Ab initio Determination of Atomic Structure and Stark broadening Parameters : Pb IV and recent results

R. Hamdi[1], N. Ben Nessib[1], M. S. Dimitrijević[2,3] and S. Sahal-Bréchot[3]

[1] Groupe de Recherche en Physique Atomique et Astrophysique, Institut National des Sciences Appliquées et de Technologie, Centre Urbain Nord B. P. No. 676, 1080 Tunis Cedex, Université de Carthage

[2] Astronomical observatory, Volgina 7, 11160 Belgrade 74

[3] Laboratoire d'Etude du Rayonnement et de la Matière en Astrophysique, UMR CNRS 8112, Observatoire de Paris-Meudon, 92195 Meudon

Introduction

- Ab initio calculation of energy levels and radiative parameters → no other data are taken from other sources.
- - Hartree-Fock with relativistic correction (Cowan 1981)

  - Scaled Thomas-Fermi potential: SUPERSTRUCTURE code (Eissner et al. 1974)

  - Fully relativistic calculation based on MCDF : GRASP code (Grant et al. 1981)
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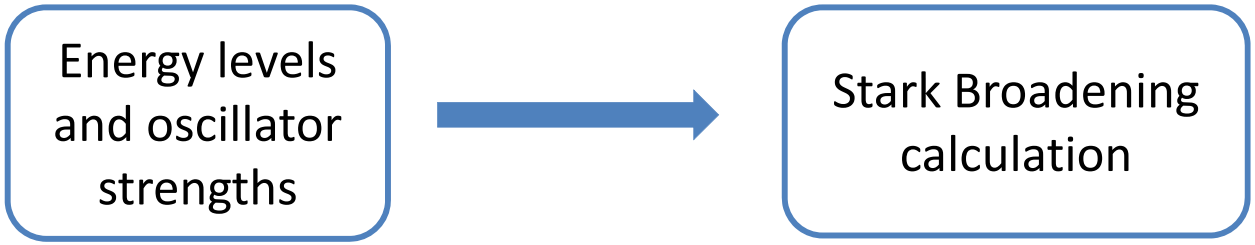


Ab initio calculation of Stark broadening parameters: atomic data are not taken from other sources

- The lack of atomic data makes Stark Broadening determination impossible
- Semiclassical perturbation method (SCP) (Sahal-Bréchot 1969 a,b) need a large set of atomic data
- Ab initio Stark broadening parameters determination: Large number of ions and transitions
- STARK-B:- database for calculated widths and shifts for isolated lines

  - devoted to modelling and spectroscopic diagnostics of stellar atmospheres and also for laboratory plasmas

- SUPESTRUCTURE code + SCP method → Si V, Ne V, Ca V
- HFR + SCP method → Pb IV

Ab initio determination of atomic data

- SUPERSTRUCTURE Code (Eissner et al. 1974)

- The wavefunctions are of configuration mixing type, and each configuration is expanded in terms of Slater states.

- P_{nl} are calculated in scaled Thomas-Fermi statistical potential $V(\lambda_l)$

- Nussbaumer & Storey (1978) : each P_{nl} is calculated in separate potential $V(\lambda_{nl})$

- Parameters λ_{nl} are determined variationally by optimizing the weighted sum of energy terms.

- Relativistic effects: Breit-Pauli Hamiltonian

$$H_{BP} = H_{nr} + H_{rc}$$

- Cowan Code (Cowan 1981)

  - RCN : single configuration radial wavefunctions

  - RCN2: multiple-configuration radial integrals, dipole integrals and Bessel integrals

  - RCG: angular factors, radiative data and collision strengths

- For electric dipole transition:

$$gf = \frac{8\pi mca_0^2\sigma}{3h} S \qquad \text{where} \qquad \sigma = \frac{|E(\gamma') - E(\gamma)|}{hc}$$

Electric dipole line strength

$$S = \left| \left\langle \gamma J \left\| P^{(1)} \right\| \gamma' J' \right\rangle \right|^2$$

- In order to calculate *gf*, we have to compute the corresponding line strength, we expand the wavefunctions $|\gamma J\rangle$ in terms of a suitable set of bases functions $|\beta J\rangle$

$$|\gamma J\rangle = \sum_{\beta} Y^{\gamma}_{\beta J} |\beta J\rangle \qquad S^{1/2}_{\gamma\gamma'} = \sum_{\beta}\sum_{\beta'} Y^{\gamma}_{\beta\beta'} \left\langle \beta J \left\| P^{(1)} \right\| \beta' J' \right\rangle Y^{\gamma'}_{\beta' J'}$$

Ab initio determination of Stark Broadening parameters

- Semi-classical perturbation approach (Sahal-Bréchot 1969 a,b) based on the founding work by Baranger (1958a,b,c) of the theory of collisional line broadening in impact approximation.

