

Polarization Profile Calculations for Plasma Diagnostics

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1 Introduction

Computer simulation techniques have been used to calculate Stark broadened profiles that can be measured by polarization spectroscopy for the two-photon transition $n = 2 \rightarrow n = 1$ (Lyman- α) of hydrogen. The plasma model and the calculation techniques used in the simulation are described in Ref.[1]. The fine structure of the level $n = 2$ has been taken into account in order to study plasmas at very low electron densities (lower than 10^{21} m^{-3}). The calculations include plasmas of pure hydrogen, pure deuterium, as well as each of these with heavier perturbers. Also considered has been the -academic- case of static perturber ions. This allows us to evaluate the effects of ion dynamics, which, for this spectral line, are of fundamental importance. The plasma conditions considered cover the range for electron densities between 4.6×10^{19} and $1.0 \times 10^{23} \text{ m}^{-3}$ and for temperatures between 2,000 and 100,000 K.

The computer simulation allows us to directly obtain the emission and absorption profiles for the two-photon transition between the levels $n = 2$ and $n = 1$ of hydrogen. The polarization profiles can be obtained from these profiles using the Kramers-Kronig relations (see p.459 of refs.[2] and [3]). The calculational technique used allows us to obtain the emission and polarization spectra simultaneously for the diagnosis of different plasma configurations. All in all, spectra have been obtained for more than 400 conditions of density, temperature and perturber mass.

2 Polarization Spectroscopy

Polarization spectroscopy is based on the measurement of the change of the polarization state of a probe wave when it passes through a studied medium [2]. Such a change is induced by a polarized pumping wave. This pumping wave changes the optical behavior of the substance. That is, it changes its refractive index and its absorption coefficient in a non-isotropic way. Up to a point, polarization spectroscopy is similar to saturation spectroscopy, which is based on the measurement of the absorption of a probe wave that passes through a substance whose optical response is changed by a pumping beam.

In the experiment studied in this work, the probe beam detects the induced susceptibility by a two-photon transition [3, 4, 5, 6] between the hydrogen atom levels of the Lyman- α transition. The pumping beam produces a transition from the state $1s$ to the virtual state $l = 1, m = 1$ (p state) because it is a σ^+ polarized beam, which gives a different saturation of the three possible states of that virtual level: only the $m = 1$ state is saturated. This is equivalent to an anisotropy in the medium, because there is no uniform population between the different m sublevels. In the same process, the probe beam is absorbed, producing a transition between the virtual level and the $n = 2$ level. The selection rule $|\Delta l| = 1$ forces the arriving level to be the $2s$ one, because there is no level with $l = 2$ in that energy interval.

3 Calculation process of the polarization profiles

The profile $A(\omega)$ of a spectral line can be readily obtained from the autocorrelation function of the atomic dipole moment by means of a Fourier transform of its average $\{ \}$ over a certain statistical ensemble [7]

$$A(\omega) = \frac{1}{\pi} \operatorname{Re} \int_0^{\infty} e^{i\omega t} \{C(t)\}, \quad C(t) = \operatorname{tr} (\mathbf{D} \cdot U^*(t) \mathbf{D} U(t)) . \quad (1)$$

The time development operator $U(t)$ obeys the following form of the Schrödinger equation under the *no-quenching* approximation:

$$ih \frac{d}{dt} U(t) = (H_0 + V(t)) U(t) , \quad (2)$$

$$V(t) = q\mathbf{E}(t) \cdot \mathbf{R} , \quad (3)$$

where H_0 includes the fine structure of the level $n = 2$. $q\mathbf{R}$ is the dipole momentum operator of the emitter, and $\mathbf{E}(t)$ is the electric microfield generated by ions and electrons surrounding it.

In this work, we are interested in the polarization profiles obtained by a two-photon absorption process. Such a spectrum is given by the addition of the squares of the absorption and the dispersion profiles [2]:

$$P(\omega) = A(\omega)^2 + D(\omega)^2 \quad (4)$$

The Kramers-Kronig relations allow us to obtain the dispersion profile from the absorption one:

$$D(\omega) = \frac{1}{\pi} \text{V.P.} \int_{-\infty}^{+\infty} \frac{A(z)}{z - \omega} dz . \quad (5)$$

Operating on it, it can be shown that

$$A(\omega) = \frac{1}{\pi} \int_0^{\infty} [\cos(\omega t) C_R(t) - \sin(\omega t) C_I(t)] \quad (6)$$

$$D(\omega) = \frac{1}{\pi} \int_0^{\infty} [\cos(\omega t) C_I(t) + \sin(\omega t) C_R(t)] \quad (7)$$

where $C_R(t) = \operatorname{Re} C(t)$ and $C_I(t) = \operatorname{Im} C(t)$.

