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

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Abstract

A new table of Stark-Zeeman line shapes is provided for plasma diagnostics in the framework of magnetic fusion research. Spectral profiles of Dα, Dβ, Dγ, Dδ, and Dε have been calculated using computer simulations in conditions relevant to tokamak edge and divertor plasmas. After a brief presentation of the calculation method, we propose an interpolation formula and we give a routine for diagnostic applications. Analyses of experimental and synthetic spectra are performed as an illustration.

Keywords:

1. Introduction

Modeling efforts have been done in the last years in order to provide a spectroscopic database for the interpretation of line spectra in magnetic fusion devices, for diagnostic purposes, for present machines as well as for ITER and the subsequent demonstration power plant DEMO. A specific issue that requires careful examination is the broadening of the hydrogen isotope lines observed in the edge and in the divertor of tokamaks. Under specific conditions ("detached regime"), the plasma located near the divertor target plates contains a large amount of neutrals in an excited state (with a principal quantum number n possibly larger than 10), which are sensitive to the plasma's microscopic electric field. The corresponding lines observed in passive spectroscopy can be used as a probe of the electron density provided a suitable

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model is used. Since the first modern treatments of Stark broadening (in particular with the works by Baranger, Griem et al. in the fifties [1, 2, 3, 4, 5]), there has been an increasing number of investigations devoted to improve the accuracy of Stark line shape-based spectroscopic diagnostics. Basically, the problem of modeling a Stark-broadened line amounts to solving an equation of the Schrödinger type with a time-dependent stochastic perturbation (Stark effect term). Whereas exact solutions exist in ideal cases and under specific assumptions (e.g. within the so-called static approximation, which is sometimes applied to the Stark effect due to the plasma ions), there is no general formula applicable in a systematic way, e.g., in a diagnostic routine. Previous analyses of spectra observed in the divertor of the ASDEX-Upgrade tokamak [6] and in TCV [7] were performed using tables obtained from the so-called model microfield method or "MMM" [8] (it provides an analytical formula for the line shape, e.g. [9, 10] for details). We present here a new table that provides a finer grid and that accounts for the presence of a magnetic field. This table is an extension of preliminary results obtained last year [11] for the deuterium Balmer γ line (Dγ). Spectral profiles of Dα, Dβ, Dγ, Dδ, and Dε have been calculated with account both for Stark broadening and for the Zeeman effect due to the magnetic field present in tokamaks. The line shapes have been calculated from a computer simulation method [12]. For a practical application, we propose an interpolation formula and we illustrate it through the analysis of an experimental spectrum and a synthetic spectrum obtained from a transport code.

2. The computer simulation method

Computer simulations for Stark broadening were developed in the seventies, with the advent of modern computers, so as to investigate ion dynamics effects on the line broadening; e.g. [13] for a review. The purpose of such simulations is to numerically reproduce the motion of the charged particles in the plasma so as to obtain the time dependent electric microfield $\mathbf{E}(t)$ at an emitter's location. While being CPU intensive, this method has the advantage of providing reference line shapes and it can be used to test the accuracy of simpler analytical models like the unified theory [14, 15] or the model microfield method [9, 8, 10]. 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:

$$I(\Delta\omega) = \frac{1}{\pi}\mathrm{Re}\int_0^\infty dt \langle \mathbf{d}_\perp \cdot U^\dagger(t)\mathbf{d}_\perp U(t)\rangle e^{i\Delta\omega t}. \quad (1)$$

$\Delta\omega = \omega - \omega_0$ denotes the frequency detuning with respect to the line position on spectrum ω_0. 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 [12] developed according to the method reported in early papers [16, 17]. 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 $\exp\{-iV(t)\Delta t/\hbar\}$, where $V = -\mathbf{d} \cdot \mathbf{E}$ is the Stark effect term taken in the interaction picture. The exponential is evaluated using the scaling and squaring method [18]. 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, e.g., if the velocity $\mathbf{v}$ is correlated with the electric field $\mathbf{E}(t)$ or if the Lorentz field $\mathbf{v} \times \mathbf{B}$ is important [19]). An example of simulated spectrum is shown in Fig. 1. The spectral profile of the Dα 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 due to a stronger Stark broadening (Fig. 2).

