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ASTRONOMY AND ASTROPHYSICS

Simple estimates for Stark broadening of ion lines in stellar plasmas

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Summary. Simple analytical expressions for estimation of Stark widths and shifts of ionized atom lines have been derived from the low temperature limit of a modified semiempirical formula.

Key words: lines: profile – atomic and molecular data

1. Introduction

In stellar atmosphere calculations, collisional broadening parameters for a large number of lines of various elements are required and they are frequently unavailable [for critical reviews of available experimental data on Stark broadening of non-hydrogenic atom and ion lines see Konjević and Roberts (1976), Konjević and Wiese (1976), and Konjević et al. (1984a, b)]. Moreover in O and B stars and white dwarfs atmospheres the Stark effect is the main pressure broadening mechanism. Even in atmospheres of relatively cool stars, such as the Sun, where line broadening caused by collisions with neutral perturbers is dominant, for higher members of spectral series the Stark effect may compete with the neutral perturber interaction on the emitter (Vince et al., 1985a, b). For evaluation of Stark broadening parameters, one can use the so-called semi-classical approach or a fully quantum mechanical theoretical approach (see e.g. Griem, 1974 and references therein), which requires elaborate calculations even for a single line. For large-scale calculations, when high accuracy for each particular line is not required, simple approximations with good average accuracy are very useful. For neutral atom lines the simplified semi-classical method (Freudenstein and Cooper, 1978; Dimitrijević and Konjević, 1986) is very convenient, while for singly ionized atoms the semi-empirical method of Griem (1968) (see also Hey, 1977; Hey and Breger, 1982) is suggested. This method has been modified recently in order to avoid an extensive set of input atomic data and extended also to multiply charged ion line widths (Dimitrijević and Konjević, 1980, 1981) and shifts (Dimitrijević and Kršljanin, 1986). Tables of calculated Stark widths of prominent lines of some doubly and triply-charged ions are given by Dimitrijević and Konjević (1981). By inspecting these tables one can determine that for typical conditions in hot stars and white dwarfs atmospheres ($T \sim 10^4$ K) the threshold value of the required Gaunt factor may be aften used in the modified semi-empirical approach for most of the intense lines in doubly – and triply – charged ion spectra. When such a situation occurs, considerable simplification of the semi-empirical method occurs (Griem, 1968). The aim of this paper is to obtain in analytical form the low temperature limit of the modified semi-empirical formulae (Dimitrijević and Konjević, 1980; Dimitrijević and Kršljanin, 1986) which can be useful for simple estimates of Stark broadening parameters of singly and multiply charged ion lines in plasmas.

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2. Theory

Stark widths and shift of isolated ion lines can be calculated e.g. from the modified semi-empirical formula (Dimitrijević and Konjević, 1980), which for the full widths (in angular frequency units) has the following form:

$$w = N\frac{8\pi}{3}\frac{\hbar^2}{m^2}\left(\frac{2m}{\pi kT}\right)^{1/2}\frac{\pi}{\sqrt{3}}\left[\boldsymbol{R}^2_{l_i,l_i+1}\tilde{g}\left(\frac{E}{\Delta E_{l_i,l_i+1}}\right) + \boldsymbol{R}^2_{l_i,l_i-1}\tilde{g}\left(\frac{E}{\Delta E_{l_i,l_i-1}}\right) + \boldsymbol{R}^2_{l_f,l_f+1}\tilde{g}\left(\frac{E}{\Delta E_{l_f,l_f+1}}\right) + \boldsymbol{R}^2_{l_f,l_f-1}\tilde{g}\left(\frac{E}{\Delta E_{l_f,l_f-1}}\right) + \sum_{i'}(\boldsymbol{R}^2_{ii'})_{\Delta n\neq 0}\,g\left(\frac{3kTn_i^3}{4Z^2E_H}\right) + \sum_{f'}(\boldsymbol{R}^2_{ff'})_{\Delta n\neq 0}\,g\left(\frac{3kTn_f^3}{4Z^2E_H}\right)\right]. \quad (1)$$

