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Tables of dipolar emission and two–photon absorption Lyman−α profiles⋆

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Abstract. This paper shows the results of calculations, obtained by computer simulation, of the Stark broadening of the dipolar Lyman−α line of hydrogen considering fine structure, of two–photon absorption profiles for the transition 1S→2S of hydrogen and of the profiles that could be obtained using two–photon polarization spectroscopy techniques for the aforementioned transition. Calculations have been carried forward for wide ranges of electron density, between 4 10^{19} and 10^{23} m^{-3} and temperature, between 2 000 and 100 000 K. We have considered ion dynamics effects with perturbers of different masses.

In this paper we give the obtained profiles and the autocorrelation functions. These autocorrelation functions could be used in order to add another broadening mechanisms before obtaining the spectral profiles.

Key words: line: profiles — plasmas

1. Introduction

Comparing precise experimental measurements of the Stark broadening in different spectral lines with the calculations of those lines using confirmed theoretical models leads us to know the perturbers' density, their temperature and the thermodynamical equilibrium between the perturbers in plasmas dominated by coulombian collisions. For these comparisons, it is necessary to have large data bases of both experimental and theoretical profiles.

The dependencies of some characteristic quantities of the profiles, whether the total width at half height (FWHM) or the depth of the central dip (DIP) for the case of very well known lines, both theoretically and experimentally, may allow us to know the orders of magnitude of the perturbers' density, at least, or the temperature of the plasma. However, comparing experimental and theoretical profiles can give very valuable information about questions such as the thermodynamical equilibrium of the different species constituting the plasma.

In this paper we give the autocorrelation functions of the emitters' electric dipolar moment, which then allows us to obtain the Lyman−α emission profiles, two–photon absorption profiles for the 1S→2S transition and the profiles that would be obtained using 1S→2S two–photon polarization spectroscopy (Danzmann et al. 1986; Seidel 1986; Grützmacher & Seidel 1989; Steiger 1993; Steiger & Grützmacher 1993; Seidel et al. 1995). These profiles can be obtained from the autocorrelation functions here. The advantage of giving the autocorrelation functions of the dipolar moment instead of the Stark profiles directly is that the first ones make it easy to operate and to consider other additional broadening mechanisms. We give the pure Stark dipolar emission and two–photon polarization profiles also obtained directly from the given autocorrelation functions.

2. Calculation process

The profiles that are shown have been obtained by computer simulation techniques using particles. The simulation process generates the microfield time sequence suffered by the emitter, which then alters the emission process. The plasma model considers an ensemble of N_p electrons and N_p ions moving along rectilinear paths with constant velocity inside a spherical volume. The emitter is placed in the center of that sphere. The plasma

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⋆ All the tables of autocorrelation functions, of dipolar emission profiles, and of polarization by two–photon absorption profiles are only available in electronic form at the CDS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via http://cdsweb.u-strasbg.fr/Abstract.html

is homogenous and isotropic. The velocities of ions and electrons are obtained using the Maxwell distribution with the equilibrium temperature T. In order to account for the correlation effects between charged perturbers, we use Debye screened electric fields. A detailed description of the simulation method can be found in Gigosos & Cardeñoso (1996). As can be seen in that reference, the simulation processes are characterized by the relationship between the mean distance between particles $r_0 = \left(\frac{3}{4\pi N_e}\right)^{1/3}$, where N_e is the electron density, and the Debye radius r_D that fixes the parameter ρ of the simulation:

$$\rho = \frac{r_0}{r_D} = \left(\frac{3}{4\pi}\right)^{1/3} \left(\frac{q^2}{\varepsilon_0 k}\right)^{1/2} \frac{N_e^{1/6}}{T^{1/2}} \ . \quad (1)$$

