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THE STARK-B DATABASE VAMDC NODE FOR SPECTRAL LINE BROADENING BY COLLISIONS WITH CHARGED PARTICLES

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Abstract. "Stark broadening" theories and calculations have been extensively developed for about 50 years. Accurate spectroscopic diagnostics and modeling require the knowledge of numerous collisional line profiles. Nowadays, the access to such data via an on line database becomes essential. The aim of STARK-B is satisfy this need. It is a collaborative project between the Astronomical Observatory of Belgrade (AOB) and the LERMA at Observatory of Paris. It is a database of widths and shifts of isolated lines of atoms and ions due to electron and ion impacts that we have calculated and published in international refereed journals. It is devoted to spectroscopic diagnostics and modeling of stellar atmospheres and envelopes, laboratory plasmas, laser equipments and technological plasmas. Hence, the domain of temperatures and densities covered by the tables is wide and depends on the ionization degree of the considered ion. STARK-B has been fully opened to the international community since fall 2008 and is a node of VAMDC. VAMDC (Virtual Atomic and Molecular Data Centre) is an European Union funded collaboration between groups involved in the generation and use of atomic and molecular data. In the present paper, we will present STARK-B, its state of development, our current projects and future plans.

Keywords: Atomic data, Line: profiles, Astronomical databases: miscellaneous, Virtual observatory tools

1 Introduction

Broadening and shifting of spectral lines emitted or absorbed by neutral or ionized atoms or molecules in a gas or a plasma can be of various physical origin. The interaction of these atoms or molecules with the surrounding particles causes the so-called pressure broadening. The interpretation of pressure broadening is important for giving informations on the medium, such as temperature, densities of the perturbers, abundances of the emitting or absorbing atoms or molecules. If these perturbers are charged particles, electrons or ions, this broadening mechanism is called "Stark" broadening and concerns various plasmas. The range of densities of interest is large: 10^{10} to 10^{23} cm^{-3}. The range of temperatures of interest is also large: 2500K to about 610^{6} K.

The theory has been extensively developed for about 50 years and is currently used for many spectroscopic diagnostics and modeling. At the same time, many laboratory experiments were developed and line broadening theory and experiments were compared and thus made together a lot of progress. Nowadays, the best agreement between theoretical and experimental results is of the order of 20%.

A number of its developments have been stimulated by the advances in astrophysics and especially stellar physics. Stark broadening is essential for interpreting the spectra of white dwarfs (e.g. Dufour et al. (2011)), since Stark broadening is the main broadening mechanism. Stark broadening is also important for interpreting and analyzing the spectra of A and B type stars and for including stratification in the modeling. Synthetic spectra achievement and modeling of stellar atmospheres and interiors require extensive sets of atomic data, including Stark broadening, and the use of databases is now indispensable. In addition, accurate spectroscopic diagnostics for laboratory plasmas, magnetic fusion plasmas (Tokamaks, e.g. ITER), inertial confinement fusion plasmas (e.g. laser LMJ) and technological plasmas (e.g. discharge lighting sources) are also needed for many lines of many ions, and Stark broadening can play an important role in the modeling. Many examples and references can be found in Dimitrijević & Sahal-Bréchot (2014).

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Hence, calculations based on a simple but enough accurate and fast methods are necessary for obtaining numerous results. Furthermore, the development of powerful computers also stimulates the development of atomic data on a large scale. Hence, Dimitrijević, Sahal-Bréchot have and coworkers updated and operated at a large scale the numerical code created and based on the impact semiclassical-perturbation theory (SCP) developed for isolated lines by Sahal-Bréchot (1969a,b, 1974); Fleurier et al. (1977), after the pioneer work by Baranger (1958a,b,c). The theory was revisited by Sahal-Bréchot et al. (2014). More than 150 papers, which concern 123 neutral and ionized atoms broadened and shifted by collisions with electrons and ions are currently issued from the first update (Dimitrijević & Sahal-Bréchot 1984).

Then, the new need of creation of an on-line database appeared in the beginning of the 21th century, particularly in correlation with the birth and the growth of virtual Observatories and to the increasing need of exchange of interoperable data. Hence, our database was designed and STARK-B (Sahal-Bréchot et al. 2014) was created: it is a database of calculated widths and shifts of isolated lines of atoms and ions due to electron and ion collisions by Dimitrijević, Sahal-Bréchot and coworkers.