$$\boldsymbol{R}^2_{ll'} \cong \left(\frac{3n}{2Z}\right)^2\frac{l_>}{2l+1}(n^2-l_>^2)\,\phi^2$$

$$\sum_{j'}(\boldsymbol{R}^2_{jj'})_{\Delta n\neq 0} \cong \left(\frac{3n_j}{2Z}\right)^2\frac{1}{9}(n_j^2+3l_j^2+3l_j+11),$$

where N and T are the electron density and electron temperature respectively, $E=3kT/2$ is the energy of perturbing electron, and $E_{jj'}=|E_{j'}-E_j|$ is the energy difference between levels j and j', $l_>=\max(l,l')$, $Z-1$ is the ionic charge ϕ is a tabulated correction factor (Bates and Damgaard, 1949; Oertel and Shomo, 1968) n is the effective principal quantum number while g (Griem, 1968) and $\tilde{g}$ (Dimitrijević and Konjević, 1980) are the effective Gaunt factors.

The comparison between experiments and the results obtained from Eq. (1) yields as an average ratio of measured to calculated widths of 1.06 ± 0.31 for doubly-, while for triply-ionized atoms this ratio is 0.92 ± 0.42 (Dimitrijević and Konjević, 1980).

When the nearest perturbing level is so far from E_j that $E/\Delta E \leq 2$ is satisfied, Griem's semi-empirical formula may be considerably simplified (Griem, 1968).

Table 1. Comparison of measured w_m and calculated Stark widths of doubly and triply ionized atoms. The values for the experimental widths w_m are normalized for electron density $N = 10^{17}$ cm^{-3}. The element, transition, multiplet number and electron temperature are given. Ratios of measured w_m to theoretical results are given in the following order: $w_{\mathrm{Eq.(1)}}$ modified semi-empirical formula Eq. (1) and $w_{\mathrm{Eq.(2)}}$ low temperature limit of same formula, Eq. (2). References: 1. Platiša et al. (1975a); 2. Purcell and Barnard (1984); 3. Platiša et al. (1975b); 4. Purić et al. (1974); 5. Platiša et al. (1977a); 6. Platiša et al. (1979); 7. Platiša et al. (1977b); 8. Platiša et al. (1975c); 9. Bogen (1972); 10. El-Farra and Hughes (1983)

