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SEMICLASSICAL CALCULATIONS OF STARK BROADENING PARAMETERS

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Resume - On présente ici une revue des calculs des largeurs et des déplacements des raies élargis par l'effet Stark, obtenus à l'aide du formalisme semiclassique-perturbations. On compare les résultats des calculs obtenus par les programmes de (i) Jones, Benett et Griem, (ii) Sahal-Bréchet et (iii) Bassalo, Cattani et Walder, et aussi, on discute la comparaison avec les résultats expérimentaux.

Abstract - A review of semiclassical calculations of Stark broadening parameters is presented. We compare the results obtained by using computer codes due to (i) Jones, Benett and Griem, (ii) Sahal-Brechot and (iii) Bassalo, Cattani et Walder. The comparison with experimental results has also been discussed.

1 - INTRODUCTION

In order to perform the calculation of a Stark Broadened line profile, the three principal ways to describe a radiating (absorbing) system are widely used, i.e. the quantum mechanical, the semiclassical or the classical approach. In the pure quantum mechanical approach, we have usually a system of non-interacting cells, containing the radiating atom and N perturbers and, we consider the whole cell as a giant molecule. However, to perform a pure quantum mechanical strong coupling calculation is very difficult and only few such calculations exist. For example the strong coupling method is used for Li I ($2s - 2p$) /1/, Ca II ($4s-4p$, and $3d - 4p$) /2 and 3/, Mg II ($3s - 3p$) /3,4/ and Be II ($2s - 2p$) /5/ lines. Recently, Seaton performed close coupling calculations for 42 transitions in Li-like ions C III, O V, Ne VII, Be II, B III, C IV, O VI, Ne VIII /6/ and for the transitions $2s^2\ ^1S - 2s2p\ ^1P^o$, $2s2p\ ^3P^o - 2p^2\ ^3P$, and $2s2p\ ^1P^o - 2p^2\ ^1D$ and 1S in C III /7/. These results, obtained as solutions of the close coupling problem which uses truncated expansions, are assumed to be correct probably within 10 percent /7/.

In spite of the existence of more refined quantum mechanical method, the semiclassical approach is still the most widely used technique for the calculation of line broadening data. Moreover, in a lot of cases such as e.g. complex spectra, heavy elements or transitions between more excited energy levels, the sophisticated quantum mechanical approach is very difficult or even practically impossible to use and, in such cases, the semiclassical approach remains the most efficient method for Stark broadening calculations.

2 - SEMICLASSICAL METHOD

Within the semiclassical model, the radiating (absorbing) atom is described quantum mechanically while perturbers are classical particles with well defined velocity (v) and impact parameter (ρ). The system of classical perturbers acts on the quantum mechanical atom via classical, time dependent interaction potential. The Schrödinger equation which is satisfied by the atomic wave functions is usually solved using the second order non stationary perturbation theory.

The existing large scale calculations of Stark broadening parameters were performed by using three different computer codes developed by (i) Jones, Bennett and Griem /8-10/: (ii) Sahal-Bréchet /11,12/ and (iii) Bassalo, Cattani and Walder /13/.

Within the frame of the semiclassical theory, half half width (w) and shift (d) of an isolated line may be expressed via S matrix as /e.g. 10/

$$w + id = N \int_0^\infty v f(v) dv \int_0^\infty 2\pi \rho d\rho (1 - S_{ii}(\rho, v) S_{ff}^{-1}(\rho, v))_{Av} \tag{1}$$

Here, N is the electron density: $f(v)$ is the Maxwellian velocity distribution function for electrons: i and f denote the initial and final atomic energy levels: and i' and f' are their corresponding perturbing levels, while $(...)_{Av}$ denotes the angular average over the directions of the colliding electron.

