Stark broadening of heavy metal spectral lines in atmospheres of chemically peculiar stars

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Abstract. Data on the Stark broadening of heavy metal spectral lines are of interest not only for laboratory but also for astrophysical plasma research as e.g. for stellar spectra analysis and synthesis. Here, we investigated theoretically the influence of collisions with charged particles on heavy metal spectral line profiles for Te I, Cr II, Mn II, Au II, Cu III, Zn III, Se III, In III and Sn III in spectra of A stars and white dwarfs. We applied semiclassical theory of Sahal-Bréchot since the most of published results in literature until now are determined using this method. When it can not be applied in an adequate way, due to the lack of reliable atomic data, we used modified semiempirical theory of Dimitrijević & Konjević, Dimitrijević & Kršljanin.

Stark broadening parameters, widths and shifts, were obtained for spectral lines of neutral emitter Te I, singly charged emitters Cr II, Mn II and Au II and doubly charged emitters Cu III, Zn III, Se III, In III and Sn III. We considered as well the contributions of different collision processes to the total Stark width in comparison with Doppler one. In this case we obtained contributions for elastic, strong and inelastic collisions for upper and lower levels.

For example, chromium lines are interesting due to their presence in stellar atmospheres, so that they give possibility to determine chromium abundance and investigate chromium stratification in stellar atmospheres and to be used for the diagnostics of stellar plasma and for more refined synthesis of stellar spectra. We consider the effect of Stark broadening on the shapes of Cr II spectral lines observed in the spectra of stars in the middle part of the main sequence. Stark broadening parameters were calculated by the semiclassical perturbation approach. For stellar spectra synthesis, the improved version SYNTH3 of the code SYNTH for synthetic spectrum calculations was used. Stark broadening parameters for Cr II spectral lines of seven multiplets belonging to 4s-4p transitions were calculated. New calculated Stark broadening parameters were applied to the analysis of Cr II line profiles observed in the spectrum of Cr-rich star HD 133792. We found that Stark broadening mechanism is very important and should be taken into account, especially in the study of Cr abundance stratification.

1. Introduction

Data on the Stark broadening of neutral atom and ion lines are of interest not only for laboratory but also for astrophysical plasma research, particularly for stellar spectra synthesis and analysis.

Numerous analyses of stellar spectra with new space techniques point to the importance of trace elements, especially in spectra of chemically peculiar stars. Therefore, determination of heavy metal spectral lines in atmospheres of these stars is relevant for laboratory and astrophysical plasma investigations. High-resolution spectra allow us to study different broadening effects using well-resolved line profiles. Stark broadening is the most important pressure broadening mechanism for A-type stars and especially for white dwarfs. Neglecting
this mechanism may therefore introduce significant errors into abundance determinations and spectra modelisation.

Tellurium lines are of astrophysical interest due to their presence in stellar atmospheres. For example, in Ref [1], is reported, that in Procyon photosphere spectrum one line of tellurium is identified, and used to determine the abundance of this element.

Data on the Stark broadening of single ionized chromium spectral lines are of interest not only for laboratory but also for astrophysical plasma research as e.g. for chromium abundances determination and opacity calculations. They have been identified in A-type star spectra, as e.g. 7 Sex [2], φ Aqu [3]. As an example, in the spectrum of φ Aqu, authors [3] identified 28 Cr II spectral lines and noted overabundance with value log Cr/H = -5.85±0.27. Particularly interesting are resonance lines investigated here, since they are often present in stellar spectra.

Ionized manganese lines are of interest for the analysis and modelling of stellar spectra as for example for HgMn stars. For plasma conditions in such star atmospheres, hydrogen is mainly ionized and Stark broadening is the main pressure broadening mechanism, influencing spectral line shapes. It is shown as well [4, 5] that in atmospheres of A stars exist conditions where Stark widths are comparable and even larger than the corresponding thermal Doppler widths.

Many examples show presence in hot stellar atmospheres of ionized gold, copper, zinc, selenium, indium, tin, rare earths and other trace elements which before the epoch of space born stellar spectroscopy were astrophysically insignificant, but now the need for their atomic data is increasing.

