Comparisons and comments on electron and ion impact profiles of spectral lines

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- Radiators : neutral atoms and ions
- <u>Collisions</u> with electrons and positive ions: *the so-called "STARK broadening"*
- Isolated lines
- What is the purpose ?

•Present: Understandable use of Stark broadening data and of the database STARK-B

•Future : STARK-C (numerical code on line) : to know how to use it (not a blackbox)

STARK-B: <u>http://stark-b.obspm.fr</u>





STARK-B

Database for "Stark" broadening of isolated lines of atoms and ions in the impact approximation http:/stark-b.obspm.fr

•SCP theory updated and operated by M.S. Dimitrijević and

S. Sahal-Bréchot

•Calculated widths and shifts: more than 140 pubs (1984-2010)

•STARK B currently developed at Paris Observatory

•the database has been opened since September 2008: 90% of the data are currently implemented

- It is a part of the atomic and molecular databases of the Paris Observatory
- Link to SerVO Serbian Virtual Observatory

•And is a part of VAMDC- Virtual Atomic and Molecular Data Centre

Scientific objectives:

Spectroscopic diagnostics, Modelling Synthetic spectra

Addresses

Astrophysics Virtual Observatories (Europe: IVOA International Virtual Observatory Alliance) Laboratory plasmas Technological plasmas







http://www.ivoa.net

VAMD

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based on the founding papers by Baranger (1958) in the impact approximation

Impact approximation

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•Collisions between radiators and perturbers act independently and are additive



Fig. 1. Full halfwidths for the K(I) 4s²S-4p²P⁰ multiplet ($\lambda = 7676.2$ Å) as a function of electron temperature; $N_e = 10^{17}$ cm⁻³. Experimental points: +, Puric *et al.* (Ref. [6]). Calculations: BG, Benett and Griem (Ref. [4]); O, Mazure and Nollez (Ref. [5]); DSB₁, present calculations (with impact ionbroadening); DSB, present calculations (quasistatic ion broadening)

> Dimitrijević & Sahal-Bréchot. **JQSRT 1987**

The impact approximation is valid if th duration of a collision or

Collision time $\rho_{typ}/v \ll$ mean interval between collisions ΔT , *i.e.*

 $\rho_{\rm tvp}/{
m v} << \Delta {
m T}$

- ρ_{typ} typical impact parameter
- typical relative velocity
- ΔT inverse of the half-width in angular frequency units: $\Delta T \approx 1/N v \sigma$

cross-section $\sigma \approx \pi \rho_{tvp}^2$ σ

$\rho_{\rm typ} << N^{-1/3}$

 $N^{-1/3} = 2 \ 10^4 \ a_0 \ at \ 10^{12} cm^{-3}$ $N^{-1/3} = 2 \ 10^3 \ a_0^{\circ} \ at \ 10^{15} \text{cm}^{-3}$ $N^{-1/3} = 200 a_0^{\circ} at 10^{18} cm^{-3}$

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H+e (low n) : $\rho_{typ} \sim 100 a_0$ H+H⁺ (low n): $\rho_{typ} \sim 2000 a_0$ al +e $\rho_{typ} \sim 10 a_0$ and more if perturbing levels are close to the levels of the studied transition Metal +e $\rho_{\rm typ}$ ~ 100 a₀ Metal +H⁺ $\rho_{\rm typ} \sim 20 \ a_0$ H or Metal+H:



based on the founding papers by Baranger (1958) in the impact approximation

Impact approximation

•Collisions between radiators and perturbers act independently and are additive

Complete collision approximation

The atom has no time to emit or absorb a photon during the collision process, the collision is not broken off

<u>Validity:</u> Collision time << inverse of the time interval between two emission (or absorption) of photons

 $\rho_{\rm typ}/{\rm v}$ << 1/ $\Delta\omega\,$ (beyond the half-width)

 $\Delta \omega$ = detuning

N.B. In the **far wings**, the atom emits photons before the perturber has any time to move: The process is **quasistatic**

⇒The effect of the perturbers are additive, and the line broadening theory becomes an application of the theory of collisions





based on the founding papers by Baranger (1958) in the impact approximation

Impact approximation

•Collisions between radiators and perturbers act independently and are additive

Complete collision approximation

Isolated lines

•Neighbouring levels do not overlap

The levels of the transition *i*-f broadened by collisions do not overlap with the neighbouring perturbing levels i' f'



