Contrib. Astron. Obs. Skalnaté Pleso **55/2**, 114 – 121, (2025)
https://doi.org/10.31577/caosp.2025.55.2.114

On the Stark broadening of O I spectral lines: comparison with experiments

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Received: January 08, 2025; Accepted: January 19, 2025

Abstract. Stark broadening parameters, line widths, and shifts have been calculated for spectral lines within the neutral oxygen spectrum for experimental conditions of published experiments to compare experiments with results of the semiclassical perturbation method. The obtained data are of particular interest in astrophysics, for instance, for the investigation of stellar spectra but also for laboratory plasma diagnostics and plasma spectra containing lines of neutral oxygen.

Key words: Stark broadening – O I – spectral lines – line profiles

1. Introduction

Data on spectral line widths and shifts broadened by fluctuating electric microfields of surrounding charged particles (Stark broadening) are useful for different topics in astrophysics (see for example Popović et al., 2001), laboratory, (Blagojević et al., 1999), fusion (Iglesias et al., 1997), and laser-produced plasma research (Sorge et al., 2000), plasma in technology (Dimitrijević & Sahal-Bréchot, 2014), laser design and development, (Csillag & Dimitrijević, 2004) etc.

Such data are particularly needed in astrophysics, for example for radiative transfer calculations, abundance determinations, and investigation, stellar spectra analysis, modelling, and synthesis, etc. (see for example Dimitrijević & Christova, 2021). They are especially needed for white dwarfs and hot subdwarfs, e.g., for DO (Dimitrijević et al., 2018), DB (Majlinger et al., 2017, 2018, 2020), DA (Majlinger et al., 2017, 2020) dwarfs and for hot subdwarfs (Hamdi et al., 2017; Chougule et al., 2020). Stark broadening data may be interesting for A and late B type stars (Majlinger et al., 2017, 2020).

Our objective here is to calculate using the semiclassical perturbation method (Sahal-Bréchot, 1969a,b; Sahal-Bréchot, Dimitrijević, & Ben Nessib, 2014), Stark widths and shifts of neutral oxygen spectral lines for plasma conditions corresponding to experimental data from the literature and to compare the obtained results with experiments of Jung (1963); Wiese & Murphy (1963); Morris & Garrison (1969); Miller & Bengtson (1970); Assous (1970); Goly et al. (1983); Goly & Weniger (1987); Sohns & Kock (1992); Mijatović et al. (1995); Gerhard et al. (2014) and Burger & Hermann (2016), to check mutually experimental data and the semiclassical perturbation theory.

2. Theory

We performed a calculation of the Stark broadening parameters of O I spectral lines within the frame of the impact semiclassical perturbation theory (Sahal-Bréchot, 1969a,b; Sahal-Bréchot, Dimitrijević, & Ben Nessib, 2014). Since it has been discussed in detail on many occasions in the references cited above, just basic formulas will be given here. The full width at half maximum (FWHM - W) and shift (d) of an isolated spectral line are given in the case of non-hydrogenic neutral atoms as:

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

$$d = N \int v f(v) dv \int_{R_3}^{R_D} 2\pi\rho d\rho \sin(2\varphi_p). \tag{1}$$

where i and f denote the initial and final level of the corresponding transition; i' and f' are perturbing levels; N perturber density; v perturber velocity, and $f(v)$ is the Maxwellian distribution of electron velocities. The inelastic cross sections $\sigma_{kk'}(v)$, $k = i, f$ are presented here by an integration of the transition probability $P_{kk'}(\rho, v)$, over the impact parameter ρ as:

$$\sum_{k' \neq k} \sigma_{kk'}(v) = \frac{1}{2}\pi R_1^2 + \int_{R_1}^{R_D} 2\pi\rho d\rho \sum_{k' \neq k} P_{kk'}(\rho, v). \tag{2}$$

The cross section for elastic collisions is given as:

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

$$\delta = (\varphi_p^2 + \varphi_q^2)^{\frac{1}{2}}. \quad (3)$$

Here, δ denotes the phase shift with components φ_p (r^{-4}) and φ_q (r^{-3}), describing contributions due to polarization and quadrupole potentials, respectively. The method of symmetrization and calculation of cut-off parameters R_1, R_2, R_3, and the Debye cut-off R_D is explained in Sahal-Bréchot (1969b).