Ion	Transition (mult. No.)	T(K)	w_m(Å) at 10^{17} cm^{-3}	$\frac{w_m}{w_{\mathrm{Eq.(1)}}}$	$\frac{w_m}{w_{\mathrm{Eq.(2)}}}$	Ref.
N III	$3s^2S-3p^2P^0$ (1)	24300	0.17	0.82	0.89	1
	$3p^2P^0-3d^2D$ (2)	24300	0.21	0.76	1.14	1
		36100	0.27	1.23	1.84	2
	$3s^4P^0-3p^4D$ (5)	24300	0.18	1.18	1.29	1
O III	$3s^3P^0-3p^3D$ (2)	25900	0.14	1.03	1.13	3
	$3s^3P^0-3p^3P$ (4)	25900	0.11	1.09	1.19	3
	$3p^3D-3d^3F^0$ (8)	25900	0.12	1.15	1.85	3
	$3p^3P-3d^3D^0$ (14)	25900	0.14	0.93	1.40	3
Si III	$4s^3S-4p^3P^0$ (2)	16400	0.38	0.67	0.57	4
		25600	0.31	0.68	0.58	5
S III	$3d^3P^0-4p^3P$ (2)	28500	0.15	1.16	1.40	6
	$3d^3D^0-4p^3P$ (8)	28500	0.17	0.96	1.12	6
	$4s^3P^0-4p^3D$ (4)	28500	0.25	0.88	0.79	6
	$4s^3P^0-4p^3P$ (5)	28500	0.20	0.86	0.77	6
	$4s^3P^0-4p^3S$ (6)	28500	0.18	0.84	0.76	6
	$4p^3D-4d^3F^0$ (15 UV)	28500	0.20	1.56	1.16	6
	$4p^3D-4d^3D^0$ (16 UV)	28500	0.20	1.64	1.20	6
	$4p^3P-4d^3D^0$ (18 UV)	28500	0.21	1.43	1.04	6
Cl III	$3d^4P-4p^4P^0$ (7)	24200	0.19	1.04	1.38	7
	$4s^4P-4p^4D^0$ (1)	24200	0.10	1.00	0.91	7
	$4s^4P-4p^4P^0$ (2)	24200	0.17	1.08	0.98	7
	$4s^4P-4p^4S^0$ (3)	24200	0.17	1.10	1.00	7
	$4s^2P-4p^2D^0$ (5)	24200	0.19	0.92	0.81	7
	$4s'^2D-4p'^2F^0$ (10)	24200	0.18	1.05	0.93	7
	$4s'^2D-4p'^2D^0$ (11)	24200	0.14	0.90	0.80	7
Ar III	$3d''^3P^0-4p''^3P$ (6)	21100	0.13	1.18	1.46	8
	$4s^5S^0-4p^5P$ (1)	21100	0.15	1.02	0.89	8
	$4s'^3D^0-4p'^3D$ (2)	21100	0.13	0.81	0.88	8
	$4s'^3D^0-4p'^3F$ (3)	21100	0.14	0.94	0.86	8
C IV	$2s^2S-2p^2P^0$ (1 UV)	58000	0.006	1.99	2.74	9
		53000	0.0027	1.09	1.18	10
Si IV	$4s^2S-4p^2P^0$ (1)	25600	0.22	0.57	0.52	5
S IV	$4s^2S-4p^2P^0$ (1)	28500	0.12	0.80	0.71	6
Ar IV	$4s^4P-4p^4D^0$ (4 UV)	20750	0.06	0.74	0.54	8
		22200	0.06	0.74	0.55	8
	$4s^4P-4p^4P^0$ (5 UV)	20750	0.06	0.76	0.55	8
		22200	0.06	0.79	0.57	8

Here, we shall perform analogous simplification of the modified semi-empirical formula, Eq. (1), for all cases when $E/\Delta E \leqq 2$. Then $g = 0.2$ and $\tilde{g} = 0.9 - 1.1/Z$. Furthermore, one can put $\phi^2 = 1$ in Eq. (1) which is a reasonable assumption for $\Delta n = 0$ (see e.g. Griem, 1974, p. 31), since exact values of ϕ^2 usually range between 0.8 and 1. If one performs the summation in Eq. (1) it is easy to obtain

$$w(\text{Å}) = 0.4430\ 10^{-8}\ \frac{\lambda^2(\text{cm})\, N(\text{cm}^{-3})}{T^{1/2}(\text{K})} \cdot \sum_{j=i,f}\left[\boldsymbol{R}_j^2 + \frac{\tilde{g}_{th} - g_{th}}{g_{th}}\left(\frac{3n_j}{2Z}\right)^2 (n_j^2 - l_j^2 - l_j - 1)\right]$$

$$\boldsymbol{R}_j^2 = \sum_{j'} \boldsymbol{R}_{jj'}^2 .$$

Since the contribution to the total line width of the transitions with $\Delta n \neq 0$ does not exceed 25% and it is compensated by assuming $\phi^2 = 1$, we can neglect them and finally obtain

$$w(\text{Å}) = 2.2151\ 10^{-8}\ \frac{\lambda^2(\text{cm})\, N(\text{cm}^{-3})}{T^{1/2}(\text{K})} \cdot \left(0.9 - \frac{1.1}{Z}\right) \sum_{j=i,f}\left(\frac{3n_j}{2Z}\right)^2 (n^2 - l_j^2 - l_j - 1), \tag{2}$$

where n_i and n_f are the effective quantum numbers of the upper and lower energy levels of the transition.

