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A table of Balmer γ line shapes for the diagnostic of magnetic fusion plasmas

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ABSTRACT

Spectral profiles of the Dγ line have been calculated in magnetic fusion plasma conditions for diagnostic purposes. This paper reports on the elaboration of a table devoted to spectroscopic applications in tokamak divertors. An overview of the method, together with the physics underlying the broadening of spectral lines, is given. A special emphasis is put on the role of the simultaneous action of the Stark and Zeeman effects.

1. Introduction

A research campaign that involves medium size tokamaks (MST1 project) has been started last year in order to broaden the already existing experimental and theoretical databases supporting the preparation of ITER and the subsequent demonstration power plant DEMO. In this paper, we report on the development of a spectroscopic database for the interpretation of hydrogen Balmer lines in conditions of high-density recombining divertor plasmas (viz. $N_e = 10^{14}$ cm^{-3} and higher), following previous works performed at Garching (ASDEX-Upgrade tokamak [1]). At such high-density plasma conditions, the spectral lines with a high principal quantum number n (say, of the order of 10) are affected by Stark broadening and can be used as a probe of the electron density (passive spectroscopy), e.g. [2–11]. An analysis of lines with a moderate quantum number such as Dγ ($n=5$) is more intricate, because the Stark broadening can be of the same order as the Doppler broadening and it can be affected by ion dynamics. Furthermore, the presence of a strong magnetic field (of the order of several teslas) results in an alteration of the energy level structure, which is not straightforward even for hydrogen due to the simultaneous action of the magnetic field and the plasma's microscopic electric field (for a recent discussion, e.g. [12]). The spectroscopic data used in [1] were obtained from the so-called model microfield method (MMM) [13] (it provides an analytical formula for the line shape, e.g. [14,15] for details). We present here a new table that provides a finer grid and that accounts for the presence of a magnetic field. Our table of line shapes has been calculated from a computer simulation method [16], following early works [17,18]. The method involves a numerical integration of the time-dependent Schrödinger equation for the hydrogen wave function under the influence of a fluctuating electric field (the plasma microfield), the latter being obtained from a particle simulation. In principle, this method can be used as a benchmark for analytical line shape models involving specific physical approximations (for a comprehensive review, e.g. [19]). Our code has been tested and validated by comparison with other codes at the "Spectral Line Shapes in Plasmas Code Comparison Workshop" (SLSP) [20]. The paper is organized as follows: Section 2 gives an overview on the Stark line shape

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formalism, Section 3 presents the simulation method, and Section 4 gives an application of the database to the calculation of a spectrum observed in a "virtual" plasma background simulated from a transport code (synthetic diagnostics).

2. Line broadening formalism

We give a summary of the formalism, along the lines of [12]. According to classical textbooks on spectroscopy (e.g. [21]), the spectral profile of an atomic line, $I(\omega,\mathbf{n})$, is given in terms of the line profile in the atom's frame of reference $I_0(\omega,\mathbf{n})$ by Doppler convolution

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

Here, ω_0 is the central angular frequency of the line under consideration, ω and $\mathbf{n}$ denote the frequency and the observation direction, respectively, and $f(\mathbf{v})$ is the atomic velocity distribution (VDF). The convolution implies that the thermal motion and the stationary-atom line shape I_0 are not correlated, i.e. we omit collisional narrowing in our treatment. 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 $I_0(\omega,\mathbf{n}) \equiv \delta(\omega-\omega_0)$] and a Voigt function if natural broadening is retained. In the general case, $I_0(\omega,\mathbf{n})$ is proportional to the Fourier transform of the atomic dipole autocorrelation function $C_\mathbf{n}(t)$, a quantity described in the framework of quantum mechanics

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

$$C_\mathbf{n}(t) = \mathrm{Tr}\{\mathbf{d}_\perp(0)\cdot\mathbf{d}_\perp(t)\rho\}. \quad (3)$$

Here, the trace is performed over the atomic states and denotes a statistical average, ρ is the projection of the density operator onto the atom's Hilbert space evaluated at initial time, the brackets $\{\cdots\}$ denote an average over the perturber trajectories (classical path approximation), and $\mathbf{d}_\perp = \mathbf{d} - (\mathbf{d}\cdot\mathbf{n})\mathbf{n}$ denotes the projection of the atomic dipole operator onto the polarization plane, in the Heisenberg picture. In (3), restrictions of this operator to the upper and lower levels of the transition are implied (no-quenching approximation). It is customary to write the autocorrelation function in terms of the evolution operator $U(t)$. Because of the identity $\mathbf{d}_\perp(t) \equiv U^\dagger(t)\mathbf{d}_\perp(0)U(t)$, a calculation of the line shape requires the knowledge of the matrix elements of $\mathbf{d}$ 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 $V(t) = -\mathbf{d}\cdot\mathbf{F}(t)$ is the time-dependent Stark effect term (Schrödinger picture) resulting from the action of the microscopic electric field $\mathbf{F}(t)$. When this term is neglected, the Schrödinger equation has the trivial solution $U(t) = \exp(-iH_0t/\hbar)$, which shows, using Eqs. (3) and (2), that $I_0(\omega,\mathbf{n})$ reduces to a set of delta functions (or Lorentzian functions if the natural broadening is retained). By contrast, the case where $\mathbf{F}(t)$ has to be retained is much trickier because there is no general exact analytical solution. The time-dependent perturbation theory yields a formal expansion (Dyson series), which is not applicable in explicit calculations because of the non-commutation of the interaction term at different times (time-ordering problem). This concerns in particular the microfield due to ions. 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). For our purposes it is convenient to have a line shape model with less restrictive approximations, in such a way to make it applicable to various plasma conditions. A good candidate is the simulation technique [17] (see also the recent review in [19]). Like the MMM, this method can be used in the elaboration of tables, e.g. [22].

3. The numerical simulation method

The purpose of "ab initio" simulations is to numerically reproduce the motion of the charged particles in the plasma so as to obtain the time dependent electric microfield $\mathbf{F}(t)$. While being CPU intensive, this method has the advantage of providing reference line shapes; e.g. it was used to test the accuracy of simpler analytical models like the unified theory or the model microfield method (see Fig. 1 for an illustration). 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; (iii) the average of the evolution operators on a set of realizations and the Fourier transform of the autocorrelation function. In the simulations performed for this work, we use a code [16] developed according to the method reported in [17,18]. 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

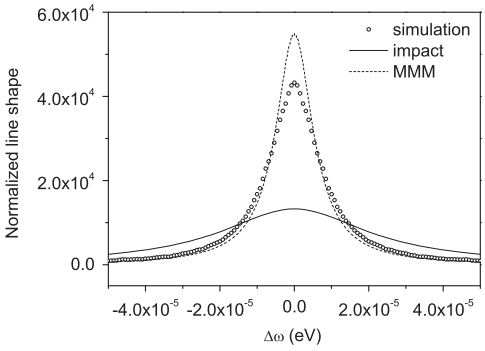

Fig. 1. Simulations serve as a reference for testing the accuracy of simpler analytical models, especially regarding the description of ion dynamics. The standard impact theory applied to ions (e.g. [16]) usually overestimates the role of microfield dynamics and yields a line width larger than that obtained from a numerical simulation. This point is illustrated here for the Lyman α line of deuterium. A plasma density of 10^{14} cm^{-3} and ion and electron temperatures of 1 eV have been assumed in the calculation, and only the Stark broadening due to ions has been retained. Also shown in the figure is the result of the model microfield method (MMM), which is closer to the simulation but still deviates from it, in the opposite sense.