3. A line shape database for diagnostics

The numerical simulation method is not appropriate for a systematic use in a diagnostic routine because it can be CPU time consuming, depending

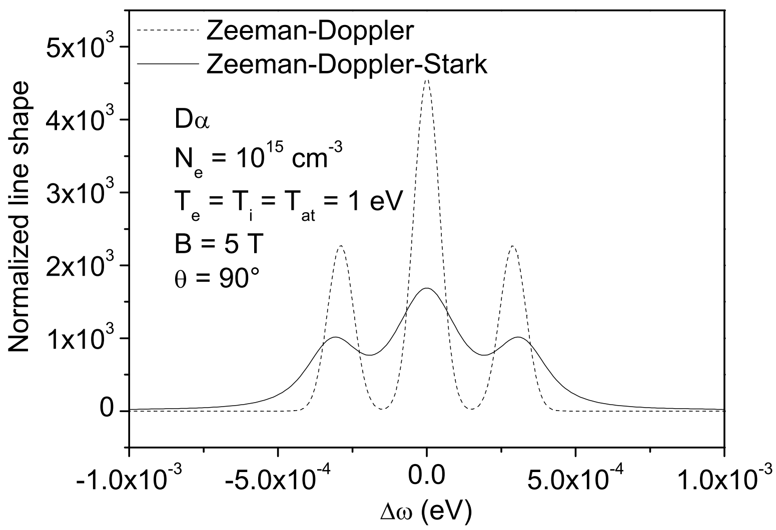

Figure 1: Plot of the Dα line shape obtained from a computer simulation, at conditions relevant to tokamak divertor plasmas at high density regimes. The Stark broadening is comparable to the Doppler broadening. The triplet structure stems from the Zeeman effect.

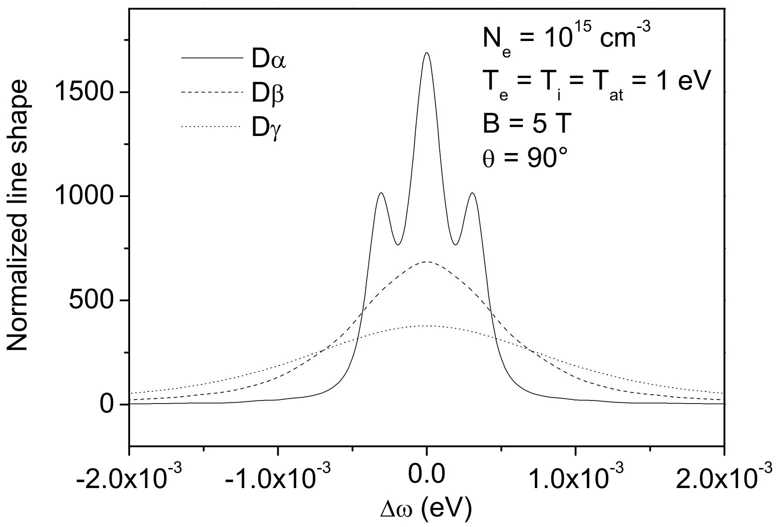

Figure 2: The Stark broadening increases with the principal quantum number and tends to mask the Zeeman triplet structure. Here, the profiles of Dα, Dβ, and Dγ have been simulated assuming the same plasma conditions as in Fig. 1.

on the plasma conditions and the spectral line under consideration. Several works have reported on the development of line shape databases constructed using this method (e.g. [20]). We present here a new database with conditions relevant to tokamak edge and divertor plasmas. Spectral profiles of the Dα, Dβ, Dγ, Dδ, and Dε lines with account of the Stark and Zeeman effects have been calculated assuming the following parameters:

$$T_e = T_i \equiv T = 0.316,\ 1,\ 3.16,\ 10,\ \text{and}\ 31.6\ \text{eV};$$
$$N = (1,\ 2.15,\ 4.64) \times (10^{13},\ 10^{14},\ 10^{15}),\ \text{and}\ 10^{16}\ \text{cm}^{-3};$$
$$B = 0,\ 1,\ 2,\ 2.5,\ 3,\ \text{and}\ 5\ \text{T}.$$