- Impact approximation: the interaction are separated in time: the duration of an interaction must be much smaller than the mean time interval between two collisions. ➡ The effect of perturbers are independent and are additive.

- Isolated lines: we are interested in "isolated lines" and exclude the case of "overlapping lines"

- The profile is Lorentzian with a FWHM

$$W = N\int vf(v)dv\left(\sum_{i'\neq i}\sigma_{ii'}(v)+\sum_{f'\neq f}\sigma_{ff'}(v)+\sigma_{el}(v)\right)$$

σ_{el} represents the contribution of elastic collisions and include Feshbach resonance when ion-electron are studied.

Ab initio SCP Stark prameters for Si V

- In Ben Nessib et al. (2004) : Stark Broadening parameters were calculated for 16 Si V multiplets.

  - Energy levels and oscillator strengths were calculated using SST code

  - Atomic model : $2s^2 2p^6, 2s^2 2p^5 3\ell, 2s2p^6 3\ell, 2s^2 2p^5 4\ell \ (\ell \leq n-1)$

  - Mean radii and mean square radii: hydrogenic approximation

  - Results were obtained for collisions with electrons and compared with values calculated with Bates & Damgaard (1949) approximation oscillator strengths.

  - The average ratio of W_{BD} and W_{sst} is 1.10

  - Proton-, ionized helium- and Si II- broadening parameters were also given.

Ab initio SCP Stark prameters for Ne V

- In Hamdi et al. (2007) Stark broadening parameters were calculated for 26 multiplets of Ne V.
- Atomic data were determined using SST code as modified by Nussbaumer & Storey (1978)

- scaling parameters depend on both quantum numbers *n* and ℓ

- Atomic model : 17 configurations

$$2s^2 2p^2,\ 2s2p^3,\ 2p^4,\ 2s^2 2p\ 3\ell$$

$$2s2p^2 3\ell,\ 2s^2 2p\ 4\ell,\ 2s2p^2 4\ell\ (\ell \le n-1)$$

Transition	T (K)	w_{SST} (Å)	d_{SST} (Å)	w_{BD} (Å)	d_{BD} (Å)
Ne v $2P$–$3S$, 173.0 Å, $C = 0.88$E+18	50,000.0	0.992E−04	0.283E−05	0.935E−04	0.449E−05
	100,000.0	0.680E−04	0.559E−05	0.664E−04	0.610E−05
	150,000.0	0.570E−04	0.633E−05	0.557E−04	0.661E−05
	200,000.0	0.507E−04	0.678E−05	0.497E−04	0.709E−05
	300,000.0	0.435E−04	0.695E−05	0.427E−04	0.729E−05
	500,000.0	0.365E−04	0.667E−05	0.359E−04	0.701E−05
Ne v $2P$–$3D$, 150.6 Å, $C = 0.55$E+18.....	50,000.0	0.874E−04	−0.283E−05	0.903E−04	−0.165E−05
	100,000.0	0.625E−04	−0.786E−06	0.653E−04	−0.101E−06
	150,000.0	0.521E−04	−0.459E−06	0.546E−04	0.133E−06
	200,000.0	0.460E−04	−0.708E−06	0.482E−04	−0.162E−06
	300,000.0	0.389E−04	−0.713E−06	0.409E−04	−0.103E−06
	500,000.0	0.320E−04	−0.414E−06	0.339E−04	0.325E−06

- $N = 10^{17}$ cm^{-3}
- Comparison between Stark widths obtained using SST oscillator strengths and Bates and Damgaard approximation oscillator strengths show that the difference is tolerable.

