Line shape models for magnetized hydrogen plasmas

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Abstract. We report on Stark-Zeeman line shape models for the diagnostic of magnetic fusion plasmas. Computer simulations, which serve as a reference for an evaluation of the ion dynamics effects, are usually CPU time consuming, so that they cannot be used in a real-time diagnostic. In this framework, a database that allows a fast evaluation of Stark-Zeeman line shapes is currently under preparation. We present preliminary results. Analytical models based on ion collision operators and suitable for strong (near-impact) ion dynamics regimes are also discussed.

1. Introduction
ITER is an international project aimed at demonstrating the feasibility of fusion as a source of energy. This machine, presently under construction in Cadarache (France), is a large scale tokamak designed so as to maintain fusion for long periods of time. It will be the first fusion device to test the integrated technologies, materials, and physics regimes necessary for the commercial production of fusion-based electricity (see the website: www.iter.org). The first plasma is planned for 2025. A Demonstration Fusion Power Reactor (DEMO) is next planned to follow ITER.

In accompaniment to ITER, research campaigns are ongoing on present tokamaks. We have taken part to a project devoted to the improvement of passive spectroscopy diagnostics involving hydrogen line shapes for a better characterization of divertor plasmas (MST1, Medium-Size Tokamak Task Force). The strong density dependence of Stark broadening renders this broadening mechanism suitable for an investigation of the divertor plasma properties in the so-called detached regime where a large amount of neutrals are present. This regime is of interest for the characterization of the plasma-wall interactions. The Stark broadening is important on lines with a high principal quantum number $n$, and it can be significant as well on lines with a small $n$ like Balmer $\alpha$ (with respect to the Doppler broadening) at the highest density regimes ($N_e \sim 10^{15}$ cm$^{-3}$); for observations, e.g. see [1,2]. In general, the Stark broadening is affected by the ion dynamics, from the near-static limit (especially on high-$n$ lines) to the near-impact limit (low-$n$ lines at a low density); this effect has to be retained in diagnostic models. The presence of a strong magnetic field (of several teslas) in tokamak plasmas yields an additional splitting due to the Zeeman effect, which has also to be retained. We report here on a database which is currently under preparation. A computer simulation method is used. Preliminary results for $D\gamma$ (deuterium Balmer $\gamma$ transition, $n = 5 \ Y \ 2$) have been obtained last year [3] for an improvement of line shape-based diagnostics of the ASDEX-Upgade tokamak divertor plasma [4]. We discuss the dependence on the magnetic field and the temperature. Analytical methods based on ion collision operator models and suitable for near-impact ion dynamics regimes are discussed.
2. Computer simulations for Stark broadening with account of Zeeman effect

Computer simulations for the investigation of ion dynamics were initiated in the late seventies and they are now widely used for Stark broadening calculations, e.g. [5–8]. Like the model microfield method (MMM) [9,10], this method can be used in the elaboration of tables, e.g. [6]. The purpose of simulations is to numerically reproduce the motion of the charged particles in the plasma so as to obtain the time dependent electric microfield $E(t)$ at the location of an emitter. While being CPU intensive, this method has the advantage of providing reference line shapes. We only give here a summary of the technique (it was discussed many times at earlier sessions of the ICSLS conference). Essentially, a numerical simulation consists of: (i) the calculation of a set of realizations for the electric field; (ii) the numerical integration of the Schrödinger equation for each realization, which provides an expression for the atomic evolution operator $U(t)$; (iii) an evaluation of the dipole autocorrelation function by ensemble averaging and a Fourier transform that provides the spectrum:

$$I(\omega) \propto \frac{1}{\pi} \text{Re} \int_0^\infty dt \langle d_+ \cdot U^\dagger(t) d_+ U(t) \rangle e^{i\omega t}.$$  \hspace{1cm} (1)

