Mem. S.A.It. Suppl. Vol. 15, 126
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Memorie della
Supplementi

Stark broadening of spectral lines of inert gases

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Abstract. We summarize our previous results for Stark broadening parameters (width and shift) with application for astrophysical purposes, especially for diagnostics of hot stars and their atmospheres. The calculated results for Stark broadening parameters of several Ar I and Ne I lines in the wide temperature range have been analyzed. The comparison of results for analogous transitions has been presented.

Key words. Atomic processes: Stark broadening, Line broadening, Plasma diagnostics

1. Introduction

Stark broadening parameters are of interest for a number of problems in astrophysics, physics and laboratory plasma. They are needed in order to solve various problems, for example, diagnostics and modeling of stellar and laboratory plasma, investigation of its physical properties and for abundance determination. These investigations provide information useful for the modeling of stellar evolution, for the processes occurring within the stellar interiors, and radiative transfer in stellar atmospheres.

Stark broadening parameters of spectral lines of inert gases can play an important role in astrophysics. From one side, helium is the most abundant element after hydrogen in the universe and reliable Stark broadening data for He lines are of particular interest in the spectroscopic study of astrophysical plasma (Dimitrijević and Sahal-Bréchot 1984). From the other side, with the development of spaceborn spectroscopy, the importance of atomic data, including the Stark broadening parameters, for trace elements like neon and argon, increases. Argon lines are observed in the optical spectrum of Be star Hen 2-90 (Kraus et al. 2005), as well as in planetary nebulae and H II regions in the two dwarf irregular galaxies Sextans A and B (Kniazev et al. 2005). For the first time, the discovery of photospheric neon and argon lines in very hot central stars of planetary nebulae and white dwarfs is reported in (Werner et al. 2007a,b). In the new NLTE model atmospheres the Stark broadening of argon lines is included (Werner et al. 2007b). Therefore, there is a need for Stark broadening results for spectral lines of inert gases. Factors governing the broadening of spectral lines in plasmas are plasma environment and atomic structure of emitting atom. Observed regularities in atomic data (wavelengths and energy levels, oscillator strengths, collision cross sec-

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Send offprint requests to: M. Christova tions and other quantities) and similarities, result in the regularities and similarities of the width and shift parameters of plasma broadened lines.

In this paper we show the similarities and regularities of Stark broadening parameters (Dimitrijević et al. 2007; Christova et al. 2009a,b) within one spectral series at high temperatures, of interest for the study of hot stars and their atmospheres. Additionally, we give a comparison of calculated Stark broadening parameters of Ne I 837.7 nm and Ar I 737.2 nm which have analogous transitions $2p^5 3d$ - $2p^5 3p$ and $3p^5 4d$ - $3p^5 4p$, respectively.

2. Theory

Within the semi-classical perturbation formalism (Sahal-Bréchot 1969a,b), the full half width (W) and the shift (d) of an isolated line originating from the transition between the initial level i and the final level f is expressed as:

$$W = 2n_e \int_0^\infty v f(v) dv \left[\sum_{i' \neq i} \sigma_{ii'}(v) + \right.$$
$$\left. + \sum_{f' \neq f} \sigma_{ff'}(v) + \sigma_{el} \right] \qquad (1)$$

$$d = \int_0^\infty v f(v) dv \int_{R_3}^{R_d} 2\pi\rho d\rho \sin 2\varphi_p \qquad (2)$$

where i' and f' are perturbing levels, n_e and v are the electron density and the velocity of perturbers respectively, and $f(v)$ is the Maxwellian distribution of electron velocities.

The inelastic cross sections $\sigma_{ii'}(v)$ (respectively $\sigma_{ff'}(v)$) can be expressed by an integration of the transition probability $P_{ii'}$ over the impact parameter ρ:

$$\sum_{i' \neq i} \sigma_{ii'}(v) = \frac{1}{2}\pi R_1^2 +$$
$$+ \int_{R_1}^{R_d} 2\pi\rho d\rho \sum_{i' \neq i} P_{ii'}(\rho, v) \qquad (3)$$

The elastic collision contribution to the width is given by:

$$\sigma_{el} = 2\pi R_2^2 + \int_{R_2}^{R_d} 8\pi\rho d\rho \sin^2 \delta \qquad (4)$$

$$\delta = \left(\varphi_p^2 + \varphi_q^2\right)^{1/2} \qquad (5)$$

The phase shifts ϕ_p and ϕ_q are due to the polarization and quadrupole potential respectively. The cut-offs parameters R_1, R_2, R_3, the Debye cut-off R_d and the symmetrization procedure are described in (Sahal-Bréchot 1969a,b).