Each time sequence of the electric microfield is used in the Schrödinger equation that establishes the evolution of the emitter atom. In that equation we have considered the fine structure for the level $n = 2$ of the hydrogen atom. From this process the autocorrelation function of the emitter dipolar momentum is calculated. An average over a large number of such processes allows us to obtain the tabulated autocorrelation functions. Gigosos & González (1998) describe in detail the calculation of the two–photon absorption profiles, $A(\Delta\omega)$, the dispersion profiles, $D(\Delta\omega)$, and two–photon polarization profiles, $P(\Delta\omega)$. As can be seen there the autocorrelation function may be written as

$$C(t) = 2C_R(t)\cos(\omega_0 t) + 2C_I(t)\sin(\omega_0 t) \quad (2)$$

so that the absorption or emission profiles, the dispersion profiles and polarization profiles may be obtained from

$$A(\Delta\omega) = \frac{1}{\pi}\int_0^\infty \mathrm{d}t[\cos(\Delta\omega t)C_R(t) - \sin(\Delta\omega t)C_I(t)] \quad (3)$$

$$D(\Delta\omega) = -\frac{1}{\pi}\int_0^\infty \mathrm{d}t[\cos(\Delta\omega t)C_I(t) + \sin(\Delta\omega t)C_R(t)] \quad (4)$$

$$P(\Delta\omega) = A(\Delta\omega)^2 + D(\Delta\omega)^2 \ . \quad (5)$$

In these expressions $\Delta\omega = \omega - \omega_0$ is the frequency displacement measured from the center of the spectral line. In our calculations that center has been considered as the distance from the medium point of the upper level $n = 2$ states to the lower level $n = 1$. When doing the Fourier transform of Eq. (2) we do not take into account how quantities such as $\int_0^\infty \mathrm{d}t \cos[(\omega+\omega_0)t]C_R(t)$ contribute to the spectrum, which would only make sense if the functions $C_R(t)$ and $C_I(t)$ had variations in time in that range of frequencies.

At time $t = 0$, $C_R(0) = 1$ so that $A(\Delta\omega)$ directly gives the areanormalized absorption or emission profile. In order to obtain the areanormalized polarization profile it is necessary to require that

$$\int_{-\infty}^{+\infty} P(\Delta\Omega)\mathrm{d}\Delta\omega = 1 \ , \quad (6)$$

which is equivalent to

$$\frac{2}{\pi}\int_0^\infty \mathrm{d}t \left(C_R(t)^2 + C_I(t)^2\right) = 1 \quad (7)$$

for the autocorrelation function. The tables for $C_R(t)$ and $C_I(t)$ given in this paper are normalized so that $C_R(0) = 1$. In order to obtain areanormalized polarization profiles, the values of $C_R(t)$ and $C_I(t)$ given in the tables should be properly renormalized according to Eq. (7).

In the simulation it has been considered that the correlation loss of the emission process, described by the $C_R(t)$ and $C_I(t)$ functions, is due exclusively to collisions with the charged particles. Whenever it may be necessary to consider aditional phenomena that were statistically independent of the Stark effect (for example collisions with neutrals or a residual Doppler effect), the supplied $C_R(t)$ and $C_I(t)$ functions may be modified in order to calculate the profiles that include all the existing phenomena. In this way, if $F(\Delta\omega)$ is the areanormalized profile due to another broadening mechanism independent of the Stark effect, we calculate the corresponding autocorrelation function using

$$B(t) \equiv B_R(t) + \mathrm{i}B_I(t) \equiv \int_{-\infty}^{+\infty} \mathrm{e}^{-\mathrm{i}\Delta\omega t} F(\Delta\omega)\mathrm{d}\Delta\omega \ . \quad (8)$$

The total autocorrelation functions that should be used in the calculations to obtain the complete profile would have, then,

$$\begin{aligned} C'_R(t) &= C_R(t)B_R(t) - C_I(t)B_I(t) \ , \\ C'_I(t) &= C_R(t)B_I(t) + C_I(t)B_R(t) \ . \end{aligned} \quad (9)$$

3. Results. Calculated lines

Here we present two sets of tables. The first includes the tables of the autocorrelation functions for dipolar emission (one photon) and for two–photon absorption obtained in the simulations. The second are the tables of the emission and polarization profiles calculated from the autocorrelation functions obtained in the simulations.

