Spectroscopic studies of highly ionized plasmas: statistical approach for atomic transitions calculations

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Plan

Purpose : study of radiative properties in plasmas
through spectroscopic methods

- **Better understanding of astrophysical explorations**, eg :
  Sun : measurement of iron opacity for stellar interior energy transport calculations (cf : *"Nature" 517, 56-59.* 2014)
- **Success on the path toward fusion energy**, eg :
  MCF : spectroscopic investigations of tungsten (W) as divertor
  (cf : *"Tungsten as a plasma facing material in fusion devices"* 2003)
  ICF : enhancement of plasma diagnostics and target design
  (cf : *"Atomic physics in Inertial Confinement Fusion"* 1998)

Why ? –> How ?

Bound-bound emission spectrum : $I(E) = \sum_{ab} I_{ab}$

I_{ab}=electron's jump between 2 energy-levels= $N_a \cdot A_{ab} \cdot E_{ab}$

where N_a= upper energy-level population (LTE=Saha-Boltzmann),

A_{ab}=dielectronic E1 transition rate, $E_{ab} = \mid E_a - E_b \mid$

Detailed level accounting : accurate ; inconvenient (highly ionized plasmas)

Atoms : several ionization stages and many open electronic sub-shells.

- spectra contain huge quantity of lines => computation time : long ;
- lines gathering in coalescing structures => high resolution : useless.

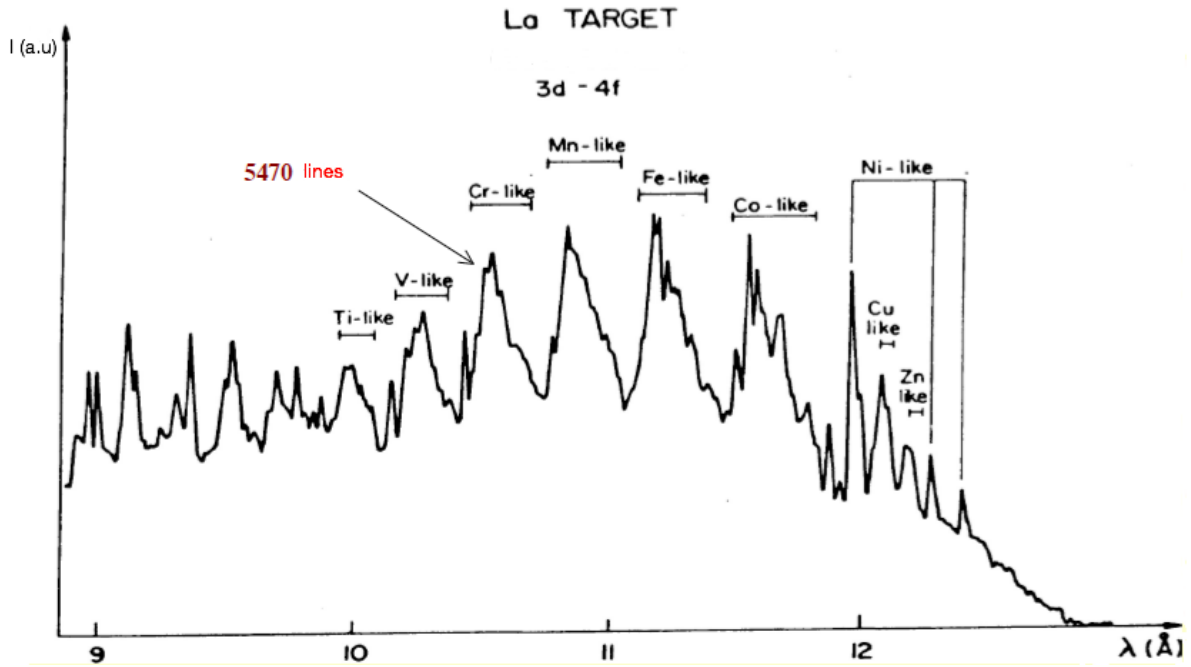
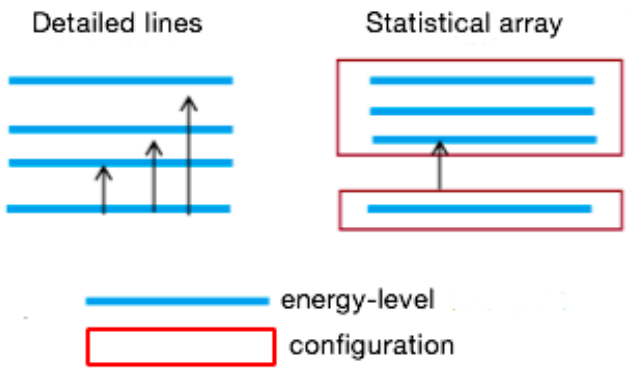


Figure : *Experimental Lanthanum (Z=75) spectrum : transition* $3d \rightarrow 4f$

Idea : regroup spectral *lines*, (i.e.$a \rightarrow b$) into transition *array*, (i.e.$C \rightarrow C'$)



