Stark broadening by Lorentz fields in tokamak edge plasmas

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Abstract.
We report calculations of hydrogen line shapes in tokamak edge plasma conditions. A special emphasis is put on the motional Stark effect that arises due to the electric field $\vec{v} \times \vec{B}$ present in the frame of reference of an atom moving at a velocity $\vec{v}$. The statistical repartition of the velocities results in a broadening of the lines, which can be significant if the upper level of the transition under consideration is high. Applications to Balmer lines are shown here.

1. Introduction
Line shape models are routinely used in magnetic fusion for diagnostic purposes, given the dependence of spectra on the plasma parameters. Hydrogen Balmer line series with a high principal quantum number $n$ (up to 10 and higher) have been observed in divertor plasmas at conditions such that a large amount of excited atoms is present (recombining “detached plasma” regime) [1, 2, 3]. It is widely recognized that an analysis of the width of such lines yields information on the electron density, given their sensitivity to Stark broadening. However, as already noticed in [1], the electron density may not be sufficiently high so that other mechanisms contribute significantly to the line broadening. The effect discussed in this work concerns the Stark broadening due to the Lorentz field $\vec{F}_L = \vec{v} \times \vec{B}$ present in the emitters’ frame of reference (motional Stark effect or MSE). Several works have reported on this effect in magnetized plasmas. Analytical expressions have been obtained for Lyman and Balmer hydrogen lines with a low upper principal quantum number $n$, in magnetic fusion conditions [4, 5], in high-density plasmas [6], and also in astrophysics [7, 8]. A rough estimate indicates that this broadening scales as $n^2 B \sqrt{T_{at}}$ (with $T_{at}$ being a characteristic atomic temperature), meaning that this additional broadening can enter in competition with the other line broadening mechanisms for lines with a sufficiently high $n$, provided the magnetic field and the atomic temperature are sufficiently high. Note, this effect is to be distinguished from the MSE splitting involved in active spectroscopic diagnostics based on highly energetic neutral beams with a strongly shifted velocity distribution function (e.g. [9]). We report here on recent investigations of high-$n$ Balmer line shapes [10] and perform new calculations of MSE broadening.

2. Line shapes in magnetized plasmas
The development hereafter follows the lines of [10]. Consider a set of atoms immersed in a magnetized plasma. The spectral profile of a line, $I(\omega, \vec{n})$, is given in terms of the line profile in...
the atom’s frame of reference $I_0(\omega, \vec{n})$ by the following integral (Doppler convolution)

$$I(\omega, \vec{n}) = \int d^3\mathbf{v} \mathcal{f}(\mathbf{v}) I_0(\omega - \omega_0 \mathbf{v} \cdot \vec{n}/c, \vec{n}). \quad (1)$$

Here, $\omega_0$ is the central angular frequency of the line under consideration, $\omega$ and $\vec{n}$ denote the frequency and the observation direction, and $\mathcal{f}(\mathbf{v})$ is the atomic velocity distribution function (VDF). For Maxwellian VDF, the line shape is a Gaussian function if there is no broadening mechanism in the atom’s frame of reference [i.e. when $I_0(\omega, \vec{n}) \equiv \delta(\omega - \omega_0)]$, and a Voigt function if natural broadening is retained. In the general case, $I_0(\omega, \vec{n})$ is proportional to the Fourier transform of the atomic dipole autocorrelation function $C_\vec{n}(t)$:

$$I_0(\omega, \vec{n}) \propto \frac{1}{\pi} \Re \int_0^\infty dt C_\vec{n}(t) e^{i\omega t}, \quad (2)$$

$$C_\vec{n}(t) = \text{Tr} \left\{ \vec{d}_\perp(0) \cdot \vec{d}_\perp(t) \rho \right\}. \quad (3)$$

