Atomic data for plasma modeling- Research projects at INFLPR

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Collaborators:

- ITM-TF AMNS (many labs.);
- QUB (P.G. Burke, V. M. Burke, M .P .Scott, A. Hibbert);
- LIXAM (A. Klisnick);

INTRODUCTION

- **The primary motivation is to provide accurate atomic data for**:
- ➢ *Fusion research ;*
- ➢ *Astrophysics*
- **Atomic processes under investigation:**
- ➢ *Electron impact excitation: Forbidden transitions*
- ➢ *Dielectronic recombination*
- ➢ *Proton impact excitation*
- **Theoretical methods and numerical codes:**
- ➢ *Plane wave Born (PWB) from GOS*
- ➢ *Perturbative: the Coulomb-Green's function for excited states*
- ➢ *Non-perturbative (non-relativistic (RMATRxx), semi-relativistic(BPRM), and full relativistic(DARC))*
- ➢ *Non –perturbative R-matrix Floquet (RMF)*
- ➢ *Cowan's suite code for heavy ions*
- **Collisional radiative calculation (ADAS)**

ATOMIC STRUCTURE CALCULATION

1) MODEL POTENTIAL

a) Bates and Damgaard approximation. (Apostol I et al., 1995, *Rom. J. Phys*. **40** 723-732)

b) the computer program SUPERSTRUCTURE (*Eissner et al 1974*) which uses a scaled Thomas-Fermi-Dirac-Amandi potential. (Stancalie et al., *Laser and Particle Beams 2006*)

c) Including CI in Multi-Configuration Hartree-Fock (MCHF) (*Frose Fischer, 1969*), or in the superposition of configurations method (Hibbert, 1975) (CIV3)(Stancalie et al. *Phys. Scr. 1999,2000, 2011*)

2) The R-MATRIX METHOD –*(Burke and Berrington, 1993)*

3) GRASP – *relativistic (Norrington , Grant 1987)*

4) **Hartree-Fock-Slater scheme** *(Cowan, 1981)*

SCATTERING CALCULATION

$$\Omega = \sum_{l=0}^{\infty} \Omega_l$$

At lower impact energies, it is very difficult to compare the different theoretical results as the most sophisticated R-matrix results have large resonance structures below many of excitation thresholds. Their effect are seen by comparing excitation rates.

a) **PERTURBATIVE APPROACH** (*Poirier, Semoune 1998)*

b) **NON-PERTURBATIVE (RMATXII, DARC, BPRM)**

FIRST-ORDER PERTURBATIVE CALCULATION IN A *SINGLE-CONFIGURATION* APPROACH for Be-like ions

- *Heisenberg approximation for He, Be-like ions* $[He]n_2l_2j_2n_1l_1$
- *A single configuration description assuming that, the Rydberg electron evolves from a bound hydrogenic state* (n_1l_1) *to a continuum state* (εl) *while, the valence electron falls from the excited state* $(n_2l_2j_2)$ *to a lower* $(n_0l_0j_0)$*;*

$$[\gamma]n_2l_2j_2n_1l_1 \longrightarrow [\gamma]n_0l_0j_0n_sl_s$$

- $H_C = H_0 + V \quad H_0 = p_0^2/2 + U(r_0) + p_s^2/2 - 1/r_s$ and $V = 1/r_0 - 1/r_s$
- $(\Omega - H_C)\, G(\Omega) = 1$ where Ω is a complex energy variable, G is the CGF

- *Nonpenetration hypothesis*

$$\left[\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} - \frac{l(l+1)}{r^2} - x^2\right]S_{n,l,x}(r) = -2nx\frac{1}{r}S_{n,l,x}(r)$$

$$S_{n,l,x}(r) = N_{n,l}(x)\exp(-xr)(2xr)^l L_{n-l-1}^{2l+1}(2xr)$$

Effective oscillator strength

$$f_{eff} = \frac{f_{eff}\,(n_1)}{n_1}$$

$$f_{eff}(n_1) = \frac{2m}{3\hbar e^2}\cdot\frac{E_s}{2J\ \ +1}\sum_{n_0,l_0,j_0,l_s}\sum_{n_s}\left|\langle n_2l_2j_2|r_2|n_0l_0j_0\rangle\right|^2\left|\left(\int_0^\infty drR(n_1l_1;r)S(k_s,n_sl_s;r)\right)\right|^2$$

'averaged excitation energy', *E*s, is given by: $E_s = E_{n_2l_2j_2} - E_{n_0l_0j_0} - 1/2n_1^2$