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





based on the founding papers by Baranger (1958) in the impact approximation

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⇒ LORENTZ PROFILE:
•width and shift ARE NOT INTRINSIC DATA
•Depend on the medium (density, temperature)







based on the founding papers by Baranger (1958) in the impact approximation

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 ⇒ LORENTZ PROFILE:
 width and shift ARE NOT INTRINSIC DATA

•Depend on the medium (density, temperature)

•Fine structure (hyperfine) components of a multiplet

The fine (hyperfine) structure can be neglected during the collision with electrons and protons

i.e. The spin (S or I) has no time to rotate (Larmor precession) during the collision). The fine structure (hyperfine) components have the same width, that of the multiplet

•N.B.: the components must be taken into account and added for interpreting the spectra if the splitting is not negligible: - case of Mn II lines (Popović et al. NAR 2008) -case of Hydrogen lines (Stehlé & Feautrier JphysB 1985, Stehlé JPhysB 1985)







based on the founding papers by Baranger (1958) in the impact approximation

Impact approximation •Collisions between radiators and perturbers act independently and are additive Complete collision approximation Isolated lines Neighbouring levels do not overlap \Rightarrow I ORENTZ PROFILE: width and shift ARE NOT INTRINSIC DATA •**Depend on the medium** (density, temperature) •Fine structure (hyperfine) components of a multiplet Interactions with charged particles Debye screening effect (at high densities) $\delta = (\phi_p^2 + \phi_q^2)^{1/2}$

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Methods of calculations of the cross-sections σ (or scattering S-matrix) -1

- Semi-classical : atom = quantum description (atomic structure), perturber= particle moving on a classical path
- + perturbation theory for the collisional transition probabilities
 - →SCP (Sahal-Bréchot, A&A1970 and further papers, 6-8 basic papers) accuracy: 20%, sometimes better, sometimes worse
 - unitarity and symmetrization of the S-matrix, adequate cut-offs
 - hyperbolae for ion-electron and ion-ion (1970),
 - complex atoms (1974), very complex (2008)
 - Feshbach resonances for ion-electron collisions (1977)
 - Updated and operated with MS. Dimitrijevic (1984 and after)
- Modified Semi-Empirical : atom = simplified quantum description (MSE)
 - $-\Rightarrow$ Dimitrijevic and colleagues, JQSRT1980 and further A&A papers)

• Quantum description in intermediate coupling: especially adapted to highly charged ions and resonance lines (Sahal-Bréchot with Elabidi & Ben Nessib (2004 and after, an also with Dubau and Cornille 2007 and after)

• **SST** (Superstructure) + **DW** (Distorted wave)





Methods of calculations of the cross-sections (i.e. scattering S-matrix) -2

Atomic structure

- Coulomb approximation with quantum defect (Bates & Damgaard 1949)
- TOPbase (R-matrix in LS coupling)
- Cowan code (HFS multi-conf with exchange and relativistic effects (by perturbations)
- SUPERSTRUCTURE (scaled Thomas-Fermi-Dirac-Amaldi potential + relativistic effects (Breit-Pauli))

Ab initio calculations

- Atomic structure coupled to the S-matrix calculation: no external data insertion
 - Interest for calculating a great number of lines (100 and more) in the SCP picture
 - Quantum picture SST+DW: homogeneous result





Remind of the semiclassical results for "Stark" broadening of isolated lines of atoms and ions in the impact approximation-1

$$W = N \int v f(v) \left(\sum_{i' \neq i} \sigma_{ii'}(v) + \sum_{f' \neq f} \sigma_{ff'}(v) + \sigma_{el}(v) \right)$$
$$\sum_{i' \neq i} \sigma_{ii'}(v) = \frac{1}{2} \pi R_1^2 + \int_{R_1}^{R_D} 2\pi \rho \, d\rho \sum_{i' \neq i} P_{ii'}(\rho, v);$$
$$d = N \int v f(v) \int_{R_3}^{R_D} 2\pi \rho \, d\rho \sin 2\phi_p;$$

$$\sigma_{el} = 2\pi R_2^2 + \int_{R_2}^{R_D} 2\pi\rho \, \mathrm{d}\rho \, \sin^2 \delta;$$

$$\delta = \left(\phi_p^2 + \phi_q^2\right)^{1/2},$$

$$\phi_p = \sum_{i' \neq i} \phi_{ii'} - \sum_{f' \neq f} \phi_{ff'}.$$

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High energies (or very small ΔE): Neutrals: $a(z) \rightarrow \ln(2/\gamma z) \sim \ln(E)$ Ions: Coulomb attraction (repulsion) decreases ($\xi \rightarrow 0, \xi \epsilon \rightarrow \rho$, neutrals) \rightarrow due to the mass and/or collider charge effect, collisions with ions can be important

