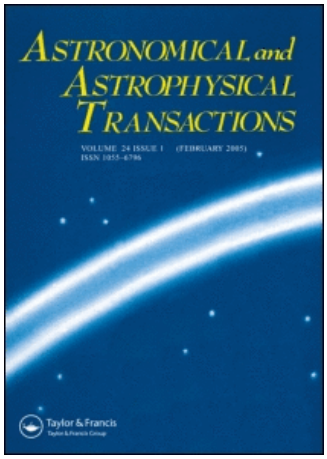

Astronomical & Astrophysical Transactions
The Journal of the Eurasian Astronomical Society
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713453505

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Online Publication Date: 01 August 1999
To cite this Article: Dimitrijević, M. S. (1999) 'Stark broadening data for stellar plasma research', Astronomical & Astrophysical Transactions, 18:1, 163 - 169
To link to this article: DOI: 10.1080/10556799908203051
URL: http://dx.doi.org/10.1080/10556799908203051

Astronomical and Astrophysical Transactions, 1999, Vol. 18, pp. 163–169
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STARK BROADENING DATA FOR STELLAR PLASMA RESEARCH

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(Received November 26, 1996)

Results of an effort to provide to astrophysicists and physicists an as much as possible complete set of Stark broadening parameters needed for stellar opacity calculations, stellar atmosphere modelling, abundance determinations and diagnostics of different plasmas in astrophysics, physics and plasma technology, are presented. Stark broadening has been considered within the semiclassical perturbation, and the modified semiempirical approaches.

KEY WORDS Lines, atomic and molecular data profiles, CP stars

1 INTRODUCTION

For a number of astrophysical problems, Stark broadening data for spectral lines of numerous atomic and ionic radiators/absorbers are needed, since the atmospheric composition of a star is not known a priori, and many interesting groups of stars exist with very peculiar abundances as compared to the Sun. Moreover, the development of space astronomy additionally stimulates interest in a very extensive list of line broadening data. For stellar plasma modelling, estimation of the radiative transfer through the stellar plasmas, especially in subphotospheric layers as well as for opacity calculations, data for especially large numbers of lines are needed. An illustrative example might be the article on the calculation of opacities for classical cepheid models (Iglesias *et al.*, 1990), where 11 996 532 spectral lines have been taken into account (45 lines of H, 45 of He, 638 of C, 54 of N, 2390 of O, 16 030 of Ne, 50 170 of Na, 105 700 of Mg, 145 200 of Al, 133 700 of Si, 12 560 of Ar and 11 530 000 of Fe), and where Stark broadening is important.

Stark broadening parameters are also needed for the determination of chemical abundances of elements from equivalent widths of absorption lines and for modelling and interpretation of stellar spectra, especially for white dwarfs and A type stars.

Results of our effort to provide to astrophysicists and physicists an as much as possible complete set of the needed Stark broadening parameters are presented here. Stark broadening has been considered within the semiclassical perturbation

(Sahal–Bréchot, 1969a,b), and the modified semiempirical approaches (Dimitrijević and Konjević, 1980).

2 THE SEMICLASSICAL PERTURBATION APPROACH

According to the semiclassical perturbation formalism (Sahal–Bréchot, 1969a,b; Fleurier *et al.*, 1977; Dimitrijević, Sahal–Bréchot and Bommier, 1991; Dimitrijević and Sahal–Bréchot, 1996a) approach, the Stark full width (W) at the intensity half maximum (FWHM) and shift (d) of an isolated spectral line, may be expressed as

$$\begin{aligned} W &= N \int v f(v)\, dv \left(\sum_{i' \neq i} \sigma_{ii'}(v) + \sum_{f' \neq f} \sigma_{ff'}(v) + \sigma_{\mathrm{el}} \right) + W_R \\ d &= N \int v f(v)\, dv \int_{R_3}^{R_D} 2\pi\rho\, d\rho \, \sin 2\phi_p \end{aligned} \tag{1}$$