STARK-B is a collaborative project between AOB and LERMA. It is currently developed at Paris Observatory and has opened on line since the end of 2008 (Sahal-Bréchot et al. 2014). It is a part of the atomic and molecular databases of the Paris Observatory, and there is a link to the Serbian Virtual Observatory (SerVO 2014). It is in free access. A mirror site is planned at AOB. STARK-B has been a node of VAMDC (Virtual Atomic and Molecular Data Centre) since the end of 2009 (Dubernet et al. 2010; Rixon et al. 2011). This FP7 European project "Research Infrastructures was created in summer 2009 for 3.5 years. It is an interoperable e-Infrastructure for exchange of atomic and molecular data. This international consortium has built an e-science interoperable platform permitting an automated exchange of atomic and molecular data.

We begun by implementing the published data of all our papers calculated through the SCP theory and code. This first stage of development of STARK-B was ended in autumn 2012.

Then, we have begun to implement the data (about 70 publications concerning 90 neutral and ionized atoms) issued from the"MSE" method developed by Dimitrijević and coworkers (Dimitrijević & Konjević 1980; Dimitrijević & Kršljanin 1986; Dimitrijević & Popović 2001). This method, more approached than the SCP one, is used when the atomic structure data are not sufficiently complete to perform an adequate semiclassical calculation.

This will be presented below, as well as the state of advancement and our program of development of the database.

2 The theory and method of calculations leading to STARK-B data

2.1 Brief outline of the assumptions and approximations of the method

Stark broadening theory is based on the founding papers by Baranger (1958a,b,c).

The impact approximation is the first basic assumption: the duration of a collision must be much smaller than the mean interval between two collisions. So the collisions between the radiating atom (or ion) act independently 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). It can break down at high densities (laser fusion plasmas for instance).

The second basic assumption is the complete collision approximation: the radiating atom has no time to emit (or absorb) a photon during the collision process. In the line center, the impact approximation and the complete collision approximation are both valid, and the line broadening theory becomes an application of the theory of collisions between the radiating atom and the surrounding perturbers. In the line wings, the complete collision approximation can break down for ion collisions. However, the contribution of ion collisions is often smaller than 10% when compared to that of electrons.

The present method is limited to the case of isolated lines: the levels of the studied transition broadened by collisions do not overlap with the neighbouring perturbing levels. So, hydrogen and hydrogenic ionic lines, some specific helium lines and some lines arising from Rydberg levels are excluded from our calculations and consequently from STARK-B.

Therefore, the impact-complete collision-isolated lines approximation leads to a Lorentz line profile characterized by a width and a shift which depend on the physical conditions of the medium (temperature and density of the perturbers). The detailed formulae, which are not repeated here, can be found in Sahal-Bréchot et al. (2014) and earlier papers. In particular, the widths are given by a sum over atom-perturber cross-sections and

an interference term multiplied by the relative velocity, followed by an average over the Maxwell distribution of relative velocities and multiplied by the density of perturbers.

Due to the impact approximation, widths and shifts are proportional to the density. However, at high densities, the Debye screening effect can be important and is taken into account in our calculations. This decreases the width and the shift which thus become not proportional to the density.

In addition, if LS coupling is valid, the different fine structure line of a same multiplet have the same width and shift, that of the multiplet (in frequency units). This is due to the fact that the electronic spin has no time to rotate during the collision and thus can be neglected for obtaining the cross-sections.

2.2 The semiclassical-perturbation (SCP) method

Most of our calculations have been performed with the semiclassical-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. (2008) for very complex atoms. The method was revisited in detail by Sahal-Bréchot et al. (2014). The numerical codes have been updated and operated by Dimitrijević and Sahal-Bréchot (Dimitrijević & Sahal-Bréchot (1984)) and further papers. When comparing to experimental results, the accuracy is about 20% for the widths but can be worse for the shifts.

For obtaining the cross-sections and the interference term which enter the calculations, we must calculate the S-matrix (the so-called collision matrix or scattering matrix). First, an atomic structure must be used and chosen for obtaining wave functions and energy levels. Second, a method of calculation of the S-matrix has to be chosen. Then, a coupling between the chosen atomic structure and the collisional part of the code is achieved for calculating Stark widths and shifts data.

