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Ion contribution to the prominent Ne I, Ar I and Kr I spectral line broadening

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Abstract. On the basis of the observed asymmetry of the measured spectral line profiles we have obtained the ion contribution to the Ne I (26 lines), Ar I (19 lines) and Kr I (20 lines) spectral line broadening due to the quasi-static ion approximation and ion-dynamical effects. The ion broadening parameters (A) and the ion dynamic coefficients (D) have been obtained directly by the use of our line deconvolution procedure which allows the determination of the basic physical properties that characterize the line profile and also the relevant plasma parameters. We are the first to publish experimental data, viz. D and A values for the Ne I, Ar I and Kr I lines. The 26 Ne I, 6 Ar I and 9 Kr I A values are the first measured data and many of them are the first published data in this field. We have found clear evidence of the quasi-static ion and ion-dynamical effects on the investigated line shapes; they play a much more important role than the approaches based on semiclassical theory provide, especially in the case of the Ne I spectral lines. This is of importance for astrophysical plasma modeling and diagnostics.

Key words. plasmas – line: profiles – atomic data

1. Introduction

Spectral line shapes represent very important sources of information about the physical conditions in the place of birth of the radiation, especially since the launch of the Hubble space telescope (Lesage & Fuhr 1999, and references therein). Many theoretical (Griem 1974, 1997; Barnard et al. 1974; Alexiou et al. 2000) and experimental studies have been dedicated to line shape investigations (Lesage & Fuhr 1999; NIST 2002; Konjević et al. 2002) (and references therein). Among these, the studies dealing with neutral spectral lines are of special interest because of the strong presence of these neutral lines in low-temperature (10 000 K–30 000 K) cosmic plasmas. Neutral spectral lines have been used to determine neon abundances in late–to mid–B stars (Sigut 1999). Neon is also present in oxygen–neon White Dwarfs (Gil–Pons & García–Berro 2001). Ar I absorption lines have been detected in the spectra of the quasar Q0347-3819 (Levshakov et al. 2002) and PG 1259 + 593 (Richter et al. 2001). Mallouris (2001) refers to the presence of Ar I lines in the spectrum of the Wolf–Rayet binary SK 108. Argon is detected in the spectrum of the damped Ly–α system of Izw 18 (Levshakov et al. 2001). Kr I lines are detected in the spectra of Translucent Clouds (Cartledge et al. 2001) and in the spectra of a number of stars (Cardelli & Meyer 1997). Moreover, in recent investigations of the spectra of Planetary Nebulae (Dinerstein 2001) it was found that krypton is one of the most abundant elements in the cosmos with Z > 32. When the Stark effect becomes important the neutral line profiles show asymmetry (Griem 1974; Barnard et al. 1974; Griem 1997). Asymmetries near the center of isolated spectral lines in plasmas can be caused by the microfield-induced quadratic Stark shifts of the energy levels of the radiating atoms. It should be mentioned that ions are not necessarily quasi-static. A dynamical treatment of ions may be found in Griem (1974) and Barnard et al. (1974). If ions are quasi-static, we generally get an asymmetric profile. As shown in Alexiou (1996), Alexiou et al. (1997) and Oks (1999) in the general case (i.e. ion dynamics) there is always an impact contribution from ions, which simply adds to (and may not be distinguished from) the electron impact contribution. The relative importance of this impact ionic contribution diminishes with increasing density. We emphasize that care must be taken in interpreting the line broadening parameters if ion impact is important, as we cannot experimentally distinguish between the electronic and ionic contributions. The ion contribution to the line shape, depending on the plasma conditions, is described by the ion broadening parameter (A) due to the quasi-static ion effect, and the ion dynamic coefficient (D) due to the ion-dynamical effect, respectively (Griem 1974;
Barnard et al. 1974; Kelleher 1981). Various theoretical papers deal with these contributions, but the number of experimental studies dedicated to these properties is limited (Jones et al. 1986, 1987; Hahn & Woltz 1990; Nikolić et al. 1998; Schinköth et al. 2000).