If one express the relevant inelastic and elastic cross sections via corresponding S matrix elements which are proportional to the transition probability $P_{jj'}$, /11,12/ one obtains the formulae which enter the computer code of Sahal-Brechet

$$2w = N \int_0^\infty v f(v) dv \left[\sum_{i' \neq i} \mathcal{G}_{ii'}(v) + \sum_{f' \neq f} \mathcal{G}_{ff'}(v) + \mathcal{G}_{el} \right], \tag{2}$$

$$d = N \int_0^\infty v f(v) dv \int_{R_3}^{R_D} 2\pi \rho d\rho \sin 2\phi_p \tag{3}$$

with

$$\sum_{j' \neq j} \mathcal{G}_{jj'}(v) = \frac{1}{2} \pi R_1^2 + \int_{R_1}^{R_D} 2\pi \rho d\rho \sum_{j' \neq j} P_{jj'}(\rho, v), \tag{4}$$

$$\mathcal{G}_{el} = 2\pi R_2^2 + \int_{R_2}^{R_D} 8\pi \rho d\rho \sin^2(\phi_p + \phi_q)^{1/2}. \tag{5}$$

The phase shifts ϕ_p and ϕ_q due respectively to the polarization potential (r^{-4}) and to the quadrupolar potential (r^{-3}) part, are given in the part 3 of Section 2 in the Ref. /11/. All the cutoffs R_1 , R_2 , R_3 and R_D are described in the part 1 of Section 3 of the Ref. /12/. The contribution of resonances in the elastic cross sections is taken into account in the ion-line-width calculations according to Ref. /14/. The formulae for the ion impact broadening are analogous but inelastic collisions are negligible.

In the computer code of Bassalo, Cattani and Walder, so called convergent theory, originally developed by Vainshtein and Sobel'man /15/ has been used. Using the similarity between the Dyson series for S matrix perturbational development and Taylor series for exponential function, this method avoid the divergence in the integration over impact parameter when ξ tends to 0 /15/.

Comprehensive calculations of Stark broadening parameters of non-hydrogenic neutral and singly ionized atom lines (helium through calcium and cesium) using the computer code of Jones, Benett and Griem, were published in 1971 and later in 1974 /8-10/. Using the same code /10/ and the version adapted by Dimitrijević for the case of multiply charged ions, data for Br I, Ge I, Hg I, Pb I, Rb I, Cd I, Zn I /16/, O II /17/, O III /18/, C III /19/, C IV /19,20/, N II, N III, N IV /21/, S III, S IV, Cl III /22/ and Ti II, Mn II /23/ have been published. Semiclassical calculations based on the method developed by Sahal-Bréchet /11,12/ exist for light elements such as C, N, Mg, Si (without the contribution of resonances /see e.g. 24 and References therein/. Data for alkali-like ions Be II, Mg II, Ca II, Sr II, Ba II may be found in Ref. /14/, while in Ref. /25/ the semiclassical and experimental data for the low-excitation Si II lines have been compared. Recently, using the same computer code, extensive calculations for 79 neutral helium multiplets /26-30/, 62 sodium /31-33/ and 51 potassium multiplets /34,35/ for perturber densities 10^{13} - 10^{19} cm^{-3} become available. Data for F I /36/, Ar II /37/, Ga II, Ga III /38/ also exist. Using this code Lanz et al /39/ published recently a set of the Si II Stark broadening parameters required for stellar analysis.

Stark width values obtained by the code of Sahal-Bréchet are in general smaller than those obtained using the code according to Griem /10/, due to the symmetrization procedure used by Sahal-Bréchet and to different lower cut-offs. This difference becomes smaller if the contribution of resonances is taken into account. In the case of the Mg II resonance lines, the experimental data of Goldbach et al /40/, chosen after the critical analysis /41/ as very reliable, agree better with the results obtained using the procedure of Sahal-Bréchet, as well as a number of experimental data in the case of the Si II multiplet 1 /25/ (see Fig. 1). However, a general conclusion is difficult to obtain /see e.g. Ref. 28/ since different assumptions involved in these two versions of the semiclassical method have different validity conditions.

