Similarities in Calculated Stark Broadening Parameters of Argon Spectral Lines

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Abstract. The similarities of the calculated Stark broadening parameters of four argon spectral lines within a spectral series 3p57d – 3p54p have been analyzed. The Stark broadening parameters have been calculated using Sahal-Bréchot theory within the semi-classical perturbation formalism. The dependences of the Stark width and shift versus the effective quantum number have been presented.

1. Introduction

The broadening of spectral lines of heavy elements in plasmas is principally determined by two factors, the plasma environment and the atomic structure of the emitting atom or ion. Since atomic structures exhibit many great regularities and similarities, one must expect the same for the width and shift parameters of plasma broadened lines. A comprehensive study and analysis of regularities and similarities of the existing experimental data for the Stark broadening parameters have been presented in [1], based on the L-S coupling scheme.

One of the most useful gases for laboratory plasmas, argon, is also interesting in astrophysics since with the development of space-borne spectroscopy, the importance of atomic data, including line broadening parameters for trace elements like argon [2], is increasing. For example argon is found in CVn binary σ2 Coronae Borealis [3], and “Chandra’s” X-ray spectra of young supernovas 1998S and 2003bg revealed an argon over-abundance [4]. Recently, argon lines are observed in the optical spectrum of the Be star Hen 2-90 [5], as well as in planetary nebulae and H II regions in the two dwarf irregular galaxies Sextans A and B [6]. Also argon abundance has been determined from spectral lines, e.g. for LSE 78, an extreme helium star [7], for the similar star BD-9º4395 [8], for DY Cen [9] and γ Peg [10], as well as for the Sun [11]. Consequently, Stark line broadening parameters for neutral and ionized argon are of interest for the modeling and investigation of astrophysical plasmas. 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 this work, the systematic trend of Stark broadening parameters of Ar I 522.1, 549.6, 603.2 and 737.2 nm spectral lines within the same spectral series with the corresponding transitions 3p57d – 3p54p, 3p56d – 3p54p, 3p55d – 3p54p and 3p54d – 3p54p has been investigated. The behavior of these parameters with the increase of the effective quantum number of the initial energy levels of the...
corresponding transition within the spectral series has been obtained. The results for Ar I 522.1, 549.6 and 603.2 are given in [12] where the calculations are oriented to laboratory plasmas. The examined perturbers are electrons, argon ions and protons. The presented calculations in this work are oriented for astrophysical purposes and the studied perturbers are electrons, protons and helium ions.

2. Theory

The Stark broadening parameters have been calculated using Sahal-Bréchot theory within the semiclassical perturbation formalism [13, 14], where the full width \( W \) at half maximum 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:

\[
W = 2n_e \int_0^{\infty} vf(v)dv \left[ \sum_p \sigma_{ii'}(v) + \sum_{f'=f} \sigma_{ff'}(v) + \sigma_{el} \right] \tag{1}
\]

\[
d = \int_0^{\infty} vf(v)dv \left[ 2\pi x d \rho \sin 2\varphi_p \right], \tag{2}
\]

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 the 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 \( \rho' \):

\[
\sum_{i'\neq i} \sigma_{ii'}(v) = \frac{1}{2} \pi R_i^2 + \int_0^R 2\pi x d \rho \sum_{i'\neq i} P_{ii'}(\rho, v). \tag{3}
\]

The elastic collision contribution to the width is given by:

\[
\sigma_{el} = 2\pi R_e^2 + \int_0^R 8\pi x d \rho \sin^2 \delta \tag{4}
\]

\[
\delta = (\varphi_p^2 + \varphi_q^2)^{1/2}. \tag{5}
\]

The phase shifts \( \varphi_p \) and \( \varphi_q \) are due to the polarization and to the quadrupole potential, respectively. The cut-off parameters \( R_1, R_2, R_3 \), the Debye cut-off \( R_d \), and the symmetrization procedure are described in [13, 14].