Recently, a modified semi-empirical formula for the shift has also been reported (Dimitrijević and Kršljanin, 1986). Since we are interested in the low temperature limit, we shall, as in previous case, neglect the collisions with $\Delta n \neq 0$. Then the simplified version of the modified semi-empirical formula for the shift is

$$d = N\,\frac{4\pi}{3}\,\frac{\hbar^2}{m}\left(\frac{2m}{\pi kT}\right)^{1/2}\frac{\pi}{\sqrt{3}}\left[\boldsymbol{R}^2_{l_i,l_i+1}\,\tilde{g}_{sh}\left(\frac{E}{\Delta E_{l_i,l_i+1}}\right) - \boldsymbol{R}^2_{l_i,l_i-1}\,\tilde{g}_{sh}\left(\frac{E}{\Delta E_{l_i,l_i-1}}\right) - \boldsymbol{R}^2_{l_f,l_f+1}\,\tilde{g}_{sh}\left(\frac{E}{\Delta E_{l_f,l_f+1}}\right) + \boldsymbol{R}^2_{l_f,l_f-1}\,\tilde{g}_{sh}\left(\frac{E}{\Delta E_{l_f,l_f-1}}\right) + \sum_k \delta_k\right]. \tag{3}$$

The sum $\sum_k \delta_k$ is not equal to zero only if perturbing levels strongly violating the assumed approximations exist, i.e. if there are levels with $|\Delta E_{jj'}| \ll |\Delta E_{n,n+1}|$. The contribution of each such level should be calculated as

$$\delta_j = \pm\,\varepsilon_j(\boldsymbol{R}^2_{jj'})\left[g_{sh}\left(\frac{E}{\Delta E_{j,j'}}\right) \pm g_{sh}\left(\frac{E}{\Delta E_{n_i,n_i+1}}\right)\right]$$

where the lower sign corresponds to $\Delta E_{jj'} < 0$ and

$$\varepsilon_j = \begin{cases} +1, j = i \\ -1, j = f. \end{cases}$$

Taking into account that $\tilde{g}_{sh} \equiv \tilde{g}$ and g_{sh} near the threshold, and applying the same procedure as for the width, we obtain, for $E/\Delta E \leqq 2$

$$d \approx 1.1076\ 10^{-8}\ \frac{\lambda^2(\text{cm})\, N(\text{cm}^{-3})}{T^{1/2}(\text{K})}\left(0.9 - \frac{1.1}{Z}\right)\frac{9}{4Z^2}\sum_{j=i,f}\frac{n_j^2\,\varepsilon_j}{2l_j+1} \cdot \left\{(l_j+1)\,[n_j^2 - (l_j+1)^2] - l_j(n_j^2 - l_j^2)\right\}. \tag{4}$$

If all levels $l_{i,f} \pm 1$ exist, an additional summation may be performed in Eq. (4) to obtain

$$d \approx 1.1076\ 10^{-8}\ \frac{\lambda^2(\text{cm})\, N(\text{cm}^{-3})}{T^{1/2}(\text{K})}\left(0.9 - \frac{1.1}{Z}\right)\frac{9}{4Z^2} \cdot \sum_{j=i,f}\frac{n_j^2\,\varepsilon}{2l_j+1}\,(n_j^2 - 3l_j^2 - 3l_j - 1). \tag{5}$$

3. Results and discussion

3.1. Widths

In order to test the equation obtained for the low temperature limit of the modified semi-empirical formula we compared first the results from Eq. (2) with the results of comprehensive width calculations for doubly and triply ionized atoms (Dimitrijević and Konjević, 1981) in which Eq. (1) is used. The discrepancy did not exceed ±30% on the average. Furthermore, in Table 1 comparison is made between the results from Eq. (1) and Eq. (2) for the experimental results obtained at electron temperatures when condition $E/\Delta E_{jj'} \leqq 2$ is satisfied. Experimental data in Table 1 are taken from Tables 1 and 2 of the paper by Dimitrijević and Konjević (1980), which have been further updated by new results.

