COMPARISONS AND COMMENTS ON ELECTRON AND ION IMPACT PROFILES OF SPECTRAL LINES

Sylvie Sahal-Bréchet¹, Milan S. Dimitrijević², Nebil Ben Nessib³

¹ Paris Observatory, LERMA CNRS UMR 8112, UPMC, 5 Place Jules Janssen, 92190 Meudon, France; sylvie.sahal-brechot@obspm.fr
² Astronomical Observatory, Volgina 7, 11060 Belgrade 38, Serbia; mdimitrijevic@aob.bg.ac.rs.
³ National Institute of Applied Sciences and Technology, University of Carthage, Tunis, Tunisia; nebil.bennessib@planet.tn

Received: 2011 August 8; accepted: 2011 August 15

Abstract. Stark broadening theory is currently operated for calculating widths and shifts of spectral lines that are needed for spectroscopic diagnostics and modeling in astrophysics, laboratory and technological plasmas. We have calculated a great number of data, obtained through the impact semiclassical perturbation theory: tables have been published for neutral atom and ion emitters, and typical temperatures, electron and ion densities. They are currently implemented in the STARK-B database which participates in the European effort within the Virtual Atomic and Molecular Data Centre. Despite of that, a great number of data are still missing. In the present paper, we revisit and compare a great number of the impact Stark widths and shifts by considering their semiclassical perturbation expressions. We also provide fitting formulae which are essential for the modeling codes of stellar atmospheres and envelopes.

Key words: atomic data – atomic processes – line: profiles – astronomical databases

1. INTRODUCTION

Pressure broadening of spectral lines arises when an atom, ion or molecule which emits or absorbs light in a gas or a plasma, is perturbed by its interactions with the other particles of the medium. In the present paper, we will consider atom or ion emitters and electron and ion colliders. This so-called Stark broadening has been extensively investigated for about 50 years. The results are now currently used for spectroscopic diagnostics and modeling. In astrophysics, with the increasing sensitivity of observations and spectral resolution in all domains of wavelengths, from far UV to infrared, it has become possible to develop realistic models of interiors and atmospheres of stars and interpret their evolution and the creation of elements through nuclear reactions. This requires the knowledge of numerous profiles, especially for trace elements, which are used as useful probes.
for abundance determinations. For white dwarfs in particular, Stark broadening is the dominant line broadening process. Hence, calculations based on a simple but enough accurate and fast method, are useful for obtaining numerous results. Ab initio calculations are a growing domain of development. Nowadays, the access to such data via an on-line database becomes crucial. This is the object of STARK-B (Sahal-Bréchot et al. 2008), which is a collaborative project between the Paris Observatory and the Astronomical Observatory of Belgrade. This database contains calculated widths and shifts of isolated lines of atoms and ions due to electron and ion collisions. It is devoted to modeling and spectroscopic diagnostics of stellar atmospheres and envelopes. In addition, it is relevant to laboratory plasmas, laser equipments and technological plasmas. It is a part of the Virtual Atomic and Molecular Data Centre (VAMDC, Dubernet et al. 2010; Rixon et al. 2010), which is a collaboration between groups involved in the generation and use of atomic and molecular data, funded by the European Union.

In the present paper, we will briefly recall the important points of the theory. Then we will revisit the orders of magnitudes and trends of the widths and shifts in the impact approximation for electron and ion colliders. This is useful for providing interpolation or extrapolation formulae for missing data, since it is impossible to calculate all the data necessary to the modeling. We will also provide fitting formulae, which are essential for the modeling codes of stellar atmospheres and stellar envelopes. The coefficients of our proposed fitting formulae will be implemented in STARK-B.

2. REMIND OF THE IMPACT LINE BROADENING FOR ISOLATED LINES

Stark broadening theory in the impact approximation is based on the founding papers by Baranger (1958a,b,c). The impact approximation is the first basic one: \( \rho \) being a typical impact parameter and \( v \) the relative velocity. The duration of a collision or collision time \( \tau = \rho/v \) must be much smaller than the mean interval between two collisions which is of the order of the inverse of the line width \( w \) (in angular frequency units). So the collisions between the radiating atom (or ion) act in dependently and are additive. It is quite always valid for electron collisions and is generally valid for collisions with positive ions in the conditions of stellar atmospheres (Sahal-Bréchot 1969a,b). The second basic approximation is the complete collision approximation: the radiating atom has no time to emit (or absorb) a photon during the collision process. In other words, the collision time \( \tau \) must be very much smaller than the time interval between two emissions (or absorptions) of photons. The latter is of the order of the inverse of the detuning \( \Delta \omega \). So, in the far wings, the atom can emit photons before the perturber has any time to move, and thus the process becomes quasistatic. In the line center, the impact approximation and the complete collision approximation are together valid, and the line broadening theory becomes an application of the theory of collisions between the radiating atom and the surrounding perturbers.

