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Spectral line shape modeling for the calculation of radiation transport in divertors

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Abstract

Radiation transport in divertor plasmas is strongly coupled to the spectral profiles of absorption and emission of the hydrogen isotopes. As a consequence an accurate description of spectral line shapes is required in order to understand the ionization equilibrium in edge plasmas. The Ly_α line gives the main contribution to reabsorption. In this work, we present a line shape model which is appropriate to describe the Ly_α line in typical divertor conditions expected in tokamaks like JET, Alcator or ITER. Our results are based on an analytical calculation, which predicts the structure and broadening of the line due to combination of fine structure, Zeeman, Stark, and Doppler effects. The model is also applied to D_α line shape and predicts that the contribution of fine structure can be significant.

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1. Introduction

The radiation of neutral hydrogen isotopes plays an important role on the ionization equilibrium in the divertor plasma of tokamaks. The photons provide an excitation mechanism for the atoms in conditions for which the plasma is not optically thin: the increase of the population of the excited states enhances ionization by collisions in the edge plasma, and the corresponding increase of electron density can then enhance 3-body recombination processes, which in turn contribute to neutral sources. The edge plasma codes generally incorporate radiation effects on population of each species by coupling transport and collisional-radiative models [1,2]. 'Species' stands here for photons, neutrals in a given energy level, ions, and electrons. These coupled models are based on a set of kinetic equations describing the evolution of the species in space and time. A Monte–Carlo calculation of photon transport involves the line shape function $I_0(\omega,v)$ [2]. This function is the probability density function of emitting or absorbing a photon with a pulsation ω, through a transition $i \rightarrow f$ between two atomic

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energy levels, shifted by Doppler effect for a given velocity v of the atom. An accurate description of $I_0(\omega,v)$ is especially needed for the Ly_α line of hydrogen isotopes because of the opacity of the plasma for this line. Reabsorption proceeds indeed from the fundamental state, which is strongly populated. It has moreover been established that the mean free path of Ly_α photons is shorter than 2 mm in the conditions of the ITER divertor [3], and simulations with the transport code EIRENE show that trapping of Ly_α photons increases the density of the ions near the target plates [4]. In this work we investigate the model which is appropriate for describing the Ly_α line shape in the various divertor conditions expected in tokamaks like JET, Alcator or ITER. We first present in Section 2 the general formalism used to describe the line shape. This formalism retains fine structure, Zeeman, Stark, and Doppler effects. We show in Section 3 that, for typical values of density and temperature found in divertors, Stark broadening can be treated by an impact theory for both ions and electrons. We present in Section 4 line shape calculations obtained with our model. We compare the structures of the line shape obtained for low and high magnetic fields, without Doppler broadening, and we show that Zeeman and fine structure effects can be of the same order. We also investigate the D_α line and, applying our model, we show that fine structure leads to a complex line shape.

2. General formalism

Let us consider the radiation emitted or absorbed by a population of atoms in a magnetized plasma. The profile $I(\omega)$ of a spectral line is given by the following formula:

$$I(\omega) = \int_{-\infty}^{+\infty} f(v) I_0(\omega, v)\,\mathrm{d}v, \tag{1}$$

where $f(v)$ is the distribution function of the projection $v = \boldsymbol{k}\cdot\mathbf{v}/\|\boldsymbol{k}\|$ of the emitter velocity $\mathbf{v}$ on the wave vector $\boldsymbol{k}$, and $I_0(\omega, v)$ is the line shape emitted or absorbed by one atom with the velocity $\mathbf{v}$. The latter is the quantity required to calculate the transport of photons with edge plasma codes. Its expression is given as follows [5]:

$$I_0(\omega, v) = \frac{1}{\pi}\mathrm{Re}\int_0^{\infty} C(t)\mathrm{e}^{\mathrm{i}\omega(1-v/c)t}\,\mathrm{d}t, \tag{2}$$

where Re denotes real part, c is the speed of light, and $C(t)$ the dipole autocorrelation function. This function is defined by

$$C(t) = \sum_{\mathrm{ii'ff'p}} \rho_\mathrm{i} D^{(p)}_{\mathrm{if}} D^{(p)^*}_{\mathrm{i'f'}} \langle\langle \mathrm{i'f'}|\{U(t)\}|\mathrm{if}\rangle\rangle. \tag{3}$$