3. Results and discussion

To calculate the Stark broadening parameters of O I spectral lines, full width at half intensity maximum (FWHM - W) and shift (d) we used the semiclassical perturbation method (Sahal-Bréchot, 1969a,b; Sahal-Bréchot, Dimitrijević, & Ben Nessib, 2014). For the electron density and temperature, we used the values for considered experiments Jung (1963); Wiese & Murphy (1963); Morris & Garrison (1969); Miller & Bengtson (1970); Assous (1970); Goly et al. (1983); Goly & Weniger (1987); Sohns & Kock (1992); Mijatović et al. (1995); Gerhard et al. (2014) and Burger & Hermann (2016). The needed set of atomic energy levels for neutral oxygen has been taken from Moore (1993). Oscillator strengths have been calculated using the method of Bates & Damgaard (1949) and the tables of Oertel & Shomo (1968).

The results obtained for Stark Full Width at Half intensity Maximum (FWHM - W) have been compared with experimental data of Jung (1963); Wiese & Murphy (1963); Morris & Garrison (1969); Miller & Bengtson (1970); Assous (1970); Goly et al. (1983); Goly & Weniger (1987); Sohns & Kock (1992); Mijatović et al. (1995); Gerhard et al. (2014) and Burger & Hermann (2016) in Table 1 and for shift in Table 2.

We can divide the obtained ratios of experimental and theoretical widths in Table 1 into three groups. The first one with ratios of experimental and theoretical widths from 1.3 up to 1.6, the second from 1.8 up to 2.2, and the third from 0.63 up to 1.22. In the first group are values from Wiese & Murphy (1963); Goly et al. (1983); Goly & Weniger (1987) and Mijatović et al. (1995). One can see that they all have estimated accuracies A, B+, and B, according to critically evaluation in Konjevic & Roberts (1976); Konjević & Wiese (1990); Konjević et al. (2002); Djurović et al. (2023). In the second group are values from Miller & Bengtson (1970); Sohns & Kock (1992); Burger & Hermann (2016). In the mentioned critical reviews, their accuracy is denoted as C+ and D. In the third group are data from Refs. Jung (1963); Morris & Garrison (1969); Assous (1970) and Gerhard et al. (2014) and accuracies are estimated as C+, C, and D. The consistency, that all experiments evaluated as best are within the same group confirms that the evaluation of accuracy in the above mentioned critical reviews is good. The difference in experimental and theoretical values is due to the influence of ion broadening. For the spectral lines in the first group, with the best accuracy, the validity condition of impact approximation is not well satisfied, and the impact semiclassical perturbation theory is not valid for

Table 1. In this Table, present calculations of Stark widths W_{th} (FWHM) are compared with experimental values (W_{exp}. References for experimental values are: 1 - Jung (1963); 2 - Wiese & Murphy (1963); 3 - Morris & Garrison (1969); 4 - Miller & Bengtson (1970); 5 - Assous (1970); 6 - Goly et al. (1983); 7 - Goly & Weniger (1987); 8 - Sohns & Kock (1992); 9 - Mijatović et al. (1995); 10 - Gerhard et al. (2014); 11 - Burger & Hermann (2016). Estimated accuracy is from Konjevic & Roberts (1976); Konjević & Wiese (1990); Konjević et al. (2002); Djurović et al. (2023). For accuracy, the letter code, as in the above-mentioned references (see for example Djurović et al. (2023)), is used: A = uncertainties with 15%; B+ = with 23%; B = with 30%;C+ = with 40%; C = with 50%; D uncertainties larger than 50%.