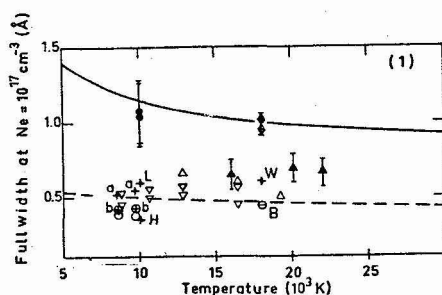


Fig. 1 - Line widths for Si II multiplet 1 at electron density 10^{17} cm^{-3} vs temperature. Experimental data: \blacktriangle , Lesage et al /25/; \circ , Konjević et al /42/; ∇ , \blacktriangledown , \triangle , Purić et al /43-45/; \bullet , Lesage et al /46/; \diamond , Chiang and Griem /47/. Theoretical data: (i) Semiclassical calculations: — Griem /10/; - - - Sahal-Bréchet /in Ref. 46/; (ii) Distorted wave calculations: \oplus Blaha

/in Ref. 47/; (iii) Semiempirical calculations: Konjević et al /42/ treating perturbing levels together (+a) and individually (+b)*; Lesage et al /46/ (+L)*; Hey /48/ (+H)*; Jones /49/ (+W).

Extensive calculations by Bassalo,Cattani and Walder obtained using the convergent semiclassical method exist for He I lines.

All three methods have been compared with critically selected experimental data for 13 He I multiplets /28/. In order to estimate the average accuracy of different methods, ratios of experimental and theoretical values have been averaged first in multiplet and then over the number of multiplets. Obtained results are presented in Table 1

Table 1 - Average accuracy of different theoretical methods compared to Stark width (W_m) and shift (d_m) experimental data for helium lines. The results in parentheses are obtained by excluding the $2p^3D - 3d^3D$ line which exhibits a strong unexplained difference between d_m and and the calculated shift (especially for d_{DSB} and d_{BG}). With DSB are denoted the data from Ref. /26/, with BCW the data from Ref. /13/ and with BG the data from Ref. /8/ (also in Ref. /10/).

	All experiments included	Experiments with C and D accuracy excluded
$(W_m/W_{DSB})_{av}$	1.17±0.04	1.17±0.02
$(W_m/W_{BCW})_{av}$	1.07±0.04	1.07±0.04
$(W_m/W_{BG})_{av}$	0.92±0.04	0.93±0.02
$(d_m/d_{DSB})_{av}$	1.20±0.13 (1.07±0.04)	1.13±0.03
$(d_m/d_{BCW})_{av}$	1.23±0.08 (1.27±0.07)	1.34±0.09
$(d_m/d_{BG})_{av}$	1.14±0.07 (1.07±0.04)	1.14±0.03

One can see that the agreement between experimental and all three semiclassical calculations is within the limits of ±20%, what is the predicted accuracy of the semiclassical method /10/. This is also well illustrated in Table 2 where average ratios of measured Stark widths and shifts to the calculated ones by using Griem's code are given.

Table 2 - Average ratios of measured and calculated linewidths (W_M/W_{th}) for various emitters in the case of various calculations according to Ref. /10/. Values in Table are from Ref. /50/ in the case of neutrals and singly charged ions and from Ref. /51/ in the case of doubly charged ions. Number of data for W and d are given under n_W and n_d ($n \geq 5$).

Element	W_M/W_{th}	d_M/d_{th}	n_W	n_d
He I	0.93	1.11	14	14
C I	0.88	1.00	18	9
N I	0.96	0.82	49	26
O I	0.93	1.03	7	5
F I	0.93	1.15	9	8

Element	W_M/W_{th}	d_M/d_{th}	n_W	n_d
Ne I	0.84	1.55	17	6
Si I	1.09	0.90	6	8
P I	1.00		10	
S I	1.09		5	
Cl I	1.10		6	
Ar I	0.86	0.81	21	15
Cs I	1.15		19	
C II	1.14		5	
N II	1.09		8	
O II	0.93		13	
Ne II	1.14		12	
Mg II	0.78	1.01	6	6
Al II	1.08		5	
Si II	0.99		6	
S II	1.03		10	
Ar II	1.00	1.15	34	26
Ca II	0.79	0.65	9	7
Ge II	1.05		7	
C III	0.76		7	
O III	0.72		6	
S III	0.73		16	
Cl III	0.74		15	

One can see that for doubly charged ions the agreement is less satisfactory and the results are consistently larger than experimental values as well as the quantum mechanical results /6,7/. If we look at a particular spectrum, the semiclassical results are of lower accuracy for first one or two lines, since in this case the possibilities of the semiclassical approach are not so good due to the significant contribution of resonances, especially in the case of charged emitters, as well as to the influence of strong and elastic collisions. In the case of singly charged ions the discrepancies between Jones, Benett and Griem's calculations /9,10/ and experimental values for Mg II and Ca II resonance lines are reason for lower (W_M/W_{th}) ratios in Table 2.