The $\perp$ symbol used here indicates that the dipole is projected onto the polarization plane; this specification is required because of the anisotropy induced by the magnetic field (Zeeman effect). In the simulations performed for this work, we have used a code [11] developed according to the method reported in early papers [5]. We consider that the ions move along straight line trajectories with constant velocities, sampled among the particles according to an equilibrium Maxwell distribution function. The electrons are not simulated here, but are described with an impact collision operator. The treatment of the correlations between ions and electrons is retained by using Debye screened fields. A cubic cell with periodic boundary conditions is considered. For each history of the electric field, the code solves the time dependent Schrödinger equation for the evolution operator $U(t)$ according to the algorithm $U(t + \Delta t) = U(t + \Delta t, t) U(t)$, with $U(t + \Delta t, t)$ being the infinitesimal evolution operator between times $t$ and $t + \Delta t$. The latter operator is approximated as $\exp \{ i \hbar [H_0 + V(t)] \Delta t / \hbar \}$ and the exponential is evaluated using the scaling and squaring method [12]. Note that the Doppler broadening is not retained in Eq. (1); it can be accounted for by convoluting Eq. (1) with the atomic velocity distribution function (except in specific conditions, viz. if the velocity $v$ is correlated with the electric field $E(t)$ or if the Lorentz field $v \cdot B$ is important, e.g. [13]). An example of simulated spectrum is shown in Fig. 1. The spectral profile of the D-\(\alpha\) (deuterium Balmer \(\alpha\)) line in conditions relevant to high density divertor plasmas is shown. As can be seen in the figure, the Stark broadening is comparable to the Doppler broadening. The magnetic field yields a Zeeman-Lorentz triplet structure, which is visible on the spectrum. This structure tends to disappear as the principal quantum number increases, in accordance with the Stark effect trend (Fig. 2).
Figure 1. Plot of the D-α line shape obtained from a computer simulation, at conditions relevant to tokamak divertor plasmas at high density regimes. The Stark broadening is comparable to the Doppler broadening. The triplet structure stems from the Zeeman effect.

Figure 2. The Stark broadening increases with the principal quantum number and tends to mask the Zeeman triplet structure. Here, the profiles of D-α, D-β, and D-γ have been simulated assuming the same plasma conditions as in Fig. 1.

A line shape database is currently under preparation for the diagnostic of divertor plasmas in detached regime. Spectral profiles of the first Balmer lines (up to $n = 7$) of deuterium have been calculated for a set of densities, temperatures, and magnetic field strengths relevant to magnetic fusion edge plasmas, in such a way to provide a table that can be used in an analysis of experimental spectra [3]. The table provides Stark-Zeeman line shapes for equal ion and electron temperatures with values comprised between 0.316 and 31.6 eV, a plasma density ranging from $10^{13}$ to $10^{16}$ cm$^{-3}$, and a magnetic field up to 5 T. The Doppler broadening is not retained in the table because the atomic...
velocity distribution can be strongly dependent of the tokamak plasma discharge under consideration (e.g., it can take the form of a superposition of Maxwellian functions with different temperatures owing to various nonthermalized populations [14,15]). Figure 3 shows an example of result: the half-width at half-maximum of the D-α line is plotted against the density for the two temperatures 1 eV and 10 eV, in the absence of a magnetic field (hence no Zeeman effect is present here). As can be seen, the width roughly follows a power law in terms of the density, and it is weakly sensitive to the temperature. Note the change in trend: according to the density value, a higher temperature can result either in a higher or a smaller line width. The former effect is expected at high densities as a result of ion dynamics broadening, whereas the line width reduction with an increasing temperature at low densities can be explained within a collisional picture (note the $T^{-1/2}$ trend of the ion collision operator). An adjustment of the plot using the empirical formula HWHM = $C \times N_e^\alpha$, with $C$ and $\alpha$ being constants, is currently ongoing, without and with the Zeeman effect. Preliminary results have indicated a power close to unity.

Figure 3. The half-width at half-maximum (HWHM) increases with the density. It roughly follows a power law. Here, the D-α HWHM is plotted against the density in the absence of a magnetic field, for the two temperatures 1 eV and 10 eV.