Here, the trace is performed over the atomic states and denotes a statistical average, $\rho$ is the projection of the density operator to the atom’s Hilbert space evaluated at initial time, the brackets $\langle ... \rangle$ denote an average over the perturber trajectories (classical path approximation), and $\vec{d}_\perp = \vec{d} - (\vec{d} \cdot \vec{n})\vec{n}$ denotes the projection of the atomic dipole operator onto the polarization plane, in the Heisenberg picture. In Eq. (3), restrictions of this operator between the upper and lower levels of the transition are implied (no-quenching approximation). Formally, this means that a projector to the final states has to be included between $\vec{d}_\perp(0)$ and $\vec{d}_\perp(t)$. We do not write it here for the sake of simplicity. It is customary to write the autocorrelation function in terms of the evolution operator $U(t)$. Because of the identity $\vec{d}_\perp(t) \equiv U(t)\vec{d}_\perp(0)U(t)$, a calculation of the line shape requires the knowledge of the matrix elements of $\vec{d}$ and an evaluation of $U(t)$. The evolution operator obeys the time-dependent Schrödinger equation

$$i\hbar \frac{dU}{dt}(t) = [H_0 + V(t)]U(t). \quad (4)$$

Here $H_0$ is the Hamiltonian including both the atomic energy level structure (with a non-Hermitian part accounting for natural broadening) and the Zeeman effect, and $V(t) = -\vec{d} \cdot \vec{F}(t)$ is the time-dependent Stark effect term (Schrödinger picture) resulting from the action of the microscopic electric field $\vec{F}(t)$. When this term is neglected, the Schrödinger equation has the trivial solution $U(t) = \exp(-iH_0 t/\hbar)$, which shows, using Eqs. (3) and (2), that $I_0(\omega, \vec{n})$ reduces to a set of delta functions (or Lorentzian functions if the natural broadening is retained). By contrast, the case where $\vec{F}(t)$ is significant is much more intricate because there is no general exact analytical solution. Several models, based on suitable approximations, have been developed in such a way to provide an analytical expression for the line shape (e.g., the impact and static approximations; the model microfield method; etc.). Fully numerical simulations can also be used.

In the presence of a magnetic field, the atom “feels” an electric field $\vec{F}_L = \vec{v} \times \vec{B}$ present in its frame of reference (Lorentz field), which results in an additional Stark effect term $-\vec{d} \cdot \vec{F}_L$ that must be retained in the Hamiltonian (motional Stark effect or MSE). The evolution operator, the autocorrelation function and thus the line profile $I_0$ depend on $\vec{v}$ [i.e. $I_0(\omega, \vec{n}) = I_0(\omega, \vec{n}; \mathbf{v})$], so that the integral in Eq. (1) is no longer a convolution. A common approximation done in the case of a strongly shifted velocity distribution function (e.g., for an energetic quasi-monokinetic neutral beam) consists in evaluating the Lorentz field at the average velocity $\bar{v}_0$. This approximation has been used for diagnostic purposes in the interpretation of MSE spectra.
in tokamaks [9]; such experiments consist in injecting a beam of neutrals, sufficiently energetic so that the MSE yields a splitting of the hydrogen lines that exceeds the other line broadening mechanisms. In a plasma with a thermal velocity distribution function (e.g., a Maxwellian function with \( \vec{v}_0 = 0 \)), the MSE splitting due to the thermal motion of the emitters (which will be referred to as thermal MSE, or TMSE in the following) is not strong enough and the corresponding effect on spectra is a broadening of the line under consideration. This broadening can be significant with respect to other line broadening mechanisms (see Fig. 1).

### 3. Calculation of spectra

We have calculated profiles of Balmer lines with a high upper principal quantum number using the simulation method. In the plasma-microfield-Stark broadening model, the ions are described as particles moving along straight lines around the emitter, in a cube with periodic boundary conditions; the initial conditions (on the positions and velocities of the perturbers) are generated randomly; correlations are retained through the use of a Debye electric field model; and the broadening due to the electrons is described with a collision operator. The Zeeman effect and the TMSE are retained through their corresponding Hamiltonians. Fine structure corrections are not retained because they are negligible on lines with a high principal quantum number. The average over the atom’s velocities Eq. (1), required for the Doppler and TMSE broadenings, is formed by random sampling using a Maxwellian VDF. Figure 2 shows a profile of the D\(_{12}\) line (Balmer 12 of deuterium) obtained assuming a plasma density of 10\(^{13}\) cm\(^{-3}\), a value of 1 eV for the temperatures \( T_i, T_e, T_{at} \), and a magnetic field of 8 T. Such plasma conditions were inferred from spectra analysis in a low-density discharge in Alcator C-Mod [1]. A line-of-sight perpendicular to the magnetic field has been assumed. The TMSE yields a significant additional broadening and more structure. In contrast, the Doppler broadening contribution is weak. This result suggests the TMSE should be accounted for in the interpretation of high-\(n\) line shapes.
4. Revisiting the Inglis-Teller formula in magnetized plasmas