The impact approximation is valid when strong collisions are separated in time, or when the duration of collisions is much shorter than the separation time between strong collisions: $C_1 = n_e \pi\rho_{typ}^3 << 1$, where ρ_{typ} is typical impact parameter for strong collisions. C_1 is the impact approximation validity criterion.

The resulting profiles are Lorentzian. This condition is well verified for electron collisions for a large range of densities. For ion collisions the impact approximation might fail, especially for high densities or low temperatures.

3. Discussion

3.1. Argon

Theoretical results for spectral lines from one spectral series

We present results for the Stark broadening coefficient of argon lines from spectral series $3p^5 nd$ - $3p^5 4p$ for n = 4 – 7: 522.1, 549.6, 603.2 and 737.2 nm. The corresponding atomic data from NIST catalogue are given in Table 1. The analysis of the contribution of particular atomic processes to the Stark broadening parameters shows a similar behavior within the spectral series.

For the considered spectral lines, we obtain the similar behavior with temperature of the total broadening coefficient ($\beta = W / n_e$) and its components. In Figure 1 we illustrate this behavior with an example for Ar I 522.1 nm spectral line. The resulting broadening coefficient is: $\beta = \beta_{in} + \beta_{el}$, where β_{in} is the contribution

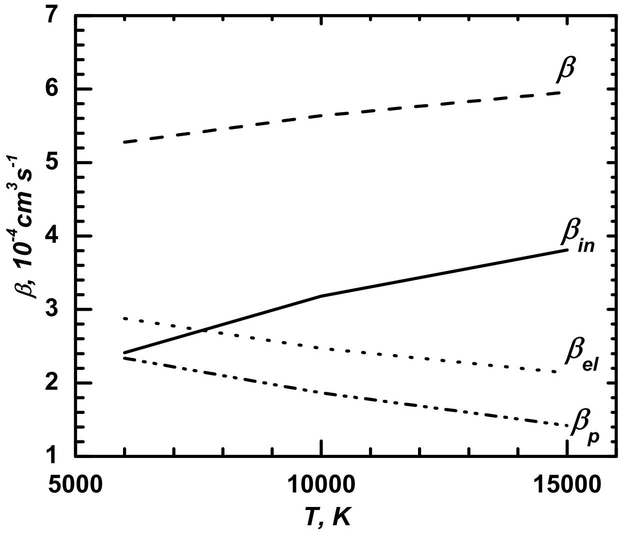

Fig. 1. Stark broadening coefficient ($\beta = W / n_e$) and its components ($\beta_{in}, \beta_{el}, \beta_p$ and β_q) versus the temperature for Ar I 522.1 nm.

Table 1. Basic data on the considered Ar I spectral lines. Here λ denotes wavelength, i and f are initial and final level of the transition (within the frame of $j - L$ coupling), i' and f' are the corresponding perturbing levels, E_i and E_f are the energy values and n* is the effective quantum number of the initial level.

λ nm	Transition (i - f)	i' levels	f' levels	E_i cm^{-1}	E_f cm^{-1}	n*
522.1	$3p^57d - 3p^54p$ $^2[7/2]^o{}_4$-$^2[5/2]_3$	5f, 6f, 7f, 8f, 9f, 5p, 6p, 7p, 8p, 9p	4s, 5s, 6s, 3d, 4d, 5d, 6d	124610	105463	6.62
549.6	$3p^56d - 3p^54p$ $^2[7/2]^o{}_3$-$^2[5/2]_3$	4f, 5f, 6f, 7f, 4p, 5p, 6p, 7p	4s, 5s, 6s, 3d, 4d, 5d, 6d	123653	105463	5.63
603.2	$3p^55d - 3p^54p$ $^2[7/2]^o{}_4$-$^2[5/2]_3$	4f, 5f, 6f, 7f, 4p, 5p, 6p, 7p	4s, 5s, 6s, 3d, 4d, 5d, 6d	122036	105463	4.65
737.2	$3p^55d' - 3p^54p$ $^2[7/2]^o{}_4$-$^2[5/2]_3$	4f, 5f, 6f, 4p, 5p, 6p	4s, 5s, 6s, 3d, 4d, 5d, 6d	119024	105463	3.68

of the inelastic collisions, β_{el} is the contribution of elastic ones, $\beta_{el} = \beta_p + \beta_q$ (β_p gives the contribution of polarisation interactions and β_q – of the quadrupole interactions).