Then we will limit our study to the case of isolated lines: the levels of the \( i \rightarrow f \) transition broadened by collisions do not overlap with the neighbouring perturbing levels which are likely to modify the broadening by introducing optical coherences. So we will consider in the present paper neither hydrogen nor hydrogenic ionic lines, nor some specific helium lines and nor some lines arising from Rydberg levels.

This leads to a Lorentz line profile characterized by a width \( w \) (full half-width at half-maximum) and a shift \( d \) which depend on the physical conditions of the
medium (temperature $T$ and density $N$ of the perturbers). Owing to the impact approximation, $w$ and $d$ are proportional to the density. The width of the $i-f$ line can be expressed as a sum over the inelastic cross-sections $\sigma_{ii'}(v)$ and $\sigma_{ff'}(v)$ ($i'$ and $f'$ are the so-called perturbing levels) and over an elastic contribution $\sigma_{el}(v)$ that are integrated over the Maxwell distribution of velocities $f(v)$. The shift can be expressed in terms of another elastic contribution, cf. Baranger (1958c).

In addition, the Debye screening effect which can be important at high densities must be taken into account. This decreases $w$ and $d$ which are thus not proportional to the density.

Finally, we will remark that the fine and hyperfine structure can be neglected during collisions with electrons. This is due to the fact that the electron spin of the atom has no time to rotate (Larmor precession) during the collision time $\tau$, because the relative velocity atom-perturber $v$ is large. Consequently, but only in $LS$ coupling, the widths and shifts due to electron collisions are equal for the different lines of a multiplet. Departures from $LS$ coupling can be important for heavy atoms or for highly charged ions and then the fine structure widths and shifts can be different. For collisions with ions, the relative velocity is smaller, and the preceding condition is not completely fulfilled for the electronic spin, but the widths and shifts of the fine structure line are not very different. In fact, the hyperfine structure is always negligible during the collisions. However, if the fine structure (or hyperfine structure) splitting is not negligible, the components must be added (taking into account their shift and their relative intensities) for obtaining the global profile. This is the case of the hyperfine Mn II lines (Popović et al. 2008) and of the fine hydrogen Balmer lines (Stehlé 1985).

3. THE SEMICLASSICAL-PERTURBATION THEORY-SCP

Most of our calculations have been performed with the semi-classical-perturbation method (SCP) developed by Sahal-Bréchot (1969a,b) and further papers: Sahal-Bréchot (1974) for complex atoms, Fleurier et al. (1977) for inclusion of Feshbach resonances in elastic cross-sections of radiating ions, and by Mahmoudi et al. (2009) for very complex atoms. The numerical codes have been updated and operated by Dimitrijević & Sahal-Bréchot (1984) and then by many further papers. The accuracy is about 20% for the widths but less for the shifts, due to oscillations in the integration over the impact parameters in the neighbourhood of the cut-off region. Other methods are briefly reminded by Sahal-Bréchot (2010).

We now focus on the physical quantities that enter the expressions of $w$ and $d$. This permits to understand their behaviours and trends as functions of atomic structure (oscillator strengths $f_{ii'}$, $f_{ff'}$, energy levels $E_i$, $E_{i'}$, $E_f$, $E_{f'}$), temperature $T$, charges of the radiating ion $Z_A$ and perturber $Z_P$, reduced mass atom-perturber $\mu$. The incoming perturber moves along a straight path (neutral radiating atom) or a hyperbola for a radiating ion (Sahal-Bréchot 1969a,b). We refer to Sahal-Bréchot (1969a,b) for all the required formulae which will not be recalled here. We will only have a look on the results. We will focus on widths because shifts are often less accurate. First, we consider the role of collision strengths.

We begin by lines of neutral atoms on the example of Mg I lines (Dimitrijević & Sahal-Bréchot 1996 and STARK-B). Figure 1 shows the width of Mg I 3s$^1S-3p^1P^o$ as a function of the temperature $T$ in K, for an electronic density of $10^{12}$ cm$^{-3}$. The difference of energy between the initial (or final) level and the closest perturbing level is $\Delta E_{\text{min}} = 8451.64$ cm$^{-1}$, and $\Delta E_{\text{min}}/kT = 1.2$ at 5000 K. Rather distant
levels are involved, hence at those temperatures inelastic collisions are completely negligible for impact ions. Elastic collisions are mostly due to the quadrupolar potential (cf. right panel of Figure 1), and since the quadrupolar contribution does not depend on the reduced mass, this explains why the width due to impact proton and the soup of ions (same charge as that of protons) are equal.

