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Contribution to the Semi-Classical and Modified Semi-Empirical Impact Stark Broadening Calculations of Singly Ionized Carbon and Oxygen Spectral Lines

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Abstract. Using the semi-classical impact perturbation theory including both dipole and quadrupole terms in the expression of electrostatic interaction between the optical electron and the perturber, we calculated widths and shifts of singly ionized carbon and oxygen spectral lines and compared with experimental results and those calculated by Griem. The impact approximation was checked for each case using the appropriate condition of validity (the collision volume must be very small compared to the inverse of the perturber density). The species of ionic perturbers depends on the plasma composition in a particular experiment. We also calculated modified semi-empirical widths using the formalism of Dimitrijević and Konjević, in order to test the applied method and the accuracy of the obtained results.

Key words. line: profiles - Atomic data

1. Introduction

The charged carbon (CII) and oxygen (OII) atoms, as emitters or absorbers, are especially important due to their presence in many kinds of cosmic sources of radiation. The abundance of the large number of ionized carbon and oxygen spectral lines in stellar plasmas make these of great importance for diagnostic purposes. In astrophysics, Stark broadening data are required e.g. for the evaluation of the physical conditions in the stellar atmospheres from the analysis of stellar spectra. Further, Stark broadening data are also required for determination of the abundances of elements and for evaluation of the radiative transfer through the stellar interior.

In the following, we will present new calculations that we have obtained with the semi-classical method of Sahal-Bréchot (1969a,b, 1974) . The aim of this paper is twofold. To provide new Stark broadening data for astrophysically important CII and OII lines and

Send offprint requests to: M. S. Dimitrijević to test the modified semiempirical approach (Dimitrijević & Konjević 1980). Also, we compared our results with available experimental and other theoretical results.

2. Stark broadening impact theory of isolated lines

2.1. Semi-classical approach

For the line corresponding to the transition between the initial level i and the final level f, the half width at half maximum w and the shift d are given by Sahal-Bréchot (1969a,b):

$$W = 2w = N_p \int_0^\infty v f(v)\, dv$$
$$\times \left(\sum_{i \neq j} \sigma_{ij}(v) + \sum_{j' \neq f} \sigma_{fj'}(v) + \sigma_{el}(v) \right) \quad (1)$$

$$d = N_p \int_0^\infty v f(v)\, dv \int_{R_3}^{R_D} 2\pi \rho d\rho \sin^2 \phi_p. \quad (2)$$

2.2. Semiempirical approach

We calculated modified semiempirical electron width using the formalism of Dimitrijević & Konjević (1980), where the mean square radius is expressed in terms of the oscillator strengths for the contribution of the collisional transitions with $\Delta n = 0$ and hydrogenic approximation is used for $\Delta n \neq 0$.

$$W = N \frac{8\pi}{3} \left(\frac{\hbar}{m}\right)^2 \left(\frac{2m}{\pi k T}\right)^{\frac{1}{2}} \frac{\pi}{\sqrt{3}} [R^2_{l_i,l_{i+1}} \widetilde{g} \left(\frac{E}{\Delta E_{l_i,l_{i+1}}}\right) +$$

$$R^2_{l_i,l_{i-1}} \widetilde{g} \left(\frac{E}{\Delta E_{l_i,l_{i+1}}}\right) + R^2_{l_f,l_{f+1}} \widetilde{g} \left(\frac{E}{\Delta E_{l_f,l_{f-1}}}\right) +$$

$$R^2_{l_f,l_{f-1}} \widetilde{g} \left(\frac{E}{\Delta E_{l_f,l_{f-1}}}\right) + \sum_{i\prime} \left(R^2_{ii\prime}\right)_{\Delta n \neq 0} g \left(\frac{3kTn_i^3}{4ZE_H}\right) +$$

$$\sum_{f\prime} \left(R^2_{ff\prime}\right)_{\Delta n \neq 0} g \left(\frac{3kTn_i^3}{4ZE_H}\right)] \quad (3)$$

For $\Delta n = 0$

$$R^2_{ij} = f_{ij} \frac{\lambda_{ij}(\text{Å})}{303.7}, \quad (4)$$

where f_{ij} is the oscillator strength between levels i and j.

When the wavelength of a particular line within the multiplet differs significantly from the averaged wavelength $\langle\lambda\rangle$ of the whole multiplet, we use, to obtain more accurate values, the following scaling (Popović et al. 2001):

$$W_{line} = \left(\frac{\lambda}{\langle\lambda\rangle}\right)^2 W. \quad (5)$$

$$d_{line} = \left(\frac{\lambda}{\langle\lambda\rangle}\right)^2 d. \quad (6)$$

In the above expression, W, d and $\langle\lambda\rangle$ are values for the multiplet, and W_{line}, d_{line} and λ refer to a particular line within the multiplet.

3. Result and discussion

The atomic energy levels and oscillator strengths for CII and OII have been taken from TOPbase (Cunto et al. 1993; Zeippen 1995). TOPbase does not provide mean square radii. Therefore we have calculated them by using the oscillator strengths and the effective quantum numbers n_i^* obtained from the TOPbase. Our calculations indicate that the impact approximation is valid for collision with electrons ($C_{impact} \simeq 10^{-3}$) and for collisions with ions ($C_{impact} \leq 10^{-1}$) (Mahmoudi et al. 2004). Konjević et al. (2002) found that the contribution due to collisions with quasistatic ions can be neglected. Our results shows that within the impact approximation, still valid under the considered plasma conditions, this contribution varies between 10% and 20%.