  ⟹ The set of oscillator strength obtained using Bates and Damgaard approximation may then be useful for Stark Broadening calculations when more reliable data are not available
- For shifts disagreements are larger: for shifts important contributions have different signs, leading to mutual concellations.

Comparison with values from Uzelac et al. (1993)

Transition	W_m (Å)	W_m/W_G	W_m/W_{DK}	W_m/W_{HB}	W_m/W_{SC}
$3s\ ^3P^o - 3p\ ^3D$, 2265.7 Å.....	0.64	1.28	1.71	1.32	1.16

- N=2.85 10^{18}cm^{-3}, T = 298,000 K
- W_m : experimental Stark width,

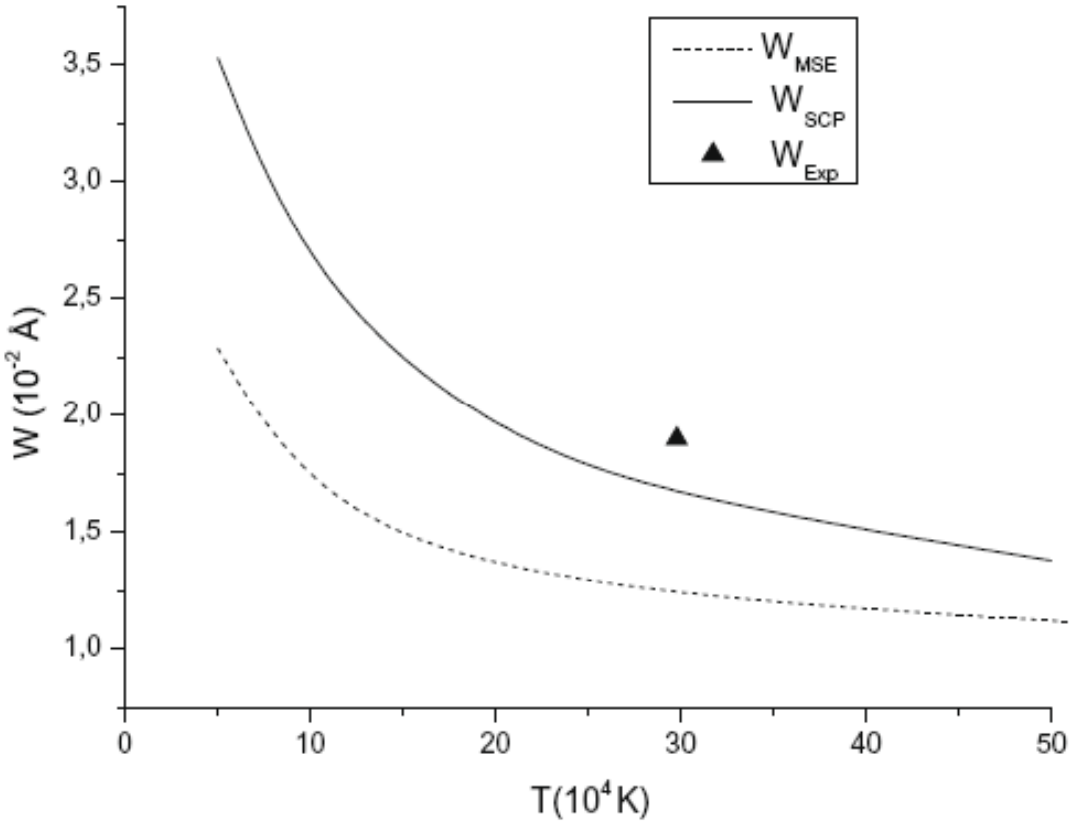
  W_G: Stark width calculated using approximate semiclassical method (Griem 1974)

  W_{DK}: Stark width calculated using modified semiempirical formula (Dimitrijević & Konjević 1980)

  W_{HB}: Stark width calculated using classical path approximation (Hey & Breger 1980)

  W_{SC}: our ab initio Stark width

Stark widths for the 3s $^3P^0$- 3p ^3D multiplet as a function of temperature
$N = 10^{17}$ cm^{-3}



- (Dot line): MSE approach from Dimitrijević (1993)
- (Solid line): ab initio SCP approach (Hamdi at al. 2007)
- Calculation were compared with experimental values from Uzelac et al. (1993)

Ab initio Stark broadening parameters of Ca V (Hamdi et al. 2010)

- Calcium is an important element in astrophysics
  - Calcium lines are detected in the atmospheres of white dwarfs (Zuckerman et al. 2003)
  - Calcium in high ionization stage (Ca X) is observed in photospheres of the hot white dwarf KPD 0005+5106 (Werner et al. 2008)
- Ab initio Stark broadening parameters were computed for 8 Ca V lines using SST atomic data.