Here, we investigated theoretically the influence of collisions with charged particles on heavy metal spectral line profiles for Te I, Cr II, Mn II, Au II, Cu III, Zn III, Se III, In III and Sn III in spectra of A stars and white dwarfs. We applied semiclassical theory [6, 7] and when it can not be applied in an adequate way, due to the lack of reliable atomic data, modified semiempirical theory [8, 9] was used.

We obtained Stark broadening parameters, widths and shifts, for spectral lines of neutral emitter Te I, singly charged emitters Cr II, Mn II and Au II and doubly charged emitters Cu III, Zn III, Se III, In III and Sn III. In the case with the available experimental and other theoretical data for the considered spectral lines we analyzed an agreement or a disagreement with our theoretical results. Also, here we considered the contributions of different collision processes to the total Stark width in comparison with Doppler one.

We consider the effect of Stark broadening on the shapes of Cr II spectral lines observed in stellar atmospheres of the middle part of the main sequence. Stark broadening parameters were calculated by the semiclassical perturbation approach. For stellar spectra synthesis, the improved version SYNT3 of the code SYNT for synthetic spectrum calculations was used. New calculated Stark parameters were applied to the analysis of Cr II line profiles observed in the spectrum of Cr-rich star HD 133792. We found that Stark broadening mechanism is very important and should be taken into account, especially in the study of Cr abundance stratification.

2. Theory
Calculations have been performed within the semiclassical perturbation formalism, developed and discussed in detail in Refs. [6, 7]. This formalism, as well as the corresponding computer code, have been optimized and updated several times [10, 11, 12, 13].

Within this formalism, the full width of an isolated spectral line of a neutral emitter broadened by electron impacts (W) can be expressed in terms of cross sections for elastic and inelastic processes as

\[
W = \frac{\lambda^2}{\pi c N} \int v f(v) dv (\sum \sigma_{i'i'}(v) + \sum_{f'\neq f} \sigma_{f'f}(v) + \sigma_{el} + W_R),
\]

(1)
and the corresponding line shift \( d \) as

\[
d = \frac{\lambda^2}{2\pi c} N \int v f(v) dv \int_{R_3}^{R_D} 2\pi \rho d\rho \sin 2\phi_p. \tag{2}
\]

Here, \( \lambda \) is the wavelength of the line originating from the transition with initial atomic energy level \( i \) and final level \( f \), \( c \) is the velocity of light, \( N \) is the electron density, \( f(v) \) is the Maxwellian velocity distribution function for electrons, \( \rho \) denotes the impact parameter of the incoming electron, and \( \phi_p \) is the phase shift due to the polarization potential. The inelastic cross sections \( \sigma_{jj'}(v) \) (where \( j = i \) or \( f \) ) and elastic cross section \( \sigma_{el} \) are determined according to Chapter 3 in [7]. The cut-offs (needed for the calculation of inelastic and elastic cross sections and the shift), included in order to maintain for the unitarity of the \( S \)-matrix, and to take into account Debye screening are described in Section 1 of Chapter 3 in [7]. \( W_R \) gives the contribution of the Feshbach resonances [14] and this term is zero if the emitters are neutral atoms. Other differences between neutral and ionized emitters is that for calculations of the cross sections rectilinear perturber paths are taken for neutral ones and hyperbolic paths for ionized species.

The formulae for the ion-impact broadening parameters are analogous to the formulae for electron-impact broadening. We note that the fact that the colliding ions could be treated using impact approximation in the far wings should be checked, even for stellar atmosphere densities.

When the semiclassical perturbation formalism can not be applied in an adequate way, due to the lack of reliable atomic data, a modified semiempirical formalism has been used.

According to the modified semiempirical (MSE) approach [for review see [15]] [8, 9] the electron impact full width at half maximum (FWHM) of an isolated ion line is given by

\[
W = N \frac{4\pi \hbar^2}{3c m^2} (\frac{2m}{\pi kT})^{1/2} \frac{\lambda^2}{\sqrt{3}} \{ \sum_{l_i \pm 1} \sum_{l_f} R_{l_i,l_f,l_i \pm 1}^2 \tilde{g}(x_{l_i,l_f,l_i \pm 1}) + \sum_{l_f \leq 1} \sum_{l_i} R_{l_i,l_f,l_f}^2 \tilde{g}(x_{l_i,l_f,l_f}) + (\sum_{l_f} R_{f f'}^2) \Delta n \neq 0 \tilde{g}(x_{f_f,n_f,n_f+1}) \} \tag{3}
\]

where \( n \) and \( \ell \) are principal and angular momentum quantum numbers, and \( R_{l_k,l_{k'}}^2, \ k = i, f \) is given by

\[
(\sum_{k'} R_{k,k'}^2) \Delta n \neq 0 = (\frac{3n_k^2}{2Z})^2 (\frac{1}{9} (n_k^2 + 3\ell_k^2 + 3\ell_k + 11) \tag{4}
\]

in the Coulomb approximation.

