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APPROXIMATE METHODS FOR STARK BROADENING CALCULATIONS FOR ASTROPHYSICALLY IMPORTANT SPECTRAL LINES

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Abstract. A review of approximate methods for calculation of spectral line profiles in hot stellar plasma has been presented. We have discussed in detail the modified semiempirical method for Stark broadening parameters determination as well as the regularities and systematic trends for interpolation of new data and critical evaluation of existing ones.

1. INTRODUCTION

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, stellar spectroscopy depends on very extensive list of elements and line transitions with their atomic and line broadening parameters.

The interest for a very extensive list of line broadening data is additionally stimulated by the development of space astronomy, since with instruments like Goddhard High Resolution Spectrograph (GHRS) on Hubble Space Telescope, an extensive amount of high quality spectroscopic information over large spectral regions of all kind of celestial objects has been and will be collected, stimulating the spectral–line–shape research. The dramatic increase of accuracy and resolution is well illustrated in Fig. 1 where the χ Lupi UV spectrum obtained by IUE and GHRS are compared

Development of computers also stimulates the need for a large amount of atomic and spectroscopic data. Particularly large number of data is needed for example for opacity calculations. 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, 2 390 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 included. Another good

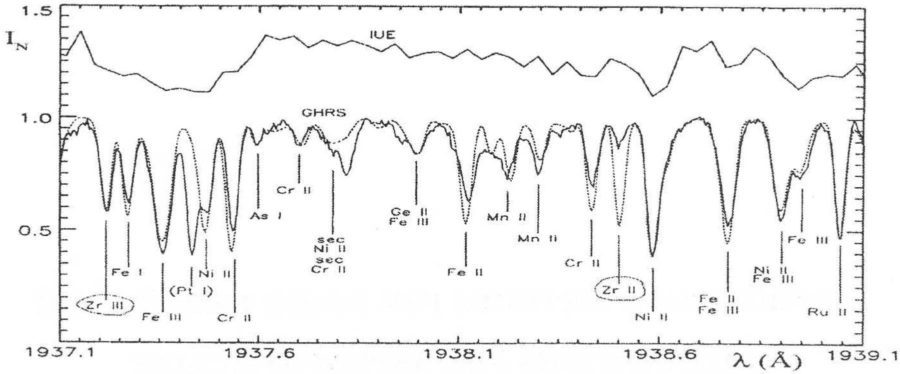

Fig. 1: The UV spectrum of χ Lupi obtained with GHRS and with IUE satellite (Leckrone et al. 1993). The resolution of GHRS spectrum is 0.0023 nm and the maximal signal to noise ratio is 95 (Brandt et al. 1999). The full line at GHRS spectrum is observed and the dotted synthesized one.

example for the need of an extensive set of atomic and spectroscopic data including Stark broadening is the modeling of stellar atmospheres. For example, PHOENIX (see Hauschildt and Baron, 1999 and references therein) computer code for the stellar modelling includes a database containing 42 x 10^6 atomic/ionic spectral lines.

Interesting investigations which shows the possibilities opened with the development of computer technology and indicating the need for as much as possible larger amount of spectroscopic and atomic data, are calculations of equivalent width changes with the age in starburst stellar clusters and galaxies (Gonzales-Delgado et al. 1999). In this research the change of particular hydrogen and helium lines equivalent widths during 500 milion years, has been calculated and compared with observations of stellar clusters and starburst galaxies. Calculations have been done in two steps. First, the population of stars of different spectral types, as a function of age are calculated, and then the profiles of the lines are synthesized by adding the different contributions from stars. For spectral line profiles synthesis the effects of natural, Stark, neutral atom impact and thermal Doppler broadening have been taken into account.

We draw attention here, that for temperatures of around 10 000 K or higher, hydrogen is mainly ionized and Stark broadening is the principal pressure broadening mechanism of spectral lines. Consequently, astronomers often need Stark broadening data for a large amount of spectral lines. In spite of the fact that very sophysticated methods for Stark broadening calculations exist, as e.g. quantum mechanical strong coupling method (see e.g. Dimitrijević et al. 1981, Dimitrijević 1996 and references therein) or semiclassical approach (see e.g. Jones et al. 1971, Benett and Griem 1971, Griem 1974, Sahal–Bréchot 1969ab), approximate approaches are often the unique way to obtain the needed information. Moreover, they may be used for the critical evaluation of existing theoretical and experimental data. The aim of this lecture is to present some of such methods, in particular methods developed in Serbia.