Preprint EFDA-JET-CP(05)02-49 *Stancalie and JET EFDA Contributors*

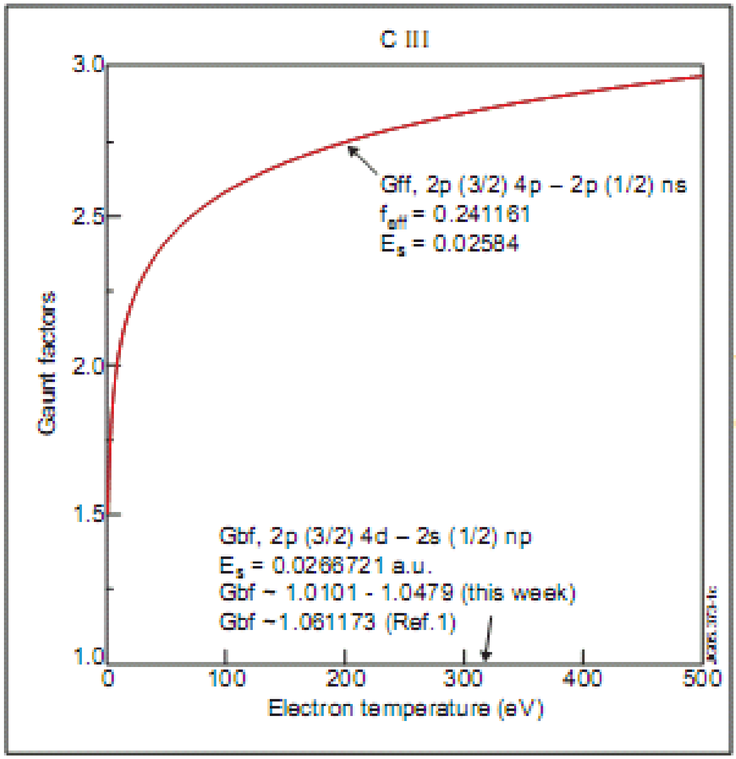


Figure 1: Bound-free (Gbf) and free-free (Gff) Gaunt factor in C^{2+}. Effective oscillator strengths averaged over continuum, f_{eff} and photon energy, E_s, in atomic units (a.u.), are given next to the curves.

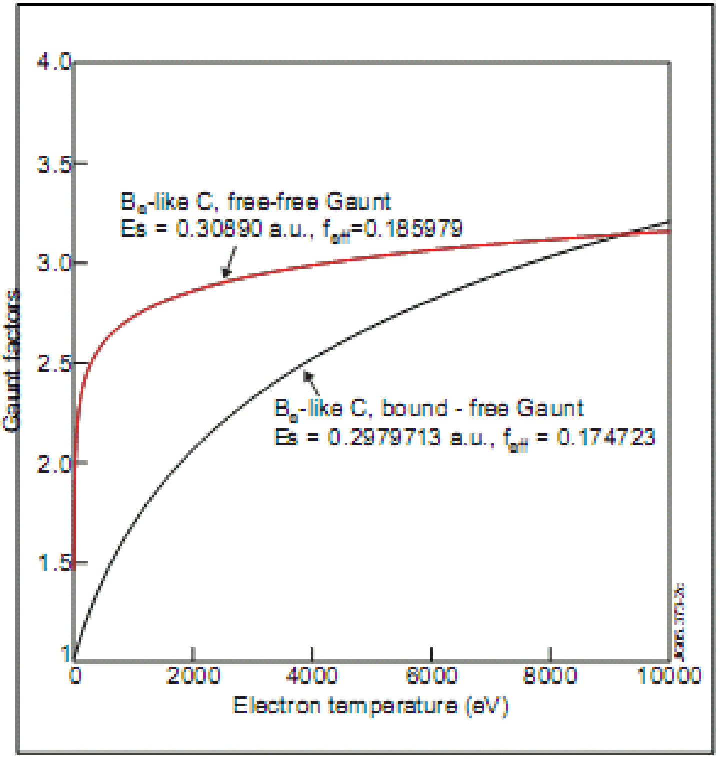
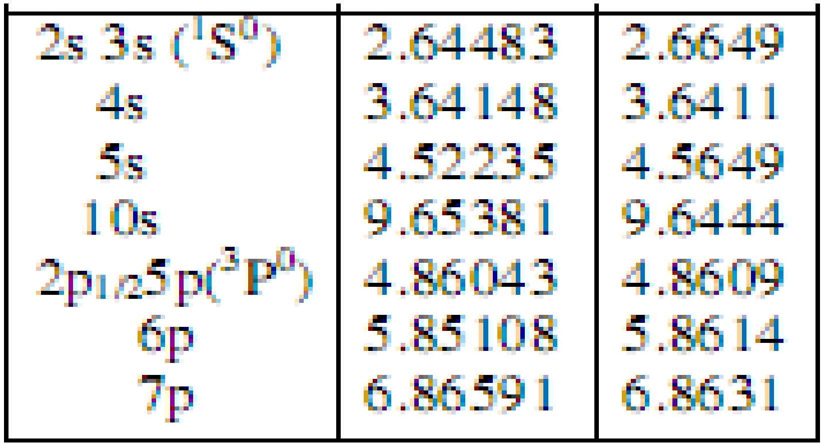