Here, $D^{(p)}_{\mathrm{if}} = \langle \mathrm{i}|D^{(p)}|\mathrm{f}\rangle$ (resp. $D^{(p)^*}_{\mathrm{i'f'}} = \langle \mathrm{i'}|D^{(p)}|\mathrm{f'}\rangle^*$) are transition matrix elements between the initial sublevels i (resp. i′) and the final sublevels f (resp. f′), $D^{(p)} = \boldsymbol{D}\cdot\boldsymbol{\varepsilon}_p$ is the projection of the emitter electric dipole $\boldsymbol{D}$ on the direction of polarization $\boldsymbol{\varepsilon}_p$, and ρ_i is the population of the initial sublevel i of the radiative transition. The quantity U is the evolution operator of the emitter in Liouville space [6]. The brackets $\{\cdots\}$ denote a statistical average over the perturbing electrons and ions of the plasma, which will be assumed to follow a classical path. The evolution operator U obeys a Liouville equation

$$\mathrm{i}\partial_t U = LU, \tag{4}$$

where L is the Liouvillian of the system. This quantity is a 'super-operator', *i.e.* an operator which acts on the space of quantum operators. Its action on an operator A is given by $LA = (HA - AH)/\hbar$, where H is the Hamiltonian of the system. The expression of L is given as follows:

$$L = L_0 + L_{\mathrm{FS}} - \boldsymbol{\mu}\cdot\boldsymbol{B} - \boldsymbol{D}\cdot\boldsymbol{E} - \boldsymbol{D}\cdot\boldsymbol{E}_\mathrm{L}, \tag{5}$$

where L_0 and L_{FS} are respectively the electrostatic Liouvillian and the fine structure term for the unperturbed emitter. The third term $-\boldsymbol{\mu}\cdot\boldsymbol{B}$ describes the interaction between the emitter magnetic momentum $\boldsymbol{\mu}$ and the magnetic field $\boldsymbol{B}$. The fourth term $-\boldsymbol{D}\cdot\boldsymbol{E}$ describes the interaction between the emitter dipole $\boldsymbol{D}$ and the plasma microfield $\boldsymbol{E}$, a function of time. The last term $-\boldsymbol{D}\cdot\boldsymbol{E}_\mathrm{L}$ describes the interaction between the emitter dipole and the Lorentz field $\boldsymbol{E}_\mathrm{L} = \mathbf{v}\times\boldsymbol{B}$ due to the motion of the emitter in the magnetic field $\boldsymbol{B}$.

Our group has previously developed a line shape code valid for arbitrary emitter and plasma conditions [7]. In the following we present a recently developed analytical model allowing for some hydrogen spectral lines an extremely fast line shape calculation. This is a mandatory requirement for radiation transport calculations using the Monte–Carlo method, where the profile has to be evaluated a large number of times.

3. Impact model for ions and electrons

The Liouville equation (Eq. (4)) has to be integrated and averaged in order to obtain $\{U(t)\}$ and then the line shape $I_0(\omega,v)$. To solve this equation we have used the impact model for both ions and electrons. This model is based on two assumptions. First, the perturbers are assumed to undergo binary collisions with the emitter. Second, the time of collision is assumed to be much smaller than the so called 'time of interest', a typical decorrelation time for the atomic dipole which can be estimated as the inverse of the typical width of the line shape. The impact theory leads to the following formula for $\{U(t)\}$ [8]:

$$\{U(t)\} = \exp[-\mathrm{i}(L_0 + L_{\mathrm{FS}} - \boldsymbol{\mu}\cdot\boldsymbol{B} - \boldsymbol{D}\cdot\boldsymbol{E}_{\mathrm{L}} - \mathrm{i}\phi_{\mathrm{i}} - \mathrm{i}\phi_{\mathrm{e}})t]. \tag{6}$$