2. MODIFIED SEMIEMPIRICAL METHOD FOR STARK BROADENING AND ASTROPHYSICAL APPLICATIONS

It is twenty two years from the formulation of the modified semiempirical (MSE) approach (Dimitrijević and Konjević 1980) for the calculation of Stark broadening parameters for non-hydrogenic ion spectral lines. Within this period the considered method has been applied successfully many times for different problems in astrophysics and physics. According to the modified semiempirical (MSE) approach (Dimitrijević and Konjević 1980, 1981, 1987, Dimitrijević and Kršljanin 1986, Dimitrijević and Popović 1993, 2001, Popović and Dimitrijević 1996a) the electron impact full width (FHWM) of an isolated ion line is given as

$$\begin{aligned} W_{MSE} = N\frac{8\pi}{3}\frac{\hbar^2}{m^2}\left(\frac{2m}{\pi kT}\right)^{1/2}\frac{\pi}{\sqrt{3}}\frac{\lambda^2}{2\pi c}\cdot\Big\{ & \sum_{\ell_i\pm 1}\sum_{A_{i'}J_{i'}}\vec{\Re}^2[n_i\ell_iA_iJ_i,n_i(\ell_i\pm1)A_{i'}J_{i'}]\widetilde{g}(x_{\ell_i,\ell_i\pm1})+ \\ & +\sum_{\ell_f\pm 1}\sum_{A_{f'}J_{f'}}\vec{\Re}^2[n_f\ell_fA_fJ_f,n_f(\ell_f\pm1)A_{f'}J_{f'}]\widetilde{g}(x_{\ell_f,\ell_f\pm1})+\Big(\sum_{i'}\vec{\Re}^2_{ii'}\Big)_{\Delta n\neq 0}g(x_{n_i,n_i+1})+ \\ & +\Big(\sum_{f'}\vec{\Re}^2_{ff'}\Big)_{\Delta n\neq 0}g(x_{n_f,n_f+1})\Big\}, \end{aligned} \tag{1}$$

and the corresponding Stark shift as

$$\begin{aligned} d_{MSE} = N\frac{4\pi}{3}\frac{\hbar^2}{m^2}\left(\frac{2m}{\pi kT}\right)^{1/2}\frac{\pi}{\sqrt{3}}\frac{\lambda^2}{2\pi c}\cdot\Big\{ & \sum_{A_{i'}J_{i'}}\sigma_{J_iJ_{i'}}\vec{\Re}^2[n_i\ell_iA_iJ_i,n_i(\ell_i+1)A_{i'}J_{i'}]\widetilde{g}_{sh}(x_{\ell_i,\ell_i+1})- \\ & -\sum_{A_{i'}J_{i'}}\sigma_{J_iJ_{i'}}\vec{\Re}^2[n_i\ell_iA_iJ_i,n_i(\ell_i-1)A_{i'}J_{i'}]\widetilde{g}_{sh}(x_{\ell_i,\ell_i-1}) \\ & -\sum_{A_{f'}J_{f'}}\sigma_{J_fJ_{f'}}\vec{\Re}^2[n_f\ell_fA_fJ_f,n_f(\ell_f+1)A_{f'}J_{f'}]\widetilde{g}_{sh}(x_{\ell_f,\ell_f+1})+ \\ & +\sum_{A_{f'}J_{f'}}\sigma_{J_fJ_{f'}}\vec{\Re}^2[n_f\ell_fA_fJ_f,n_f(\ell_f-1)A_{f'}J_{f'}]\widetilde{g}_{sh}(x_{\ell_f,\ell_f-1})+\Big(\sum_{i'}\vec{\Re}^2_{ii'}\Big)_{\Delta n\neq 0}g_{sh}(x_{n_i,n_i+1})- \\ & -2\sum_{i'(\Delta E_{ii'}<0)}\sum_{A_{i'}J_{i'}}\vec{\Re}^2(n_i\ell_iA_iJ_i,n_i\ell_{i'}A_{i'}J_{i'})g_{sh}(x_{\ell_i,\ell_{i'}})-\Big(\sum_{f'}\vec{\Re}^2_{ff'}\Big)_{\Delta n\neq 0}g_{sh}(x_{n_f,n_f+1})+ \\ & +2\sum_{f'(\Delta E_{ff'}<0)}\sum_{A_{f'}J_{f'}}\vec{\Re}^2(n_f\ell_fA_fJ_f,n_f\ell_{f'}A_{f'}J_{f'})g_{sh}(x_{\ell_f,\ell_{f'}})+\sum_k\delta_k\Big\} \end{aligned} \tag{2}$$

where the initial level is denoted as i and the final one as f and the square of the matrix element
$\{\vec{\Re}^2[n_k\ell_k A_k J_k, (\ell_k \pm 1)A_{k'} J_{k'}], \quad k = i, f\}$ is

$$\vec{\Re}^2[n_k\ell_k A_k J_k, n_k(\ell_k \pm 1)A'_k J'_k] = \frac{\ell_>}{2J_k+1} Q[\ell_k A_k, (\ell_k \pm 1)A'_k] Q(J_k, J'_k)[R^{n_k^*(\ell_k \pm 1)}_{n_k^*\ell_k}]^2 \tag{3}$$