where N is the electron density, $f(v)$ the Maxwellian velocity distribution function for electrons, ρ denotes the impact parameter of the incoming electron, i and f denote the initial and final atomic energy levels, and i', f' their corresponding perturbing levels, while W_R gives the contribution of the Feshbach resonances (Fleurier *et al.*, 1977). The inelastic cross-section $\sigma_{j,j'}(v)$ can be expressed by an integral over the impact parameter of the transition probability $P_{jj'}(\rho, v)$ as

$$\sum_{j' \neq j} \sigma_{jj'}(v) = \frac{1}{2}\pi R^2 + \int_{R_1}^{R_D} \sum_{j \neq j'} P_{jj'}(\rho, v), \quad j = i, f \tag{2}$$

and the elastic cross-section is given by

$$\begin{aligned} \sigma_{\mathrm{el}} &= 2\pi R_2^2 + \int_{R_2}^{R_D} 8\pi\rho\, d\rho \, \sin^2 \delta \\ \delta &= (\phi_p^2 + \phi_q^2)^{1/2}. \end{aligned} \tag{3}$$

The phase shifts ϕ_p and ϕ_q due respectively to the polarization potential (r^{-4}) and to the quadrupolar potential (r^{-3}), are given in Section 3 of Chapter 2 in Sahal–Bréchot (1969a). R_D is the Debye radius. All the cut-offs R_1, R_2, R_3 are described in Section 1 of Chapter 3 in Sahal–Bréchot (1969b).

The semiclassical perturbation approach has been tested on critically selected experimental data for helium (Dimitrijević and Sahal–Bréchot, 1985) and it was found that the averaged ratio of experimental and theoretical data is 1.17 ± 0.04 for widths and 1.07 ± 0.04 for shifts, which is well within the limits of 20 percent, the predicted accuracy of the semiclassical method (Griem, 1974).

3 THE MODIFIED SEMIEMPIRICAL METHOD

According to the modified semiempirical method (Dimitrijević and Konjević, 1980; Dimitrijević and Konjević, 1981, Dimitrijević and Kršljanin, 1986; Dimitrijević and Konjević, 1987; Dimitrijević, 1988a,b), the electron impact full width (FHWM) of an ion line is given as

$$W_{\mathrm{MSE}} = N\frac{8\pi}{3}\frac{\hbar^2}{m^2}\left(\frac{2m}{\pi kT}\right)^{1/2}\frac{\pi}{\sqrt{3}}\cdot\left\{\sum_{l_i\pm1}R^2[n_il_i,n_i(l_i\pm1)]\tilde{g}\left(\frac{E}{\Delta E_{l_i,l_i\pm1}}\right)\right.$$
$$+\sum_{l_f\pm1}R^2[n_fl_f,n_f(l_f\pm1)]\tilde{g}\left(\frac{E}{\Delta E_{l_f,l_f\pm1}}\right)+\left(\sum_{i'}R^2_{ii'}\right)_{\Delta n\neq0}g(x_{n_i,n_i+1})$$
$$\left.+\left(\sum_{f'}R^2_{ff'}\right)_{\Delta n\neq0}g(x_{n_f,n_f+1})\right\}, \tag{4}$$