The quantities ϕ_{i} and ϕ_{e} are the collision operators, respectively for ions and electrons. Their expressions have been established for hydrogen in [8] ($\alpha = i$ for ions, $\alpha = e$ for electrons)

$$\phi_\alpha = 2\sqrt{\pi}N_\alpha\rho_{\mathrm{W}\alpha}^2 v_\alpha\left(1 + \left(\frac{r}{n^2}\right)^2\int_{y_\alpha}^{\infty}\frac{\mathrm{e}^{-y}\mathrm{d}y}{y}\right), \tag{7}$$

where N_α stands for the density and $v_\alpha = (2T_\alpha/m_\alpha)^{1/2}$ for the thermal velocity, T_α and m_α being respectively the temperature and the mass. The quantity r is the position operator of the atomic electron, in units of Bohr radius. The Weisskopf radius $\rho_{\mathrm{W}\alpha}$ defines the typical distance below which strong collisions occur, and is given by $\rho_{\mathrm{W}\alpha} = (2/3)^{1/2}\hbar n^2/m_{\mathrm{e}}v_\alpha$ [8], where n is the principal quantum number of the transition upper level. The integral describes weak collisions, *i.e.* occurring for distances larger than $\rho_{\mathrm{W}\alpha}$. The cutoff y_α has been introduced so as to take into account Debye shielding. It is defined by $y_\alpha = (\rho_{\mathrm{W}\alpha}/\lambda_{\mathrm{D}\alpha})^2$, where $\lambda_{\mathrm{D}\alpha} = (\varepsilon_0 T_\alpha/N_\alpha \mathrm{e}^2)^{1/2}$ is the Debye length. For $N_{\mathrm{i}} = N_{\mathrm{e}}$ and $T_{\mathrm{i}} = T_{\mathrm{e}}$, the matrix elements of the ion collision operator ϕ_{i} are about 60 times larger than those of ϕ_{e} for deuterium because of the mass ratio $(m_{\mathrm{i}}/m_{\mathrm{e}})^{1/2}$.

As mentioned before, the impact model is valid provided that the time of collision of each charged particle, $\tau_{c\alpha} \approx N_\alpha^{-1/3}/v_\alpha$, is much smaller than the time of interest τ_{i}. The condition for electrons is always satisfied for Ly_α line with $10^{12}\,\mathrm{cm}^{-3} \leqslant N_{\mathrm{e}} \leqslant 10^{15}\,\mathrm{cm}^{-3}$ and $1\,\mathrm{eV} \leqslant T_{\mathrm{e}} \leqslant 100\,\mathrm{eV}$, typical ranges of density and temperature in divertors. The condition is satisfied for deuterium ions, except in a domain of high density and low temperature values, for which the ratio $\tau_{\mathrm{ci}}/\tau_{\mathrm{i}}$ exceeds 20% (Fig. 1). In the latter case the effect of the ion microfield cannot be described by the impact model anymore. The line shape can then be computed with the PPP code,

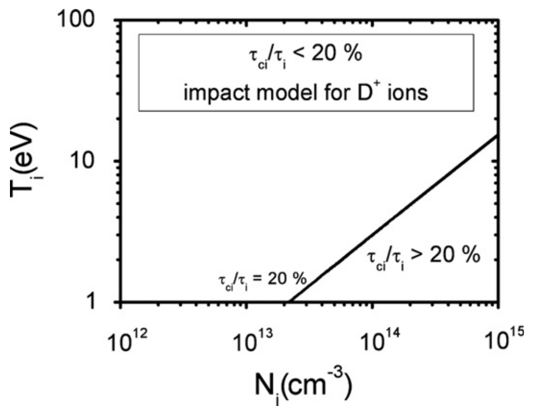

Fig. 1. Validity domain of the impact model of ions of deuterium for the Ly_α line.

which includes a numerical model based on the frequency fluctuation model (FFM) [7]. We will next consider conditions of density and temperature for which the impact model for ions is valid. Taking Eq. (3) and inserting the formal expression of $\{U(t)\}$, the line shape is given by a matrix inversion

$$I_0(\omega,v) = -\frac{1}{\pi}\mathrm{Im}\sum_{\mathrm{ii'ff'p}}\rho_{\mathrm{i}}D_{\mathrm{if}}^{(p)}D_{\mathrm{i'f'}}^{(p)^*}\langle\langle \mathrm{i'f'}|A^{-1}(\omega,v)|\mathrm{if}\rangle\rangle, \tag{8}$$

where $A(\omega,v) = \omega(1 - v/c) - L_0 - L_{\mathrm{FS}} + \boldsymbol{\mu}\cdot\boldsymbol{B} + \boldsymbol{D}\cdot\boldsymbol{E}_{\mathrm{L}} + i\phi_{\mathrm{i}} + i\phi_{\mathrm{e}}$.