3 - MULTIPLY CHARGED IONS

With the increase of the ionization degree, increases the importance of the short range effects since perturbers come closer to the emitter due to larger Coulomb attraction making the validity of the classical path approximation more questionable. The comparison /53/ of different experimental and theoretical results is presented for 2s - 2p C IV multiplet in Fig. 2 and for 3s - 3p C IV line ($\lambda = 5801.3\text{\AA}$) in Table 3. One can see that the agreement is not so good as in the case of neutrals and singly charged ions. However, the agreement becomes better for higher temperatures. This can be explained by the fact that the distance between the perturbing levels and the initial and final levels is larger for multicharged ions than in the case of singly charged ions. Therefore, elastic collisions are more important than inelastic ones, and elastic collisions are due to close interactions which are not well treated by the perturbation theory. At high temperatures or for excited levels, inelastic collisions become important: they are due to more distant interactions and the perturbation theory may give correct results. It can be noticed that quantum close coupling calculations become difficult to perform for high levels, owing to the number of involved channels.

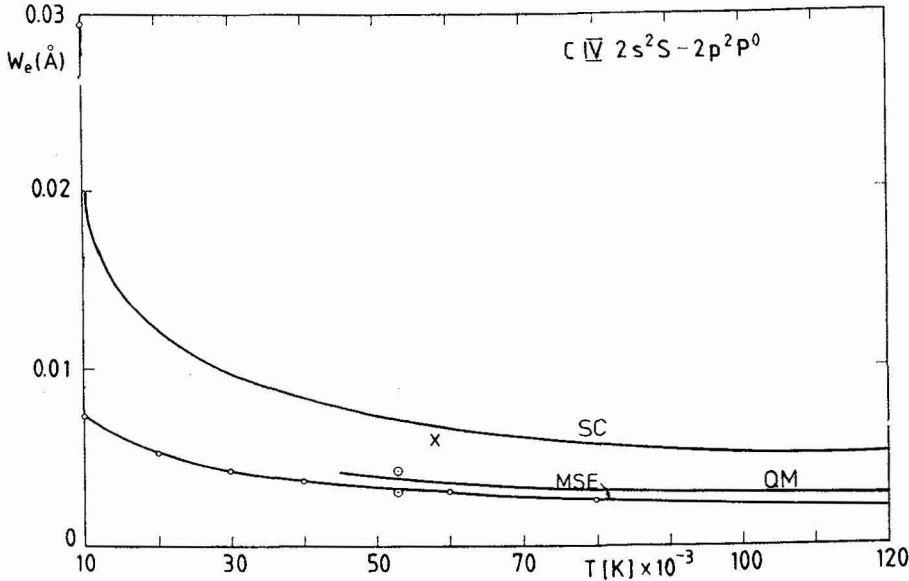


Figure 2 - Theoretical and experimental Stark widths (FWHM) for C IV $2s^2S - 2p^2P^0$ multiplets as function of temperature: SC=Semiclassical calculations, Dimitrijević, Sahal-Bréchet (1990) /52/; QM=Quantum close coupling calculations, Seaton (1988) /6/; MSE- Modified semiempirical calculations, Dimitrijević, Konjević (1980) /53/; Experimental data : X=Bogen (1972) /54/; O=El-Farra, Hughes (1983) /55/.

Table 3 - Experimental (W_M) and calculated (W_{th}) Stark widths (FWHM) for the transition C IV, $3s^2S_{1/2} - 3p^2P^0_{3/2}$ ($\lambda = 5801.3\text{\AA}$) at an electron density of $1.8 \cdot 10^{18} \text{ cm}^{-3}$ and $kT = 12.5 \text{ eV}$.