The quadrupole component (β_q) depends only on the initial and final states of the emitter and does not depend on the temperature and perturber density. It is not included in the figure, since from the behavior of β_{el} and β_p it is easy to conclude on its behavior too.

For all these lines the total coefficient and the component due to inelastic interac-

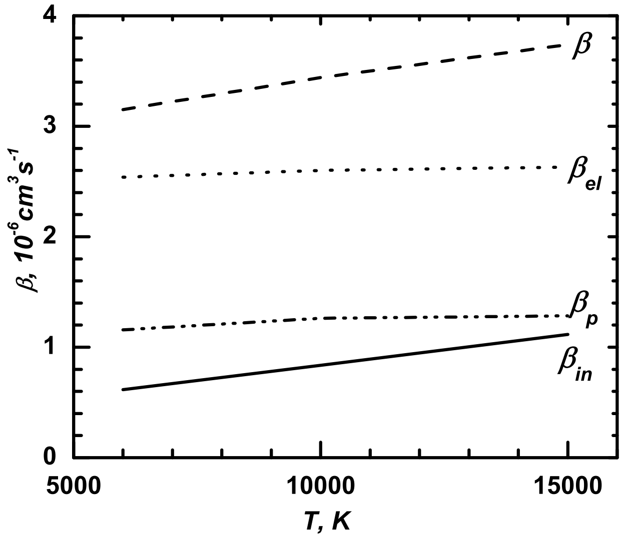

Fig. 2. Stark broadening coefficient ($\beta = W / n_e$) and its components (β_{in}, β_{el}, β_p and β_q) versus the temperature for Ar I 696.5 nm.

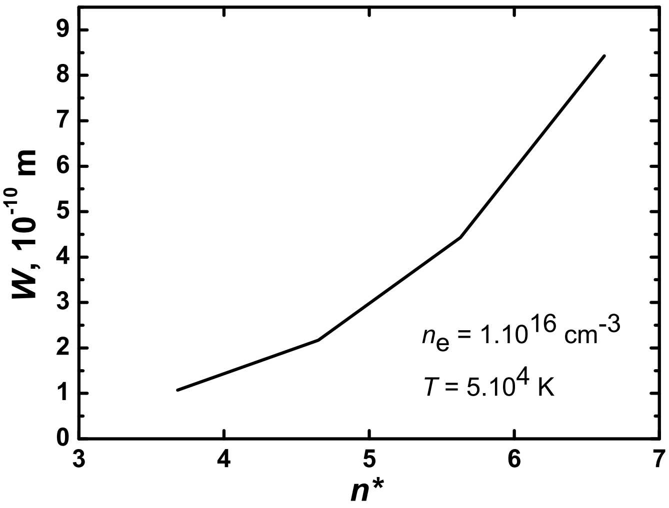

Fig. 3. Electron impact widths of Ar I spectral lines within the spectral series versus effective quantum number of the initial energy level for electron density of 10^{16} cm^{-3} and temperature of 5.10^4 K.

tions increase with the temperature, while β_p and β_{el}, respectively decrease with T. It means that the principal contribution to the broadening of these lines comes from inelastic collisions between emitters and surrounding particles. This contribution gives the trend of the total broadening coefficient in whole temperature interval.

The contribution of elastic collisions is dominated by the polarization interactions

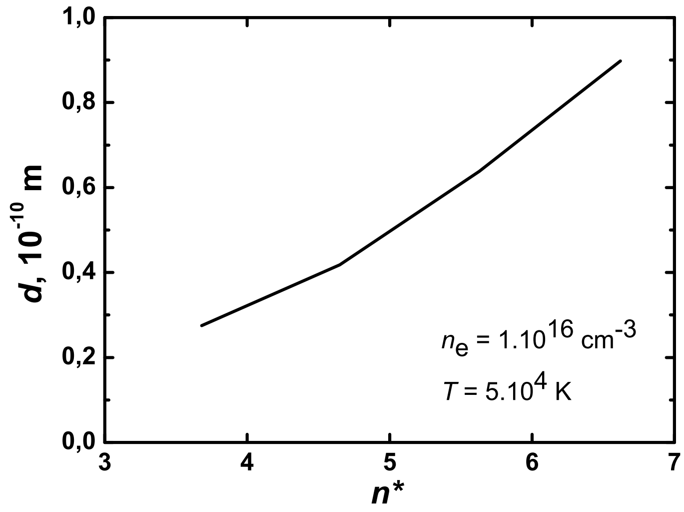

Fig. 4. Electron impact shifts of Ar I spectral lines within the spectral series versus effective quantum number of the initial energy level for electron density of 10^{16} cm^{-3} and temperature of 5.10^4 K.

