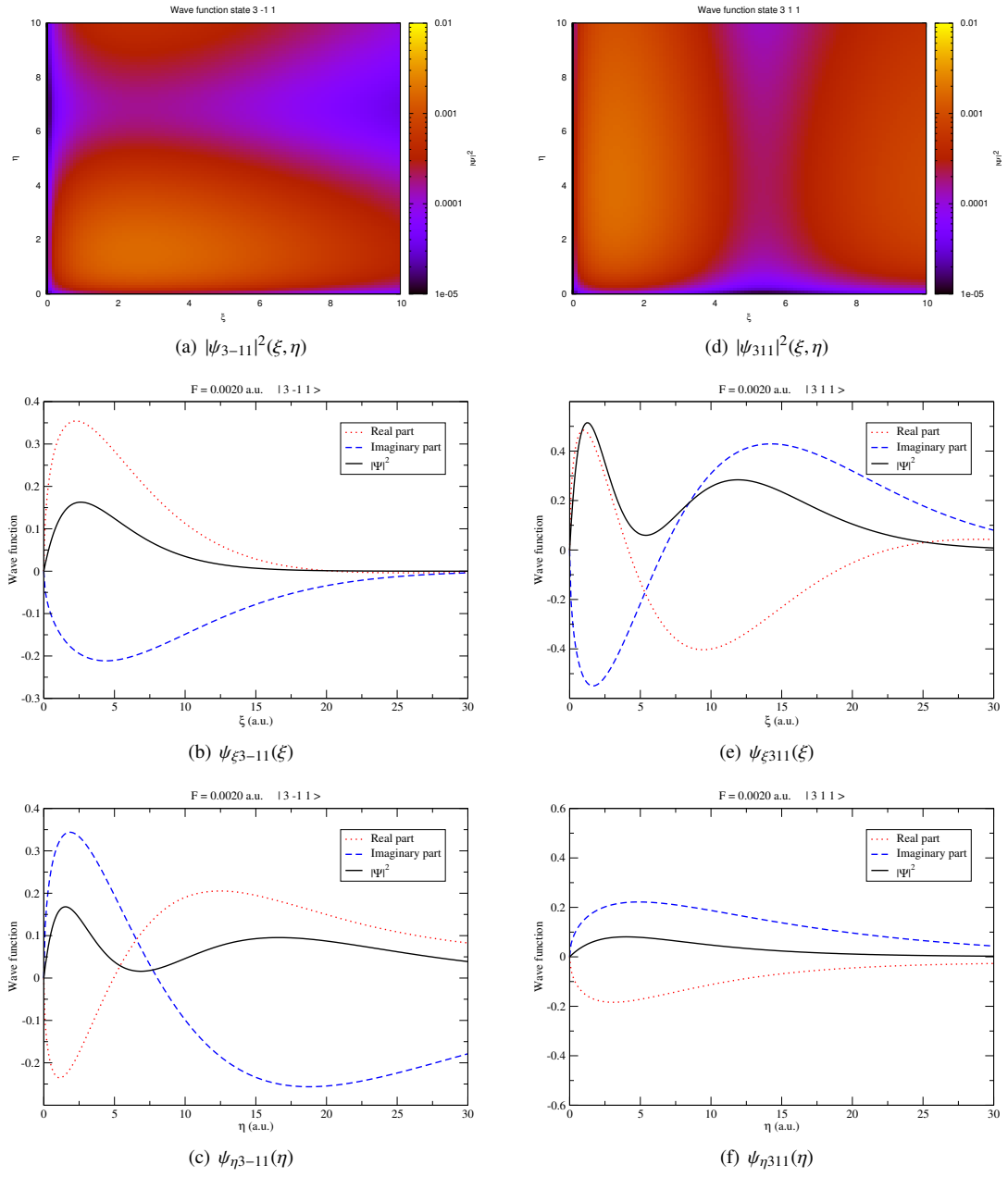


(a) $|\psi_{3-20}|^2(\xi,\eta)$ (d) $|\psi_{320}|^2(\xi,\eta)$

(b) $\psi_{\xi 3-20}(\xi)$ (e) $\psi_{\xi 320}(\xi)$

(c) $\psi_{\eta 3-20}(\eta)$ (f) $\psi_{\eta 320}(\eta)$

Figure 2.5: (Colour on line) Wave function of the Stark states $|3\ -2\,0\rangle$ and $|3\,2\,0\rangle$ for a field intensity of $F = 0.0020$ a.u..