Also,
$\ell_> = \max(\ell_k, \ell_k \pm 1)$ and

$$(\sum_{k'} \vec{\Re}^2_{kk'})_{\Delta n \neq 0} = (\frac{3n_k^*}{2Z})^2 \frac{1}{9}(n_k^{*2} + 3\ell_k^2 + 3\ell_k + 11) \tag{4}$$

In Eqs. (1) and (2)

$$x_{\ell_k,\ell_{k'}} = \frac{E}{\Delta E_{\ell_k,\ell_{k'}}}, \quad k = i, f;$$

and $E = \frac{3}{2}kT$
is the electron kinetic energy and $\Delta E_{\ell_k,\ell_{k'}} = |E_{\ell_k} - E_{\ell_{k'}}|$ is the energy difference between levels ℓ_k and $\ell_k \pm 1$ $(k = i, f)$,

$$x_{n_k,n_k+1} \approx \frac{E}{\Delta E_{n_k,n_k+1}},$$

where for $\Delta n \neq 0$, the energy difference between energy levels with n_k and n_k+1, $\Delta E_{n_k,n_k+1}$ is estimated as $\Delta E_{n_k,n_k+1} \approx 2Z^2 E_H / n_k^{*3}$, $n_k^* = [E_H Z^2 / (E_{ion} - E_k)]^{1/2}$ is the effective principal quantum number, Z is the residual ionic charge (for example Z=1 for neutrals) and E_{ion} is the appropriate spectral series limit.

If we have an oscillator strength, e.g. from literature, the corresponding matrix element may be calculated as

$$\vec{\Re}^2_{k,k'} \approx 3\frac{E_H}{E_{k'} - E_k} \cdot f_{k'k} \qquad (E_{k'} > E_k), \quad k = i, f$$

or

$$\vec{\Re}^2_{k,k'} \approx 3\frac{E_H}{E_k - E_{k'}} \frac{2k'+1}{2k+1} \cdot f_{kk'} \qquad (E_{k'} < E_k), \quad k = i, f \tag{5}$$

where $f_{k'k}$ (for $E_{k'} > E_k$) and $f_{kk'}$ (for $E_{k'} < E_k$) are oscillator strengths and E_H is the hydrogen ionization energy.

Possible configuration mixing may be taken into account (see e.g. Dimitrijević and Popović 1993) if one represents $\vec{\Re}^2_{\alpha\beta}$ as

$$\vec{\Re}^2_{\alpha\beta} = K_\alpha \cdot \vec{\Re}^2_{\alpha\alpha'} + K_\beta \cdot \vec{\Re}^2_{\beta\beta'}, \tag{6}$$

where K_α and K_β are mixing coefficients for two configurations and $K_\alpha + K_\beta = 1$.

In Eqs. (1 – 4) N and T are electron density and temperature, respectively, while $Q(\ell A, \ell' A')$ and $Q(J, J')$ are multiplet and line factors. The value of A depends on the coupling approximation (see e.g. Dimitrijević and Popović 1996a). In the case of the LS coupling approximation, applied here, $A = L$, for the jK approximation $A = K$ and for the jj approximation $A = j$. The $[R^{n^*_k \ell_k \pm 1}_{n^*_k \ell_k}]$ is the radial integral, and with $g(x)$ (Griem 1968), $\widetilde{g}(x)$ (Dimitrijević and Konjević 1980) and $g_{sh}(x)$ (Griem 1968), $\widetilde{g}_{sh}(x)$ (Dimitrijević and Kršljanin 1986) are denoted the corresponding Gaunt factors for width and shift, respectively. The factor $\sigma_{kk'} = (E_{k'} - E_k)/|E_{k'} - E_k|$, where E_k and $E_{k'}$ are the energy of the considered and its perturbing level. The sum $\sum_k \delta_k$ is different from zero only if perturbing levels with $\Delta n \neq 0$ strongly violating the assumed approximations exist, so that they should be taken into account separately, and may be evaluated as

$$\delta_i = \pm \vec{\Re}^2_{ii'} [g_{sh}(\frac{E}{\Delta E_{i,i'}}) \mp g_{sh}(x_{n_i, n_i+1})], \tag{7}$$

for the upper level, and

$$\delta_f = \mp \vec{\Re}^2_{ff'} [g_{sh}(\frac{E}{\Delta E_{f,f'}}) \mp g_{sh}(x_{n_f, n_f+1})], \tag{8}$$

for the lower level. In eqs. (7) and (8) the lower signs correspond to $\Delta E_{kk'} < 0$, $k = i, f$.