1- Inelastic cross-section:
Neutral atom, straight path:

$$\sigma_{ii}(E) = 8\pi a_0^2 \frac{2I_H^2}{E \Delta E_{ii}} f_{ii} \frac{\mu}{m_e} Z_p^2 (a(z_{max}) - a(z_{min})) + (strong.coll.).$$

$$\mu \text{ reduced mass atom-perturber}$$

$$Z_A \text{ charge o the radiating atom}$$

$$Z_P \text{ charge of the collider}$$

$$\rho \text{ impact parameter}$$

$$\varepsilon \text{ eccentricity of the hyperbola}$$

$$a \text{ half-major axis o$$

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Remind of the semiclassical results for "Stark" broadening of isolated lines of atoms and ions in the impact approximation- 2

2-Elastic contributions to the width:
2-1- Neutral atom, straight path:
Polarization potential (or quadratic)
Low energies (analytic)

$$W = 0.61 \ 10^{-8} N \left(\alpha_i - \alpha_f\right)^{2/3} Z_P^{4/3} \ T^{-1/6} \left(\frac{m_e}{\mu}\right)^{1/6}$$
$$\alpha_i = 4a_0^3 \sum_{i' \neq i} f_{ii'} \left(\frac{I_H}{\Delta E_{ii'}}\right)^2$$

Medium energies (more complicate)

 $\varphi_{i} = \sum_{i' \neq i} \frac{2I_{H}^{2}}{E \Delta E_{ii'}} f_{ii'} \frac{\mu}{m_{e}} \frac{a_{0}^{2}}{\rho^{2}} Z_{P}^{2} (B(z))$

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High energies $B(z) \rightarrow \pi z^2 \exp(-2/\gamma z)$ The width increases with μ , $Z_{P,}$ and small $\Delta E_{ii'}$ 2-Elastic contribution to the width
 2-2- Neutral atom, straight path:
 Quadrupole potential
 Analytic solution

 $W = 1.21 \, 10^{-7} \, N \, Z_P \, (\text{coef})$

coef is the mean square root of a linear combination of the means square radius of the i and f levels)

W does depend on the charge of the perturber but not of its mass

For low levels (ΔE_{ii} , large) the quadrupole potential dominates the elastic contribution

For high levels the polarization contribution dominates





Remind of the semiclassical results for "Stark" broadening of isolated lines of atoms and ions in the impact approximation- 3

3-Elastic contributions to the width:
 3-1- ion : hyperbolic path
 Polarization potential (or quadratic)
 Not analytic

$$\varphi_i = \sum_{i' \neq i} \frac{I_H^2}{E \Delta E_{ii'}} f_{ii'} \frac{\mu}{m_e} \frac{a_0^2}{a^2 \varepsilon^2} Z_P^2 \Big(B(\xi, \varepsilon) \Big)$$

High energies: $\xi \rightarrow 0, \xi \epsilon \rightarrow \rho$ $B(\xi, \epsilon) \sim B(z)$ 3-Elastic contributions to the width: 3-2- ion : hyperbolic path Quadrupole potential Not analytic - Collision rate ~ $(\mu/m_e)^{1/2}/Z_a^2$ for the repulsive case





Influence of collision strengths - neutral atoms -1

Mg I 3s ¹S -3p 1P^o: resonance line, low levels involved.





Contribution of the polarization potential (in percent of the elastic contribution)

Inelastic collisions are completely negligible for ion collisions Elastic collisions are mostly due to the quadrupole potential

> $\Delta E_{min} = \Delta E (4s-3p) = 8451.64 \text{ cm-1}$ $\Delta E_{min}/kT = 1.18 \text{ at } 5000 \text{ K}$ $f_{jj'} = 0.1623$



Astronomical Observatory, Belgrafe



Influence of collision strengths - neutral atoms -2





-The relative contribution of ion collisions increases with *n* and the ion width becomes higher than the electron width -the inelastic contribution of ion collisions increases -The contribution of the quadrupole term is less than 4% for electron and less than 1% for ion collisions

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Influence of collision strengths - radiating ions -1

AI XI 2s ²S-2p ²P^o: resonance line, low levels involved.