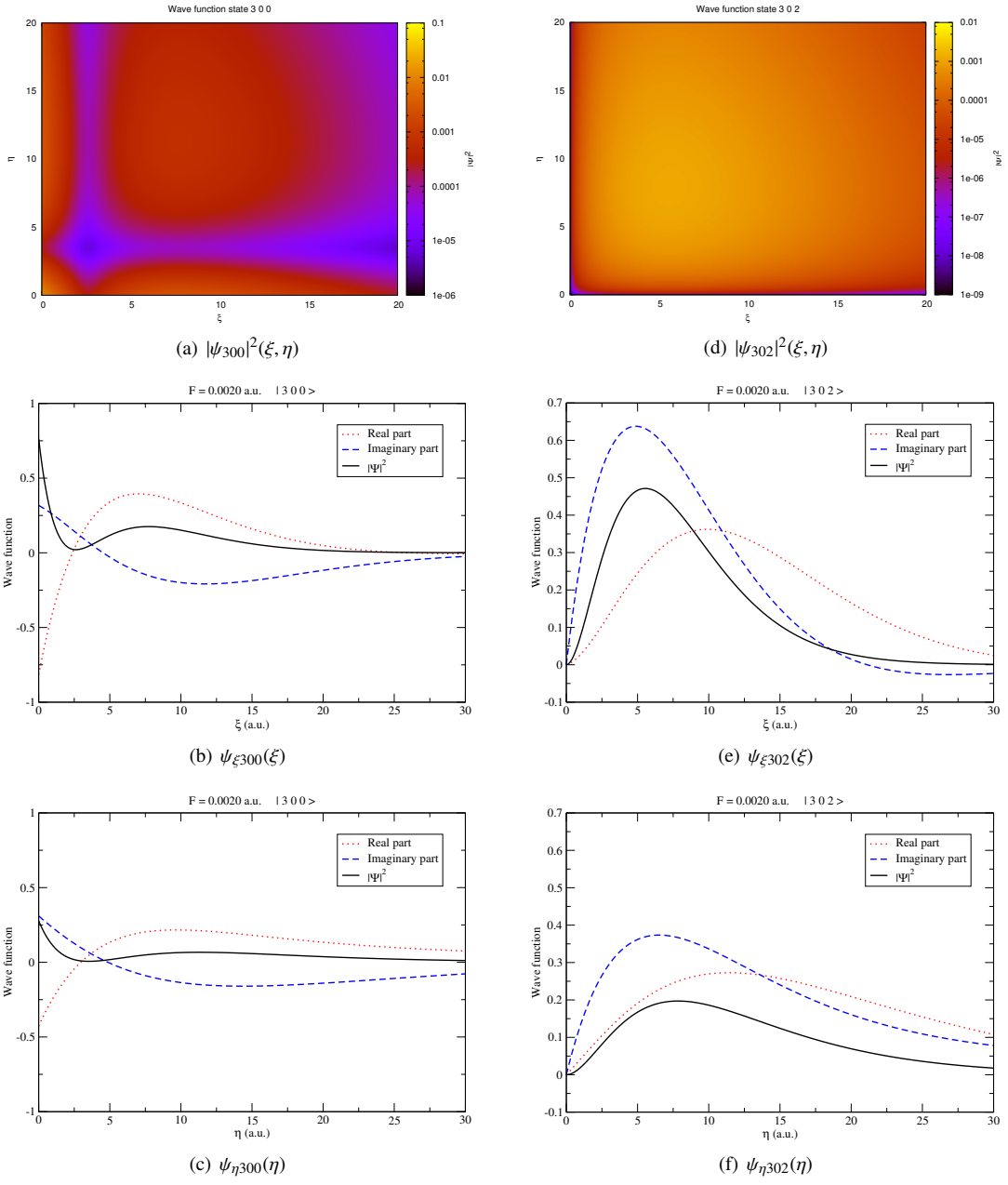


(a) $|\psi_{3-11}|^2(\xi,\eta)$ (d) $|\psi_{311}|^2(\xi,\eta)$

(b) $\psi_{\xi 3-11}(\xi)$ (e) $\psi_{\xi 311}(\xi)$

(c) $\psi_{\eta 3-11}(\eta)$ (f) $\psi_{\eta 311}(\eta)$

Figure 2.6: (Colour on line) Wave function of the Stark states $|3\ -1\,1\rangle$ and $|3\,1\,1\rangle$ for a field intensity of $F = 0.0020$ a.u..



(a) $|\psi_{300}|^2(\xi,\eta)$ (d) $|\psi_{302}|^2(\xi,\eta)$

(b) $\psi_{\xi 300}(\xi)$ (e) $\psi_{\xi 302}(\xi)$

(c) $\psi_{\eta 300}(\eta)$ (f) $\psi_{\eta 302}(\eta)$

Figure 2.7: (Colour on line) Wave function of the Stark states $|\,3\,0\,0\,\rangle$ and $|\,3\,0\,2\,\rangle$ for a field intensity of $F = 0.0020$ a.u..

2.3.2 Experimental measurements of Charge Exchange cross sections in ASDEX Upgrade (work packages 8-4)

The following work was conducted in collaboration with F. Guzmán, R. Mc Dermott, M. Sertoli, R. Dux.

In literature we can find two data sets for theoretical calculations of charge exchange cross sections for Ar^{18+}, Ar^{17+} and Ar^{16+}, for Oak Ridge National Lab [14] and from Universidad Autónoma de Madrid [15]. Both data strongly disagree, so it was proposed by F. Guzmán an experiment in ASDEX Upgrade to measure these cross sections. A comparison of data between soft X-rays and Charge Exchange Spectroscopy was used to determine the cross sections. For the data analysis it was used the code CHarge exchange tool for Impurity Concentration Analysis (CHICA) created by R. Mc Dermott and which read the data for beam charge exchange and thermal charge exchange cross sections prepared by L. F. Menchero.

2.3.3 Other activities (work packages 8-4, 9-1)

Determination of impurity concentration through Charge Exchange Spectroscopy

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