In comparison with the full semiclassical approach (Sahal-Bréchot 1969ab, Griem 1974) and the Griem's semiempirical approach (Griem 1968) who needs practically the same set of atomic data as the more sophysticated semiclassical one, the modified semiempirical approach (Dimitrijević and Konjević 1980, 1981, 1987, Dimitrijević and Kršljanin 1986, Dimitrijević and Popović 1993, 2001, Popović and Dimitrijević 1996a) needs a considerably smaller number of such data. 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 $\ell_{if} = \ell_{if} \pm 1$, since all perturbing levels with $\Delta n \neq 0$, needed for a full semiclasical investigation or an investigation within the Griem's semiempirical approach (Griem 1968), are lumped together and approximately estimated. Here, n is the principal and ℓ the orbital angular momentum quantum numbers of the optical electron and with i and f are denoted the initial and final state of the considered transition.

Due to the considerably smaller set of needed atomic data in comparison with the complete semiclassical (Sahal-Bréchot 1969ab, Griem 1974) or Griem's semiempirical (Griem 1968) methods, the MSE method is particularly useful for stellar spectroscopy depending on very extensive list of elements and line transitions with their atomic and line broadening parameters where it is not possible to use sophysticated theoretical approaches in all cases of interest.

The MSE method is also very useful whenever line broadening data for a large number of lines are required, and the high precision of every particular result is not so important like e.g. for opacity calculations or plasma modeling. Moreover, in the case of more complex atoms or multiply charged ions the lack of the accurate atomic data needed for more sophysticated calculations, makes that the reliability of the semiclassical results decreases. In such cases the MSE method might be very interesting as well.

3. SYMPLIFIED MSE FORMULA

For the 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 dipolly allowed transition can occur from or to initial (i) or final (f) energy level of the considered line, is so far, that the condition $x_{\mathrm{jj}'} = E/|E_{\mathrm{j}'} - E_{\mathrm{j}}| \leq 2$ is satisfied. In such a case full width at half maximum is given by the expression (Dimitrijević and Konjević 1987):

$$W(\mathring{A}) = 2.2151 \times 10^{-8} \frac{\lambda^2(\mathrm{cm}) N(\mathrm{cm}^{-3})}{T^{1/2}(\mathrm{K})} (0.9 - \frac{1.1}{Z}) \sum_{\mathrm{j=i,f}} (\frac{3n_{\mathrm{j}}^*}{2Z})^2 (n_{\mathrm{j}}^{*2} - \ell_{\mathrm{j}}^2 - \ell - 1). \quad (15)$$

Here, N and T are the electron density and temperature respectively, $E = 3kT/2$ is the energy of perturbing electron, $Z - 1$ is the ionic charge and n the effective principal quantum number. This expression is of interest for abundance calculations, as well as for stellar atmospheres research, since the validity conditions are often satisfied for stellar plasma conditions.

Similarly, in the case of the shift

$$d(\mathring{A}) = 1.1076 \times 10^{-8} \frac{\lambda^2(\mathrm{cm}) N(\mathrm{cm}^{-3})}{T^{1/2}(\mathrm{K})} (0.9 - \frac{1.1}{Z}) \frac{9}{4Z^2} \times$$

$$\times \sum_{\mathrm{j=i,f}} \frac{n_{\mathrm{j}}^{*2} \varepsilon_{\mathrm{j}}}{2\ell_{\mathrm{j}} + 1} \{(\ell_{\mathrm{j}} + 1)[n_{\mathrm{j}}^{*2} - (\ell_{\mathrm{j}} + 1)^2] - \ell_{\mathrm{j}}(n_{\mathrm{j}}^{*2} - \ell_{\mathrm{j}}^2)\}. \quad (16)$$

If all levels $\ell_{\mathrm{i,f}} \pm 1$ exist, an additional summation may be performed in Eq. (16) to obtain

$$d(\mathring{A}) = 1.1076 \times 10^{-8} \frac{\lambda^2(\mathrm{cm}) N(\mathrm{cm}^{-3})}{T^{1/2}(\mathrm{K})} (0.9 - \frac{1.1}{Z}) \frac{9}{4Z^2} \sum_{\mathrm{j=i,f}} \frac{n_{\mathrm{j}}^{*2} \varepsilon_{\mathrm{j}}}{2\ell_{\mathrm{j}} + 1} (n_{\mathrm{j}}^{*2} - 3\ell_{\mathrm{j}}^2 - 3\ell_{\mathrm{j}} - 1), \quad (17)$$

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

4. TESTS AND APPLICATIONS FOR DETERMINATION OF STARK BROADENING PARAMETERS

The modified semiempirical approach has been tested several times on numerous examples (Dimitrijević 1990a). In order to test this method, selected experimental data for 36 multiplets (7 different ion species) of triply–charged ions were compared with theoretical linewidths. The averaged values of the ratios of measured to calculated widths are as follows (Dimitrijević and Konjević 1980): for doubly charged ions 1.06 ± 0.32 and for triply–charged ions 0.91 ± 0.42. The assumed accuracy of the MSE approximation is about ±50%, but it has been shown in Popović and Dimitrijević (1996b, 1998) and, Dimitrijević and Popović (2001) that the MSE approach, even in the case of the emitters with very complex spectra (e.g. Xe II and Kr II), gives very good agreement with experimental measurements (in the interval ±30%). For example for Xe II, $6s - 6p$ transitions, the averaged ratio between experimental and theoretical widths is 1.15 ± 0.5 (Popović and Dimitrijević 1996b).