Figure 2: Gaunt factors for C^{2+} at given photon energy, E_s, in atomic units, versus T_e in eV.

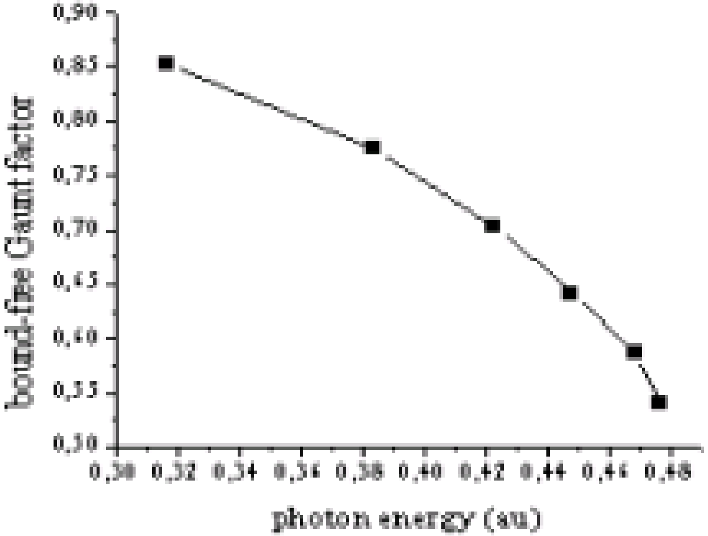
$$G = 1 + f_{eff} \ln\left|1 + \frac{E4Ry}{\chi_1}\right| \qquad \chi_1 = Ry / n_1^2 \qquad Ry = 13.6eV$$

Effective quantum numbers: perturbative and non-perturbative (Berrington et al, Phys Scr.1998) calculation (C 2+)



2s 3s ($^1S^0$)	2.64483	2.6649
4s	3.64148	3.6411
5s	4.52235	4.5649
10s	9.65381	9.6444
$2p_{1/2}5p(^3P^0)$	4.86043	4.8609
6p	5.85108	5.8614
7p	6.86591	6.8631

Fig. 1. Bound-free Gaunt factor for $1s^22p_{3/2}3p$-$1s^22p_{3/2}ns$ series



Autoionization

$$\Gamma = 2\pi \sum_{n_0 l_0 j_0 l} \left| A_1 + A_2 \right|^2$$

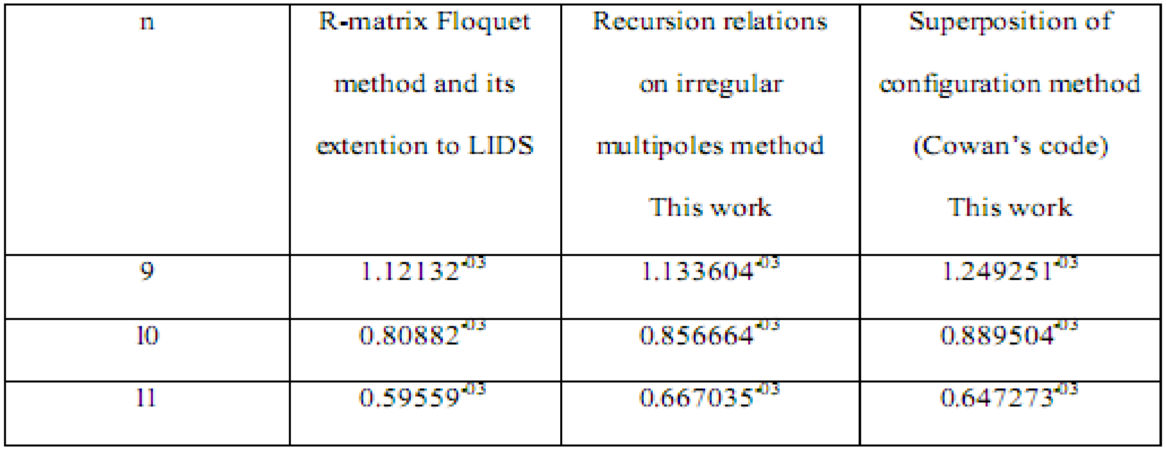
$$A_1 = \sum_{t \geq l} \Omega\left(l_2, j_2, l_1; l_0, j_0, l; k; t\right) \times \left\langle n_2 l_2 j_2 \middle| r^t \middle| n_0 l_0 j_0 \right\rangle \left\langle n_1 l_1 \middle| r^{-t-1} \middle| \varepsilon l \right\rangle$$