 $\Delta E_{min} = \Delta E (3s-2p) = 1.8446 \ 10^{6} \text{ cm-1}$ $\Delta E_{min}/kT = 2.564 \ \text{at} \ 500 \ 000 \ \text{K}$ $f_{ii'} = 0.0212$ $\Delta E (3d-2p) = 1.9085 \ 10^{6} \text{ cm-1}$ $\Delta E/kT = 2. \ 65 \ \text{at} \ 500 \ 000 \ \text{K}$ $f_{ii'} = 0.667$ Collisions with ions: guadrupole poter

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- -Collisions with ions: quadrupole potential prevails.
- Coulomb repulsion high : ion collision width small







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Influence of collision strengths - radiating ions - 2

AI XI 5s-2p: high levels involved.





 $-\Delta E_{min} = \Delta E (5s-2p) = 1.0 \ 10^4 \ cm-1$ $\Delta E_{min}/kT = 1.39 \ 10^{-2} \ at \ 500 \ 000 \ K$ $f_{ii} = 0.33$

-Collisions with ions: the polarization potential prevails, quadrupole part negligible .

-- Coulomb repulsion small : The ion collision width increases





Influence of collision strengths - 3 Behaviour with the charge of the perturber

from STARK-B and Dimitrijević, SAJ 1999





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Influence of atomic structure - 1

1- Asymptotic trends: Coulomb approximation:

Line strength $S(i, j) \sim f_{iij} / \Delta E_{ij}$

 $\Delta n = 0 \qquad S(i, j) \sim n^4 / Z^5 \quad (Z = \text{effective charge} = Z_A + 1) \\ \Delta n \neq 0 \qquad S(i, j) \sim 1 / Z^2$

Energy

 Z^2/n^2 (in Rydberg)

Spin-orbit hamiltonian ~ $2(Z\alpha)^2 / [(nl (2l+1)(l+1]))$

Distance between two fine structure levels (doublet) ~ $Z^4/(n^3 I(l+1))$

2- Importance of configurations interaction and relativistic effects (spin orbit...)







Influence of atomic structure - 3 Behaviour with the charge of the radiating ion (width in ang.freq. units)



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Fig. 20. Present quantum: \circ and present SCP: \blacktriangle Stark widths (in angular frequency units) of the transition $3s {}^{2}S_{1/2}-3p {}^{2}P_{3/2}^{\circ}$ for ions from C IV to P XIII as a function of log Z. Results are given for $N_{e} = 1.8 \times 10^{18} \text{ cm}^{-3}$ and $T_{e} = 14.51 \times 10^{4} \text{ K}$. Solid line: linear fit of the quantum results, dashed line: linear fit of the SCP results.

From Elabidi et al. EPJD 2009



Systematic trends Shift: Variation with the charge of the radiating ion



Fig. 1. The behavior of the reduced shift $|d|(Å)/(Å)^2$ for(——) electron- and (----) proton-impact for the 2s-2p transition along the lithium isoelectronic sequence. Z denotes the residual charge as "seen" by the optical electron (Z = 1 for neutrals, 2 for singly charged ions, etc.). The electron density is 10^{17} cm⁻³ and the temperature 500,000 K.

Astrophysical Applications of Powerful New Databases ASP Conference Series, Vol. 78, 1995 S. J. Adelman and W. L. Wiese (eds.)

(MSD &SSB 1995)

Stark Broadening of Al XI Spectral Lines





CII in hot DQ White Dwarfs with carbon atmosphere Ab initio Stark broadening calculations: 1- SCP+TOPBase/R-matrix and systematic trends 2- Width: Variation with the principal quantum number



CII in hot DQ White Dwarfs with carbon atmosphere Comparisons between atomic data used: Example of the width 426.7 nm 3d ²D_{3/2} - 4f ²F_{5/2}

T = 2 10⁴ K Ne = 10¹⁷ cm⁻³

Total width at half-maximum in nm:

•TOPBase/R-matrix levels and TOPBase/R-matrix line strengths:	0.142
•TOPBase/R-matrix levels and Bates & Damgaard line strengths:	0.142
•NIST levels and TOPBase/R-matrix line strengths:	0.137
•VALD data (not very different from NIST levels and NIST line strengths :	0.137

•N.B. The wavlength given by TOPBASE is 429.9 nm

Thus, what can we conclude from this example?