The database is available online as a single zipped folder containing 3000 files. For the sake of simplicity, only line shapes in observation perpendicular ($I_\perp$) and parallel ($I_{//}$) to the magnetic field are given; a reconstruction of the spectral profile at a given angle θ is obtained by forming the relation $\sin^2\theta \times I_\perp + \cos^2\theta \times I_{//}$. For diagnostic purposes, an interpolation FORTRAN program is provided as a supplementary file. The following formula is used:

$$\begin{aligned} I(N,T,B,\theta,\Delta\omega) \;&=\; 3\log\left(\frac{N}{N_0}\right) I_{10}(B,\theta,\Delta\omega) + 2\log\left(\frac{T}{T_0}\right) I_{01}(B,\theta,\Delta\omega) \\ &\quad + \left[1 - 3\log\left(\frac{N}{N_0}\right) - 2\log\left(\frac{T}{T_0}\right)\right] I_{00}(B,\theta,\Delta\omega). \quad (2) \end{aligned}$$

It takes advantage of the logarithmic scale used for the density and temperature. The '0' and '1' indices refer to the grid point immediately below and above the input density and temperature (N,T), i.e., $N_0 \leq N < N_1$ and $T_0 \leq T < T_1$. The shortcut notation $I_{ab}(B,\theta,\Delta\omega) = I(N_a,T_b,B,\theta,\Delta\omega)$ is used with $a,\ b = 0,\ 1$. For the magnetic field, we exploit the linear dependence on B of the Zeeman lateral components and perform a rescaling of the $\Delta\omega$ values. The quantity I_{ab} evaluated at $(B,\Delta\omega)$ can be estimated as follows (θ is not written for the sake of simplicity):

$$I_{ab}(B,\Delta\omega) = \frac{B-B_0}{B_1-B_0} \times \frac{B_1}{B} I_{ab}\left(B_1, \Delta\omega\frac{B_1}{B}\right) + \frac{B_1-B}{B_1-B_0} \times \frac{B_0}{B} I_{ab}\left(B_0, \Delta\omega\frac{B_0}{B}\right). \quad (3)$$

The first fraction present in front of each term denotes a weight in a proportion respective to the distance of the next point on the B grid and the second fraction denotes a normalization factor associated to the $\Delta\omega$ rescaling. The formula needs to be modified in the case where the magnetic field is in the first interval ($B_0 \leq B < B_1$ with $B_0 \equiv 0$ and $B_1 \equiv 1$ T) in order to avoid a numerical divergence. The following relation can be used

$$I_{ab}(B, \Delta\omega) = I_{ab}\left(B_1, \Delta\omega \frac{B_1}{B}\right) + \left(1 - \frac{B}{B_1}\right) \times I_{ab}(B_0, \Delta\omega). \tag{4}$$

It becomes formally identical to $I_{ab}(B_0 = 0, \Delta\omega)$ at the $B \to 0$ limit. Figure 3 shows an example of application of the routine. An experimental spectrum of the Dε line observed in the divertor of ASDEX-Upgrade [21] is analyzed using the database. The principal quantum number is sufficiently high so that the Zeeman effect is masked and the Stark effect is the dominant broadening mechanism. Furthermore, the spectral profile is weakly dependent on the temperature. A density adjustment assuming a given temperature of 1 eV and leaving the density as the only adjustable parameter yields a value of 8×10^{14} cm^{-3}, which falls in the typical range expected in divertor plasmas at high-density conditions.

4. Application to synthetic diagnostics

A common problem that occurs in the interpretation of passive spectroscopy signals is the non-uniformity of the emission zone along the line-of-sight. The formation of a spectral line results from the emission of atoms that are located in regions with different values of N_e, T_e etc., which makes the interpretation of spectra intricate. In recent years, modeling efforts have been carried out with the purpose of analyzing spectra observed in a virtual plasma background obtained from a transport code (synthetic diagnostics, e.g. [22]). A major difficulty in this task is the elaboration of a line shape model sufficiently general and accurate to be applicable to the wide range of values covered by the plasma parameters on the line-of-sight. Our database would provide an interesting approach because it involves no restrictive physical approximation on the atomic physics (namely: the time-dependent Schrödinger equation is solved) and it allows for a systematic evaluation of the emission spectra along the line-of-sight. As an illustration, we consider here an application to a virtual plasma background calculated from the SolEdge2D-EIRENE code in conditions relevant to the divertor of the WEST tokamak [23]. The same plasma background as in [11] is considered; Fig. 4 shows an example of density and temperature spatial profiles calculated on a line-of-sight crossing the divertor region at the densest location. The spectral profile