In order to complete as much as possible the needed Stark broadening data, Belgrade group (Milan S. Dimitrijević, Luka Č. Popović, Vladimir Kršljanin, Dragana Tankosić, Nenad Milovanović, Zoran Simić, Miodrag Dačić, Zorica Cvetković, Predrag Jovanović) used the modified semiempirical method to obtain the Stark width and in some cases shift data for a large number of spectral lines for the different atom and ion species. Up to now:

6 Fe II, 4 Pt II, 16 Bi II, 12 Zn II, 8 Cd II, 18 As II, 10 Br II, 18 Sb II, 8 I II, 20 Xe II, 138 Ti II, 3 La II, 16 Mn II, 14 V II, 6 Eu II, 37 Kr II, 6 Y II, 6 Sc II, 4 Be III, 4 B III, 13 S III, 8 Au II, 8 Zr II, 53 Ra II, 3 Mn III, 10 Ga III, 8 Ge III, 4 As III, 3 Se III, 6 Mg III, 6 La III, 5 Sr III, 8 V III, 210 Ti III, 9 C III, 7 N III, 11 O III, 5 F III, 6 Ne III, 8 Na III, 10 Al III, 5 Si III, 3 P III, 16 Cl III, 6 Ar III, 30 Zr III, 20 Co III 2 B IV, Cu IV, 30 V IV, 14 Ge IV, 7 C IV, 4 N IV, 4 O IV, 2 Ne IV, 4 Mg IV, 7 Si IV, 3 P IV, 2 S IV, 2 Cl IV, 4 Ar IV, 3 C V, 50 O V, 12 F V, 9 Ne V, 3 Al V, 6 Si V, 11 N VI, 28 F VI, 8 Ne VI, 7 Na VI, 15 Si VI, 6 P VI, and 1 Cl VI transitions have been calculated (see Dimitrijević and Popović 2001 and references therein). The shift data for 16 Bi II, 12 Zn II, 8 Cd II, 18 As II, 10 Br II, 18 Sb II , 8 I II, 20 Xe II, 5 Ar II, 6 Eu II, 14 V II, 8 Au II, 14 Kr II and 138 Ti II transitions have been calculated (see Dimitrijević and Popović 2001 and references therein). Moreover, 286 Nd II Stark widths have been calculated (Popović et al. 2001b) within the symplified modified semiempirical approach.

Calculations within the modified semiempirical approach, for comparison with experimental data or testing of the theory have been performed also for Stark widths for 14 Al I, 46 Al II, 12 Al III (Heading et al. 1997), 1 C IV, 1 N V, 1 O VI (Böttcher et al. 1988, Glenzer et al. 1992), 1 Ne VIII (Glenzer et al. 1992), 3 N III, 3 O IV, 3 F V, 2 Ne VI (Glenzer et al. 1994), 12 C IV (Ackermann et al. 1985), 4 C II, 5 N II, 3 O II, 4 F II, 3 Ne II (Blagojević et al. 1999), 1 N II (Milosavljević et al. 1999), 8 S II (Djeniže et al. 1990), 2 Ne VII (Wrubel et al. 1996), 4 N III, 2 F V (Blagojević et al. 1996), 2 Ne III, 2 Ar III, 2 Kr III, 2 Xe III (Konjević 1995), 3 Si III (Dimitrijević 1983), 3 Ne III, 2 Ar III, 2 Kr III, 2 Xe III (Konjević and Pittman 1987) transitions. Moreover, in Kobilarov and Konjević (1990) Stark widths and shifts for 2 Cl II and 6 Ar III lines have been calculated.

5. APPLICATION TO THE INVESTIGATION OF "ZIRCONIUM CONFLICT" IN χ LUPI STAR ATMOSPHERE

The electron-impact broadening is the main broadening mechanism in A and B type star atmospheres (see e.g. Popović et al. 1999). The electron-impact broadening data are needed for various problems in astrophysics, as e.g. for diagnostic and modeling of stellar plasma, investigation of its physical properties and for abundance determination. These investigations provide us with useful information for modeling of stellar evolution. As an example, the abundances study in stellar atmospheres provides evidences for the chemical composition of the stellar primordial cloud, processes occurring within the stellar interior, and the dynamical processes in stellar atmosphere.