More data for Maxwell integrated thermal charge exchange were added to the data basis in order to be used by the code CHICA, for Ar^{18+}, B^{5+}, He^{2+}, Li^{3+}, C^{6+}, N^{7+}, Ne^{10+} with hydrogen in excited $n = 2$ state.

New files for charge exchange data (work packages 9-1)

Some data files stored in the ADAS data base for charge exchange cross sections *adf01* were improved. Data for argon *qcx#h0_ornl#ar18.dat* and *qcx#h0_uam#ar18.dat* and for nitrogen calculated by K. Igenbergs *qcx#h0_en2_aoc#n7.dat* were modified. The values for the calculated cross sections remained unchanged, and the modification remained in the values of the extrapolation parameters α for the capturing main quantum number n'.

$$\sigma(n') \;=\; \sigma(n_0)\left(\frac{n'}{n_0}\right)^{\alpha}, \tag{2.1}$$

where n_0 is the last shell tabulated. The method used was a linear regression of the cross sections of the last tabulated n' shells, preferred to the method used by ADAS up to the date, which was a simple quotient of the last two n' shells tabulated.

$$\log\sigma(n') \;=\; \log\sigma(n_0) \;+\; \alpha\,\log\left(\frac{n'}{n_0}\right), \tag{2.2}$$

taking n' between n_1 and n_0, tabulated data. The compromise remained in what values of n_1 to take for the regression, due to the tendency (2.1) fulfils only asymptotically and a value of n_1 too low will make not to reproduce this behaviour, and a quite large value of n_1, closed to n_0 will not give enough data. We tried several values of n_1 for each tabulated collision energy and we kept the lowest one such the obtained correlation coefficient had a reasonable value ($1 - r < 10^{-2}$). The values of α changed respect the old ones, and this led to a change in the effective emission coefficients *adf12*. New derived data files *adf12* were calculated with these new *adf01* files. These new data were used in the experiment of charge exchange cross sections of Ar and other impurity concentration works in ASDEX Upgrade [16].