The aim of this work is to present the A and D values of the prominent Ne I, Ar I and Kr I spectral lines useful in the diagnostics of various laboratory and cosmic plasmas. On the basis of the precisely recorded spectral line profiles and their observed asymmetries we have obtained the A and D values by the use of our deconvolution procedure described in Milosavljević & Poparić (2001); Milosavljević (2001) and already applied to the prominent He I lines (Milosavljević & Djeniže 2002). It includes a new advanced numerical procedure for the deconvolution of the theoretical asymmetric convolution integral of a Gaussian and a plasma broadened spectral line profile $J_{\lambda,R}(\lambda)$. This method gives complete information on the plasma parameters from a single recorded spectral line. The method determines all line broadening and plasma parameters (electron density ($N$) and electron temperature ($T$)) self-consistently and directly from the shape of spectral lines without any assumptions or prior knowledge. All one needs to known is the instrumental width of the spectrometer. It should be pointed out that this deconvolution procedure is very useful in the case of astrophysical plasmas where direct measurements of the relevant plasma parameters are impossible.

We have obtained the ion contribution to the Ne I (26 lines), Ar I (19 lines) and Kr I (20 lines) spectral lines broadening due to the quasi-static ion approximation and ion–dynamical effects. Our D values for the Ne I, Ar I and Kr I lines are the first experimental data. The 26 Ne I, 6 Ar I and 9 Kr I A values are the first measured data and many of them are the first published data in this field.

2. Theoretical background

The total line Stark FWHM (full-width at a half intensity maximum, $W_l$) is given as

$$W_l = W_e + W_i,$$

(1)

where $W_e$ and $W_i$ represent the electron and ion contributions, respectively. For a non–hydrogenic, isolated neutral atom line the ion broadening is not negligible and the line profiles are described by an asymmetric $K$ function (see Eq. (6) in Sect. 3 and in Milosavljević & Poparić 2001). The total Stark width ($W_l$) may be calculated from the equation (Griem 1974; Barnard et al. 1974; Kelleher 1981):

$$W_l \approx W_e(1 + 1.75AD(1 - 0.75R)),$$

(2)

where

$$R = \sqrt{\frac{36 \cdot \pi \cdot e^6 \cdot N}{(K T)^3}},$$

(3)

is the ratio of the mean ion separation to the Debye length. $N$ and $T$ represent electron density and temperature, respectively. $A$ is the quasi-static ion broadening parameter (see Eq. (224) in Griem 1974) and $D$ is a coefficient of the ion-dynamic contribution with the established criterion:

$$D = \frac{1.36}{1.75 \cdot (1 - 0.75 \cdot R)} \cdot B^{1/3}$$

for

$$B < \left( \frac{1.36}{1.75 \cdot (1 - 0.75 \cdot R)} \right)^3;$$

or

$$D = 1 \quad \text{for} \quad B \geq \left( \frac{1.36}{1.75 \cdot (1 - 0.75 \cdot R)} \right)^3,$$

(4)

where

$$B = A^{1/3} \frac{4.03 \times 10^{-7} \cdot W_e[\text{nm}]}{(d[\text{nm}])^2} \cdot (N[\text{m}^{-3}])^{2/3} \cdot \sqrt{\frac{\mu}{T_e[K]}} < 1;$$

(5)

is the factor with atom-ion perturber reduced mass $\mu$ (in amu) and gas temperature $T_e$. When $D = 1$ the influence of the ion–dynamical effect is negligible and the line shape is treated using the quasi-static ion approximation. From Eqs. (1)–(6) it is possible to obtain the plasma parameters ($N$ and $T$) and the line broadening characteristics ($W_e$, $W_i$, $A$ and $D$). One can see that the ion contribution, expressed in terms of the $A$ and $D$ parameters directly determine the ion width ($W_i$) component in the total Stark width (Eqs. (1), (2)).

3. Numerical procedure for deconvolution

The proposed functions for various line shapes, Eq. (6) are of the integral form and include several parameters. Some of these parameters can be determined in separate experiments, but not all of them. Furthermore, it is impossible to find an analytical solution for the integrals, and methods of numerical integration have to be applied. This procedure, combined with the simultaneous fitting of several free parameters, causes the deconvolution to be an extremely difficult task and requires a number of computer supported mathematical techniques. Particular problems are the convergence and reliability of the deconvolution procedure, which are closely connected with the quality of experimental data.

$$K(\lambda) = K_o + K_{\text{max}} \int_{0}^{\infty} \exp(-r^2) \left[ \int_{0}^{\infty} \frac{H_0(\beta)}{1 + (2^{-\lambda - \lambda_o} - \frac{H_0(\beta)}{W_o})} \cdot \beta^2 \cdot d\beta \right] \cdot dt;$$

(6)