3. Analytical line shape models for radiation transport simulations

A few years ago, investigations were carried out in order to provide analytical formulas for Stark-Zeeman line shapes suitable for a fast evaluation in radiation transport simulations. This concerns the Lyman α and Lyman β lines in particular, given the short absorption length they provide (the corresponding photons can be absorbed after traveling over less than 1 mm; e.g. [16] for a mean free path estimate; see also [17,18] for experimental observations). The corresponding atom excitation can play an important role on the ionization-recombination balance. In this framework, simulations of the coupled plasma-atom-radiation transport are presently ongoing [19]. The EIRENE code utilized in the magnetic fusion community (see www.eirene.de) employs a kinetic Monte Carlo method for a description of the Lyman line radiation. Photons are described as point-like particles performing random walks and interacting with the atoms according to prescribed statistical properties. The spectral line shape function presented in Eq. (1), when normalized to unity, provides a key quantity for the generation of the photon frequency (in an emission event) or its path length (when dealing with absorption). The broadening of the Lyman lines with a low principal quantum number is usually
governed by the Doppler effect. The Zeeman effect provides a correction either visible in the Lorentz triplet form or as an additional broadening if the magnetic field is not sufficiently strong. The Stark effect, which is usually visible in the wings, provides a significant additional broadening on the whole spectrum at the highest density conditions \( N_e > 10^{15} \text{ cm}^{-3} \), e.g. [20]). Several approaches were used to model the Stark-Zeeman spectral profile in the atomic frame of reference (see [20] and Refs. therein). Because of the low principal quantum number, the ions are in a strong dynamics regime, which renders their description tricky. An example of approach that can used for the lowest densities is the impact approximation adapted to ions. The ratio \( b_W/r_0 \) between the ion Weisskopf radius and the mean interparticle distance is smaller than 10% at \( N_e = 10^{13} \text{ cm}^{-3} \) and \( T_{ei} = 1 \text{ eV} \), suggesting that the binary assumption can be used as a reasonable approximation. We have adapted the early approaches to impact broadening developed by Griem et al. to ionic perturbers [11]. The original treatment of hydrogen line broadening (Griem-Kolb-Shen 1959 model [21]) cannot be applied in a strictly sense due to the Zeeman energy degeneracy removal, but it can be readily adapted following the same method as for helium lines (Griem-Baranger-Kolb-Oertel 1962 model [22]). Figure 4 shows an example of application to Lyman \( \alpha \). The computer simulation result (where many perturbers are retained) is also shown. The collision operator model is in a good agreement with the simulation.

![Figure 4](image_url)

**Figure 4.** Plot of the Lyman \( \alpha \) blue lateral component calculated using an impact model for ions, at conditions such that the binary assumption can be used as a reasonable approximation. The Doppler broadening is not retained here. The Zeeman energy degeneracy removal is accounted for through the GBKO method (see text). As can be seen, the model is in a good agreement with the simulation.

E. Oks made criticisms during the ICSLS conference regarding both the impact model we used and computer simulations [23], with the claim that his models \( \tilde{\text{GT}} \) and \( \tilde{\text{AGT}} \) are more accurate. The \( \tilde{\text{GT}} \) and \( \tilde{\text{AGT}} \) are nothing but a reformulation of the impact theory, which involves a binary approximation like the older models by Griem et al. The subtlety mentioned by Oks concerns the interaction picture used in his theories. In a previous study [24], we pointed out an inconsistency in Oks theories, which can be avoided readily (in technical points: this concerns the description of the strong collisions). A cut-off procedure in the evaluation of integrals, as done in the models by Griem et al., would be appropriate.
4. Conclusion

The operation of magnetic fusion devices requires passive spectroscopy diagnostics in the edge plasma region. In this framework, we are developing a database for the interpretation of the hydrogen Balmer lines in conditions of recombining divertor plasmas. This database accounts for the simultaneous action of the Zeeman and Stark effects, and it can be used for a density diagnostic routine involving Stark broadening. In the framework of radiation transport simulations, analytical formulas for Stark-Zeeman line shapes in the atomic frame of reference are suitable. An example of method concerns the impact theory adapted to ions. Comparisons to computer simulations have indicated that the use of a collision operator model following early (Griem et al.) approaches is appropriate when the emitter-perturber interactions are binary. Extensions to non-binary interactions can be performed using kinetic theory methods [25–27].

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