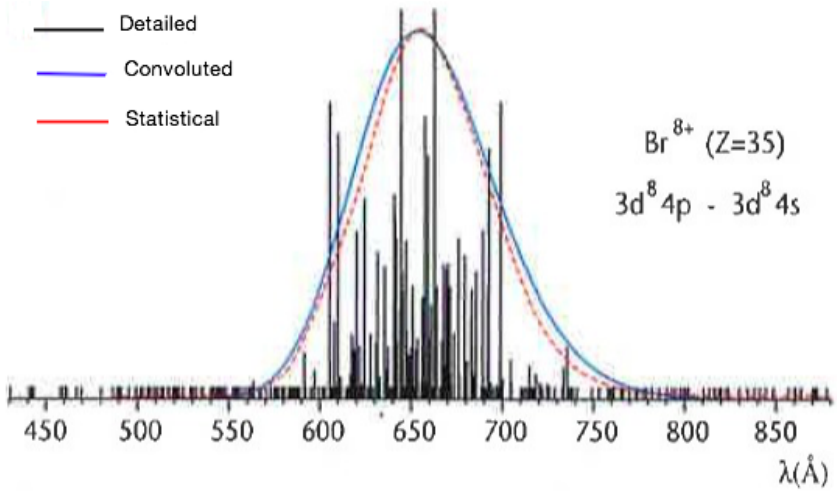


Figure : *(cf. "Chocs" Bauche et al. 2008)*

Comments on spectrum of $3d^8 4p \rightarrow 3d^8 4s$ array :

- Detailed lines $\not\Rightarrow$ provide directly global features (eg : central position, FWHM, etc) –> need convolution for identification
- Very good agreement between detailed-convoluted spectrum and statistical one => reliability of statistical calculation

Simulation results of statistical arrays by the *Flexible Atomic Code*

Number of levels and transitions between detailed and statistical calculations :

Output FAC	Lev-D	Trans-D	Lev-S	Trans-S
Account	61	359	9	6

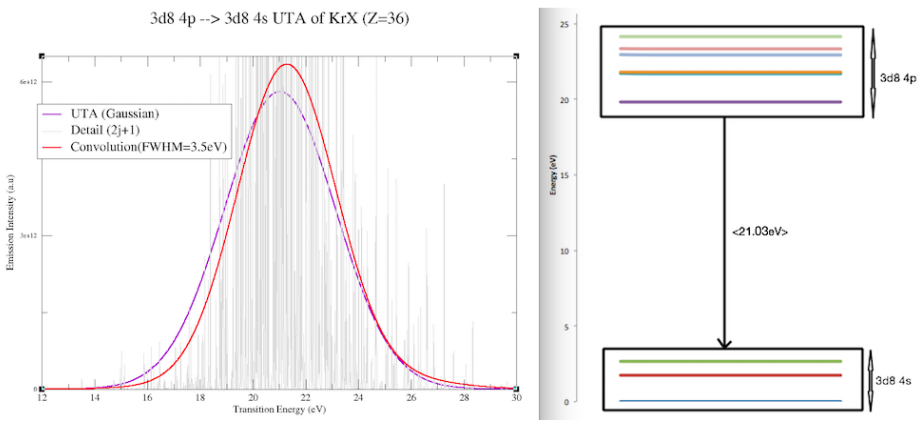


Figure : Transition array in Krypton (Z=36) plasma : electrostatic interaction dominates over spin-orbit interaction

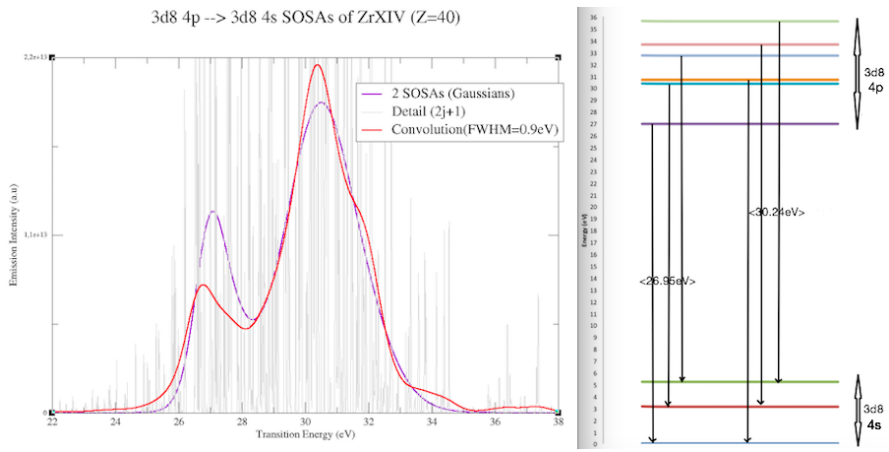


Figure : Spin-orbit split in Zirconium (Z=40) plasma into 2 sub-arrays : $3d^2 4p_{1/2} \rightarrow 3d^2 4s$; $3d^2 4p_{3/2} \rightarrow 3d^2 4s$.

Theoretical model to build up transition arrays

Statistical configuration average procedure

- *Theory of transition array* : consider a line spectrum as a *distribution*, characterized by a set of distribution moments :

$$\mu_n(C - C') = \sum_{mm'} \frac{(< m' \mid H \mid m' > - < m \mid H \mid m >)^n \cdot w_{mm'}}{W} \quad (1)$$

  - where the sum runs over all states m, m' of configurations C, C' respectively ;
  - $m - m'$ E1-transition strength : $w_{mm'} =< m \mid D \mid m' >^2$, the whole array transition strength : $W = \sum_{mm'} w_{mm'}$.
- Then, the spectrum is directly represented by a Gaussian curve : n=1 : average energy ; n=2 : FWHM.

Objective : To access global features directly, dispensing with detailed accounting

Self-critical summary

Regarding to the *Flexible Atomic Code* :

- Take knowledge of numerous option choices –> edit input files
- Use output data –> write post-processor

but, what's inside the script ?

Work forward

- Gain insight into the *theory of transition array* ($\langle m|H|m\rangle$ calculations in the 1st and 2nd quantization formalisms)
- Implement further statistical options in the Flexible Atomic Code
- Compare spectra from statistical simulations to experimental ones

Thanks for your attention !