Table 2. Comparison of experimental and theoretical Stark widths of analogous transitions of doubly ionized inert gases, multiplets $ns\,^3S^0 - np\,^3P$: w_m – experimental data (Konjević and Pittman, 1984) and $w_{\text{Eq.(1)}}$ and $w_{\text{Eq.(2)}}$ calculated ones using Eqs. (1) and (2) respectively

Ion	Wavelength	Temperature	Full width in Å units at $N = 10^{17}\ \text{cm}^{-3}$		
	(Å)	(K)	w_m	$w_{\text{Eq.(1)}}$	$w_{\text{Eq.(2)}}$
Ne III	2677.90	34000	0.063	0.052	0.049
	2678.64	34000	0.062	0.052	0.049
Ar III	3509.33	27500	0.160	0.153	0.174
	3514.18	27500	0.148	0.153	0.174
Kr III	3564.23	26000	0.160	0.168	0.194
Xe III	3780.98	27000	0.222	0.235	0.267

From Table 1 the average ratio of experimental w_m and calculated values from Eq. (1) and (2) are 1.01 and 1.04, respectively. Finally, in Table 2 are given the results obtained from Eqs. (1) and (2) together with recently measured Stark widths (Konjević and Pittman, 1984) of analogous transitions of doubly ionized inert gases. Here, the condition $E/\Delta E_{jj'} \leqq 2$ is always satisfied and the agreement between two sets of calculated data is within $\pm 15\%$, while the discrepancy with the experiment does not exceed 21%. Therefore, on the basis of comparisons in Tables 1 and 2 we estimate that the results of Eq. (2) for widths of doubly- and triply-ionized atoms agree with experiment within $\pm 40\%$. The experimental results for higher ionization stages are not available for comparison.

3.2. *Shifts*

The possibilities of the theory and expected accuracy in the case of shifts are considerably smaller than for the line widths (see e.g. Dimitrijević et al., 1981; Griem, 1974). In Figs. 1–3 comparison is made between various experimental results for Be II $2s^2S-2p^2P^0$, Mg II $3p^2P^0-4s^2S$ and Ca II $4s^2S-4p^2P^0$ lines, calculations according to Eq. (4) and other theoretical calculations. On the basis of the comparison of data in Figs. 1–3 one can conclude that the agreement of the proposed simple method with experimental results is at least comparable with more elaborate approaches.

We believe that simple formulae, Eqs. (2) and (4), will be adequate when astrophysicists require a large number of ion line widths of doubly and triply charged ions due to the Stark broadening. The estimate requires only the knowledge of atomic data for ionization potentials, energy levels and orbital quantum numbers of the upper and lower level of the considered transition. However, before using Eqs. (2) and (4), the condition $E/\Delta E_{jj'} \leqq 2$ should be checked, and if this condition is not satisfied Eqs. (1) or (3) must be used.