The available abundance analysis for early-type stars show that about 10% - 20% of A and B stars have abundance anomalies, including anomalies in isotopic compositions

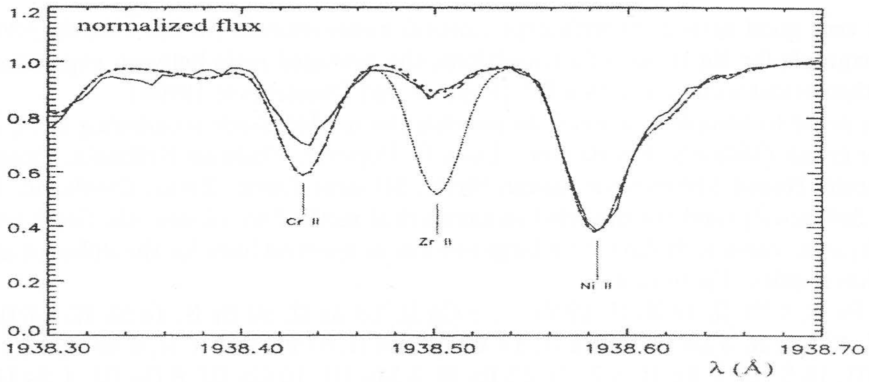

Fig. 2: The UV spectrum of the χ Lupi star within the 193.83 nm - 193.87 nm wavelength range. With the full line is denoted the spectrum obtained by GHRS. With the dotted line is shown the synthesized Zr II 4d5s5p $v^2D^o_{3/2}$ - $4d^25s$ $a^2D_{3/2}$ $\lambda = 193.85$ nm line obtained for zirconium abundance $\log(N_{\rm Zr}/N_{\rm H}) = -8.12$. These abundance value is obtained from Zr III lines. With - - - is denoted synthesized spectrum for zirconium abundance $\log(N_{\rm Zr}/N_{\rm H}) = -9.1$, and with larger dots for $\log(N_{\rm Zr}/N_{\rm H}) = -9.0$ (Leckrone et al. 1993).

(Leckrone et al. 1993). The abundance anomalies in these stars, called CP stars, have been caused by different hydrodynamical processes in the outer stellar layers (aided and mitigated by magnetic fields, weak stellar winds, turbulence, rotation mixing, etc.). In order to investigate these processes, atomic data for numerous lines of numerous emitters are needed.

For example the zirconium lines are present in spectra of HgMn stars (Cowley and Aikman 1975, Heacox 1979, Leckrone et al. 1993, Sikström et al. 1999). It is interesting that the zirconium abundance determination from weak Zr II optical lines and strong Zr III lines (detected in UV) is quite different (see Leckrone et al. 1993, Sikström et al. 1999) in HgMn star χ Lupi. This is illustrated in Fig. 2, where the UV spectrum of the χ Lupi star within the 193.83 nm - v 193.87 nm wavelength range is shown. With the full line is denoted the spectrum obtained by GHRS. With the dotted line is shown the synthesized Zr II 4d5s5p $v^2D^o_{3/2}$ - $4d^25s$ $a^2D_{3/2}$ $\lambda = 193.85$ nm line obtained for zirconium abundance $\log(N_{\rm Zr}/N_{\rm H}) = -8.12$. These abundance value is obtained from Zr III lines. With - - - is denoted synthesized spectrum for zirconium abundance $\log(N_{\rm Zr}/N_{\rm H}) = -9.1$, and with larger dots for $\log(N_{\rm Zr}/N_{\rm H}) = -9.0$ (Leckrone et al. 1993).

It is so called "zirconium conflict" and it was supposed by Sikström et al. (1999) that this difference is probably due to non adequate use of stellar models, e.g. if the influence of non-LTE effects or if diffusion is not taken into account.

Zirconium, often overabundant in HgMn stars (see Heacox 1979), is one member of Sr-Y-Zr triad, which is vital for the study of s-process nucleosynthesis and has been pointed as presenting a non-nuclear abundance pattern in HgMn stars. The most obvious interpretations of this anomaly are with the help of diffusion theory or with inclusion of non-LTE effects. However, it is of interest also to investigate the

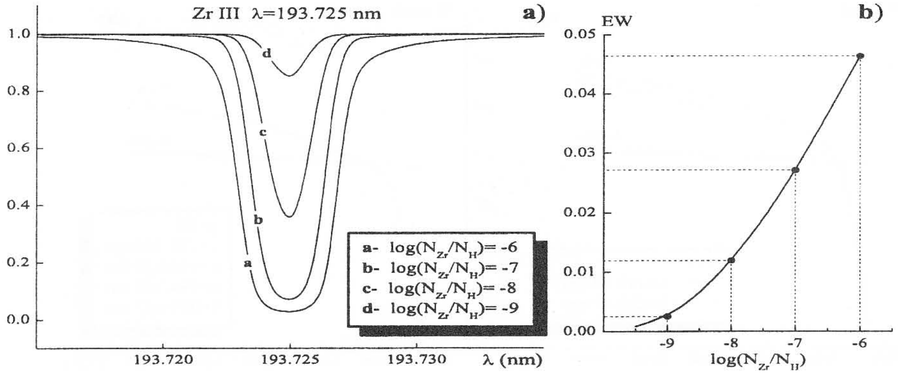

Fig. 3: The change of the Zr III 4d^2 ^{3}P$_1$ - 4d5p ^{3}P$^o_0$ λ = 193.725 line profile due to the change of the zirconium abundance $\log(N_{\mathrm{Zr}}/N_{\mathrm{H}})$ for stellar atmospheres model with T_{eff} = 10500 K, $\log g$ = 4.0 and the turbulence velocity V_t = 0.0 km s^{-1} (**a**). In (**b**), the equivalent width as a function of the zirconium abundance is shown.