The Inglis-Teller limit is the upper principal quantum number $n$ of the last distinguishable line in a series before the lines merge into the continuum. A simple formula is provided by equating the half separation between two consecutive energy levels $\Delta E \simeq E_I/n^3$ (with $E_I$ being the Rydberg ionization energy) to the Stark width $(3/2)n^2e\alpha_0F_0$ associated with the plasma microfield $F_0$ (see details in [11]). Using the Holtsmark formula for the microfield yields the following relation

$$N_n^{15/2} \simeq 0.027 a_0^{-3},$$

which provides an estimate of the density $N$ in terms of the upper principal quantum number $n$ of the last line. Such a procedure, with a relation similar to Eq. (5) (apart from a multiplicative factor in the right-hand side [12]), was followed by the authors in [1] to estimate the plasma density. The Inglis-Teller formula should be reconsidered in the case where a magnetic field is present, because the TMSE can dominate the plasma-microfield-Stark broadening. Replacing $F_0$ by the Lorentz field $F_L$ estimated at the thermal velocity yields a relation that does not contain the density, but the magnetic field-strength and the atomic temperature instead:

$$n^{10} B^2T_{at} \simeq 1.5 \times 10^{14} m_{at} / m_p.$$

Here the temperature is expressed in eV and the other quantities are in SI units. This expression could serve as a diagnostic of $T_{at}$. For example, applying it to the low-density discharge reported in [1] with $n > 16$ and $B = 8$ T yields a temperature smaller than 5 eV, which is in the range expected from the Doppler analysis performed in [1]. Note, the Zeeman effect, not considered here, can be significant with respect to the TMSE. The derivation of a more accurate formula, which accounts for this effect, could be done along the lines of the analytical model reported in [10].

5. Conclusion

We have presented an investigation of atomic line shapes broadened due to the thermal motional Stark effect (TMSE) at conditions relevant to magnetic fusion experiments, following
a recent work [10]. If the magnetic field is sufficiently strong, the TMSE broadening enters in competition with the usual (Doppler, Zeeman, and plasma-microfield-Stark) broadening mechanisms considered in diagnostic models. We have confirmed this by numerical simulations of Balmer lines with a high principal quantum number. An adaptation of the Inglis-Teller formula to the Lorentz field has also been considered and it has been shown that it also provides the correct order of magnitude for the temperature. The analysis of high-\(n\) hydrogen spectra can be used to reinforce the usual diagnostics for the atomic temperature that utilize Doppler-broadened lines. Our work has focused on the plasma discharges in Alcator C-Mod reported in [1] because the high-\(n\) Balmer lines observed in this machine and the strong magnetic field present therein are also expected in the ITER divertor (detached plasma regime). The diamagnetic quadratic Zeeman effect, not considered in this paper, may be significant on high-\(n\) lines (e.g. [13]) and should be investigated in details in a future work.

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References
[1] Welch B L, Griem H R, Terry J, Kurz C, LaBombard B, Lipschultz B, Marmar E and McCracken G 1995 Phys. Plasmas 5 4246
[2] Wenzel U, Behringer K, Carlson A, Gafert J, Napiontek B and Thoma A 1999 Nucl. Fusion 39 873
[3] Koubiti M, Loch S, Capes H, Godbert-Mouret L, Marandet Y, Meigs A, Stamm R and Summers H 2003 J. Quant. Spectrosc. Radiat. Transfer 81 265
[4] Isler R C 1976 Phys. Rev. A 14 1015
[5] Breton C, Michelis C D, Finkenthal M and Mattioli M 1980 J. Phys. B: At. Mol. Phys. 13 1703
[6] Hoe N, Grumberg J, Caby M, Leboucher E and Coulaud G 1981 Phys. Rev. A 24 438
[7] Brillant S, Mathys G and Stehlé C 1998 Astron. Astrophys. 339 286
[8] Stehlé C, Brillant S and Mathys G 2000 Eur. Phys. J. D 11 491
[9] Donné A J H et al. 2007 Nucl. Fusion 47 S337
[10] Rosato J, Marandet Y and Stamm R 2014 J. Phys. B: At. Mol. Opt. Phys. 47 105702
[11] Inglis D R and Teller E 1939 Astrophys. J. 90 439
[12] Griem H R 1964 Plasma Spectroscopy (McGraw-Hill)
[13] Hey J D, Chu C C and Mertens P 2002 AIP Conf. Proc. 645 26