Transition	λ [Å]	T [K]	N [10^{17} cm^{-3}]	W_{exp}	W_{th}	$\frac{W_{exp}}{W_{th}}$	Acc.	Ref.
$2p^4\ ^3P$-$(^4S^o)3s^3S^o$	1303.5	13600	1.32	0.01848	0.0175	1.06	D	3
$2p^4\ ^3P_2$-$(^4S^o)3s^3S^o_1$	1302.17	12500	1	0.0233	0.013	1.79	C+	8
$2p^4\ ^3P_1$-$(^4S^o)3s^3S^o_1$	1304.86	12500	1	0.0233	0.013	1.79	C+	8
$2p^4\ ^3P_0$-$(^4S^o)3s^3S^o_1$	1306.03	12500	1	0.0233	0.013	1.79	C+	8
$3s\ ^5S^o_2$-$(^4S^o)3p^5P_3$	7771.94	11000	1	1.05	0.544	1.93	C+	11
		11200	1	0.64	0.547	1.17	C+	10
$3s\ ^5S^o_2$-$(^4S^o)3p^5P_2$	7774.17	11000	1	1.05	0.544	1.93	C+	11
$3s\ ^5S^o_2$-$(^4S^o)3p^5P_1$	7775.39	11000	1	1.05	0.544	1.93	C+	11
$3s\ ^5S^o$-$(^4S^o)4p^5P$	3947.3	11580	0.397	0.62	0.416	1.49	B+	7
		12080	0.57	0.83	0.606	1.37	B	2
		12500	0.784	1.20	0.842	1.43	B+	7
		13570	0.441	0.64	0.486	1.32	B	7
$3s\ ^3S^o$-$(^4S^o)4p^3P$	4368.3	10100	0.191	0.39	0.249	1.57	B	6
		10600	0.240	0.51	0.317	1.61	A	9
		10960	0.312	0.67	0.416	1.61	A	9
		11580	0.397	0.78	0.539	1.45	B+	7
		11800	0.45	0.59	0.614	0.96	C	1
		12080	0.57	1.08	0.784	1.38	B	2
		12500	0.784	1.44	1.09	1.32	B+	7
		12700	0.713	1.37	0.996	1.38	B	6
		13800	1.11	1.36	1.59	0.86	C	1
$3s\ ^3S^o$-$(^4S^o)5p^3P$	3692.4	12080	0.57	2.72	1.81	1.50	C	2
$3p\ ^5P$-$(^4S^o)4d^5D^o$	6157.3	11000	1	37.2	16.7	2.23	D	4
		11800	0.45	5.05	8.05	0.63	D	1
		13800	1.11	12.2	18.4	0.66	D	1
$4s\ ^5S^o$-$(^4S^o)4p^5P$	27645.2	11200	0.291	22	20.5	1.07	C	5
$4p\ ^5P$-$(^4S^o)4d^5D^o$	26520.4	11200	0.291	107.5	108	0.995	C	5
$4p\ ^3P$-$(^4S^o)4d^3D^o$	30973.0	11200	0.291	185.0	152	1.22	C	5

the ion contribution, so a theory of unified type or a quasistatic method should be used for ions. To approximately estimate this influence, we calculated line widths due to collisions with Ar II ions (working gas in this experiment) for plasma conditions corresponding to the experiment in Mijatović et al. (1995), with the best accuracy, labeled as A, but for transitions 3s $^3S^o$-$(^4S^o)3p^5P$ and 3s $^5S^o$-$(^4S^o)3p^5P$. We obtained that the widths due to electron impacts should be increased by 30.5% and 29.0% respectively. If we increase the line widths of 3s $^3S^o$-$(^4S^o)4p^5P$ for 30%, the ratio of experimental and theoretical values will

Table 2. Same as in Table 1, but for shift *d*.