and the corresponding Stark shift as

$$d = N\frac{4\pi}{3}\frac{\hbar^2}{m^2}\left(\frac{2m}{\pi kT}\right)^{1/2}\frac{\pi}{\sqrt{3}}\cdot\left\{\varepsilon_{l_i,l_{i+1}}R^2[n_il_i,n_i(l_i+1)]\tilde{g}_{\mathrm{sh}}\left(\frac{E}{\Delta E_{l_i,l_{i+1}}}\right)\right.$$
$$-\varepsilon_{l_i,l_{i-1}}R^2[n_il_i,n_i(l_i-1)]\tilde{g}_{\mathrm{sh}}\left(\frac{E}{\Delta E_{l_i,l_{i-1}}}\right)$$
$$-\varepsilon_{l_f,l_{f+1}}R^2[n_fl_f,n_f(l_f+1)]\tilde{g}_{\mathrm{sh}}\left(\frac{E}{\Delta E_{l_f,l_{f+1}}}\right)$$
$$+\varepsilon_{l_f,l_{f-1}}R^2[n_fl_f,n_f(l_f-1)]\tilde{g}_{\mathrm{sh}}\left(\frac{E}{\Delta E_{l_f,l_f-1}}\right)+\left(\sum_{i'}R^2_{ii'}\right)_{\Delta n\neq0}g_{\mathrm{sh}}(x_{n_i},x_{n_i+1})$$
$$-2\sum_{i'(\Delta E_{ii'}<0)}R^2_{ii',\Delta n\neq0}g_{\mathrm{sh}}\left(\frac{E}{\Delta E_{n_i,l_i,n_{i'}l_{i'}}}\right)-\left(\sum_{f'}R^2_{ff'}\right)_{\Delta n\neq0}g_{\mathrm{sh}}(x_{n_f},x_{n_f+1})$$
$$\left.+2\sum_{f'(\Delta E_{ff'}<0)}R^2_{ii',\Delta n\neq0}g_{\mathrm{sh}}\left(\frac{E}{\Delta E_{n_f,l_f,n_{f'}l_{f'}}}\right)+\sum_k\delta_k\right\} \tag{5}$$

where the square of the matrix element $\{R^2[n_kl_k,n_k(l_k\pm1)],\ k=i,f\}$ is

$$R^2[n_kl_k,n_k(l_k\pm1)]=\left(\frac{3n_k^*}{2Z}\right)^2\frac{l_>}{2l_k+1}(n_k^{*2}-l_k^2)\Phi^2(n_{l_k-1}^{*2},n_{l_k}^{*2},l_k) \tag{6}$$

and

$$\left(\sum_{k'}R^2_{kk'}\right)_{\Delta n\neq0}=\left(\frac{3n_k^*}{2Z}\right)^2\frac{1}{9}(n_k^{*2}+3l_k^2+3l_k+11). \tag{7}$$

Here $l_>=\max(l_k,l_{k'})$, and l denotes the angular momentum quantum number.

In equations (4)–(7) Φ^2 is the Bates–Damgaard factor tabulated e.g. in Oertel and Shomo (1968), $g(x)$, $g_{\mathrm{sh}}(x)$ and $\tilde{g}(x)$, $\tilde{g}_{\mathrm{sh}}(x)$ are the semiempirical (Griem, 1968)

and the modified semiempirical (Dimitrijević and Konjević, 1980; Dimitrijević and Kršljanin, 1986) Gaunt factors for Stark width and shift, respectively. The factor $\varepsilon_{kk'} = (E_{k'} - E_k)/|E_{k'} - E_k|$, where E_k and $E_{k'}$ are the energy of the considered level and its pertubing level. The sum $\sum_k \delta_k$ is different from zero only if perturbing levels strongly violating the assumed approximations exist and may be evaluated as

$$\delta_i = \pm R^2_{ii'}[g_{\rm sh}\left(\frac{E}{\Delta E_{i,i'}}\right) \mp g_{\rm sh}(x_{n_i,n_i+1})], \tag{8}$$

for the upper level, and

$$\delta_f = \mp R^2_{ff'}[g_{\rm sh}\left(\frac{E}{\Delta E_{f,f'}}\right) \mp g_{\rm sh}(x_{n_f,n_f+1})], \tag{9}$$

for the lower level. In equations (8) and (9) the lower signs correspond to

$$\Delta E_{jj'} < 0; \quad x_{n_k,n_k+1} \approx 3kTn^{*3}_k/(2Z^2E_H),$$

where $\Delta E_{kk'} = |E_k - E_{k'}|$, n_k is the principal quantum number, n^*_k the effective principal quantum number, $E = 3kT/2$ and $(Z-1)$ is the ionic charge.

The modified semiempirical approach needs a considerably smaller amount of atomic data than full semiclassical or quantum mechanical calculations. In fact, if there are no perturbing levels strongly violating the assumed approximation, for e.g. the line width calculations, we need only the energy levels with $\Delta n = 0$ and $l_{if} = l_{if} \pm 1$, since all perturbing levels with $\Delta n \neq 0$, needed for a full semiclassical investigation, are lumped together and approximately estimated.