$$A_2 = \sum_{n_p l_p j_p l_s} \sum_{l_1 \geq 1 l_2 \geq 1} \left\langle n_2 l_2 j_2 \middle| r^{t_1} \middle| n_p l_p j_p \right\rangle \left\langle n_p l_p j_p \middle| r^{t_2} \middle| n_0 l_0 j_0 \right\rangle$$

$$\times \Omega\left(l_2, j_2, l_1; l_p j_p, l_s; k; t_1\right) \times \Omega\left(l_p, j_p, l_s; l_0, j_0, l; k; t_2\right) \times \sum \int_\nu \left\langle n_1 l_1 \middle| r^{-t_1-1} \middle| \nu l_s \right\rangle \frac{1}{E_s - E(\nu)} \left\langle \nu l_s \middle| r^{-t_2-1} \middle| \varepsilon l \right\rangle$$

$$E_s = E_{n_2 l_2 j_2} - \frac{\varsigma^2}{2n_1^2} - E_{n_p l_p j_p}$$

type $1s^2 2pns(^1P^0)$, n = 9 -11, in Al^{10+}. (*a^{-b} reads $a \times 10^{-b}$*).



n	R-matrix Floquet method and its extention to LIDS	Recursion relations on irregular multipoles method This work	Superposition of configuration method (Cowan's code) This work
9	1.12132^{-03}	1.133604^{-03}	1.249251^{-03}
10	0.80882^{-03}	0.856664^{-03}	0.889504^{-03}
11	0.59559^{-03}	0.667035^{-03}	0.647273^{-03}

Stancalie, Laser and Particle Beams, 2009

OLD WORKS on DR

- **Prior to 1990, theory and experiments did not agree for the gain values in X-ray lasers with Li-like ions**

➢ *Influence of dielectronic recombination on gain of X-ray lasers with Li-like ions (Stancalie et al. , 1995 IOP Conf Ser 140): semi-classical*

- **Prior to 2000, no satisfactory mathematical and physical formulation in the case of damping effect on DR**

$$\varepsilon_{nl} \rightarrow \varepsilon_{nl} - \frac{i}{2}\sum_{f} \Gamma_{i \rightarrow f}$$

➢ *GOS calculation in Li-like Al (Stancalie V., Burke V.M., Sureau A. Phys Scr.1999)*

➢ *Fine-structure atomic data using RMATXI (Stancalie,Phys Scr. 2000)*

- **New formalism has been proposed** *(Stancalie V, Burke P.G., Burke V.M., Conf on Xray lasers, J. Phys.IV 2000) for non-perturbative treatment of DR*
- **Working ions: Li-like Al and C ions**

RECENT WORKS on DR and AUTOIONIZATION

Ab initio NON-PERTURBATIVE TREATMENT

- **Consequently we have developed new model calculation that retains the essential ingredients of the full R-matrix Floquet theory, namely, a bound state coupled nonperturbatively by the field to an autoionizing state and to the continuum**

(*Stancalie V, Physics of Plasmas* ***12****(2005)043301,12(2005)100705*).

$$e^- + X^{Z}\,(1s^2 2s(^2S^e)) \Leftrightarrow X^{(Z-1)+**}(1s^2 2p n'l') \rightarrow$$
$$X^{(Z-1)+*}(1s^2 2s\, n'l') + h\nu$$

- **Structure using CIV3**
- **Scattering: R-matrix**
- **Damping effect : Floquet method**
- **Results: LIDS positions, and rates**