2.2.1 The chosen atomic structure

In our earlier papers, the Coulomb approximation with quantum defect (Bates and Damgaard 1949), improved for high levels by Van Regemorter et al. (1979), were used, together with measured or calculated energy levels, e.g. Kramida et al. (2014) or other tables.

In the more recent papers modern *ab initio* methods are used. Modern atomic structure computer codes or their data obtained from a database can be downloaded on line. Thus the calculations of widths and shifts can be made from the beginning to the end without any additional external input or experimental adjustment. Then, the chosen atomic structure package enters our computer semi-classical code and that allows, when these methods are applicable, to obtain widths and shifts for several hundreds of lines in a same run. We have used:

- TOPbase, the Opacity Project atomic database, contains accurate calculated oscillator strengths and energy levels for abundant neutral and ionized atoms relevant for astrophysics. They have been obtained within the close-coupling scattering theory by means of the R-matrix method with innovative asymptotic techniques (Cunto et al. 1993). LS coupling is assumed. So, TOPbase data have been especially useful for light and low and moderately ionized atoms and ions: e.g. Larbi-Terzi et al. (2012) for C II lines.

- The Cowan code (Cowan 1981) is an online atomic structure package consisting of a set of computer programs for calculation of energy levels, radiative transition wavelengths and probabilities, etc. The Hartree-Fock-Slater multi-configuration expansion method with statistical exchange is the normal option since it is most computationally efficient. The relativistic corrections are treated by perturbations. So this method is especially suited to moderately heavy atoms which are little and moderately ionized: e.g. Hamdi et al. (2013) for Pb IV lines.

- SUPERSTRUCTURE (SST) (Eissner et al. 1974) is well suited for medium and highly charged ions. The wave functions are determined by diagonalization of the nonrelativistic Hamiltonian using orbitals calculated in a scaled Thomas-Fermi-Dirac-Amaldi potential. Relativistic corrections are introduced according to the Breit-Pauli approach. Atomic data are obtained in intermediate coupling: e.g. Ben Nessib et al. (2004) for Si V lines, and Hamdi et al. (2007) for Ne V lines.

Si V and Ne V line widths and shifts data have been calculated with both Bates & Damgaard and SST atomic data. The difference does not exceed 30%. C II widths and shifts data have been calculated with both TOPbase and Bates and Damgaard atomic data, and the difference does not exceed a few percent, except when

configuration interaction plays an important role by allowing a forbidden transition. This remark is for giving an idea of the importance of the chosen atomic structure for obtaining Stark broadening data.

2.2.2 The semiclassical approximation for obtaining the S-matrix, the cross-sections and the interference term

The basic formalism has been revisited in detail by Sahal-Bréchot et al. (2014). The perturber is considered as a classical particle moving along a classical path unperturbed by the interaction with the radiating atom: straight paths for neutral radiators, hyperbolic paths for ion-electron and ion-ion collisions. Then the S-matrix has been obtained within the second order perturbation theory. The needed cross-sections are obtained through integration over the impact parameter of the transition probabilities. The needed cut-offs are determined in order to maintain the unitarity of the scattering S- matrix, and Debye screening is taken into account. This permitted to create a very fast computer code, which can now work on a personal laptop: one night of calculation is sufficient to obtain data for one or two hundred lines of a same neutral or ionized atom, and for a set of about 5 temperatures and 5 densities. For the purposes of STARK-B, this semiclassical-perturbation treatment is adapted and gives results with a sufficient accuracy (about 20%). This is especially the case if the perturbing levels are not too far from the levels of the studied line.

2.3 The MSE method

The"MSE" method developed by Dimitrijević and coworkers (Dimitrijević & Konjević 1980; Dimitrijević & Kršljanin 1986; Dimitrijević & Popović 2001) is more approached than the SCP one. It can be used when the atomic structure data are not sufficiently complete to perform an adequate semiclassical calculation. it uses a simplified atom quantum description, and the cross-sections are calculated by means of an effective Gaunt factor (Van Regemorter 1962; Griem 1968) revisited, and modified for ions with a charge $Z > 1$. The accuracy of the results is about 30-40%. Indeed, due to its simplicity, the MSE method is much faster than the SCP one.