($\beta_{el} >> \beta_q$). We note that: (i) the contribution of polarization interactions increases with effective quantum number; (ii) the principal contribution to the Stark broadening – 85% is due to the collisions with electrons.

For comparison, in the Figure 2 is shown the behavior of broadening coefficients for Ar I 696.5 nm line, which does not belong to the considered spectral series. The interactions which most contribute to the broadening of this line are the elastic ones. Their contribution practically does not vary with temperature. Namely the increase with T is very small. In this case, we found that the polarization and quadrupole components have the same values.

This means that the quadrupole contribution is larger for spectral lines emitted from lower energy levels. The smallest component in the total broadening for Ar I 696.5 nm is due to inelastic collisions between emitters and perturbers, four times lower than β_{el}. The conclusion is that the average free-electron energy is not so high for enough inelastic transitions to produce larger inelastic collision contribution to the line profile at the examined temperature interval. For this argon line, with low laying upper energy level, the contribution of collisions with ions is up to 30%. Therefore, for the considered transition involving lower energy levels, the quadrupole interactions and ion collisions play an important role in the total broadening, while the contribution of inelastic collisions is smallest. However, since the increase of β_{in} with temperature is largest, it gives the temperature trend to the β.

Often, the modeling of astrophysical objects needs atomic data for thousands and sometimes millions transitions. It is difficult and cumbersome to calculate the Stark broadening parameters for all these lines, so that methods enabling interpolation and extrapolation of the calculated results on the basis of similarities and systematic trends are of interest.

For example we can obtain new Stark broadening parameters from regularities within spectral series. In the next two figures we present the electron impact Stark width (Fig. 3) and shift (Fig. 4) for the argon lines (see Table 1) from the considered spectral series. Since, one of aims of this work is the applicability of Stark broadening results in the case of hot stars, we give our data for the temperature of 50 000 K, which is typical for DO white dwarfs where Stark broadening is important.

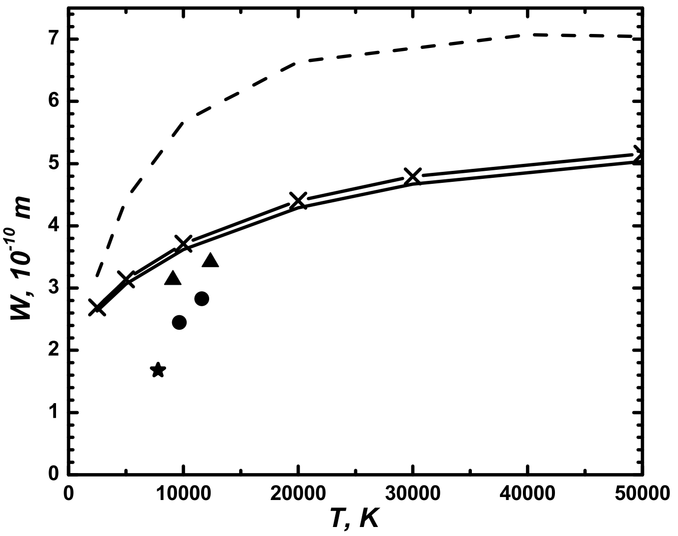

Fig. 5. Stark width of Ar I 549.6 nm versus temperature for electron density of 10^{16} cm^{-3}. (Theoretical results: dashed line - Griem (1964); solid line - Dimitrijević et al. (2007) for impact-electrons and impact-ions; solid line and cross symbols - Dimitrijević et al. (2007) for impact-electrons and quasistatic-ions; single symbols: experimental results from critical reviews (Lesage (2009) and references therein)