Resonant single-photon ionization in Li-like ions

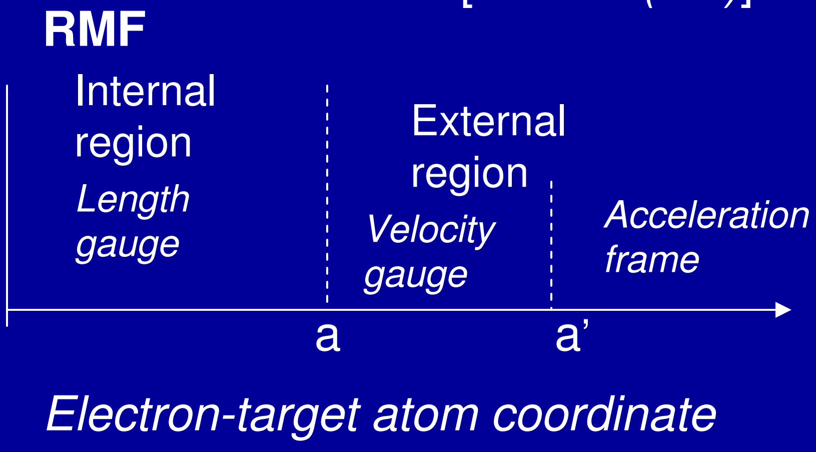
$X^{Z+}[1s^2 2s(^2S^e)] + e^-$

↓↑

$X^{(Z-1)**}[1s^2 2pn'l](^1P^0)$

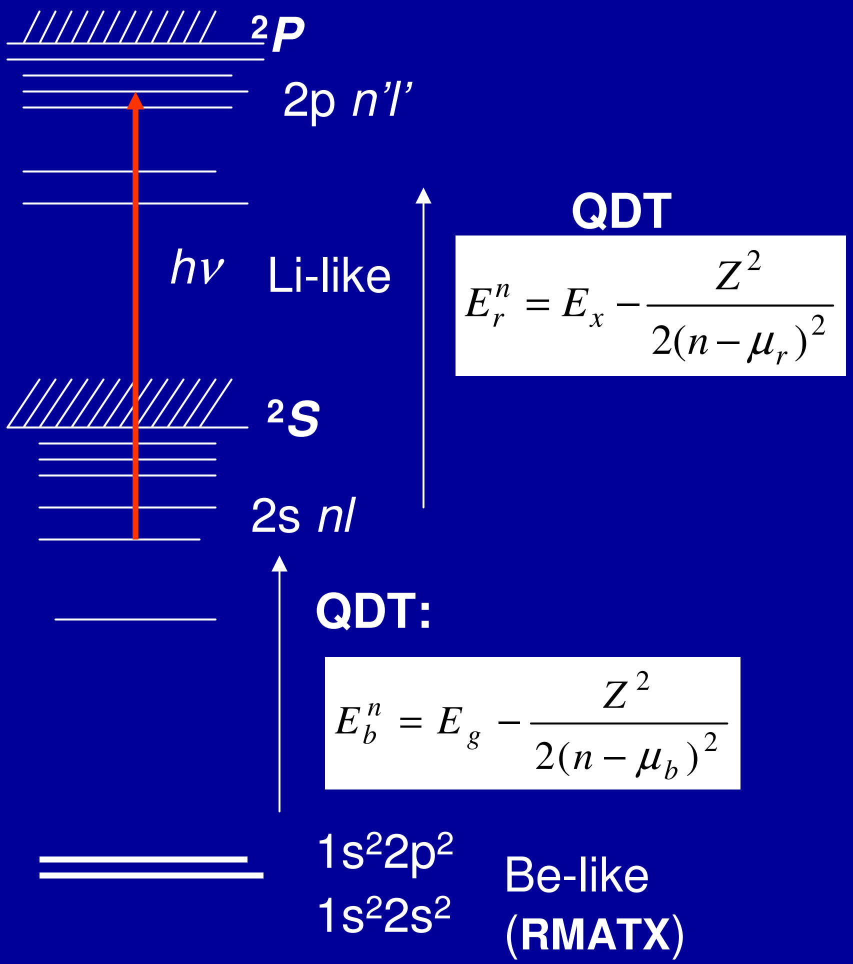
$h\nu$ ↓ ↑ I, ω

$X^{(Z-1)*}[1s^2 2sn'l(^1S^0)]$



RMF

Electron-target atom coordinate



QDT

$$E_r^n = E_x - \frac{Z^2}{2(n-\mu_r)^2}$$

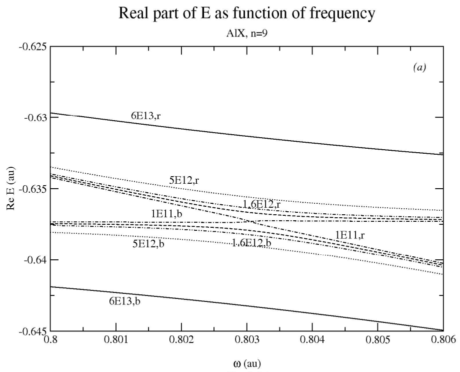
QDT:

$$E_b^n = E_g - \frac{Z^2}{2(n-\mu_b)^2}$$

The resulting complex energies: LIDS structures in C^{2+}

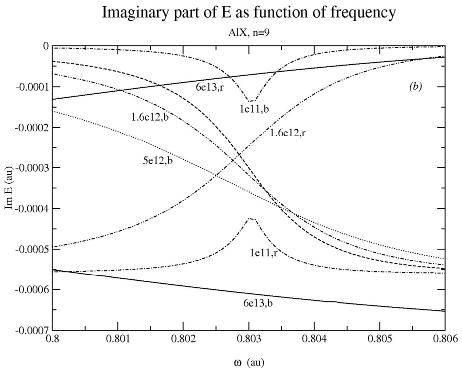
$$2E_{1,2} = E_a + E_g - \omega - i(\Gamma_a + I\gamma)/2 \pm \Omega$$

$$\Omega = \{[d - i(\Gamma_a - I\gamma)/2]^2 + \Gamma_a I\gamma[q-i]^2\}^{1/2}$$


Real part of E as function of frequency

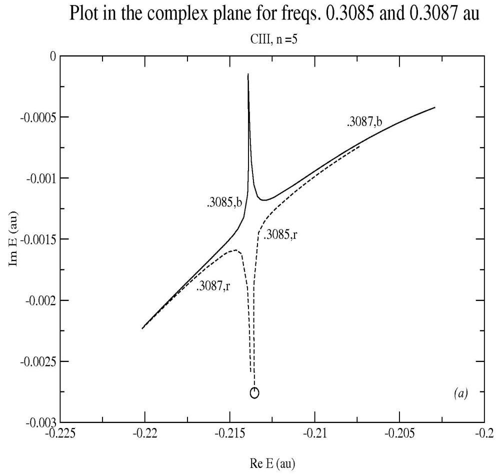
AlX, n=9

Fig. 3 *(a)*


Imaginary part of E as function of frequency

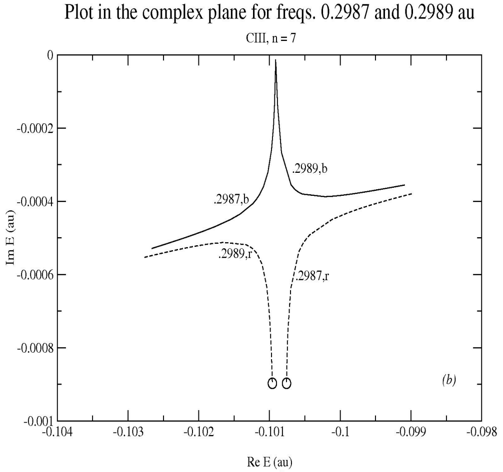
AlX, n=9

Fig. 3 *(b)*


Plot in the complex plane for freqs. 0.3085 and 0.3087 au

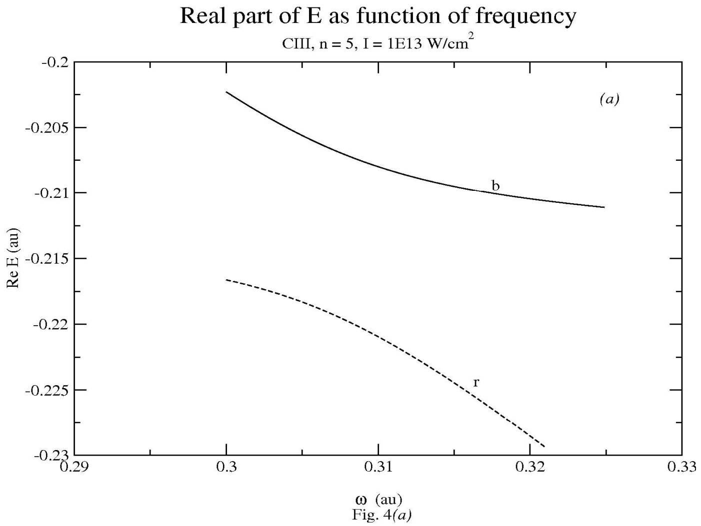
CIII, n =5

Fig. 2*(a)*