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

26 Sep.-5 Oct. 2012	ADAS-EU course, CEA Cadarache, France: participated in the ADAS course lectures and tutorials.
24-26 Sept. 2012	ADAS Workshop, CEA Cadarache, France: presented talk ‘Motional Stark Effect models’.

2.3.5 Conference papers and published papers

K. Gál, G. Pautasso, K. Lackner, J. Neuhauser, M. Bernert, L. Fernández Menchero and ASDEX Upgrade Team. Simulations of the gas evolution during MGI. EPS-ICPP 2012 / Europhysics Conference Abstracts 36F, P-2086 (2012)

R. Dux, B. Geiger, R. M. Mc Dermott, L. Menchero, T. Pütterich, E. Viezzer and ASDEX Upgrade team. Impurity density determination using charge exchange and beam emission spectroscopy at ASDEX Upgrade EPS-ICPP 2012 / Europhysics Conference Abstracts 36F, P-2049 (2012)

F. J. Casson, C. Angioni, R. Dux, B. Geiger, R. M. Mc Dermott, L. Menchero, A. G. Peeters, C. Veth, and ASDEX Upgrade team Progress in the theoretical description and experimental characterisation of impurity transport in ASDEX Upgrade EPS-ICPP 2012 / Europhysics Conference Abstracts 36F, P-1080 (2012)

F. J. Casson, C. Angioni, R. Dux, B. Geiger, R. M. Mc Dermott, L. Menchero, A. G. Peeters, C. Veth, and ASDEX Upgrade team Progress in the theoretical description and experimental characterisation of impurity transport in ASDEX Upgrade [16]

L. Fernandez-Menchero and H. P. Summers. 'Stark effect in neutral hydrogen by direct integration of the Hamiltonian in parabolic coordinates' [13].

2.4 Hugh Summers

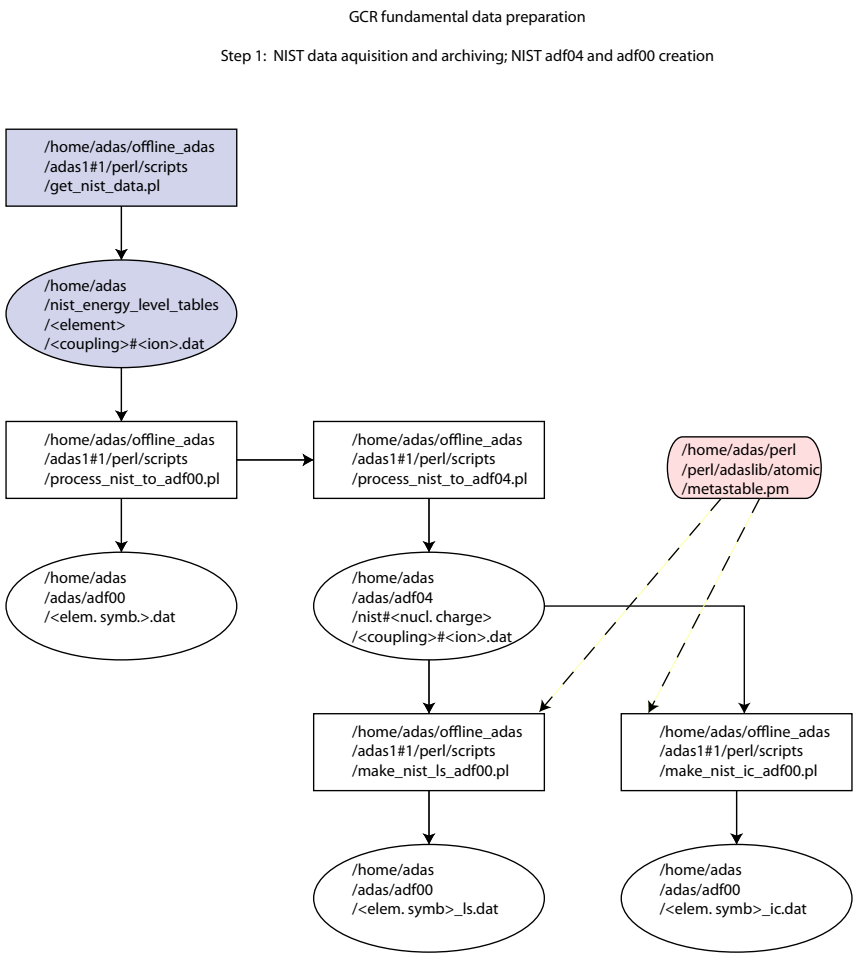
2.4.1 Acquistion of NIST energy level data for ADAS data refinement (work packages 27-1, 27-2)