The impact approximation is valid when the duration of collisions is much shorter than the separation time between strong collisions (collisions whose resulting phase shift is bigger than 1 rad):

\[
n_e \rho_{op} \ll 1, \tag{6}
\]

where \( \rho_{op} \) is the typical impact parameter for strong collisions.

The resulting profiles are Lorentzian. For ion collisions the impact approximation might fail, especially for high densities or low temperatures. Within the impact approximation the ion broadening contribution has a Lorentzian shape and the total full width or shift is simply the sum of the corresponding full widths or shifts for electron and ion broadening. If the impact approximation is not applicable to ion broadening, it is possible to apply the quasistatic approximation given by Griem in [15]. Then the ion broadening parameters obtained within the quasistatic approximation, denoted here with the index \( iq \), are:

\[
W_{iq} = 1.75.10^{-4} n_e^{1/4} A[1 - 0.068n_e^{1/6}T^{-1/2}] W_e \tag{6}
\]

\[
d_{iq} = 10^{-4} n_e^{1/4} A[1 - 0.068n_e^{1/6}T^{-1/2}] W_e, \tag{7}
\]

where \( W_e \) is the impact contribution of electrons to the total width, \( T \) is in Kelvin, and \( n_e \) in cm\(^3\). \( A \) is the quasistatic parameter, defined in [15] as follows:

\[
A = \left( \frac{eF_0^2}{\hbar W_e} \alpha_0 - \alpha_f \right)^{3/4}, \tag{8}
\]
where \( F_0 = 2 \pi \left( \frac{4}{15} \right)^{2/3} \frac{e \nu_{ei}^{2/3}}{\alpha_i} \) is the normal field strength. The polarizability of the initial level \( \alpha_i \) (resp. \( \alpha_f \) is the polarizability of the final level) is expressed as:

\[
\alpha_i = 4a_0^3 \sum_{i \neq f} f\nu_i \left( \frac{I_{ii}}{\Delta E_{ii}} \right)^2, \tag{9}
\]

where \( a_0 \) is the Bohr radius, \( f\nu_i \) is the oscillator strength, and \( I_{ii} \) is the ionization energy of hydrogen.

3. Results

The calculations were performed for particular lines within multiplets (spin-orbital interaction is included). The most appropriate \( j-L \) coupling scheme for argon atoms has been used. The values of the energy levels have been taken from the NIST catalogue \([16]\). The oscillator strengths \((j-L)\) coupling have been calculated within the Bates & Damgaard approximation. The calculations have been made for a set of temperatures \((2.5 - 5.0) \times 10^4 \) K at a perturber (electrons, protons and helium ions) density of \(10^{16} \) cm\(^{-3}\).

In this work we present the calculated Stark broadening parameters for the Ar I 737.2 nm spectral line. In table 1 the wavelengths of the studied argon lines, the corresponding transitions in \( j-L \) coupling, the perturbing levels \( i' \) and \( f' \), the energy values, and the effective quantum number of the initial level are presented.

Table 1. Basic data on the considered Ar I spectral lines. Here \( \lambda \) denotes the wavelength, \( i \) and \( f \) are the 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.

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

The results are presented in table 2 for the Ar I 737.2 nm argon line. The calculated Stark widths (full width at half intensity maximum) \( W \) and shifts \( d \) for collisions with electrons \((W_e, d_e)\), \( \text{He}^+ \) ions \((W_{\text{He}^+}, d_{\text{He}^+})\), and protons \((W_p, d_p)\) are given. The ratio \( C/W \) gives the value of the maximum density for which the line is isolated for the corresponding perturber.