For astrophysical purposes, of particular interest might be the simplified semiempirical formula (Dimitrijević and Konjević, 1987) for Stark widths of isolated, singly, and multiply charged ion lines applicable in the cases when the nearest atomic energy level ($j' = i'$ or f') where a dipole allowed transition can occur from or to the initial (i) or final (f) energy level of the considered line, is so far, that the condition $x_{jj'} = E/|E_{j'} - E_j| \leq 2$ is satisfied. In such cases the full width at half maximum is given by the expression (Dimitrijević and Konjević, 1987):

$$\begin{aligned} W(\text{Å}) &= 2.2151 \times 10^{-8} \frac{\lambda^2(\text{cm})N(\text{cm}^{-3})}{T^{1/2}(\text{K})}\left(0.9 - \frac{1.1}{Z}\right) \\ &\times \sum_{j=i,f}\left(\frac{3n^*_j}{2Z}\right)^2 (n^{*2}_j - l^2_j - l - 1). \end{aligned} \tag{10}$$

Similarly, in the case of the shift

$$\begin{aligned} d(\text{Å}) &= 1.1076 \times 10^{-8} \frac{\lambda^2(\text{cm})N(\text{cm}^{-3})}{T^{1/2}(\text{K})}\left(0.9 - \frac{1.1}{Z}\right)\frac{9}{4Z^2} \\ &\times \sum_{j=i,f} \frac{n^*_j\varepsilon^2_j}{2l_j+1}(l_j+1)[n^{*2}_j - (l_j+1)^2] - l_j(n^{*2}_j - l^2_j), \end{aligned} \tag{11}$$

where $\varepsilon = +1$ if $j = i$ and -1 if $j = f$.

If all levels $l_{i,f} \pm 1$ exist, an additional summation may be performed in equation (11) to obtain

$$d(\text{Å}) = 1.1076 \times 10^{-8} \frac{\lambda^2(\text{cm}) N(\text{cm}^{-3})}{T^{1/2}(\text{K})} \left(0.9 - \frac{1.1}{Z}\right) \frac{9}{4Z^2} \times \sum_{j=i,f} \frac{n_j^* \varepsilon_j^2}{2l_j + 1} (n_j^{*2} - 3l_j^2 - 3l_j - 1). \quad (12)$$

The averaged values of the ratios of measured to calculated widths for the modified semiempirical approach are (Dimitrijević and Konjević, 1980): for doubly charged ions 1.06±0.32 and for triply charged ions 0.91±0.42. The modified semiempirical approach has been tested several times on numerous examples (Dimitrijević, 1990). For singly charged ions, results obtained with the modified semiempirical approach are similar to results obtained with the Griem's semiempirical formula (Griem, 1968). However, while in order to apply the Griem's semiempirical formula one needs the same atomic data set as for the full semiclassical calculations, for the modified semiempirical formula this data set is minimized, so that it is applicable. It is also useful when it is not possible to apply more sophisticated approaches, due to the lack of reliable atomic data.