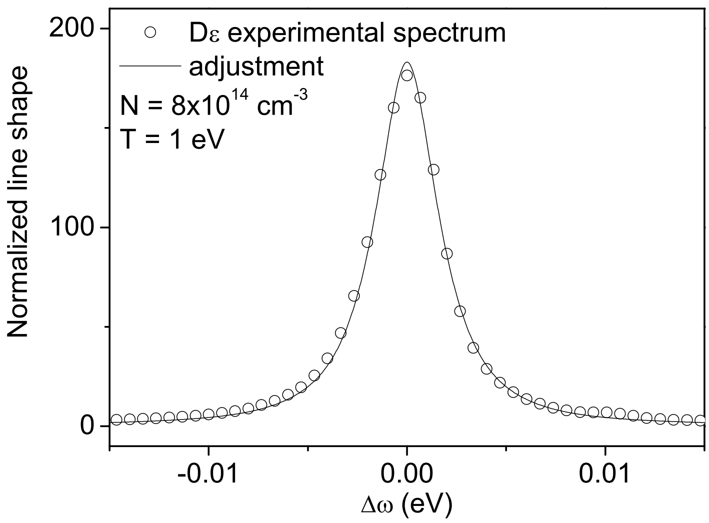

Figure 3: Adjustment of an experimental spectrum observed in the divertor of ASDEX-Upgrade using the line shape database. The line broadening is weakly dependent on the temperature. Assuming a given temperature of 1 eV and leaving the density as the only adjustable parameter yields a value of 8×10^{14} cm^{-3}, which falls in the typical range expected in divertor plasmas at high-density conditions.

of Dα resulting from integration on this line-of-sight has been calculated using the database. The Doppler broadening, which is important on this line, has been retained through a numerical convolution. The excited level ($n = 3$) population has been estimated using the same collisional-radiative model as in [22]. The simulated spectrum is close to that obtained at the densest location on the line-of-sight (see Fig. 5). We have performed an adjustment of this simulated Dα spectrum using the database and assuming $T_e = T_{\rm at} \equiv T$, B, θ, and N_e as four independent parameters. A χ^2 minimization routine based on a genetic algorithm has been used [24]. As can be seen in Fig. 6, the adjustment is in a good agreement with the simulated spectrum. The obtained values for the magnetic field and the angle coincide with the local values on the emission zone with an accuracy better than 10%. A relatively good estimate is also obtained for the temperature and density, with a deviation to the local values of 30% and 40%, respectively. This deviation is in part due to the $T_e = T_{\rm at}$ assumption done in the adjustment and it can be mitigated through the use of a more accurate model. Values within the same order of magnitude are obtained from the analysis of other lines (Fig. 7).

5. Conclusion

The operation of magnetic fusion devices requires passive spectroscopy diagnostics in the edge plasma region. In this work, we have elaborated a new database for the interpretation of the first hydrogen Balmer lines in conditions of high-density recombining divertor plasmas. This database accounts for the simultaneous action of the Zeeman and Stark effects. The applicability of the database has been illustrated through experimental and synthetic diagnostics. The results indicate that the apparent spectral profile as it results from line-of-sight integration can serve as a diagnostic for the plasma parameters at the densest location. An extension of this work to the modeling of Balmer lines in the presence of a stronger magnetic field is currently in preparation for applications to the ITER divertor (B will attain values up to 8 T). Specific effects due to the thermal Lorentz electric field are expected [19] and will be investigated. An extension of the database to white dwarf stellar atmosphere conditions in an astrophysical framework is also planned.