The addition of the *GCR theme* to ADAS-EU and the associated increase in the precision of *adf04* data sets for medium-weight element collisional-radiative modelling requires a more systematic method for the refinement of level energies in the ADAS data bases.

Atomic structure codes, such as AUTOSTRUCTURE, do not achieve spectroscopic precision of energy level prediction. For this precision, which is essential for ionisation potentials, metastable energies and diagnostic spctrum lines, the National Institute of Standards, NIST, has for many years assembled all available reference information on energy levels. This key resource is drawn on by ADAS, when available, to revise lower precision calculated data. PERL scripts download NIST energy level tables for all ions of elements, archive them and strip out key data,namely, ionisation potentials, ground and metastable level configurations, outer quantum numbers and energies into the ADAS data format *adf00*. Other scripts strip out excited energy level data for reassembly in ADAS data format *adf04*. This first step, which comprises three parts, is shown schematically in figures 2.8, with the first part highlighted in blue. The elements are divided into three categories - light, medium-weight and heavy - as shown in these tables. Only selected elements in the medium-weight and heavy elements are handled, although light elements (up to zinc) are complete. Information is given at the foot of each schematic on how a user may execute the extraction. A PERL script library has been prepared which executes the various steps. Note that NIST *adf04* datasets comprise only the energy level list and do not contain transition data. Therefore they are not viable for population modelling by, for example, ADAS208. These data sets are used in a merging process with complete theoretical *adf04* datasets to adjust the theeoretical level energies to precise NIST values. The merging procedures are described later.

Script	Current location	Local checks		
		Txt	Opr	svn
nist_get_data.pl	/home/adas/offline_adas/adas1#1/	y	y	y
process_nist_to_adf00.pl	/home/adas/offline_adas/adas1#1/	y	y	y
process_nist_to_adf04.pl	/home/adas/offline_adas/adas1#1/	y	y	y
make_nist_ls_adf00.pl	/home/adas/offline_adas/adas1#1/	y	y	y
make_nist_ic_adf00.pl	/home/adas/offline_adas/adas1#1/	y	y	y

The next step is merging of two *adf04* specific ion datasets so that, for example, best energy level data can be chosen from one and collisional data from another. The principal case is NIST-derived *adf04* data set, as above, without col-



Notes: 1. *metastable.pm* defines the metastables for each isoelectronic sequence - complete to Fe-like
2. For g*et_nist_data.pl* execution, at the command line type:
nist_get_data.pl --nistroot=/home/<uid>/nist_energy_level_tables -- coupling=<coupling>
--userpostfix=<code> --element=<element name>
3. *<coupling>* is *ls* or *ic*. *<uid>* is *adas* for central ADAS production and no *userpostfix* is supplied
.

Figure 2.8:

lisional cross-section data and an automatically produced AUTOSTRUCTURE *adf04*. Such merging can be difficult due to missing levels and breakdown of quantum numbers in mixed configuration and intermediate coupling situations. A new merging alogorithm has been created to implement this. It executes a detailed analysis of each data set so that level group shifts can be evaluated and exploited in the matching. A further PERL script *process_merge_nist_adf04.pl* has been prepared which executes the merge step.