4. Line shape calculation

We have performed an analytical calculation of the Ly_α line shape of deuterium. Our method is based on analytical inversion of the 16×16 A-matrix in Eq. (8), using properties of linear algebra, assuming the initial sublevels to be equally populated, and neglecting the contribution of the Lorentz field $\boldsymbol{E}_{\mathrm{L}}$, which is less than 10%. The resulting line shape is a sum of 10 Lorentzian functions:

$$I_0(\omega,v) = \sum_{j=1}^{10}K_j L_\gamma(\Delta\omega - \omega_j), \tag{9}$$

where $\Delta\omega = \omega(1-v/c)$. The expressions of the frequency ω_j, the amplitude K_j and the width γ of each Lorentzian are given in Appendix.

We have done calculations of the Ly_α line shape for different values of B. For low magnitudes, at about 1 T, the structure of the line shape is complex, and exhibits 10 components, resulting from a competition between fine structure and Zeeman effects

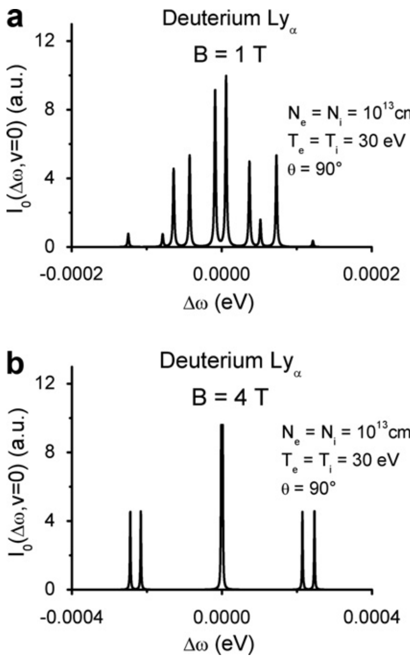

Fig. 2. Fine structure and Zeeman effects on Ly_α line shape of deuterium, with $N_e = N_i = 10^{13}$ cm^{-3}, $T_e = T_i = 30$ eV, $\theta = 90°$, for (a) $B = 1T$, (b) $B = 4T$.

(Fig. 2(a)). When B increases, the Zeeman effect becomes dominant, and the line shape tends toward a Lorentz triplet when $B \geqslant 2$ T. Fig. 2(b) shows the line shape with $B = 4$ T.

We have also calculated the profile of the D_α line for cases where fine structure is of the same order as the Zeeman effect. This line, corresponding to the transition $3 \rightarrow 2$, would be involved in a detailed calculation of the opacity, and is moreover of interest for divertor diagnostics. Being interested here by the structure of the line, we have computed the profile of D_α without Doppler broadening. This requires a 188×188 matrix inversion, for which we have used the PPP code. Fig. 3 shows the result for $B = 4$ T, and demonstrates the complex structure of this line due to fine structure.

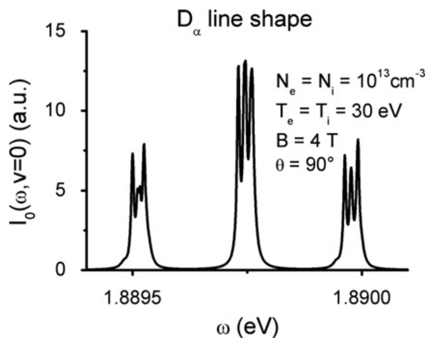

Fig. 3. Fine structure and Zeeman effects on D_α line shape, with $B = 4T, \theta = 90°$, $N_e = N_i = 10^{13}$ cm^{-3}, and $T_e = T_i = 30$ eV.