3 The STARK-B database

3.1 Description of the database

The homepage proposes several menus, among which "Introduction", "Data Description" and "Access to the Data". "Introduction" recalls the approximations and methods of calculation. "Data Description" describes the data that are in the files. "Access to the Data"provides a graphical interface: first, the user clicks on the wished element in the Mendeleev periodic table and then on the ionization degree of interest. Yellow cells contain data, while grey cells are empty. Next, with a few clicks, the user chooses the colliding perturber(s), the perturber density, the transition(s) defined by quantum numbers and the plasma temperature(s). The user can also make a query by domain of wavelengths instead by transitions. Then a table displaying the widths and shifts is generated. Bibliographic references are given and linked to the publications via the SAO/NASA ADS Physics Abstract Service (2014) and/or within DOI if available. The publications can be freely downloaded if the access is not restricted. The widths and shifts data can be downloaded in ASCII and in VOTable format (XML format), adapted to Virtual Observatories.

Since STARK-B is devoted to spectroscopic diagnostics and modeling of various plasmas in astrophysics, laboratory physics, technology and other topics, the range of temperatures and densities in the tables is wide and vary with the ionization degree of the considered ion. The temperatures vary from several thousands Kelvin for neutral atoms to several millions for highly charged ions. The perturber densities vary from 10^{12} cm^{-3} to several 10^{22}cm^{-3}. The data model (in particular the identification of the line transitions) follows the VAMDC standards, in order to allow interoperability with other atomic databases included in the Virtual Atomic and Molecular Data Center. The transitions are defined by configurations, terms, J-values, and wavelengths. The multiplet number is also often included and taken from the NIST database (Kramida et al. 2014). In addition, the widths and shifts data are provided in units of wavelengths (Å) and not in angular frequency units. It must be noticed that the wavelengths displayed in STARK-B are calculated from the energy levels that are used as input data in the SCP computer code. Consequently, the tabulated wavelengths are most often different from the measured ones, especially if the used energy levels are theoretically calculated: this is especially the case for the atomic structure data originating from TOPBase, SST or Cowan code. So, if widths and shifts data are needed for measured wavelengths ($\lambda_{measured}$), or for fine structure data whereas the data are only provided for multiplets, one has to multiply the STARK-B data by $(\lambda_{measured}/\lambda_{STARK-B})^2$.

In our tables, a positive shift is towards the red and a negative one towards the blue.

When the impact approximation approaches its limit of validity, a warning (an asterisk) is introduced at the left of the data. If the impact approximation is not valid, there is only an asterisk and no data in the corresponding cell. The isolated line approximation, which can approach its limit of validity at high densities is also checked in the tables. This is commented on the menu "Data description".

3.2 Implementation of the published SCP data

During the first stage of STARK-B development (from the end of 2008 to the end of 2012), we have implemented all the Stark broadening parameters calculated and published by means of the SCP computer code. Currently, the database contains SCP widths and shifts for spectral lines of the following elements and ionization degrees:

Ag I, Al I, Al III, Al XI, Ar I, Ar II, Ar III, Ar VIII, Au I, B II, B III, Ba I, Ba II, Be I, Be II, Be III, Br I, C II, C III, C IV, C V, Ca I, Ca II, Ca V, Ca IX, Ca X, Cd I, Cd II, Cl I, Cl VII, Cr I, Cr II, Cu I, F I, F II, F III ,F IV, F V, F VI, F VII, Fe II, Ga I, Ge I, Ge IV, He I, Hg II, I I, In II, In III, K I, K VIII, K IX, Kr I, Kr II, Kr VIII, Li I, Li II, Mg I, Mg II, Mg XI, Mn II, N I, N II, N III, N IV, N V, Na I, Na X, Ne I, Ne II, Ne II, Ne III, Ne IV, Ne V, Ne VIII, Ni II, O I, O II, O III , O IV, O V, O VI; O VII, P IV, P V, Pb IV, Pd I, Rb I, S III, S IV, S V, S VI, Sc III, Sc X, Sc XI, Se I, Si I, Si II, Si IV, Si IV, Si V, Si VI, Si XI, Si XII, Si XIII, Sr I, Te I, Ti IV, Ti XII, Ti XIII, Tl III, V V, V XIII, Y III, Zn I.