In Eq. (3)

\[
x_{l_k,l_{k'}} = E/\Delta E_{l_k,l_{k'}} \tag{5}
\]

\( k = i, f \) where \( E = \frac{3}{2} kT \) is the electron kinetic energy and

\[
\Delta E_{l_k,l_{k'}} = |E_{l_k} - E_{l_{k'}}| \tag{6}
\]

is the energy difference between levels \( \ell_k \) and \( \ell_k \pm 1 \) \((k = i, f)\). Also

\[
x_{n_k,n_k+1} \approx E/\Delta E_{n_k,n_k+1}, \tag{7}
\]

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.
\[ \Delta E_{n_k,n_k+1} \approx 2Z^2 E_H/n_k^3. \]  

(8)

In Eq. (4) the effective principal quantum number is defined by

\[ n_k^* = [E_H Z^2/(E_{ion} - E_k)]^{1/2}, \]

(9)

\[ Z \] is the residual ionic charge i.e. the charge of the rest of atom as “seen” by optical electron (for example \( Z = 1 \) for neutral atoms, 2 for singly charged ions etc), and \( E_{ion} \) is the appropriate spectral series limit.

In Eq. (3) \( T \) is the electron temperature, while \( g(x) \) [16] and \( \tilde{g}(x) \) [8] denote the corresponding effective Gaunt factors.

In comparison with the semiclassical perturbation approach [6, 7], the modified semiempirical approach requires much less atomic input data. In fact, if there are not perturbing levels strongly violating the assumed approximation, we only need 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 semiclassical calculation are lumped together and estimated approximately. If for the nearest perturbing levels the condition \( E/\Delta E \leq 2 \) is satisfied the simplified version of the Eq. (3) [9] can be used.

3. Results and discussions

We obtained Stark widths and shifts of four Te I multiplets [17] by using the semiclassical perturbation method for a perturber density of \( 10^{16} \text{cm}^{-3} \) and temperatures from 2500 up to 50000 K. As an example of the influence of Stark broadening in atmospheres of hot stars we present in Fig. 1 Stark widths for the 5125.2 Å multiplet compared with Doppler widths for a model: \( T_{eff} = 10000 \text{K}, \log g = 4.5 \) of A type star atmosphere [18]. Even if Doppler broadening dominates the line centre, Stark broadening may influence line wings. There is no experimental or other theoretical data for the comparison with the calculated Stark broadening parameters of Te I spectral lines.

![Figure 1. Thermal Doppler and Stark widths for Te I 6s \(^5\)S\(_0\) - 7p \(^5\)P (5125.2 Å) multiplet as functions of Rosseland optical depth for an A type star (\( T_{eff} = 10000 \text{K}, \log g = 4.5 \)). It is interesting that the Stark broadening mechanism is absolutely dominant in comparison with the thermal Doppler mechanism in deeper layers of the stellar atmosphere (\( \log \tau > 0.8 \)).](image)

New Stark broadening parameters for seven strongest 4s - 4p Cr II multiplets for a perturber density of \( 10^{14} \text{cm}^{-3} \) and temperatures from 2500 up to 100000 K [19] and nine resonant 3d\(^5\) - 3d\(^4\) 4p Cr II multiplets for a perturber density of \( 10^{17} \text{cm}^{-3} \) and temperatures from 2500 up to 100000 K have been determined within the semiclassical perturbation approach. In order to demonstrate one possibility for their usage in astrophysical plasma research, obtained results have been applied to the analysis of the Stark broadening influence on stellar spectral line shapes. For example, we synthesized resonant Cr II 4588.2 Å line profile using SYNTH code [20] and, DIPOS program package, for the corresponding equivalent width, for a model atmosphere with \( T_{eff} = 8750 \text{K} \) and \( \log g = 4.0 \) as a function of chromium abundance. One can see, that the
influence of Stark broadening increases in line wings and with chromium abundance as expected. Also, one can see that in A type CP stars exist atmospheric layers where Doppler and Stark widths are comparable, so that the influence of Stark broadening is important.