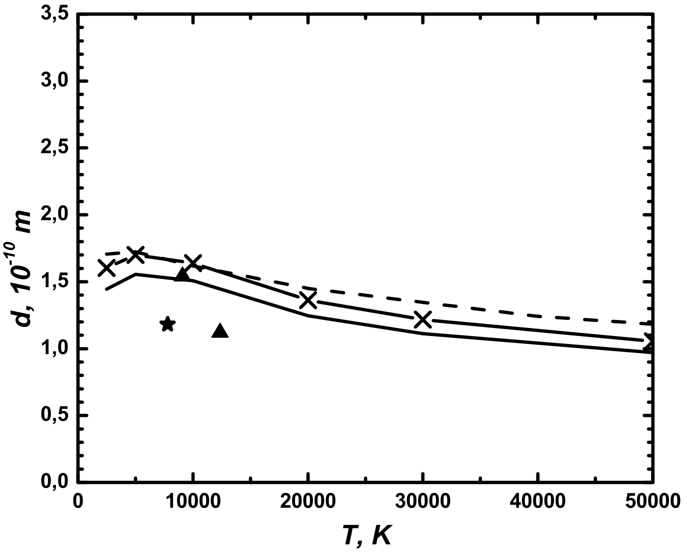

Fig. 6. Stark shift of Ar I 549.6 nm versus temperature for electron density of 10^{16} cm^{-3}. (Theoretical results: dashed line - Griem (1964); solid line - Dimitrijević et al. (2007) for impact-electrons and impact-ions; solid line and cross symbols - Dimitrijević et al. (2007) for impact-electrons and quasistatic-ions; single symbols: experimental results from critical reviews (Lesage (2009) and references therein)

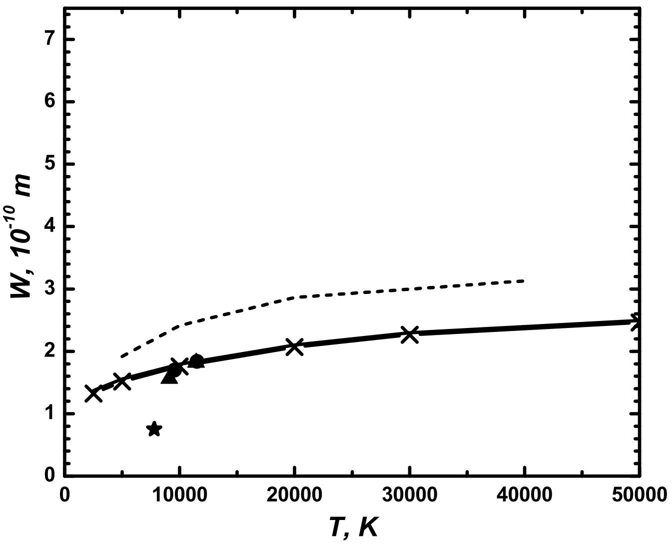

Fig. 7. Stark width of Ar I 603.2 nm versus temperature for electron density of 10^{16} cm^{-3}. (Theoretical results: dashed line - Griem (1974); solid line - Dimitrijević et al. (2007) for impact-electrons and impact-ions; solid line and cross symbols - Dimitrijević et al. (2007) for impact-electrons and quasistatic-ions; single symbols: experimental results from critical reviews (Lesage (2009) and references therein)

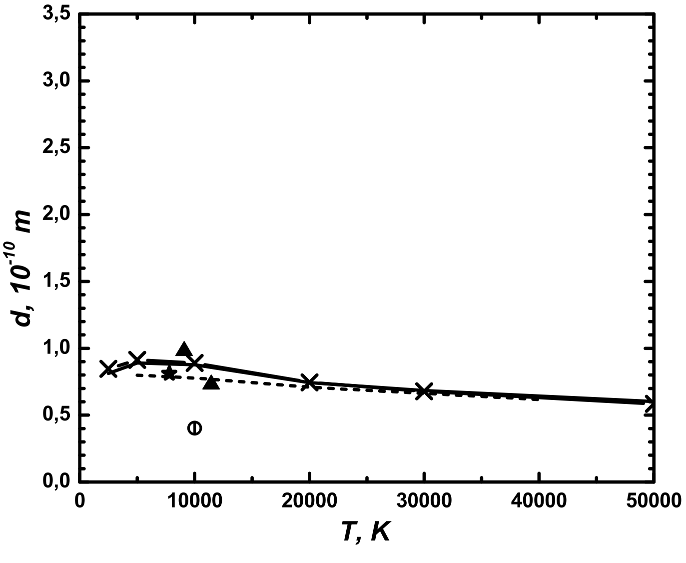

Fig. 8. Stark shift of Ar I 603.2 nm versus temperature for electron density of 10^{16} cm^{-3}. (Theoretical results: dashed line - Griem (1974); solid line - Dimitrijević et al. (2007) for impact-electrons and impact-ions; solid line and cross symbols - Dimitrijević et al. (2007) for impact-electrons and quasistatic-ions; single symbols: experimental results from critical reviews (Lesage (2009) and references therein))