Here $K_o$ is the baseline (offset) and $K_{\text{max}}$ is the maximum intensity (for $\lambda = \lambda_o$) (Milosavljević & Poparić 2001). $H_0(\beta)$ is an electric microfield strength distribution function of normalized field strength $\beta = F/F_o$, where $F_o$ is the Holtsmark field strength. $A (\alpha = A^{1/3})$ is the static ion broadening parameter and is a measure of the relative importance of ion and electron broadenings. $R$ is the ratio of the mean distance between the ions to the Debye radius (see Eq. (3)), i.e. the Debye shielding
Table 1. Various discharge conditions: C-bank capacity (in μF), U-bank voltage (in kV), H-plasma length (in cm), Φ-tube diameter (in mm), P-filling pressure (in Pa). \( N^{\exp} \) (in 10^{22} \text{ m}^{-3}) and \( T^{\exp} \) (in 10^1 \text{ K}) denote experimental electron density and temperature, respectively obtained at a moment when the line profiles were analyzed. \( N^C \) (in 10^{22} \text{ m}^{-3}) and \( T^C \) (in 10^1 \text{ K}) represent averaged electron density and averaged electron temperature obtained by using our line deconvolution procedure (Milosavljević & Poparić 2001).

<table>
<thead>
<tr>
<th>Emitter</th>
<th>Working gas</th>
<th>Exp.</th>
<th>C</th>
<th>H</th>
<th>Φ</th>
<th>P</th>
<th>( N^{\exp} )</th>
<th>( N^C )</th>
<th>( T^{\exp} )</th>
<th>( T^C )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ne1</td>
<td>pure neon</td>
<td>a1</td>
<td>14</td>
<td>1.5</td>
<td>7.2</td>
<td>5</td>
<td>133</td>
<td>6.7 ± 7%</td>
<td>7.0 ± 12%</td>
<td>33.0 ± 6%</td>
</tr>
<tr>
<td>Ne1</td>
<td>pure neon</td>
<td>a2</td>
<td>14</td>
<td>2.5</td>
<td>7.2</td>
<td>5</td>
<td>133</td>
<td>8.8 ± 7%</td>
<td>9.2 ± 12%</td>
<td>36.5 ± 6%</td>
</tr>
<tr>
<td>Ar1</td>
<td>72% Ar + 28% He</td>
<td>b1</td>
<td>14</td>
<td>1.5</td>
<td>7.2</td>
<td>5</td>
<td>133</td>
<td>6.7 ± 7%</td>
<td>6.9 ± 12%</td>
<td>16.5 ± 11%</td>
</tr>
<tr>
<td>Ar1</td>
<td>97% Ar + 3% H2</td>
<td>b2</td>
<td>14</td>
<td>1.5</td>
<td>7.2</td>
<td>5</td>
<td>67</td>
<td>7.0 ± 7%</td>
<td>7.3 ± 12%</td>
<td>16.0 ± 11%</td>
</tr>
<tr>
<td>Kr1</td>
<td>pure krypton</td>
<td>c</td>
<td>14</td>
<td>1.5</td>
<td>7.2</td>
<td>5</td>
<td>133</td>
<td>7.1 ± 7%</td>
<td>7.4 ± 12%</td>
<td>16.2 ± 11%</td>
</tr>
</tbody>
</table>

The electron density and temperature obtained by using our line deconvolution procedure (Milosavljević & Poparić 2001). For the Ar1 lines no theoretical A values exist.

5. Discussion

5.1. Neon spectral lines

Our \( A^{\exp} \) and \( D^{\exp} \) values are the first measured data in this field. Our \( A^{\exp} \) values are much higher than Griem’s \( A^G \) data by up to a factor 3–6. Extreme disagreement was found in the case of the 703.241 nm and 724.517 nm spectral lines belonging to the lower lying 3s–3p transition. In this case the theoretical \( A^G \) values are very low and lie far below our measured data by up to a factor 15. The obtained \( D^{\exp} \) values are relatively high (at our plasma conditions) and multiply the quasi-static ion effect by about 2.2 times (on average) in the case of all investigated Ne1 lines.

We have found that the ion contribution to the Ne1 spectral line profiles plays a more important role than the theoretical semiclassical approximation (Griem 1974) provides.