We will continue to implement the new results of calculations as soon as they are published. The description of newly added data with the date of importation appears under the menu "Updates". Also all updates with the date of the first importation and the importation of revised data are noted. Moreover, for further enquiries or user support, there is the menu "Contact" with the possibility to send an e-mail with questions to the corresponding persons.

3.3 Fitting formulae as functions of temperature

The beginning of stage 2 STARK-B development was devoted to implement fitting coefficients of the tabulated data with temperature. In fact, he theory of Stark broadening shows that the line widths decrease with temperature as $T^{-1/2}$ for ionized emitters at low temperature, and to $\log(T)/T^{1/2}$ for both neutral and ionized atoms at high temperatures. However, in astrophysics, especially for the modeling of stellar atmospheres, this is not sufficient. Fitting formulae and coefficients as functions of temperature for every line are needed, since such fitting coefficients are more efficient for the use in the computer codes for stellar atmosphere modeling than tabulated widths and shifts for a set of temperatures.

Consequently, in order to enable a more adequate use of STARK-B for stellar modeling, we derived (Sahal-Bréchot et al. 2011) a simple and accurate fitting formula based on a least-square method, which is logarithmic and represented by a second degree polynomial:

$$\begin{aligned} \log(w) &= a_0 + a_1 \log(T) + a_2 \left(\log(T)\right)^2, \\ d/w &= b_0 + b_1 \log(T) + b_2 \left(\log(T)\right)^2. \end{aligned} \tag{3.1}$$

It can be noted that Dimitrijević et al. (2007) proposed the fitting formula $w = C + AT^B$, but the present one is more accurate, due to the second degree term of the expansion. It should be also noted that none of them have a real physical sense.

Then, for each table of widths and shifts, a complementary table was added, with coefficients a_0, a_1, a_2 and b_0, b_1, b_2, obtained by using the above equations for the corresponding fitting with the temperature. These fitting coefficients can also be downloaded in ASCII and in VOTable format, and can be included in the computer codes for stellar atmospheres modeling.

We plan also to develop other fitting formulae as functions of perturber densities in order to make easier the use of data on high densities needed for white dwarf atmospheres and subphotospheric layers modeling.

3.4 The current development of STARK-B: implementation of MSE data

Since the end of 2013, we have begun to implement our Stark broadening data obtained with the Modified SemiEmpirical method. We recall that this approach is convenient for emitters where atomic data are not sufficiently complete to perform an adequate semiclassical perturbation calculation.

Up to now, Stark line widths and in some cases also shifts of the following emitters spectral lines:

Ag II, Al III, Al V, Ar II, *Ar III*, Ar IV, As II, As III, Au II, *B III*, B IV, Ba II, Be III, Bi II, Bi III, Br II, C III, C IV, *C V*, Ca II , Cd II, *Cd III*, Cl III, *Cl IV*, *Cl VI*, Co II, *Co III*, Cu III, Cu IV, Eu II, Eu III, F III, F V, F VI, Fe II, Ga II, *Ga III*, *Ge III*, *Ge IV*, I II, Kr II, Kr III, La II, La III, Mg II, Mg III, Mg IV, *Mn II*, *Mn III*, N II, N III, N IV, N VI, Na III, Na VI, Nd II, Ne III, Ne IV, Ne V, Ne VI, O II, O III, O IV, O V, P III, P IV, *P VI*, Pt II, *Ra II*, S II, S III, S IV, Sb II, Sc II, Se III, Si II, Si III, Si IV, Si V, Si VI, Sn III, Sr II, Sr III, Ti II, Ti III, V II, V III, V IV, Xe II, Y II, Zn II, Zn III, Zr II.

The data were inserted in the beginning of 2014 for the elements written in italics.

4 Future developments of STARK-B and conclusion

As soon as new data will be calculated and published, they will be added to the database. The implementation of our quantum data will be another future stage (e.g. Elabidi et al. (2008, 2009) and further papers). The further developments also concern insertion of little apps (fitting along principal quantum number for a given multiplet, charge of the ion collider along isoelectronic sequences, of the radiating ion, homologous ions...) by using fittings or systematic trends in order to obtain data that are missing on the database. In a more distant future, we would plan to put the SCP code on line.

The continuation of such developments and services of powerful and constantly updated online databases, like STARK-B, is crucial.

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