For each case considered in the simulation we present four files: 1) The autocorrelation function of the dipolar emission processes in the transition from level $n = 2$ to level $n = 1$. 2) The autocorrelation function of the two photon absorption process in the transition from the $n = 1$ to the $n = 2$ level. 3) Stark broadened spectral profiles of the Lyman alpha dipolar emission with fine structure. 4) Stark broadened profiles that could be obtained in a two–photon polarization spectroscopy experiment for the same transition, along with fine structure.

As the simulation processes include ion dynamics effects, each one of these files has the results that correspond to five different values of the reduced mass μ of the emitter–perturber pair. More precisely, each file includes the results corresponding to $\mu = 0.5$, 0.8, 0.9, 1.0 and 2.0 (measured in units of proton mass).

The tables are ordered according to the parameter ρ that characterizes the simulations. For the same value of ρ the tables are organized in increasing values of the electron density.

Table 1. Correlation function file `r30n2133.c1p` for dipolar emission with $\rho = 0.30$ and $\log(N_e) = 21.33$

```
#
# Correlation function : Lyman alpha dipolar emission
#
#       Density       :   Ne = 2.154435e+21 m-3
#       Temperature   :   T  =        11597 K
#       Time step     :   dt = 1.946181e-13 s
#
#
#  t (s)             mu = 0.50            mu = 0.80            mu = 0.90            mu = 1.00            mu = 2.00
#-------------|--------------------|--------------------|--------------------|--------------------|--------------------|
#              |    C_R       C_I   |    C_R       C_I   |    C_R       C_I   |    C_R       C_I   |    C_R       C_I   |
#{
 0.000e+00      1.000000  0.000000   1.000000  0.000000   1.000000  0.000000   1.000000  0.000000   1.000000  0.000000
 1.946e-13      0.996433 -0.001490   0.996746 -0.001383   0.996792 -0.001365   0.996405 -0.001337   0.996937 -0.001184
 3.892e-13      0.987534 -0.003716   0.987854 -0.003609   0.987982 -0.003591   0.988408 -0.003564   0.989033 -0.003411
 5.839e-13      0.976362 -0.005932   0.977025 -0.005828   0.977273 -0.005812   0.977388 -0.005783   0.978459 -0.005634
 7.785e-13      0.963521 -0.008137   0.964044 -0.008034   0.964347 -0.008018   0.965012 -0.007996   0.966267 -0.007849
 9.731e-13      0.949281 -0.010319   0.950040 -0.010229   0.950334 -0.010216   0.950929 -0.010193   0.952710 -0.010056
 1.168e-12      0.934227 -0.012483   0.934875 -0.012400   0.935289 -0.012392   0.936131 -0.012375   0.938186 -0.012250
 1.362e-12      0.918276 -0.014614   0.919032 -0.014549   0.919573 -0.014545   0.920290 -0.014531   0.922882 -0.014428
. . .
. . .
. . .
 4.924e-11     -0.000424  0.000005   0.002230 -0.000034   0.000156 -0.000732  -0.001274  0.000681  -0.003001 -0.000208
 4.943e-11     -0.000712 -0.000033   0.002000 -0.000035   0.000101 -0.000727  -0.001585  0.000683  -0.003222 -0.000262
 4.963e-11     -0.001210 -0.000088   0.001752 -0.000019   0.000099 -0.000694  -0.001769  0.000720  -0.003302 -0.000210
#}
```