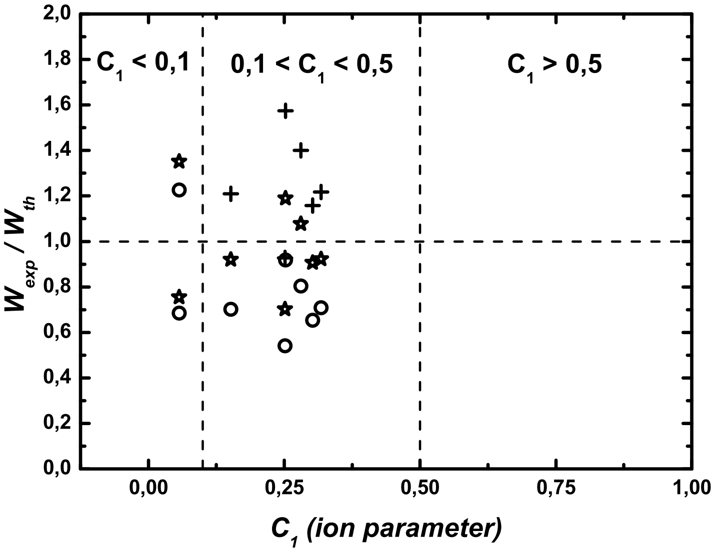

Fig. 9. Ratio of experimental and theoretical (○ according to Griem's theory, ★ Sahal-Bréchot theory with impact ions, + according to Sahal-Bréchot theory with quasistatic ions) Stark widths for Ar I 696.5 nm versus the validity criterion of the impact approximation for ions (the impact approximation for ions is valid if the parameter C_1 is small compared to unity).

Also for example, temperatures around 50 000 K are typical for Be star Hen 2-90.

One can see that the behavior of the electron impact widths and shifts within the considered spectral series is so regular, therefore interpolation and extrapolation of new data is possible.

Comparison with other theoretical and experimental results

In Figures 5-8 the calculations of Dimitrijević et al. (2007) for the Stark broadening parameters of studied spectral lines in pure argon gas are compared with those published by Griem (1974, 1964) and with the experimental widths and shifts, with estimated accuracy A or B, from published critical reviews (see Lesage (2009) and references therein). For lines, where there are no results in Griem (1974), corresponding data from Griem (1964, 1962) were used.

For the Ar I 549.6 and 603.2 nm spectral lines the impact approximation is not valid for ions under all experimental conditions (Dimitrijević et al. 2007) in the relevant papers (Lesage (2009) and references therein on critical reviews for earlier period).

In Figures 5-8, the electron-impact width from Dimitrijević et al. (2007) is presented once with impact ion contribution, and once with quasistatic, so that two curves may be compared. The theoretical results for Stark broadening obtained in Dimitrijević et al. (2007) are closer to the experimental points for these lines.

The difference between curves with total Stark broadening parameters with impact and quasistatic ion broadening is small. For 549.6 nm, one obtains smaller widths and shifts with impact ions (Figures 5, 6). The shift values for 549.6 nm from Griem (1964) are in very good agreement with impact-electrons + quasistatic-ions values in Dimitrijević et al. (2007), and coincide for temperatures up to 20000 K. In fact, for 603.2 nm the broadening and shift values in the cases of impact and quasistatic ions obtained in Dimitrijević et al. (2007) are the same (see Figures 7, 8). Shift values from Sahal-Bréchot theory are a little bit

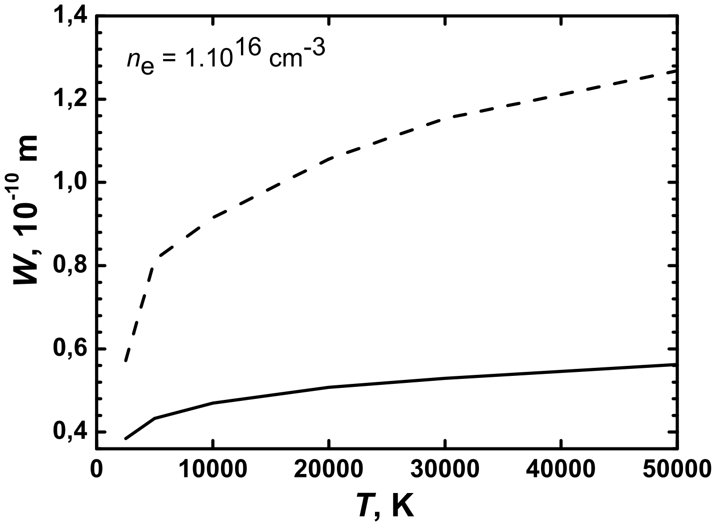

Fig. 10. Electron impact width of: Ne I 837.7 nm (solid line) and Ar I 737.2 nm (dashed line) spectral lines versus the temperature for electron density of 10^{16} cm^{-3}.