Table 1 shows the increasing contribution of impact ions when higher levels are involved. It displays the ratio of the width due to electron collisions to the width due to Fe II collisions as a function of $T$ for Mg I $n+1, l+1 - n, l$, with $l = n$. The width due to impact ions becomes higher than that due to impact electrons.

Table 1. Mg I $n+1, l+1 - n, l$, with $l = n$: the ratio of the widths due to electron collisions to the width due to Fe II collisions as a function of $T$ (in $10^3$ K). $N = 10^{10}$ cm$^{-3}$.

<table>
<thead>
<tr>
<th>$T$ (10$^3$ K)</th>
<th>$6h - 5g$</th>
<th>$7i - 6h$</th>
<th>$8j - 7i$</th>
<th>$9k - 8j$</th>
<th>$10l - 9k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>5.08</td>
<td>3.59</td>
<td>2.30</td>
<td>1.440</td>
<td>0.720</td>
</tr>
<tr>
<td>4.5</td>
<td>4.35</td>
<td>2.80</td>
<td>1.71</td>
<td>0.998</td>
<td>0.474</td>
</tr>
<tr>
<td>6.0</td>
<td>3.97</td>
<td>2.48</td>
<td>1.45</td>
<td>0.800</td>
<td>0.400</td>
</tr>
</tbody>
</table>

Figure 2 shows the details of the contributions for two lines: Mg I $5q^1G - 6h^1H^0$, where the closest perturbing level is such as $\Delta E_{\text{min}} = 89.04$ cm$^{-1}$, and Mg I $9k - 10l$, where $\Delta E_{\text{min}} = 0.04$ cm$^{-1}$. The inelastic contribution of impact ions increases, and the contribution of the quadrupole term becomes negligible: it is less than 4% for electrons and less than 1% for ions.

Then we consider the case of ion lines on the example of the Li-like Al XI ion (Dimitrijević & Sahal-Bréchat 1994 and STARK-B). We begin with the case of the resonance line $2s - 2p$ (Figure 3), $\Delta E_{\text{min}} = 1.8446 10^6$ cm$^{-1}$, and $\Delta E_{\text{min}}/kT = 2.6$ at 5 $10^5$ K. Coulomb repulsion is high for colliding ions, and their contributions are less than 10%. The quadrupole part of the elastic contribution is predominant. Proton contribution is higher than He III contribution at high temperatures, ow-
Electron and ion impact spectral line profiles

Fig. 2. Left panel: Mg I 5g1G − 6h1Hσ. Right panel: Mg I 9k − 10l. The line widths $w$ in angular frequency units as a function of the temperature $T$ in K, the electronic density is $10^{18}$ cm$^{-3}$. Full lines are for total widths, dashed lines for inelastic contributions, dotted lines for elastic contributions, circles for electrons; triangles for Fe II ions.

Fig. 3. Al XI 2s2S − 2p2Pσ. The line widths $w$ are in angular frequency units, $N = 10^{18}$ cm$^{-3}$. Full lines are for total widths, dashed lines for inelastic contribution; dotted lines for elastic contributions; dot-dashed lines for quadrupole contribution, dotted lines without circles for Feshbach resonances, circles for electrons, diamonds for protons, triangles for He III ions. Left panel is for impact electrons, right panel – for impact ions.

ning to the decrease of the Coulomb repulsion. For elastic electron collisions, the quadrupole part is dominant, but Feshbach resonances are important at low temperatures. The case of the 2p − 5s line is completely different, because the 5s level is rather close to the 5p one: $\Delta E_{\text{min}}/kT = 1.39 \times 10^{-2}$ at 5 $10^5$ K. So the Coulomb repulsion is rather small for colliding ions, and the ionic width increases and becomes higher than the one due to electrons. The highest contribution is due to He III. This is due to the charge- and the reduced mass- effect. This is shown in Figure 4. The polarization potential prevails for elastic collisions because the involved levels are high.

This study explains why the widths due to impact ions of Cr I lines (Dimitrijević et al. 2005) are larger than the widths due to electrons: there are perturbing levels that are very close to the upper ones (4.26 and 14.14 cm$^{-1}$). This abnormal situation is due to configuration interaction effects.

Concerning the behaviour with the charge of the perturber, the widths and the shifts increase linearly with $Z_P$ (e.g., Dimitrijević 1999), as expected by the SCP formulae.
Second, we consider the effect of atomic structure and the charge of the radiating ion $Z_A$. It is expected that the width increases as $n^4$ when the principal quantum number $n$ increases. This is shown in Figure 5.

The widths are predicted to vary as $Z_{\text{eff}}^{-2}$, with $Z_{\text{eff}} = Z_A + 1$. Fig. 20 of Elabidi et al. (2009) shows a $-1.84$ slope for the $3s - 3p$ transitions from C IV to P XIII.