4 RESULTS AND DISCUSSION

A review of the semiclassical Stark broadening parameter calculations based on the method developed by Sahal-Bréchot (1969a,b), together with the corresponding references exists in Dimitrijević (1996). During our efforts over more than twenty years to provide the reliable semiclassical Stark broadening data needed in astrophysics, we have calculated as a function of the temperature and in most of cases as a function of the perturber density as well the corresponding parameters for 79 neutral helium multiplets, 62 sodium, 51 potassium, 61 lithium, 25 aluminium, 24 rubidium, 3 paladium, 19 berrylium (see references in Dimitrijević, 1996), 270 magnesium (see references in Dimitrijević, 1996 and Dimitrijević and Sahal-Bréchot, 1996b), 33 strontium (Dimitrijević and Sahal-Bréchot, 1996c,d), 31 selenium (Dimitrijević and Sahal-Bréchot, 1996e,f), 14 barium (Dimitrijević and Sahal-Bréchot, 1997b, 1996g), 28 Ca II, 30 Be II (see references in Dimitrijević, 1996), 29 Li II (see references in Dimitrijević, 1996 and Dimitrijević and Sahal-Bréchot, 1996a), 52 Mg II (see references in Dimitrijević, 1996 and Dimitrijević and Sahal-Bréchot, 1995a, 1997a), 3 Fe II (see references in Dimitrijević, 1996), 2 Ni II (Dimitrijević and Sahal-Bréchot, 1995b), 64 Ba II (Dimitrijević and Sahal-Bréchot, 1996g, 1997b), Be III, B III (Dimitrijević and Sahal-Bréchot, 1996h,i), 23 Al III, 10 Sc III, 10 Ti IV, 39 Si IV, 90 C IV (see references in Dimitrijević, 1996), 114 P IV (Dimitrijević and Sahal-Bréchot, 1997c, 1996j), 5 O IV, 19 O V (see references in Dimitrijević, 1996 and Blagojević *et al.* 1996), 30 N V (see references in Dimitrijević, 1996), 25 C V, 51 P V (Dimitrijević and Sahal-Bréchot, 1995c, 1996k), 30 O VI, 21 S VI, 10 F VII,

20 Ne VIII, 8 Na IX, 7 Al XI and 9 Si XII (see references in Dimitrijević, 1996) multiplets become available.

Data for particular lines of F I, Ar II, Ga II, Ga III, Si II, Cl I, Br I, I I, Cu I, Hg II, N III, F V (see references in Dimitrijević, 1996) and S IV (Dimitrijević *et al.* 1996) also exist.

In order to achieve better accuracy, only transitions where for upper and lower level accurate data for all possible dipole allowed transitions with at least $\Delta n = 0, \pm 1, \pm 2$ exist, were selected. If additional reliable data on energy levels exist, they are included as well in the calculations. The accuracy of the method is estimated to be ± 20 percent. However, generally shifts are of smaller accuracy than widths. This is particularly significant when shifts are much smaller than widths, since then cancelations between important contributions with different signs may occur, and the accuracy decreases.

The modified semiempirical approach (Dimitrijević and Konjević, 1980; Dimitrijević and Konjević, 1981, Dimitrijević and Kršljanin, 1986; Dimitrijević and Konjević, 1987; Dimitrijević, 1988a,b) has been used as well for the calculation of Stark broadening parameters of astrophysically important spectral lines, as well as the lines important for laboratory plasma and laser produced plasma diagnostics and modelling, especially for radiators where there is not a sufficiently complete atomic data set for reliable semiclassical calculations. The width data for the most intensive lines for the following atom and ion species were calculated by us with the help of the modified semiempirical approach: Ti II, Mn II, Fe II, Bi II, Pt II, Zn II, Cd II, As II, Br II, Sb II, I II (see references in Dimitrijević, 1996), Xe II (Popović and Dimitrijević, 1996a), Sc II, Y II, Zr II (Popović and Dimitrijević, 1996b), S III (Dimitrijević *et al.*, 1996), Cu IV, Be III, B III, B IV, C III, C IV, N III, N IV, O III, O IV, F III, Ne III, Ne IV, Na III, Mg IV, Al III, Si III, Si IV, P III, P IV, S III, S IV, Cl III, Cl IV, Ar III, Ar IV, C V, N VI, O V, F V, F VI, Ne V, Ne VI, Al V, Si V, P VI, Cl VI and the shift data for Bi II, Zn II, Cd II, As II, Br II, Sb II, I II (see references in Dimitrijević, 1996), Xe II (Popović and Dimitrijević, 1996a), and Ar II lines. Since the accuracy of the shift calculations is lower, shift values are not given when experimental data enabling an additional checking, are not availlable.

We hope that the obtained set of semiclassical Stark broadening data for a large number of radiators will be of help for various problems in astrophysics, physics and plasma technology.

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