5.2. Argon spectral lines

Our \( A^{\exp} \) are higher than the uniquely theoretical \( A^G \) values, by about 80% (on average). The A data obtained by Schinköth et al. (2000) for 15 Ar1 lines (in the 4s–4p transition) show similar behavior. Our ion dynamic coefficients \( D^{\exp} \) show dependence on the upper level energy of the transition. They are higher for the low lying transitions (4s–4p). In these cases the ion dynamic effect (at our plasma conditions) multiply the quasi-static ion effect by about 3 times. In the cases of high–lying transitions (4p–4d, 4p–5d and 4p’–6d) the ion dynamic effect is negligible (\( D \sim 1.2 \)) within the accuracy of the measurements.

5.3. Krypton spectral lines

Our \( A^{\exp} \) values can be separated into two groups. In the first group are the higher A values (from 0.06651 up to 0.07428) corresponding to the lines in the 5s–5p transitions.

parameter and \( W_e \) is the electron width (FWHM) in the \( j_{\lambda,R} \) profile (Griem 1974).

For the purpose of the deconvolution iteration process we need to know the value of \( K \) (Eq. (6)) as a function of \( \lambda \) for every group of parameters (\( K_{\max}, \lambda_0, W_e, W_G, R, A \)). \( W_G \) is defined in Eq. (2.3) of Milosavljević & Poparić (2001). The used numerical procedure for the solution of Eq. (6) is described in earlier publications (Milosavljević & Poparić 2001; Milosavljević 2001; Milosavljević & Djeniže 2002). It should be noted that to apply this deconvolution and fitting method some assumptions or prior knowledge about plasma conditions are necessary. For each emitter ionization stage one needs to know the electric microfield distribution, in order to fit the \( K \) functions. In the cases of quasi-static or quasi-static and dynamic broadening, our fitting procedure gives the electron impact width (\( W_e \)), static ion broadening parameter (A) and, finally the dynamic ion broadening parameter (D).

4. Experiment and results

A linear low-pressure pulsed arc (Milosavljević et al. 2000, 2001; Milosavljević & Djeniže 2002; Djeniže et al. 1992, 2002) has been used as a plasma source. A pulsed discharge was driven in a quartz discharge tube at different inner diameters and plasma lengths. The used tube geometry and corresponding discharge conditions are presented in Table 1.

Spectroscopic observations of spectral lines were made end-on along the axis of the discharge tube and the profiles were recorded by a step-by-step technique. The used experimental procedures are described in Milosavljević et al. (2001) and in Djeniže et al. (2002) for the Ne1 lines, in Milosavljević (2001) for the Ar1 lines and in Milosavljević et al. (2000) for the Kr1 lines, together with the applied diagnostic methods. The experimentally obtained electron densities (\( N^{\exp} \)) and electron temperatures (\( T^{\exp} \)) are presented in Table 1 together with those (\( N^C \) and \( T^C \)) obtained using our line deconvolution procedure. It should be pointed out that the values \( N^{\exp} \) and \( N^C \), and \( T^{\exp} \) and \( T^C \) show excellent mutual agreement (within ±3% on average) providing confirmation of the validity of the used deconvolution procedure.

Our experimentally obtained quasi-static ion broadening parameters (\( A^{\exp} \)) and ion dynamic coefficients (\( D^{\exp} \)) are presented in Tables 2–4 together with the available theoretical \( A^G \) values taken from Griem (1974). The necessary atomic data were taken from NIST (2002) and Striganov & Sventickij (1996). For the Kr1 lines no theoretical A values exist.
The second group comprises the lower A values (from 0.05004 up to 0.05492) corresponding to the lines in the higher lying 5s–6p transitions.

It turns out that our \( A^{\exp} \) values show small internal scatter within the mentioned groups. They lie within ±7% of the mean value. A similar behavior is also shown by A values from Schinköth et al. (2000) in the 5s–5p transitions. Their scatter is ±6%.

The normalized A values obtained in Schinköth et al. (2000) are about 34% higher than ours. But, taking into account the difference between electron temperatures (10 000 K and 17 000 K) in the two experiments this discrepancy is really lower than 34% and can be estimated to be 20%. Thus, one can conclude that tolerable agreement exists among our A values and those from Schinköth et al. (2000).

It should be pointed out that our A values in the Kr I 5s–6p transitions are the unique data in this field. Our \( D^{\exp} \) values are the first obtained data in this field. We have found that the ion dynamic effect plays a significant role in the Kr I line broadening (at our plasma conditions) and multiplies the quasi-static ion effect by about 1.5 times (on average) in the case of the 5s–5p transition.