Now let us look at the influence of the chosen atomic structure for the SCP calculations. Larbi-Terzi et al. (2009), on the example of the widths of the C II $3d-nf$ series, have shown that the differences in the results are very weak (less than 1%) when the Coulomb approximation with quantum defect (Bates & Damgaard 1949) oscillator strengths are used, compared to the TOPBASE R-matrix calculations (Cunto et al. 1973). In fact, C II is a simple atom and a simple atomic structure is sufficient. However, when highly charged ions or moderately charged ions like Si V (Ben Nessib et al. 2004) or Ne V (Hamdi et al. 2007) are concerned, the choice of a good atomic structure becomes important. For these two ions, the difference
electron and ion impact spectral line profiles

Fig. 6. Example of fitting corresponding to Equation (1) for Mg I 4f$^1$F$^o$ − 6g$^1$G at 10$^{11}$ cm$^{-3}$. Left panel is the line width, right panel is the shift/width, the x-axis is the temperature in K. Dots are the results of the SCP calculations; electron collisions. Fitting is shown as the full line. The fitting coefficients (a, b, c), $\chi^2$ and $R^2$ are given in the insert.

can attain 25–30% between the Bates & Damgaard approximation and the more sophisticated method SUPERSTRUCTURE (Nussbaumer & Storey 1978).

Finally, the behaviour of the fine structure widths of a multiplet are not very sensitive to the fine structure splitting: for the 3s − 3p multiplets of the Li-like series, the ratio of the widths of the two components attains 1.12 only for P XIII (Elabidi et al. 2009). This is quite negligible by looking at the accuracy of the calculations.

4. FITTING FORMULAE AS THE FUNCTIONS OF TEMPERATURE

The theory and the SCP formulae show that the widths vary as $T^{-1/2}$ at low temperature and as $\log(T)/T^{1/2}$ at high temperatures (e.g., see Elabidi et al. 2009). But this is not sufficient for the users. Astrophysics need fitting formulae and coefficients as functions of temperature for each line. In fact, such fitting coefficients are easier to enter the computing codes than tables providing widths and shifts for a set of temperatures. So, for the astrophysical needs, we have obtained a simple but accurate fitting formula based on the least-squares method. It is logarithmic + second degree polynomial:

$$\log(w) = a_0 + a_1 \log(T) + a_2 [\log(T)]^2,$$
$$d/w = b_0 + b_1 \log(T) + b_2 [\log(T)]^2.$$ (1)

Another fitting formula, $w = C + AT^B$, was proposed by Dimitrijević et al. (2007). The present one is more accurate, due to the second degree term of the expansion. However, none of them have a real physical sense.

Figure 6 shows an example of such fitting for Mg I 4f$^1$F$^o$ − 6g$^1$G at 10$^{11}$ cm$^{-3}$ (Dimitrijević & Sahal-Bréchot 1996, and other related papers cited in STARK-B). The fit is excellent for the width, but not so good for the shift: this happens due to the fact that the accuracy of the shift calculation can be low at small shifts. This bad shift example has been deliberately chosen for testing the accuracy of the fitting formula.

The present coefficients will be placed at STARK-B in a near future under the form of complementary tables for each line.
5. CONCLUSION

We hope that the present study will help the users to interpret the results of SCP calculations, to obtain interpolated and extrapolated data that are absent in the STARK-B tables, and to include the provided fitting coefficients into their modeling codes for stellar atmospheres and interiors.

ACKNOWLEDGMENTS. A part of this work was supported by VAMDC. VAMDC is funded under the 7th Framework Program, grant agreement No. 239108. This work was also supported by the cooperation agreement between Tunisia (DGRS) and France (CNRS) (project code 09/R 13.03, No. 22637), by the Programme National de Physique Stellaire (INSU-CNRS), by the Paris Observatory and by the project No. 176002 of the Ministry of Education and Science of Serbia.

REFERENCES
Baranger M. 1958a, Phys. Rev., 111, 481
Baranger M. 1958b, Phys. Rev., 111, 494
Baranger M. 1958c, Phys. Rev., 112, 885
Dimitrijević M. S., Sahal-Bréchat S. 1984, JQSRT, 31, 301
Dimitrijević M. S. 1999, Serbian AJ, 159, 65
Dubernet M. L., Boudon V., Culhane J. L. et al. 2010, JQSRT, 111, 2151; http://www.vamdc.eu
Elabidi H., Ben Nessib N., Sahal-Bréchat S. 2009, EPJD, 54, 51
Fleurier C., Sahal-Bréchat S., Chapelle J. 1977, JQSRT, 17, 5954
Mahmoudi W., Ben Nessib N., Sahal-Bréchat S. 2008, EPJD, 47, 7