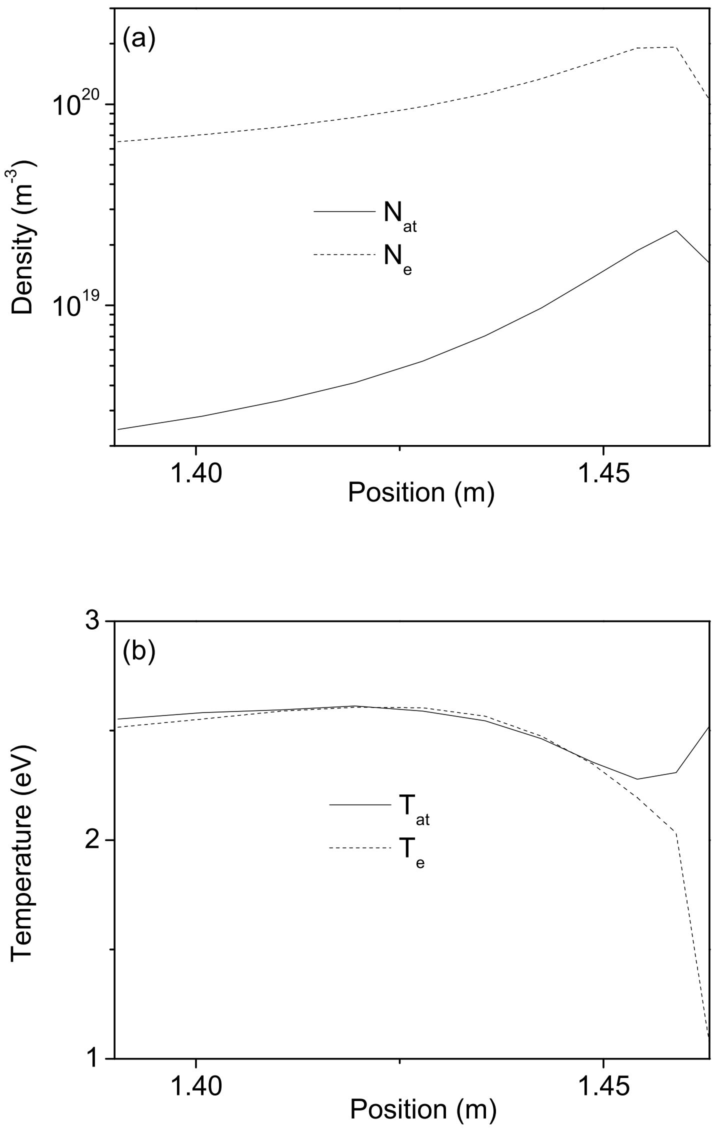

Figure 4: Calculated spatial profiles of the densities and temperatures on a line-of-sight crossing the divertor of WEST (geometry details are reported in [11]). The right side corresponds to the wall. Note a slight increase of the atomic temperature near the wall, which denotes the presence of a population due to reflection.

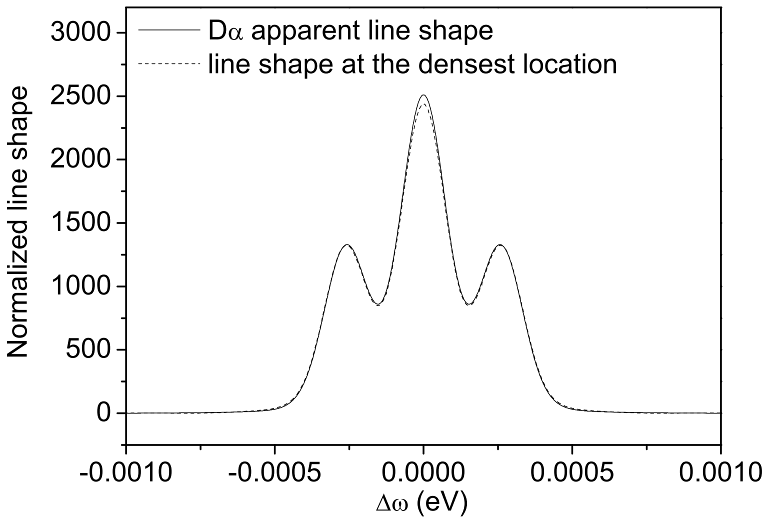

Figure 5: The apparent Dα spectrum, i.e. resulting from line-of-sight integration, is close to that obtained at the densest location on the line-of-sight.