Transition	T(kK)	w_e	d_e	w_{H^+}	d_{H^+}	w_{He^+}	d_{He^+}
$3p^4\ ^3P\text{-}3s3p^5\ ^3P^\circ$	50.	0.19E-2	-0.28E-3	0.76E-5	-0.95E-5	0.14E-4	-0.94E-5
694.6 Å	100.	0.14E-2	-0.17E-3	0.20E-4	-0.18E-4	0.30E-4	-0.18E-4
C= 0.69E+20	150.	0.11E-2	-0.14E-3	0.30E-4	-0.26E-4	0.42E-4	-0.24E-4
	200.	0.95E-3	-0.14E-3	0.40E-4	-0.31E-4	0.49E-4	-0.28E-4
	300.	0.78E-3	-0.12E-3	0.51E-4	-0.39E-4	0.61E-4	-0.34E-4
	500.	0.62E-3	-0.11E-3	0.70E-4	-0.50E-4	0.72E-4	-0.42E-4

Ab initio Stark broadening parameters of Pb IV

- Triply ionized Lead Pb IV belong to gold isoelectronic sequence

  - Pb IV is a candidate for spectroscopic detection in hot DA white dwarfs (Vennes et al. 2005)

  - O'Toole (2004) reported the discovery of strong photospheric resonance lines of several heavy elements in the UV spectra of more than two dozen sdB and sdOB stars at temperature ranging from 22000 K up to 40 000 K. Among these lines, several correspond to Pb IV ones.

- **HFR + SCP:** ⟹ several lines of the type $5d^{10}$ nl – $5d^{10}$ n'l'

- Atomic model: 43 configurations

$5d^96s^2$, $5d^96p^2$, $5d^{10}ns$ ($6\leq n\leq 11$), $5d^{10}nd$ ($6\leq n\leq 11$), $5d^{10}ng$ ($5\leq n\leq 11$), $5d^96s7s$, $5d^96s6d$ (even parity)
and $5d^{10}np$ ($6\leq n\leq 11$), $5d^{10}nf$ ($5\leq n\leq 11$), $5d^{10}nh$ ($6\leq n\leq 11$), $5d^96s6p$ (odd parity).

$Transition$	$T(kK)$	W_e	d_e	W_{H+}	d_{H+}	W_{He+}	d_{He+}
	20	0.66E-02	-0.85E-04	0.31E-03	-0.24E-04	0.39E-03	-0.23E-04
$6s\ ^2S_{1/2} - \ 8p\ ^2P_{3/2}$	30	0.58E-02	-0.39E-04	0.39E-03	-0.34E-04	0.47E-03	-0.32E-04
$\lambda = 385,5$ Å	50	0.51E-02	-0.53E-04	0.48E-03	-0.51E-04	0.52E-03	-0.45E-04
C= 0.20E+19	100	0.45E-02	-0.32E-04	0.55E-03	-0.72E-04	0.59E-03	-0.62E-04
	200	0.41E-02	-0.29E-04	0.61E-03	-0.91E-04	0.64E-03	-0.75E-04
	400	0.37E-02	-0.35E-04	0.65E-03	-0.11E-03	0.66E-03	-0.89E-04

- Such temperatures are of interest for sdB and sdBO subdwarfs and hot white dwarfs
- We also specify the parameter *C.* We can consider the line as isolated up to perturber density equal to *C/W*
- $V \times N << 1$: the impact approximation is valid.

  - when the impact approximation is not valid, the ion broadening may be estimated using the quasistatic approach

  - In the region where neither approximation is valid, a unified-type theory should be used

Conclusions

- Ab initio determination of Stark broadening parameters allows us to overcome the probleme of lack of atomic data.

- our study of the Pb IV ion will be continued: a comparison between different methods will be made (SC – SE –MSE), and also comparison with other works (theoretical and experimental)

THANK YOU FOR ATTENTION