contribution of the differences of Zr II and Zr III Stark broadening parameters to the zirconium conflict.

In Popović et al. (2001a), the electron-impact broadening parameters calculation of two astrophysically important Zr II and 34 Zr III lines has been performed, in order to test the influence of this broadening mechanism on determination of equivalent widths and to discuss its possible influence on zirconium abundance determination.

Atomic energy levels needed for calculations have been taken from Reader and Acquista (1997) and from Charro *et al.* (1999). Obtained results have been used to see how much the electron-impact broadening can take part in so called "zirconium conflict" in the HgMn star χ Lupi. In order to test the importance of the electron-impact broadening effect in determination of zirconium abundance, Popović et al. (2001a) have synthesized the line profiles of Zr II, λ=193.8 nm and Zr III, λ=194.0 nm using SYNTH code (Piskunov 1992) and the Kurucz's ATLAS9 code for stellar atmosphere model (Kurucz 1993) T_{eff} = 10500 K, $\log g$ =4.0 and the turbulence velocity V_t = 0.0 km s^{-1} , i.e. with the stellar models with similar characteristics as in the case of χ Lupi (T_{eff} =10650 K and $\log g$ =3.8, see e.g. Leckrone et al. 1999). These lines have been choosen, because they have been usually used for abundance determination. The reason is that the lines have small wavelength displacement and they are well resolved (Leckrone et al. 1993). The change of the Zr III 4d^2 ^{3}P$_1$ - 4d5p ^{3}P$^o_0$ λ = 193.725 line profile due to the change of the zirconium abundance is shown in Fig. 3a, while in Fig. 3b the equivalent width as a function of the zirconium abundance is shown.

Popović et al. (2001a) have calculated the equivalent widths with the electron-impact broadening effect and without it for different abundances of zirconium. The obtained results for ZrIII[194.0nm] and ZrII[193.8nm] lines show that the electron-broadening effect is more important in the case of higher abundance of zirconium. The equivalent width increases with abundance for both lines, but the equivalent width for ZrIII[194.0nm] line is more sensitive than for ZrII[193.8nm] line. It may cause error in abundance determination in the case when the electron-impact broadening

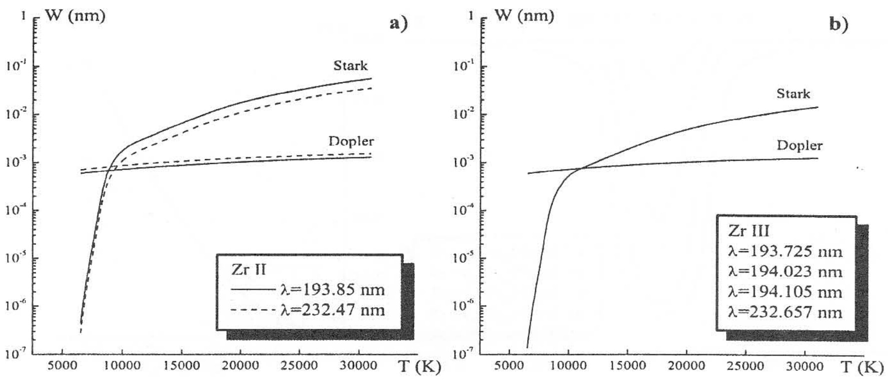

Fig. 4: The behaviour of Stark and Doppler widths (FWHM) with temperature, for stellar atmosphere model with T_{eff} =10500 K, $\log g$=4.0 and V_t = 0.0 km s^{-1} for a) Zr II 4d5s5p v^{2}D$^o_{3/2}$ - 4d^{2}5s a^{2}D$_{3/2}$ λ = 193.85 nm (full line—) and Zr II 4d5s5p v^{2}F$^o_{5/2}$ - 4d^{2}5s b^{2}G$_{7/2}$ λ = 232.47 nm (broken line) and b) Zr III 4d^2 ^{3}P$_1$ - 4d5p ^{3}P$^o_0$ λ = 193.725 nm, Zr III 4d^2 ^{1}G$_4$ - 4d5p ^{1}F$^o_3$ λ = 194.023 nm, Zr III 4d^2 ^{3}P$_2$ - 4d5p ^{3}P$^o_2$ λ = 194.105 nm i Zr III 4d^2 ^{3}P$_1$ - 4d5p ^{3}P$^o_1$ λ = 194.657 nm. In Fig. 4b, dependence for all indicated lines is not shown since it is approximately the same.

effect is not taken into account. In any case synthesizing of these two lines in order to measure the zirconium abundance without taking into account the electron-impact widths will give that with the ZrIII[194.0nm] the abundance of zirconium is higher than with the ZrII[193.8nm] line. However, this effect cannot cause the difference of one order of magnitude in abundance.