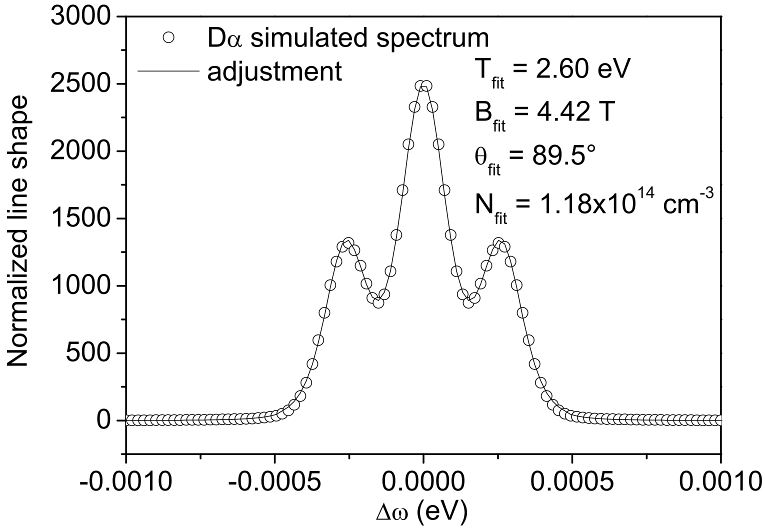

Figure 6: Adjustment of the simulated Dα spectrum using the line shape database with Doppler convolution. The obtained values for the parameters are close to those at the densest location.

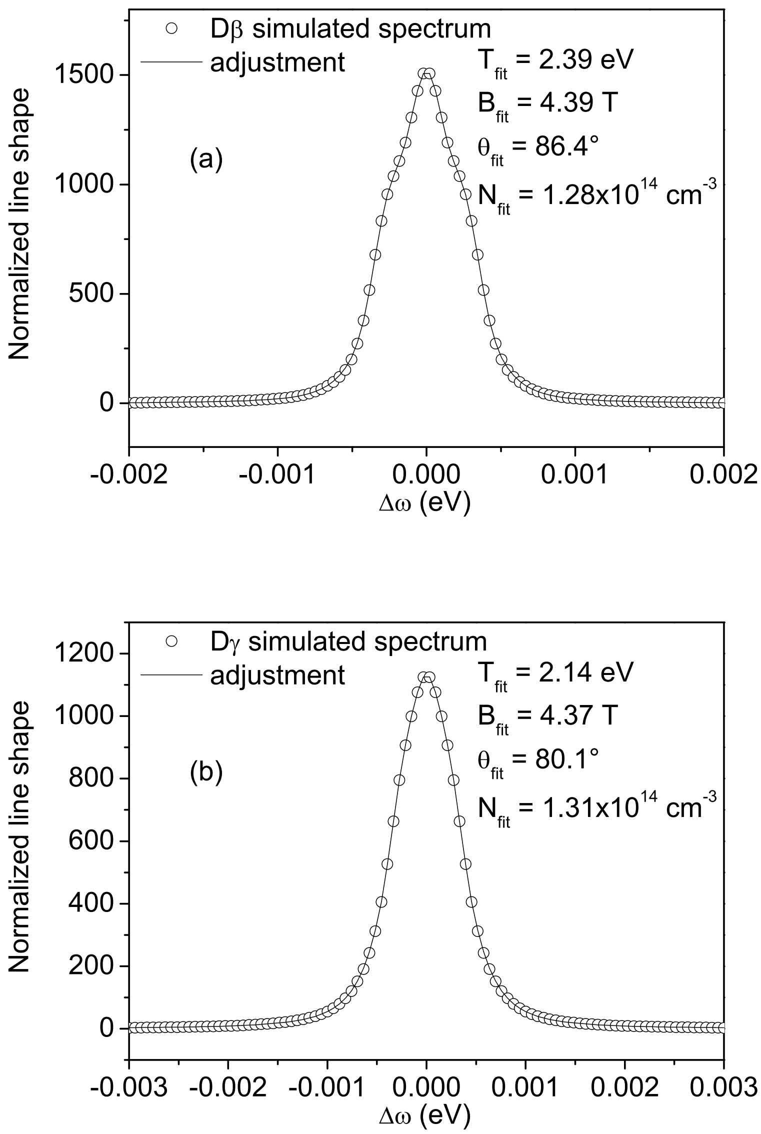

Figure 7: Adjustment of the Dβ and Dγ spectra using the same model. The local values are also obtained within a good accuracy here.

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References

[1] M. Baranger, Simplified quantum-mechanical theory of pressure broadening, Phys. Rev. 111 (1958) 481.

[2] M. Baranger, Problem of overlapping lines in the theory of pressure broadening, Phys. Rev. 111 (1958) 494.

[3] A. C. Kolb, H. R. Griem, Theory of line broadening in multiplet spectra, Phys. Rev. 111 (1958) 514.