•The choice of the energy levels have the greatest effect.

- •The choice of the oscillator strengths are less important probably because we have a summation over many levels and it is a rather simple atom
- •Owing to the accuracy of the SCP method, all these results are consistent.

•This encourages us to pursue the use of atomic structure tables when they are available for calculating many many numerous data (e.g. more than 1000 lines for C II!) with an automatic procedure







Comparison of Stark impact widths:

 fine structure components - widths due to electrons and to ions collisions: importance of configuration interaction and of departure from LS coupling *

•Example of Cr I lines

- Contribution of ions are larger than that of electrons at high temperatures
- Widths and shifts of fine structure lines are different
 - Cr I 7P⁰₄ –7D₄ 5329.14 Å
 - Cr I 7P⁰₄ –7D₅ 5328.32 Å

Dimitrijević et al., *A*&*A* 2005 SCP+ Bates &Damgaard with experimental energy levels In Cr-rich Ap star (deeper layers)

* Only for the levels in this case

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 $\Delta E (3d^{5}.(^{6}S).4d e^{7}D_{4} - 3d^{5}.(^{6}S).5p \times ^{7}P^{\circ}_{3}) = 4.26 \text{ cm}^{-1}$ $\Delta E (3d^{5}.(^{6}S).4d e^{7}D_{5} - 3d^{5}.(^{6}S).5p \times ^{7}P^{\circ}_{4}) = 14.14 \text{ cm}^{-1}$



According to Elabidi, Sahal-Bréchot and Ben Nessib, 2009 SST (intermediate coupling) and quantum scattering matrix (DW)

Z (charge of the ion)

Distance between 3/2 and 1/2 ~ Z⁴/[*n*³(*l*+1)*l*]





Behaviours with the temperature T: Asymptotic limits

Radiating ions at low energies: $W \approx T^{-1/2}$

SCP calculations with SST atomic structure (after Elabidi, Sahal-Bréchot and Ben Nessib, 2009)



Behaviours with the temperature T: Asymptotic limits

Neutral radiating atoms and ions at high energies:Bethe approximation $W \approx Log_n(T) / T^{1/2}$

Elabidi & Sahal-Bréchot, 2010, EPJD

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Figure 1. Quantum electron impact width of the Mg X 3s $^2\mathrm{S}_{1/2}-3p$ $^2\mathrm{P}_{3/2}$ transition as a function of $\ln(T)/\sqrt{T}$ for the temperature range $[1.6\times10^4-5\times10^6~\mathrm{K}]$ at density $N_e=10^{18}~\mathrm{cm}^{-3}.$



Behaviour of the width with temperature and comparison between SCP, quantum calculations and

experiments

Elabidi, Sahal-Bréchot and Ben Nessib: 2009, *EPJD*, **54**, 51

White circles O: our quantum calculations (SSt+DW)

Black triangles ▲: our SCP calculations with SST atomic structure

Black circles ● and ▼ : quantum close-coupling calculations (should be the best ones)

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Fig. 1. Stark width W as a function of the electron temperature for the C IV $3s \ ^2S_{1/2}$ - $3p \ ^2P_{3/2}^{\circ}$ transition at an electron density $N_e = 10^{18} \text{ cm}^{-3}$. Present work: \circ , CCC [19]: •, SCP [2,41]: ▲, S [15]: ▼. Experimental values: [24]: *, [2]: ×, [21]: +. Notations are the same as those of Table 1.

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Fitting formula (variation with the temperature T) Interest for modelling of stellar atmospheres and synthetic spectra on a large scale

8th SCSLSA, Divčibare, Serbia, June 6-10 2011

No physical sense! But very accurate !!!

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```
Find a, b ,c:
Logarithmic + 2nd degree polynomial fitting
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Width:
W = 10^{(a_0 + a_1 + \log(x) + a_2 + \log(x) + \log(x))}
```

```
Shift:
We fit d/w as
d/w = (b_1 + b_2 * \log(x) + b_3 * \log(x) * \log(x))
```

x is proportional to the temperature

Cf the fitting W = a T^b



Now we are currently introducing this fitting into STARK-B









Astronomical Observatory, Belgrade



Thank you for your attention