Plot in the complex plane for freqs. 0.2987 and 0.2989 au

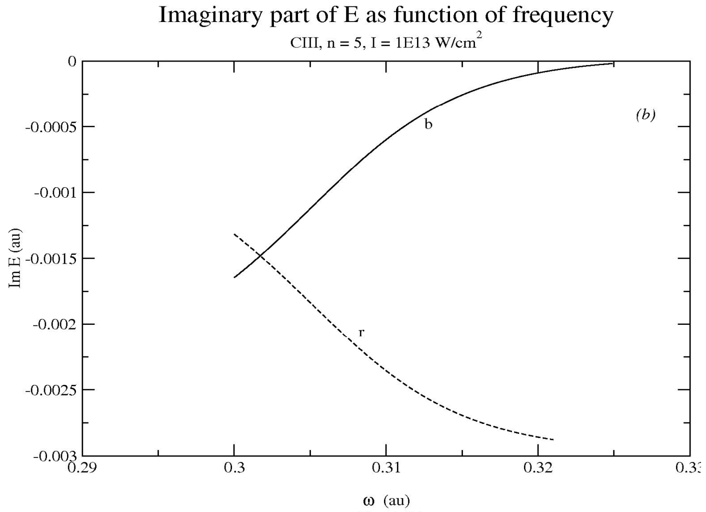
CIII, n = 7

Fig. 2 *(b)*


Real part of E as function of frequency

CIII, n = 5, I = 1E13 W/cm^2

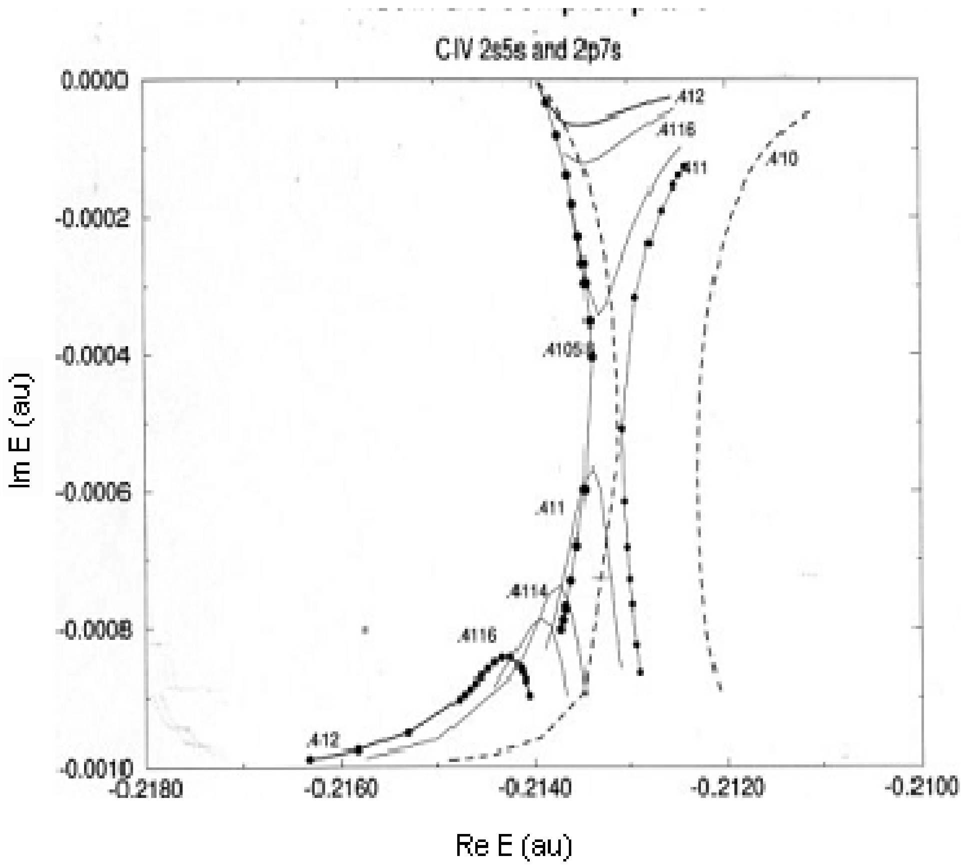
Fig. 4*(a)*


Imaginary part of E as function of frequency

CIII, n = 5, I = 1E13 W/cm^2

Fig. 4 *(b)*

First theoretical demonstration of $\Delta n = 2$ radiative transition



	E_b(au)		E_a(au)
n	This work	OP	
5	-.21394	-.21518	.09496
6	-.13801	-.13849	.15984
7	-.10091	-.10106	.19794
8	-.07656	-.07664	.22221
9	-.06001	-.060059	.23861
10	-.04828	-.0483	.25021
11	-.03967	-.03967	.25872
12	-.03317	-.03315	.26514