[4] M. Baranger, General impact theory of pressure broadening, Phys. Rev. 112 (1958) 855.

[5] H. R. Griem, A. C. Kolb, K. Y. Shen, Stark broadening of hydrogen lines in a plasma, Phys. Rev. 116 (1959) 4.

[6] S. Potzel, R. Dux, H. W. Müller, A. Scarabosio, M. Wischmeier, ASDEX Upgrade team, Electron density determination in the divertor volume of ASDEX Upgrade via Stark broadening of the Balmer lines, Plasma Phys. Control. Fusion 56 (2014) 025010.

[7] K. Verhaegh, B. Lipschultz, B. P. Duval, J. R. Harrison, H. Reimerdes, C. Theiler, B. Labit, R. Maurizio, C. Marini, F. Nespoli, U. Sheikh, C. K. Tsui, N. Vianello, W. A. J. Vijvers, TCV team, MST1 team, Spectroscopic investigations of divertor detachment in TCV, http://arxiv.org/abs/1607.04539.

[8] C. Stehlé, Stark broadening of hydrogen Lyman and Balmer in the conditions of stellar enveloppes, Astron. Astrophys. Suppl. Ser. 104 (1994) 509.

[9] A. Brissaud, U. Frisch, Theory of Stark broadening - II Exact line profile with model microfield, J. Quant. Spectrosc. Radiat. Transfer 11 (1971) 1767.

[10] S. Günter, A. Könies, Diagnostics of dense plasmas from the profile of hydrogen spectral lines in the presence of a magnetic field, J. Quant. Spectrosc. Radiat. Transfer 62 (1999) 425.

[11] J. Rosato, H. Bufferand, M. Koubiti, Y. Marandet, R. Stamm, A table of Balmer γ line shapes for the diagnostic of magnetic fusion plasmas, J. Quant. Spectrosc. Radiat. Transfer 165 (2015) 102.

[12] J. Rosato, Y. Marandet, H. Capes, S. Ferri, C. Mossé, L. Godbert-Mouret, M. Koubiti, R. Stamm, Stark broadening of hydrogen lines in low-density magnetized plasmas, Phys. Rev. E 79 (2009) 046408.

[13] E. Stambulchik, Y. Maron, Plasma line broadening and computer simulations: A mini-review, High Energy Density Phys. 6 (2010) 9.

[14] D. Voslamber, Unified model for Stark broadening, Z. Naturforsch. 24a (1969) 1458.

[15] E. W. Smith, J. Cooper, C. R. Vidal, Unified classical-path treatment of Stark broadening in plasmas, Phys. Rev. 185 (1969) 140.

[16] R. Stamm, D. Voslamber, On the role of ion dynamics in the Stark broadening of hydrogen lines, J. Quant. Spectrosc. Radiat. Transfer 22 (1979) 599.

[17] R. Stamm, E. W. Smith, B. Talin, Study of hydrogen Stark profiles by means of computer simulation, Phys. Rev. A 30 (1984) 2039.

[18] C. Moler, C. V. Loan, Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later, SIAM Rev. 45 (2003) 3.

[19] J. Rosato, Y. Marandet, R. Stamm, Stark broadening by Lorentz fields in magnetically confined plasmas, J. Phys. B: At. Mol. Opt. Phys. 47 (2014) 105702.

[20] M. A. Gigosos, V. Cardeñoso, New plasma diagnosis tables of hydrogen Stark broadening including ion dynamics, J. Phys. B: At. Mol. Opt. Phys. 29 (1996) 4795.

[21] S. Potzel, private communication.

[22] J. Rosato, V. Kotov, D. Reiter, Modelling of passive spectroscopy in the ITER divertor: the first hydrogen Balmer lines, J. Phys. B: At. Mol. Opt. Phys. 43 (2010) 144024.

[23] H. Bufferand, G. Ciraolo, Y. Marandet, J. Bucalossi, P. Ghendrih, J. Gunn, N. Mellet, P. Tamain, R. Leybros, N. Fedorczak, F. Schwander, E. Serre, Numerical modelling for divertor design of the WEST device with a focus on plasma-wall interactions, Nucl. Fusion 55 (2015) 053025.

[24] P. Charbonneau, Genetic algorithms in astronomy and astrophysics, Astrophys. J. Suppl. Ser. 101 (1995) 309.