The comparison with different measured Stark FWHM (Full Width at Half Maximum) W_m and calculated values at various electron temperatures and electron densities are shown in Table 1, where calculated $\frac{\Delta S}{S}$ ratios are also included. This ratio is a measure of the completeness of the set of perturbing levels with respect to the sums of dipole matrix elements

Table 1. Comparison of experimental and theoretical Stark line widths for the C II transition array $2s^2 3s - 2s^2 3p$. Experimental Stark width – W_m (FWHM); ratio of the measured width to the electron-impact Stark width of Griem – W_m/W_{eG}; ratio of the measured width to the electron-impact Stark width – W_m/W_e; the semi-classical total-impact Stark width – W_{SC}; ratio of the measured width to the modified semiempirical electron width – W_m/W_{MSE}. References: a – (Blagojević et al. 1999); b – (Srećković et al. 2000)

Multiplet	λ(Å)	T(K)	$N_e(10^{17}cm^{-3})$	W_m(Å)	$\frac{W_m}{W_{eG}}$	$\frac{W_m}{W_e}$	W_{SC}(Å)	$\frac{W_m}{W_{MSE}}$	$\frac{\Delta S}{S}$	Ref
^{2}S-^{2}P^0	6578.05	17100	0.25	0.213	0.81	0.80	0.305	0.78	0.12	a
		17500	0.23	0.200	0.83	0.83	0.279	0.80	0.12	a
		17800	1.96	2.198	1.07	1.07	2.385	1.05	0.12	b
		18800	0.31	0.265	0.82	0.83	0.370	0.82	0.12	a
		19500	1.44	1.128	0.75	0.77	1.713	0.77	0.12	b
		20500	0.98	0.862	0.85	0.87	1.159	0.88	0.12	b
	6582.88	17100	0.25	0.227	0.87	0.86	0.305	0.83	0.12	a
		17500	0.23	0.206	0.86	0.85	0.279	0.83	0.12	a
		17800	1.96	2.145	1.04	1.04	2.389	1.02	0.12	b
		18800	0.31	0.265	0.82	0.83	0.370	0.82	0.12	a
		19500	1.44	1.198	0.80	0.82	1.715	0.81	0.12	b
		20500	0.98	0.860	0.85	0.87	1.160	0.88	0.12	b

Table 2. Calculated shifts for the OII $3s - 3p$ multiplet: semi-classical (Griem 1974) values d_D calculated by Dimitrijević (1982) and our calculation within the semi-classical approach (Sahal-Bréchot 1969a,b) d_e. With λ_m is denoted the averaged wavelength for the multiplet.

Multiplet	λ_m Å	T K	N_e $10^{17}cm^{-3}$	d_e Å	d_D Å
^{4}P–^{4}P^0	4341	20000	1.0	-0.0070	-0.0812
		30000	1.0	-0.0075	-0.0686
		60000	1.0	-0.0084	-0.0592
		80000	1.0	-0.0078	-0.0574
^{4}P–^{4}S^0	3736	20000	1.0	-0.0055	-0.0589
		30000	1.0	-0.0043	-0.0538
		60000	1.0	-0.0047	-0.0383
		80000	1.0	-0.0048	-0.0290

and it is calculated by Mahmoudi et al. (2005). One can notice that our data are in agreement, within the experimental accuracy and with data calculated on the basis of the simplified semi-classical approach of Griem (1974).

One can see also from Table 1 that the MSE results are in good agreement with experiments and more sophisticated theoretical calculations (Mahmoudi et al. 2004; Griem 1974) for all considered experimental conditions (T and N_e). Indeed the ratio $\frac{W_m}{W_{MSE}}$ and $\frac{W_m}{W_e}$ shows in average an agreement within 20% and 16% respectively. This is well within the error bars of the semiempirical and the modified semiempirical methods estimated to be ±50% (Griem 1974; Dimitrijević & Konjević 1980) which is a very good agreement especially taking into account that the needed atomic data set is much smaller than for more sophisticated semi-classical calculations.

The Table 2 shows a large difference between our Stark shifts calculations and those of Dimitrijević (1982): our data have the same sign but they are ten times higher. This discrepancy can be explained by taking into account the sensitivity of the shift calculations to the oscillator strengths and atomic energy data (Mahmoudi et al. 2005b), especially when shift is much smaller than width, indicating the mutual cancellations of particular contributions with different signs. Dimitrijević (1982) used *LS* coupling and the Coulomb approximation to perform the one-electron model for oscillator strengths, whereas our values have been taken from the "TOPbase" atomic data given by the "Opacity Project". On the other hand the number of perturbing levels which are included in the calculation has an appreciable influence in the resulting shift. If one omits some of them, erroneous results may appear.

4. Conclusion

We have calculated Stark broadening data of CII and OII by using the semi-classical approach (Sahal-Bréchot 1969a,b) and the modified semiempirical method (Dimitrijević & Konjević 1980). We found that the ratio of experimental and our theoretical values is in average in agreement within 20%, which is well within the estimated error bars of this method (±50%), with several exceptions of the order of 50% (Mahmoudi et al. 2005). The found agreement of experimental and semi-classical values, demonstrates that the investigated method can be used for the CII and OII Stark width calculations, especially when more sophisticated methods are not applicable in an adequate way.

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