![Figure 2. Comparison of the Cr II 4588.2 Å line profile ("a") without Stark broadening contribution and with this contribution for different Cr abundances log Cr/H : ("b") Solar one, ("c") -3.75, ("d") -3.25, ("e") -2.75. The atmosphere model: $T_{\text{eff}}$ = 8750 K and log $g$ = 4.0.](image)

Large differences between previous calculations of the Mn II spectral line Stark widths [21, 22] and a recent experiment in [23] are considered in [24]. In order to do so, new semiclassical perturbation calculations of the Stark broadening parameters of three spectral lines within Mn II 3d$^5$4s a$^5$S -3d$^5$4p z$^5$P$^o$ and three within Mn II 3d$^5$4s a$^5$S - 3d$^5$4p z$^5$P$^o$ multiplets, are performed. The influence of hfs on the Stark broadening parameters determination as a possible reason of disagreement is discussed also, on the example of Mn II 260.6455 nm and 259.4497 nm lines. Namely, measured and calculated values taking into account the hfs effect are compared. We found that this effect can not explain the large discrepancy between experiment and theory. Other possible reasons for disagreement like the configuration interaction are discussed as well. The new semiclassical perturbation calculations, more sophisticated than previous ones, performed by using the modified semiempirical theory, are in better agreement with experiment, but a large difference up to a factor 2.39 for the width, still exist. Also, the obtained results were used for the investigation of the influence of Stark broadening on Mn II spectral line profiles in DB and DA white dwarfs, see Fig. 3. It was demonstrated the importance to take into account Stark broadening mechanism for the analysis of DB white dwarf spectra. The obtained data and conclusions are of interest for a number of problems in stellar and Solar physics, like spectrum analysis and synthesis, radiative transfer and modelling of sub photospheric layers.

![Figure 3. Thermal Doppler and Stark widths for Mn II a$^5$S - z$^5$P$^o$ spectral line for a DB and DA white dwarf atmosphere model with $T_{\text{eff}}$ = 15000 K and log $g$ = 8, as a function of optical depth $\tau_{5150}$.](image)

We reviewed and compared our experimental [25] and theoretical [26] Au II Stark widths. The new measurements and calculations are in course in order to obtain a better agreement between experimental and theoretical values.
Table 1. Experimental [25] and theoretical [26] Stark widths are compared in Table 1: \( W_m/W_{th} \) ratio of experimental [25] and theoretical [26], \( W_m'/W_{th} \) ratio of new experimental and theoretical results.

| \( \lambda(A) \) | \( W_m(A) \) | \( W_m/W_{th} \) | \( W_m'(A) \) | \( W_m'/W_{th} \) |
|-----------------|-------------|-----------------|-------------|-----------------|
| 1921.00         | 0.0338      | 1.15            | 0.0173      | 0.96            |
| 2043.54         | 0.0372      | 1.12            | 0.0179      | 0.87            |
| 2215.64         | 0.0424      | 0.38            | 0.0759      | 1.10            |
| 2263.63         | 0.1006      | 1.16            |             |                 |
| 2291.41         | 0.0408      | 0.35            | 0.0759      | 1.03            |
| 2315.75         | 0.0498      | 0.33            | 0.0816      | 1.05            |
| 2353.53         |             | 0.1518          |             |                 |
| 2802.04         | 0.0438      | 0.24            | 0.1105      | 0.98            |
| 2819.79         | 0.0452      | 0.25            | 0.1108      | 0.97            |
| 2822.35         |             | 0.1422          |             | 1.03            |
| 2837.85         | 0.0454      | 0.25            | 0.1077      | 0.93            |
| 2846.92         | 0.1335      | 0.96            |             |                 |
| 2894.32         | 0.1291      | 0.90            |             |                 |
| 2904.22         | 0.0434      | 0.21            | 0.1055      | 0.85            |
| 2994.80         | 0.0442      | 0.21            | 0.1070      | 0.83            |