For the atmospheres of the main branch stars the total Stark width \( W \) and shift \( d \) are approximately:

\[
W = W_e + 0.9W_p + 0.1W_{\text{He}^+}, \tag{10}
\]

\[
d = d_e + 0.9d_p + 0.1d_{\text{He}^+}. \tag{11}
\]
Table 2. Stark broadening parameters for Ar I 737.2 nm for a perturber (electrons, helium ions, and protons) density of $10^{16}$ cm$^{-3}$ and temperatures from 2500 up to 50000 K.

| Perturbers are: | Electrons | Ionized helium | Protons |
|----------------|-----------|----------------|---------|
| Transition     | $T$ ($10^3$ K) | $W_e$ (0.1 nm) | $d_e$ (0.1 nm) | $W_{He^+}$ (0.1 nm) | $d_{He^+}$ (0.1 nm) | $W_p$ (0.1 nm) | $d_p$ (0.1 nm) |
| $4d^2[7/2]_4$ | 2.5       | 0.572          | 0.367     | -                 | -                 | 0.171      | 0.787$\times10^{-1}$ |
| $4p^2[5/2]_3$ | 5         | 0.646          | 0.425     | 0.168             | 0.0756            | 0.182      | 0.980$\times10^{-1}$ |
| 737.2 nm       | 10        | 0.739          | 0.428     | 0.176             | 0.0917            | 0.193      | 0.117 |
| $C = 0.65\times10^{19}$ | 20       | 0.871          | 0.371     | 0.185             | 0.108             | 0.205      | 0.136 |
| $4d^2[7/2]_4$ | 30        | 0.964          | 0.318     | 0.19              | 0.117             | 0.213      | 0.148 |
| $4p^2[5/2]_3$ | 50        | 1.07           | 0.275     | 0.198             | 0.13              | 0.224      | 0.163 |

In figures 1 and 2 the temperature dependences of the electron impact width and shift (electron density $10^{16}$ cm$^{-3}$) of Ar I 737.2 nm are illustrated.

**Figure 1.** Electron impact width of the Ar I 737.2 nm spectral line versus the temperature for a $10^{16}$ cm$^{-3}$ electron density.

**Figure 2.** Electron impact shift of the Ar I 737.2 nm spectral line versus the temperature for a $10^{16}$ cm$^{-3}$ electron density.

The contributions of the different collisions between emitters and perturbers (inelastic and elastic (polarization) collisions) in the Stark width of the examined argon lines from one spectral series show a similar behavior versus the temperature. One example for this behavior is presented in figure 3 for the Ar I 522.1 nm argon line. The broadening coefficient ($\beta = W / n_e$) and their components ($\beta_{in}$ – contribution of inelastic collisions, $\beta_{el}$ – contribution of elastic collisions, and $\beta_{p}$ – contribution of polarization (the polarization interactions are elastic ones) collisions) have been analyzed. The inelastic component increases with the temperature while the elastic and polarization ones decrease for the argon lines from the studied series. The quadruple component ($\beta_{q}$) depends only by the initial and final states of the emitters and does not depend on the temperature and perturber density, and is not included in the figure.
Figure 3. Stark broadening coefficient for Ar I 522.1 nm ($\beta = W / n_e$) and their components: $\beta = \beta_{\text{in}} + \beta_{\text{el}}$, where $\beta_{\text{in}}$ is the contribution of the inelastic argon emitter-perturber collisions, $\beta_{\text{el}}$ is the contribution of elastic ones, $\beta_{\text{al}} = \beta_{\text{in}} + \beta_{\text{el}}$ ($\beta_p$ gives the contribution of polarisation interactions and $\beta_q$ – of the quadruple interactions). The quadruple interactions do not depend on the temperature and the perturber density so it is not presented in the figure.

In figures 4 and 5 the electron impact width and shift, respectively, are given. From one side, the argon spectral lines are broadened mainly due to the collisions with electrons, usually. From the other side, it is more correct to study the width and shift trends of the spectral lines for each kind of perturbers separately.

One can see that the behavior of the electron impact widths and shifts within the considered spectral series is so regular, that interpolation and extrapolation of new data is possible. The complete
analysis of the results of this paper and the comparison with other theoretical and experimental data available in the literature will be given in [17].

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