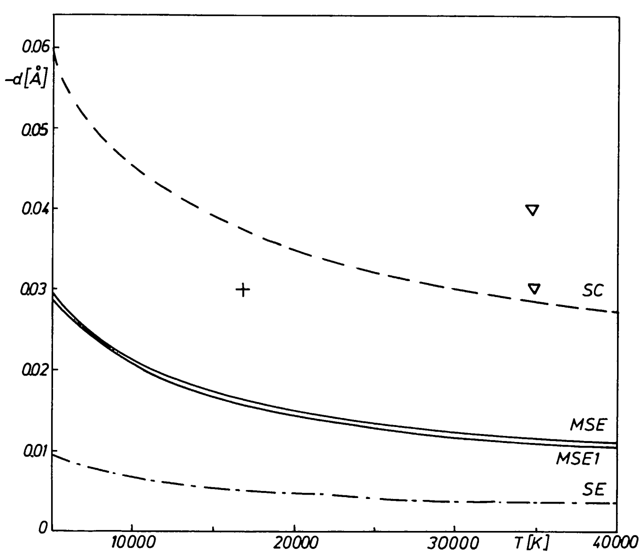

Fig. 1. Stark shifts for Be II $2s^2S-2p^2P^0$ multiplet. Calculations: MSE – modified semi-empirical (Dimitrijević and Kršljanin, 1986); MSE1 – present results; SE – semi-empirical according to Griem (1968); SC – semi-classical, Jones et al. (1971); QM – quantum mechanical, Barnes and Peach (1970). Experimental points: + – Purić and Konjević (1972); △ – Hadžiomerspahić et al. (1973); △ – Roberts and Barnard (1972); ○ – Fleurier et al. (1977); □ – Helbig and Kusch (1972)

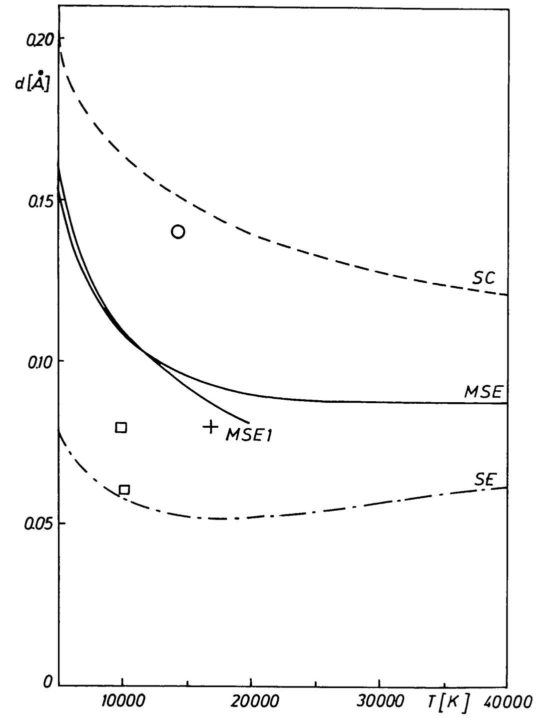

Fig. 2. Stark shifts for Mg II $3p^2P^0-4s^2S$ multiplet. Notation is the same as in Fig. 1

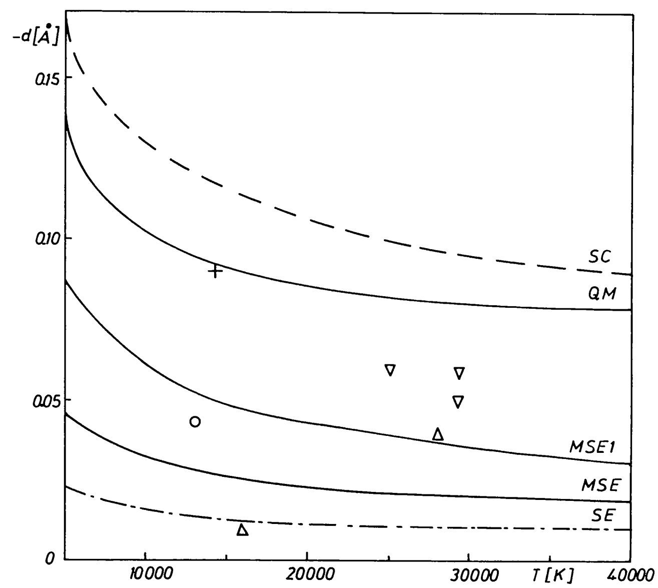

Fig. 3. Stark shifts for Ca II $4s^2S-4p^2P^0$ multiplet. Notation is the same as in Fig. 1

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