2.4.2 Using new hybrid dielectronic data for medium/heavy species (work package 28-2)

The extensions to AUTOSTRUCTURE to handle hybrid systems with metastable resolved parents and *n*-shell and *nl*-shell bundled recombined states has been put in place by Badnell. It is an key solution to the problem of the increasing size and complexity of state-selective dielectronic data for isoelectronic systems beyond Mg-like and can be consistent with detailed treatment of the near threshold resonances which matter for low temperature dielectronic recombination in photoionised astrophysical plasmas. We have found through the ADAS-EU sub-contract measurement of the DR crosss-ection for W^{+20} discussed in report SUBC1 that such low-lying resonances can have a very large and expected effect even at the high temperatures of electron excited plasmas. The bundling of the hybrid method condenses the

long resonance series in a manner tuned to generalised collisional-radiative population modelling, but still allows the restricted low level resonance analysis. This development is designed for medium/heavy species and produces *adf09* datasets of a slightly different format from before. The necessary re-writing of the acquisition routine *xxdata_09.for* has been completed. With the above developments of this subsection, the previous subsections and the *bbgp* methods summarised in the report SCIENCE7, a full infrastructure for extended generalised collisional-radiative modelling for intermediate weight species has been completed. Full details are in PUBL6.

Figure 2.9: Illustration of spectral comparison and adjustment of spectra for identification. The widget is self adjusting dependent on how many theoretical and experimental spectra are to be compared.

2.4.3 Diatomic rovibronic band emission modelling and display (work package 19-1, 19-2)

Whereas the vibronic collisional-radiative modelling of H_2 isotopomers satisfies the ADAS-EU work package requirements, it is only directly applicable to theoretical plasma modelling. Spectral diagnostic studies of molecules, which in practice are limited to homonuclear (especially H_2 isotopomers) and heteronuclear (especially CH and BeH isotopomers) diatomics require rotational emission predictions for comparision with observations. An additional capability, called ADAS908, has been constructed to allow simulation of complete rovibrational band structures and their comparison with experimental spectra. The rovibrational energies are obtained from parametric expansions supplemented by specific energy level data where available, held in ADAS data format *mdf02* in subdirectories */pickett* and */behr*. The *pickett* form is used for heternuclear diatomics with the data laid out in the manner required for the *CALCAT* code. The *behr* form is laid out in the manner adopted by Behringer and is used only for the H_2 isotopomers. The codes *run_pickett.pro* and *run_behr.pro* generate the required sets of rovibrational band wavelengths and relative spectral intensities. It is to be noted that rotational sub-populations are Boltzmann at some some effective rotational temperature. The effective temperature includes a correction for upward projection from the ground vibronic state based on Franck-Condon factors. There is no true rotational collisional-radiative model. The vibronic collisional-radiative populations are multipliers on the relative intensities obtained here. A further component of the *ADAS908* package is a theoretical/experimental comparator widget illustrated in figure 2.9.

2.4.4 Science evaluation meetings (work package 22-2)

Four working visits were arranged in the last two months of this period to examine and critically evaluate large code developments. These included the molecular H_2 vibronic collisional-radiative model and associated database carried out by Guzman. For this purpose there were two, two-week periods at EFDA-JET by Dr. Guzman, the second overlapping with a one-week visit by Prof. K Behringer as specialist is spectroscopy of molecular species in fusion plasma. The third working visit was by Menchero and concerned his new atomic model for the motional Stark modified hydrogen beam atoms. This advanced model, which is a direct solution of the Scrdoinger equation for the atom in a strong field, built on a complete basis of Laguerre state in parabolic coordinates, and using the complex rotation method for rsoance identification, gives the proper zero-prder solution and includes field ionisation consistently from the beginning. The fourth visit of one week, was by Dr. Palmeri coinciding with a visit by Prof. Badnell to investigate whether optimised Cowan atomic structure solutions prepared by the Mons-Hainaut team for ADAS-EU can be realised identically by AUTOSTRUCTURE. To achieve this would be an important prize, since it would allow us to lift the quality of collisional data entering the neutral and near-neutral heavy atom collisional-radiative modelling from plane-wave Born to distorted wave. These evaluations were overseen and coordinated by Prof. Summers.

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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