$W_M(\text{\AA})$	$W_{th}(\text{\AA})$	Reference
10.0		/56/
	7.38	/52/
	7.98	/10/
	6.01	/53/
	5.45	/57/
	6.09	/58/
	10.80	/59/
	5.32	/6/

Therefore the two methods are complementary: at low temperatures and for lines between low levels, quantum close coupling calculations are necessary if one needs a good accuracy: the semiclassical approximation can not give better than a factor of two. At high temperatures or for lines originating from high levels the semiclassical approximation can give correct results when close coupling calculations become unoperative.

With the increase of the ionization degree the contribution of the ion-impact broadening also decrease. In astrophysical investigations broadening by the radiator interaction with protons is the most important and also, such results give an upper limit since the proton collisions are the most effective in comparison with the heavier ionic species. In Table 4 the validity condition of the impact approximation for proton-impact broadening in the case of the O V (1371Å) $2p^2\ ^1D - 2s2p\ ^1P$ line /60/ is presented. We can see that only for the plasma conditions $N_e = 10^{22}\text{cm}^{-3}$ and $T = 2$ and $3 \times 10^5\text{K}$ the validity of impact approximation becomes questionable in the line center.

Table 4 - The validity of the impact approximation for proton collisions in the case of O V (1371Å) $2p^2\ ^1D - 2s2p\ ^1P$ line /60/. (The time of interest for line broadening/the line width) $\ll 1$ (see Refs. /11,12/).

$T(K)$ N_e (cm^{-3})	1.2×10^5	2×10^5	3×10^5
10^{18}	0.9×10^{-4}	1.3×10^{-4}	1.4×10^{-4}
10^{20}	0.9×10^{-2}	1.3×10^{-2}	1.3×10^{-2}
10^{22}	0.1	0.6	0.9

In Table 5 the semiclassical calculations /60/ of widths are compared for the same O V line. One can see that the proton width is very small compared to the electron width. This is due to the Coulomb repulsion which increases with the radiating ion charge.

Table 5 - The electron- and proton-impact widths (FWHM) for O V (1371Å) $2p^2\ ^1D - 2s2p\ ^1P$ line at $N_e = 10^{20}\text{cm}^{-3}$ and at different temperatures.

Temperature (K)	8.0×10^4	1.2×10^5	2.0×10^5	3.0×10^5
Electron-impact width (Å)	4.6	3.8	3.0	2.5
Proton-impact width (Å)	0.06	0.1	0.17	0.22

A quasistatic calculation in the wings /60/ shows that the proton contribution becomes completely negligible. In the examined case the Franck-Condon turning point falls inside the classical - ly forbidden region determined by the Coulomb repulsion /60/.

4 - CONCLUDING REMARKS

Generally, the width data are more reliable than the shift data, since shift calculations are more sensitive to the small variations of various parameters. The reason is because shifts are smaller than widths and produced in average by more distant collisions. Roberts /61/ performed an analysis of the width and shift values convergence as a function of the number of perturbing levels, demonstrating that in the case of the shift, even the sign may be changed if an insufficient number of perturbing levels is used.

This is also illustrated in Figs. 3 and 4 (from Ref. /1/). Here, we have sums of relative contributions to width and shift for the various angular momenta ℓ of the colliding electron.

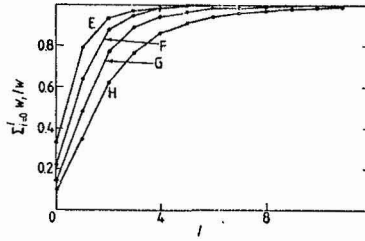


Fig. 3 - Convergence of the sum $\sum_{i=1}^l W_i/W$ in the semiclassical approximation as a function of l . The curves E, F, G and H refer to temperatures of 2500, 5000, 10000 and 20000 K respectively.

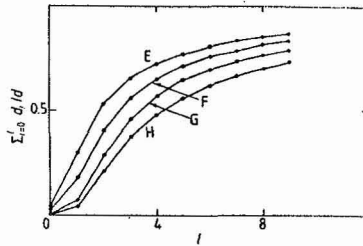


Fig. 4 - Convergence of the sum $\sum_{i=1}^l d_i/d$ in the semiclassical approximation as a function of l . Otherwise the same notation.

We can see that in the case of the shift the convergence is not so good as in the case of the width. Consequently, larger computational efforts are needed in order to obtain a good accuracy for the shift.

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