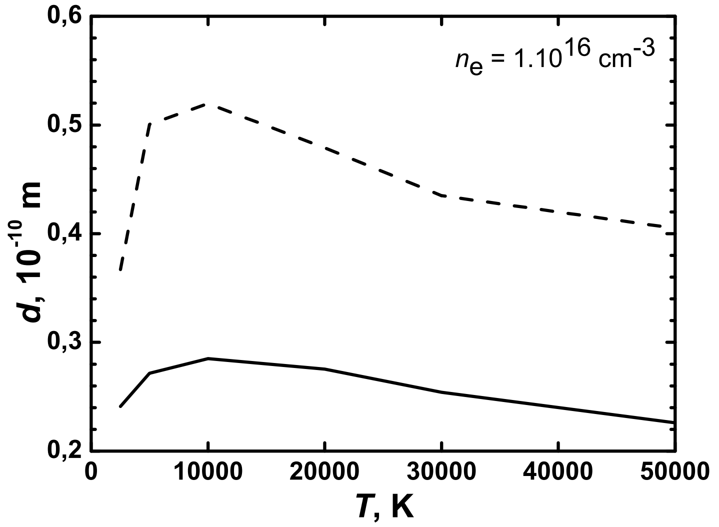

Fig. 11. Electron impact shift of: Ne I 837.7 nm (solid line) and Ar I 737.2 nm (dashed line) spectral line versus the temperature for the electron density of 10^{16} cm^{-3}.

larger, then Griem's calculated ones, for temperatures up to 20000 K and practically equal for higher temperatures.

The Ar I 696.5 nm spectral line is one of the most used argon lines for the diagnostic purposes. It is well isolated, visible and intense. This explains the great interest for it. This line is usually applied to measure the electron densities over 1.10^{16} cm^{-3}. In Figure 9 the ratios of measured widths for this line and

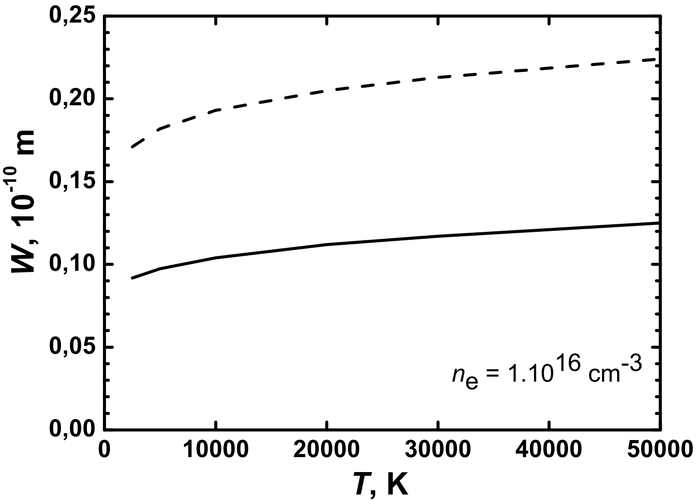

Fig. 12. Impact width due to protons collisions of: Ne I 837.7 nm (solid line) and Ar I 737.2 nm (dashed line) spectral lines versus the temperature for electron density of 10^{16} cm^{-3}.

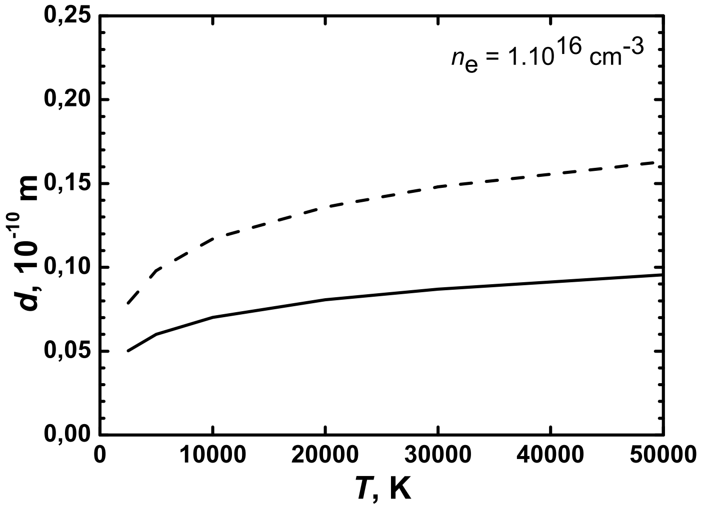

Fig. 13. Impact shift due to proton collisions of: Ne I 837.7 nm (solid line) and Ar I 737.2 nm (dashed line) spectral line versus the temperature for the electron density of 10^{16} cm^{-3}.