Position and width of doubly excited states

n	*d* (au)	ω_{LIDS} (au)	Re(E_{LIDS}) (au)	Im(E_{LIDS}) (au)	Γ (meV)
5	0.30890	0.3086	-0.21385	-0.001362	148.1856
6	0.29785	0.2977	-0.1379	-0.0007165	77.9552
7	0.29885	0.2988	-0.1009	-0.00045	48.96
8	0.29877	0.2988	-0.07660	-0.000299	32.5312
9	0.29862	0.2986	-0.06000	-0.000210	22.848
10	0.29849	0.2985	-0.0483	-0.000145	15.776
11	0.29839	0.2984	-0.0397	-0.000108	11.7504
12	0.29831	0.2983	-0.03318	-0.0000905	9.8464

Scaling with n

n	I_{LIDS}(W/cm^2)	$n^{*3}Ei(LIDS)$
5	*5.5 10^{11}*	*0.17*
6	*1.9 10^{11}*	*0.15*
7	*0.9 10^{11}*	*0.15*
8	*0.4 10^{11}*	*0.15*
9	*0.25 10^{11}*	*0.15*
10	*0.2 10^{11}*	*0.15*
11	*0.04 10^{11}*	*0.14*
12	*0.07 10^{11}*	*0.16*

Comparison

n	Γ^a (meV) (*Stancalie 2005*) *RMF results*	Γ^a (meV) *Berrington, K., Pelan, J., Quigley, L., Physica Scripta 57 (1998) 549 – 555) RMAT*
5	150	138
6	81	74
7	49	44
8	32	28
9	21.8	19
10	15.6	-
11	11.6	-
12	8.8	-

Consequences of LIDS

- trapping of population at some non zero field intensity; Population transfer from the excited to autoionizing state

Scaling for the Lithium isoelectronic sequence

1) Effect of the target being a highly charged ion is that of **Z^2** scaled energies and therefore frequencies;

2) Imaginary part of LIDS energy varies as **$1/n^3$**;

3) Autoionization probability shows a Z dependence for *n =9-12:*

Γ^a (AlX)/Γ^a (CIII)= $(11/4)^{0.333}$= **1.4** which is the ratio of the nuclear charge screened by the 1s electrons, at power 1/3

3) Radiative width in channel *n* shows usually scaled Z relation

$$B^n = \frac{\Gamma^{r,n}}{\Gamma^{a,n}}$$

STUDY OF OPACITY EFFECTS ON HYDROGEN (H-α and Ly-β) and Li-LIKE OXYGEN EMISSION LINES

ADAS package

- We have investigated the influence of opacity on hydrogen (H-α and Ly-β) and Li-like oxygen emission lines from the RFP EXTRAP T2R plasma *(Stancalie & Rachlew, Phys.Scr.2002)*
- Simulation of the total radiated power [Y.Corre, et.al., Phys.Scr.71(2005)]

Atomic structure calculation.

ADAS yields atomic data for Li-like O based on a 41-state RMPS calculation that includes 9 spectroscopic terms of the configurations $1s^2nl$ (n=2-4) and the 32 pseudo states $1s^2nl$ (n =5 -12, l = 0-3) in close coupling expansion.

Collisional radiative calculation (ADAS)

Opacity calculation using escape factor approximation (ADAS)

Concluding remarks and future plans

- A general formulation of DR process, including damping effect in a consistent way, has been developed. These data are to be compared with existing experimental measurements for Li-like ions and $\Delta n = 0, 2$ transitions rate.
- The inclusion of negative energy resonances in the general program of DR for plasma modeling
- The use of full relativistic Dirac-Atomic R-matrix Code for radiative and autoionization rates for atomic carbon and its ions.
- A special attention will be paid to perturbative approach in describing autoionization from high Rydberg states with large angular momentum
- The accuracy of atomic data: Calculated energy separations; Comparison between length and velocity forms of the oscillator strength;Fine-tuning energy levels; Convergence of results;