6. Conclusion

We have found a clear influence of the quasi-static ion and ion dynamic effects on the investigated spectral line shapes; they play a much more important role than the semiclassical theory provides, especially for the Ne I spectral lines, where our \( A^{\exp} \) values are much higher than theoretical \( A^G \) values. The observed ion dynamic effect, at our plasma conditions, multiplies the quasi-static ion contribution by up to a factor 3 for the Ar I (lower multiplets) lines and by up to a factor 2 for the Ne I lines. This can play an important role for the use of these lines for astrophysical plasma modeling or for diagnostic purposes.

Acknowledgements. This work is a part of the project “Determination of the atomic parameters on the basis of the spectral line profiles” supported by the Ministry of Science, Technologies and Development of the Republic of Serbia. S. Djeniža is grateful to the Foundation “Arany János Közalapítvány” Budapest, Hungary.
Table 3. Same as in Table 2 but for the 19 Ar I spectral lines (see also Table 1).

<table>
<thead>
<tr>
<th>Exp.</th>
<th>Tran.</th>
<th>Multiplet</th>
<th>λ (nm)</th>
<th>A&lt;sup&gt;exp&lt;/sup&gt;</th>
<th>A&lt;sup&gt;G&lt;/sup&gt;</th>
<th>D&lt;sup&gt;exp&lt;/sup&gt;</th>
<th>Tran.</th>
<th>Multiplet</th>
<th>λ (nm)</th>
<th>A&lt;sup&gt;exp&lt;/sup&gt;</th>
<th>A&lt;sup&gt;G&lt;/sup&gt;</th>
<th>D&lt;sup&gt;exp&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>b&lt;sub&gt;1&lt;/sub&gt;</td>
<td>4s–4p’</td>
<td>[3/2]&lt;sup&gt;1&lt;/sup&gt;–[1/2]&lt;sub&gt;0&lt;/sub&gt;</td>
<td>750.387</td>
<td>0.0636</td>
<td>2.489</td>
<td>4p–4d’</td>
<td>[1/2]&lt;sup&gt;1&lt;/sup&gt;–[3/2]&lt;sub&gt;0&lt;/sub&gt;</td>
<td>591.209</td>
<td>0.1419</td>
<td>1.030</td>
<td></td>
<td></td>
</tr>
<tr>
<td>b&lt;sub&gt;2&lt;/sub&gt;</td>
<td>4s–4p’</td>
<td>[1/2]&lt;sup&gt;1&lt;/sup&gt;–[1/2]&lt;sub&gt;0&lt;/sub&gt;</td>
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<td></td>
</tr>
<tr>
<td>b&lt;sub&gt;1&lt;/sub&gt;</td>
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<td>b&lt;sub&gt;2&lt;/sub&gt;</td>
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<td>[3/2]&lt;sup&gt;1&lt;/sup&gt;–[3/2]&lt;sub&gt;0&lt;/sub&gt;</td>
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<td>591.209</td>
<td>0.1419</td>
<td>1.030</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 4. Same as in Table 2 but for the 20 Kr I spectral lines (see also Table 1).

| Exp. | Transition | Multiplet | λ (nm) | A<sup>exp</sup> | D<sup>exp</sup> | Transition | Multiplet | λ (nm) | A<sup>exp</sup> | D<sup>exp</sup> |
|------|------------|-----------|--------|-----------------|------------|------------|-----------|--------|-----------------|------------|-------------|
| c    | 5s–5p’     | [3/2]<sup>2</sup>–[3/2]<sub>0</sub> | 758.741 | 0.074 | 1.464 | 5s–5p’ | [1/2]<sup>1</sup>–[1/2]<sub>0</sub> | 828.105 | 0.070 | 1.580 |
| c    | 5s–5p’     | [3/2]<sup>2</sup>–[3/2]<sub>0</sub> | 758.741 | 0.074 | 1.464 | 5s–5p’ | [1/2]<sup>1</sup>–[1/2]<sub>0</sub> | 828.105 | 0.070 | 1.580 |
| c    | 5s–5p’     | [3/2]<sup>2</sup>–[3/2]<sub>0</sub> | 758.741 | 0.074 | 1.464 | 5s–5p’ | [1/2]<sup>1</sup>–[1/2]<sub>0</sub> | 828.105 | 0.070 | 1.580 |
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| c    | 5s–5p’     | [3/2]<sup>2</sup>–[3/2]<sub>0</sub> | 758.741 | 0.074 | 1.464 | 5s–5p’ | [1/2]<sup>1</sup>–[1/2]<sub>0</sub> | 828.105 | 0.070 | 1.580 |

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