calculated ones (according to Griem's (Griem 1964) and Sahal-Bréchot theory with impact and quasistatic ion contribution) versus the parameter C_1 for ion perturbers are presented. C_1 is the impact approximation validity criterion (C_1 should be much less than one. We use here less or equal to 0.1). The values of C_1 correspond to the experimental n_e and T conditions, according to (Konjević et al 2002). The majority (six) of experimental widths fall within the transitional range (from impact to quasistatic regime for ion perturbers, $0.5 > C_1 > 0.1$),

Table 2. Basic data for the considered Ne I spectral line. Here λ denotes wavelength, i and f are initial and final level of the transition (within the frame of $j - L$ coupling), i' and f' are the corresponding perturbing levels, E_i and E_f are the energy values and n* is the effective quantum number of the initial level.

λ nm	Transition (i - f)	i' levels	f' levels	E_i cm^{-1}	E_f cm^{-1}	n*
837.7	$2p^53d' - 2p^53p$ $^2[7/2]^o_4 - ^2[5/2]_3$	4f, 5f, 3p, 4p, 5p	3s, 4s, 5s, 3d, 4d, 5d	161590.3	149657.0	2.98

two – in the impact regime ($C_1 < 0.1$) and there are no data for $C_1 > 0.5$, when only the quasistatic approximation is applicable. The both theories predict similar values in the impact regime. One can see that in average the Griem's theory overestimates the experimental Stark widths in the transitional range. The Sahal-Bréchot theory gives better results in this region. The ratio values for impact ions (Dimitrijević et al. 2007) are near to unity in the second region, while those for quasistatic ions (Dimitrijević et al. 2007) are underestimated.

A comprehensive study of the experimental Stark broadening of Ar I 696.5 nm, published over the period of 30 years was reported in Pellerin et al. (1996) yielding $W = 0.0814$ nm ± 5.0%, normalized to $n_e = 10^{17}$ $cm^{-3}$and $T = 13\,000$ K. There is a good agreement between this value and our calculated Stark width using Sahal-Bréchot theory which is 0.0857-0.0884 nm ± 30%.

The good agreement between available experimental results in the literature and our calculated Stark broadening parameters shows that the Stark theoretical data can be applied for modeling of stellar atmospheres of hot stars and for the analysis and synthesis of their spectra. One advantage of the results in Dimitrijević et al. (2007) is that the results for Stark broadening parameters for ions and protons are given in impact approximation which is often more appropriate in the case of hot stars.

A comparison of analogous neon and argon transitions

We will consider now Stark broadening for analogous transitions on the example of spectral lines: Ne I 837.7 nm $2p^53d$ - $2p^53p$ and Ar I 737.2 nm $3p^54d$ - $3p^54p$. The corresponding atomic data for neon transition are given in Table 2.

In the next four figures we give a comparison of their calculated Stark broadening parameters in order to study the variation of the width and shift of spectral line from analogues transitions. In Figures 10 and 11 the electron impact width and shift are presented as a function of temperature.

The Stark width due to collisions with electrons of the argon line is larger from 1.5 to 2.3 times than the neon one, while the corresponding Stark shift ratio vary from 1.5 to 1.8 in the whole temperature range. In Figures 12 and 13 the proton-impact widths and shifts are given.

The contribution of proton collisions in the Stark width for argon line is around 1.9 greater than those for neon line. The corresponding ratio for the Stark shift due to proton collisions slowly increases from 1.6 to 1.7. It is obvious that the difference of electron impact parameters for considered analogous transitions is larger than that of the protons.

4. Conclusion

The good agreement between available experimental results in the literature and our calculated Stark broadening parameters shows that the Stark theoretical data can be applied for the modeling of stellar atmospheres of hot stars and their spectra.

The observed similarities and regularities of Stark broadening parameters of spectral line within a spectral series can be used to obtain new data.

The study of Stark widths and shifts of spectral lines belonging to analogous transitions needs further efforts.

Acknowledgements. This work is a part of the project 146 001 “Influence of collisional processes on astrophysical plasma lineshapes” supported by the Ministry of Science and Technological development of Serbia. Partial support by the Technical University – Sofia was also given.

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