For example, the influence of Stark broadening on Cu III, Zn III and Se III spectral lines in DB white dwarf atmospheres was also investigated by [27] for 4s\(^2\)F - 4p\(^2\)G\(^o\) (\(\lambda=1774.4\) Å), 4s\(^3\)D - 4p\(^3\)P\(^o\) (\(\lambda=1667.9\) Å) and 4p5s\(^3\)P\(^o\) - 5p\(^3\)D (\(\lambda=3815.5\) Å) by using the corresponding model with \( T_{eff} = 15000 \) K and \( \log g = 7 \) [28]. For the model atmosphere of the DB white dwarfs the prechosen optical depth points at the standard wavelength \( \lambda_s=5150 \) Å(\(\tau_{5150}\)) are used in [28] and in [27]. As one can see in Fig. 4, for the plasma conditions in the DB white dwarf atmospheres, thermal Doppler broadening is much less important compared to Stark broadening. For example the Stark width of the Se III 3815.5 Å line is larger than the Doppler one by up to two orders of magnitude within the range of optical depths considered. Much larger Stark widths in DB white dwarf atmospheres in comparison with A type stars are the consequence of larger electron densities due to much larger \( \log g \) and larger \( T_{eff} \), so that electron-impact (Stark) broadening is more effective.

Figure 4. Thermal Doppler and Stark widths for Cu III 4s\(^2\)F - 4p\(^2\)G\(^o\) (\(\lambda=1774.4\) Å), Zn III 4s\(^3\)D - 4p\(^3\)P\(^o\) (\(\lambda=1667.9\) Å) and Se III 4p5s\(^3\)P\(^o\) - 5p\(^3\)D (\(\lambda=3815.5\) Å) spectral lines for a DB white dwarf atmosphere model with \( T_{eff} = 15,000 \) K and \( \log g = 7 \), as a function of optical depth \( \tau_{5150} \).

In order to see the influence of Stark broadening mechanism for In III and Sn III spectral lines in stellar plasma conditions, we have calculated Stark widths for a [18] A type star (\( T_{eff} = 10000 \) K; \( \log g = 4.5 \)) atmosphere model and compared them with Doppler ones. We found
that exist photospheric layers where Doppler and Stark widths are comparable and even where the Stark width is dominant and must be taken into account. Also, for the same atmosphere model, we present here in Fig. 5. Stark widths and contributions of different collision processes to the total Stark width in comparison with Doppler one.

Cr II lines in the spectrum of the Ap star HD 133792, for which careful abundance and stratification analysis has recently been performed in [29] were analyzed in [19]. HD 133792 has an effective temperature of $T_{\text{eff}}=9400$ K, log $g=3.7$, and a mean Cr overabundance $+2.6$ dex relative to the solar Cr abundance [29]. All calculations were carried out with the improved version SYNTH3 of the code SYNTH for synthetic spectrum calculations. Stark damping parameters were introduced in the spectrum synthesis code. The stratified Cr distribution in the atmosphere of HD 133972 derived by [29] was used. Figure 6 shows a comparison between the observed line profiles of Cr II lines 3403.30 Å and synthetic calculations with the Stark parameters from paper by [19](full line) and those from [30] (dashed line).

Figure 5. Thermal Doppler, total Stark width and contributions of different collisional processes to the total Stark width of Sn III 5226.2 Å for a model: $T_{\text{eff}}=10000$ K, log $g=4.5$ [18] of an A type star, as a function of the Rosseland optical depth. In this case, elastic and strong collisions and inelastic collision from upper levels have a similar contribution to the full Stark width as well as the similar behaviour with temperature.

Figure 6. Comparison between the observed Cr II 3403.30 line profile (dots) and synthetic calculations with the Stark parameters from paper by [19](full line) and those from [30] (dashed line).

Figure 7. Comparison between the observed Cr II 3421.20, 3422.73 lines profile (dots) and synthetic calculations with the Stark parameters from paper by [19](full line) and those from [30] (dashed line).
development of space born spectroscopy, building of giant telescopes of the new generation
and increase of accuracy of computer codes for modelling of stellar atmospheres. The Cr II
lines analyzed in [19] are particularly suitable for such purpose since they have good clean wings
where the influence of Stark broadening is the most important.

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