Table 2. One photon dipolar emission profile `r30n2133.d1p` with $\rho = 0.30$ and $\log(N_e) = 21.33$

```
##################################################{
#
# Dipolar with fine structure
# Electronic density = 2.154e+21 (m-3)
# Plasma temperature =     11597 (K)
# rho                =     0.300
#
##########}
##########{
#|DeltaL  (m)| mu = 0.50  | mu = 0.80  | mu = 0.90  | mu = 1.00  | mu = 2.00  |
#|-----------|------------|------------|------------|------------|------------|
  -3.4908e-12  2.2128e+10   2.3266e+10   2.3207e+10   2.2948e+10   2.1884e+10
  -3.4635e-12  2.2548e+10   2.3693e+10   2.3652e+10   2.3364e+10   2.2291e+10
  -3.4363e-12  2.2980e+10   2.4129e+10   2.4107e+10   2.3788e+10   2.2711e+10
  -3.4090e-12  2.3423e+10   2.4574e+10   2.4572e+10   2.4222e+10   2.3142e+10
  -3.3818e-12  2.3878e+10   2.5029e+10   2.5048e+10   2.4666e+10   2.3587e+10
. . .
. . .
. . .
   3.4295e-12  2.1248e+10   2.2617e+10   2.2692e+10   2.2338e+10   2.1815e+10
   3.4567e-12  2.0872e+10   2.2248e+10   2.2316e+10   2.1952e+10   2.1409e+10
##################################################}
```

The autocorrelation function files have, then, eleven columns, the first one corresponding to the time step (in seconds), followed by five pairs of columns corresponding to the five values of μ. Each pair is formed by the $C_R(t)$ and $C_I(t)$ parts of the autocorrelation function. The name of the files are `rXXnYYYY.c1p` or `rXXnYYYY.c2p`, where `XX` and `YYYY` correspond, respectively, to $100 \times \rho$ and to $100 \times \log(N_e)$, ρ and N_e being the values of the parameter ρ and of the electron density for which the calculation was made. The `c1p` and `c2p` mean, respectively, correlation function for one photon emission and correlation function for two–photon absorption. An example of a correlation function file is given in Table 1.

The profile files have six columns, where the first one is the displacement in wavelength measured in meters from the wavelength that corresponds to the transition from the center of the fine structure sublevels of the level $n = 2$ to the level $n = 1$. The other five columns show the areanormalized profiles obtained for the five values of μ.

Table 3. Temperature of the plasma – in K – of the simulation conditions considered

$\log N_e$	ρ								
m^{-3}	0.10	0.15	0.20	0.25	0.30	0.40	0.50	0.60	0.70
19.67	29041	12907	7260	4647	–	–	–	–	–
20.00	37508	16670	9377	6001	4168	–	–	–	–
20.33	48444	21531	12111	7751	5383	–	–	–	–
20.67	62568	27808	15642	10011	6952	3910	–	–	–
21.00	80809	35915	20202	12929	8979	5051	3232	2245	–
21.33	104369	46386	26092	16699	11597	6523	4175	2899	–
21.67	–	59910	33699	21568	14978	8425	5392	3744	–
22.00	–	77377	43525	27856	19344	10881	6964	4836	3553
22.33	–	–	56214	35977	24984	14054	8994	6246	4589
22.67	–	–	–	46466	32268	18151	11617	8067	5927
23.00	–	–	–	60013	41676	23443	15003	10419	7655

The tabulated profiles give only the central part of the transition (to more or less $\frac{1}{10}$ of the peak intensity), because the plasma model employed in the simulation does not allow calculations far away from the center of the line. The name of the profiles files are `rXXnYYYY.d1p` or `rXXnYYYY.p2p`, where `XX` and `YYYY` have the same meaning as before, and the `d1p` and `p2p` mean, respectively, one photon dipolar emission profile and two–photon polarization profile. An example of a profile file is given in Table 2.

Table 3 summarizes the cases considered in the simulations and indicates the equilibrium temperature of the plasma for each value of ρ and N_e.

The values of $C_R(t)$ and $C_I(t)$ given in the tables are those obtained directly from the computer simulations. However, the profiles given in the tables have been calculated from a smoothed autocorrelation function. These smooth functions have been obtained fitting their last channels to functions like

$$A e^{-\gamma t} \cos(\omega t + \varphi) \; . \tag{10}$$

In addition, this fit avoids the appearance of a $\mathrm{sinc}(\Delta\omega)$ convolved in the Fourier transform.

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