Transition	λ [Å]	T [K]	N [10^{17} cm^{-3}]	d_{exp}	d_{th}	$\frac{d_{exp}}{d_{th}}$	Acc.	Ref.
3s $^5S^o$-($^4S^o$)4p^{5}P	3947.3	11580	0.397	0.05	0.0308	1.62	D	7
		12080	0.57	-0.13	0.0457	-2.84	B	2
		12500	0.784	0.09	0.0645	1.40	D	7
3s $^5S^o_2$-($^4S^o$)3p$^5P_3$	7771.94	11000	1	0.15	0.160	0.94	C	11
		11200	1	0.14	0.159	0.88	C+	10
3s $^5S^o_2$-($^4S^o$)3p$^5P_2$	7774.17	11000	1	0.15	0.160	0.94	C	11
3s $^5S^o_2$-($^4S^o$)3p$^5P_1$	7775.39	11000	1	0.15	0.160	0.94	C	11
3s $^3S^o$-($^4S^o$)4p^{3}P	4368.3	10600	0.240	0.10	0.113	0.88	A	9
		10960	0.312	0.13	0.146	0.89	A	9
		11580	0.397	0.12	0.184	0.65	C+	7
		11800	0.45	0.16	0.208	0.77	C	1
		12080	0.57	0.20	0.263	0.76	B	2
		12500	0.784	0.27	0.359	0.75	C+	7
		13800	1.11	0.36	0.528	0.68	C	1
3p ^{5}P-($^4S^o$)4d$^5D^o$	6157.3	11800	0.45	4.3	2.88	1.49	D	1
		13800	1.11	9.9	6.08	1.63	D	1
3s $^3S^o$-($^4S^o$)5p^{3}P	3692.4	12080	0.57	0.18	-0.187	-0.96	C	2
4p ^{5}P-($^4S^o$)4d$^5D^o$	26520.4	11200	0.291	42.9	37.7	1.14	C	5

be 1.24 instead of 1.61, which is within the errors of experiment and theory. So we can conclude that we recommend the experimental values from the first group and that they are confirmed by our calculation and analysis.

If we look at Table 2, where the experimental and theoretical results for shift are presented, we can notice that shift values are much smaller than the corresponding widths. Namely, as a difference with the width calculations where all contributions are positive, in the case of the shift we have positive and negative contributions, and if there is their mutual cancellation, shifts are smaller. If they are much smaller than the corresponding widths, like in the present case, the accuracy of theoretical calculations is smaller and also, the experiment has more difficulties. The majority of the shifts in Table 2 have values of ratios of experimental and theoretical shifts between 0.68 and 0.95. Only for 3947.3 Å multiplet in Goly & Weniger (1987), 6157.3 Å multiplet in, Jung (1963) and 26520.4 multiplet in Assous (1970) shift ratios have values within the range 1.14 - 1.63. An exception are the results in Wiese & Murphy (1963), who obtained the shift with a different sign from theoretical ones. In the case of 3s $^5S^o$-($^4S^o$)4p^{5}P transition, in the experiment of Goly & Weniger (1987) the shift is positive as in the present calculations, but its accuracy is denoted as "D". Since the shift is much smaller than width the new experiments are needed for this transition. The sign of the shift, different from the theoretical one is in Ref. Wiese & Murphy (1963), also for the transition 3s $^3S^o$-($^4S^o$)5p^{3}P. However in this case, due to close perturbing atomic energy level 4d^{3}D, which is lower than the level 5p^{3}P, the shift must be negative as it is obtained theoretically, while in the experiment, it is positive. In this case, also, new measurements would be of interest.

4. Conclusion

The Stark broadening parameters, including spectral line FWHM and shifts, have been calculated for O I lines reported in the literature using the impact semiclassical perturbation theory (Sahal-Bréchot, 1969a,b; Sahal-Bréchot et al., 2014). The obtained results were compared with the experimental data, and the corresponding agreement was discussed to further verify the experimental data considered. These results were compared with the experimental data, and the level of agreement was analyzed to further validate the experimental conclusions. Strong broadening data for neutral oxygen spectral lines are valuable for stellar spectrum analysis and synthesis, stellar atmosphere modeling, laboratory plasma diagnostics, and various plasma technological applications.

Acknowledgements. This article is based upon work from COST Action CA21136 Addressing observational tensions in cosmology with systematics and fundamental physics (CosmoVerse) supported by COST (European Cooperation in Science and Technology).

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