Although the "zirconium conflict" in HgMn star χ Lupi cannot be explained only by this effects, one should take into account that this effect may cause errors in abundance determination. Moreover in Fig 4 is demonstrated that Stark broadening is comparable with Doppler broadening or dominant broadening mechanisms for temperatures around 10 000 K and higher.

6. OTHER ASTROPHYSICAL APPLICATIONS

The modified semiempirical method and Stark broadening parameters calculated within this approach have been applied in astrophysics e.g. for the determination of carbon, nitrogen and oxygen abundances in early B-type stars (Gies and Lambert 1992) magnesium, aluminium and silicon abundances in normal late-B and HgMn stars, from co-added IUE spectra (Smith 1993) and elemental abundances in hot white dwarfs (Chayer et al. 1995ab), investigations of abundance anomalies in stars (Michaud and Richer 1992), elemental abundance analyses with DAO spectrograms for 15 - Vulpeculae and 32 - Aquarii (Bolcal et al 1992), radiative acceleration calculation in stellar envelopes (LeBlanc and Michaud 1995, Gonzales et al. 1995ab, Alecian et al. 1993, Seaton 1997), consideration of radiative levitation in hot white dwarfs (Char et al. 1995, Chayer et al. 1995ab), quantitative spectroscopy of hot stars (Kudritzki and Hummer 1990), non - LTE calculations of silicon - line strengths in B - type stars (Lennon et al. 1986), stellar opacities calculations and study (Iglesias et al. 1990, Iglesias and Rogers 1992, Rogers and Iglesias 1992, 1995, 1999, Seaton 1993, Mostovych et al. 1995), atmospheres and winds of hot stars investigations (Butler 1995), investigation of Ga II lines in the spectrum of Ap stars (Lanz et al. 1993). Stark broadening data calculated within the modified semiempirical method entered in a critical overview of atomic data for stellar abundance analysis (Lanz and Artru 1988), and a catalogue of atomic data for low-density astrophysical plasma (Golovatyj et al. (1997), Stark broadening parameter regularities and systematic trends research (Glenzer et al. 1992, 1994, Wrubel et al. 1998, Purić et al. 1987, 1988a-d, Purić 1996)... The modified semiempirical method entered also in computer codes, as e. g. OPAL opacity code (Rogers and Iglesias 1995), handbooks (Peach 1996, Vogt 1996) and monographs (Gray 1992, Griem 1997, Konjević 1999).

In order to make the application and usage of our Stark broadening data obtained within the semiclassical and modified semiempirical approaches more easier, we are organizing them now in a database BELDATA.

7. REGULARITIES AND SYSTEMATIC TRENDS

When reliable data do not exist, the knowledge on regularities and systematic trends of line broadening parameters can be used for quick acquisition of new data especially when high accuracy of each particular value is not needed.

Regularities and systemic trends for the widths of isolated non−hydrogenic spectral lines in plasmas have been studied in a number of papers (see for example Purić et al. 1980, 1987, 1988a-d, 1991, Konjević and Dimitrijević, 1981, Dimitrijević 1982, Wiese and Konjević 1982, 1992, Lakićević and Purić 1983, Dimitrijević 1985, Vitel et al. 1988, Dimitrijević and Popović 1989, Dimitrijević and Peach 1990, Djeniže et al. 1990, Glenzer et al. 1992, 1994, Purić 1996, Wrubel et al. 1998, Purić and Šćepanović 1999). The aim of such studies is to find out if regularities and systematic trends can be used to predict line widths and to critically evaluate experimental data. With the suitable use of the knowledge of regularities and systematic trends, we might use the existing experimental and theoretical values for the interpolation of new data needed in stellar spectroscopy. One must take into account however, that the validity of systematic trends and line broadening data is limited to the plasma conditions for which they are derrived and extrapolations are of low accuracy.

At the end, it is interesting to emphasize that the Stark broadening research is a developed research field in Yugoslavia, which has a critical mass of scientists. In Dimitrijević (1990b, 1991, 1994, 1997, 2001) reviewing spectral line shapes investigations in Yugoslavia and Serbia within 1962 - 2000 periode, it is shown that during this periode 1427 (1222 by serbian authors) bibliographic items have been published by 179 Yugoslav authors (152 from Serbia, 26 from Croatia and 1 living in France). Majority of these articles concern Stark broadening.

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