5. Conclusion

Detailed line shape studies are required for accurate modeling of radiation transport in divertor conditions. Here, we have investigated the Ly_α transition because the latter is responsible for most of the reabsorption. We have developed an analytical model which allows very fast numerical evaluation of the line shape. The Ly_α line appears as a set of 10 components resulting from a competition between fine structure and Zeeman effects. Stark broadening is described in our model by the impact theory, which is valid for a wide domain of density and temperature values found in divertors. Our line shape calculations are now used to model the transport of photons by the Monte–Carlo code EIRENE [9]. Their inclusion should improve the accuracy of ionization equilibrium calculation in the divertor plasma. Further work could consist in developing the same kind of analytical calculation for the Ly_β line, which is the second contributor to the reabsorption. This would entail a 36×36 matrix inversion. We have also investigated the D_α line shape and, using the PPP code, we have shown that fine structure leads to a complex structure of the line profile. In this case, an analytical calculation is out of reach, and rapid numerical techniques would have to be developed so as to use accurate line shapes in a radiative transport calculation. Another possible future development of our work would consist in investigating Stark broadening in conditions for which the impact approximation is no longer valid.

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Appendix

The Ly_α line shape is described in Eq. (9) as a sum of 10 Lorentzian functions with a central pulsation ω_j, an amplitude K_j, and a width γ. The width is a matrix element of the sum of the collision opera-

Table 1
Central pulsation ω_j and associated amplitude K_j of each Lorentzian function with $C_\theta = (1+\cos^2\theta)/2$, $S_\theta = \sin^2\theta$, $\omega_\pm = \omega_{FS}/4 \pm \omega_Z/2$, $\omega_{1\pm} = \omega_{FS}/4 \pm 3\omega_Z/2$, and $\omega_{2\pm} = (9\omega_{FS}^2 + 4\omega_Z^2 \pm 4\omega_{FS}\omega_Z)^{1/2}/4$

ω_j	$2\,\omega_+$	$2\omega_-$	$-\omega_{1-} + \omega_{2+}$	$-\omega_{1-} - \omega_{2+}$	$-\omega_{1+} + \omega_{2-}$
K_j	C_θ	C_θ	$C_\theta(1 - \omega_+/\omega_{2+})/2$	$C_\theta(1 + \omega_+/\omega_{2+})/2$	$C_\theta(1 - \omega_-/\omega_{2-})/2$
ω_j	$-\omega_{1+} - \omega_{2-}$	$-\omega_+ + \omega_{2+}$	$-\omega_+ - \omega_{2+}$	$-\omega_- + \omega_{2-}$	$-\omega_- - \omega_{2-}$
K_j	$C_\theta(1 + \omega_-/\omega_{2-})/2$	$S_\theta(1 + \omega_+/\omega_{2+})/2$	$S_\theta(1 - \omega_+/\omega_{2+})/2$	$S_\theta(1 + \omega_-/\omega_{2-})/2$	$S_\theta(1 - \omega_-/\omega_{2-})/2$

tors $\phi_i + \phi_e$. Its expression, derived from Eq. (7), is given by the following formula:

$$\gamma = \sum_{\alpha=i,e} \frac{12N_\alpha\sqrt{\pi}}{v_\alpha}\left(\frac{\hbar}{m_e}\right)^2\left(\frac{16}{9} + \int_{y\alpha}^{\infty}\frac{e^{-y}dy}{y}\right). \qquad (10)$$

The amplitudes and the central pulsations depend on the magnitude B of the magnetic field and on the angle $\theta = (\boldsymbol{B},\boldsymbol{k})$ between the magnetic field and the wave vector. To express these quantities we introduce the parameters $\omega_Z = eB/2m_e$ and $\omega_{FS} = \alpha^2 E_I/24\hbar$, where α is the fine structure constant and E_I is the energy of ionization of the hydrogen. The value of each pulsation ω_j and each amplitude K_j is given in Table 1.

References

[1] H.A. Scott, M.L. Adams, Contrib. Plasma Phys. 44 (2004) 51.
[2] D. Reiter, S. Wiesen, M. Born, Plasma Phys. Control. Fusion 44 (2002) 1723.
[3] D.E. Post, J. Nucl. Mater. 220–222 (1995) 143.
[4] V. Kotov et al., Contrib. Plasma Phys. 46 (2006) 635.
[5] M. Baranger, Phys. Rev. 111 (1958) 481.
[6] U. Fano, Phys. Rev. 131 (1963) 259.
[7] B. Talin et al., Phys. Rev. A 51 (1995) 1918.
[8] H.R. Griem, A.C. Kolb, K.Y. Shen, Phys. Rev. 116 (1959) 4.
[9] D. Reiter et al., J. Nucl. Mater., these Proceedings, doi:10.1016/j.jnucmat.2007.01.213.