In a computer simulation process, a microfield time sequence is obtained for some selected plasma conditions, and the numerical integration of equations (2) is a previous step to the calculation of $\{C(t)\}$.

The simulated plasma is made up of a set of N_p independent ions and N_p independent electrons placed at random inside a spherical volume in such a way that the homogeneity of the

spatial distribution of particles is guaranteed. Both electrons and ions move along straight line trajectories with a Maxwellian velocity distribution, as established in the μ -ion model [8]. The emitting atom is located at the center of the simulation sphere. Details of the particle substitution technique can be found in Ref. [1]. The electric field of the set of simulated ions and electrons is determined at the center of the sphere and readily carried to the system of differential equations on which the calculation of the evolution operator of the emitter finally depends. Debye screening has been included in the calculation of the electric field to account for the correlation effects between charged particles of different sign.

The results obtained for low densities yield a dependence of the width and shape of the spectrum with density and temperature that fits very well with an impact model of the broadening, both electronic and ionic (see Fig. 1).

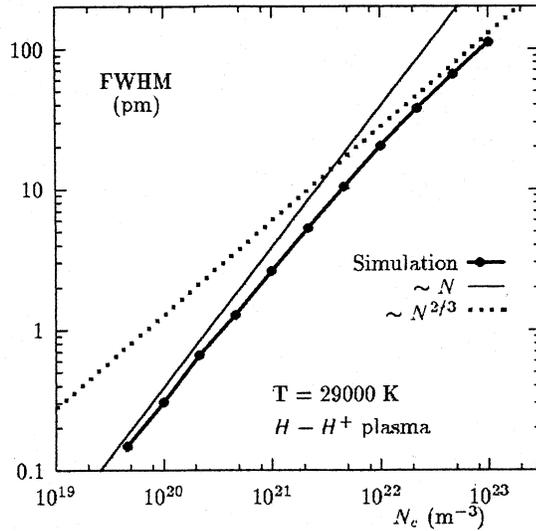


Figure 1: Dependence of the full width at half maximum (FWHM) with the electron density. For low densities, the trend is linear with N_e , which is characteristic of impact broadening.

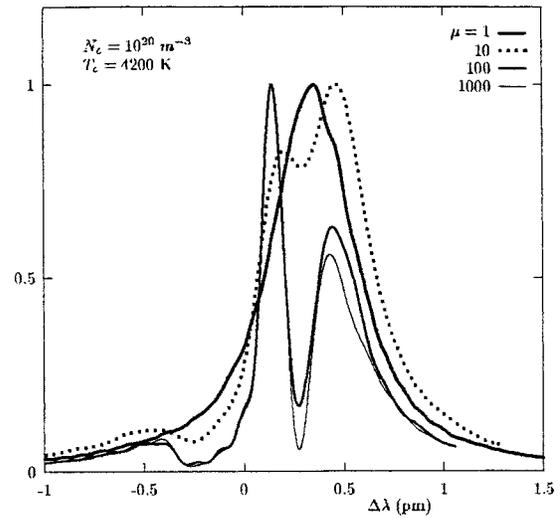


Figure 2: Polarization spectra by two-photon absorption. The effect of the reduced mass μ of the emitter-perturber pair is shown.

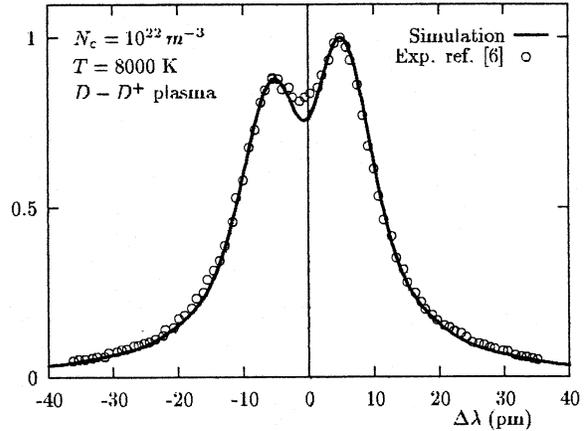
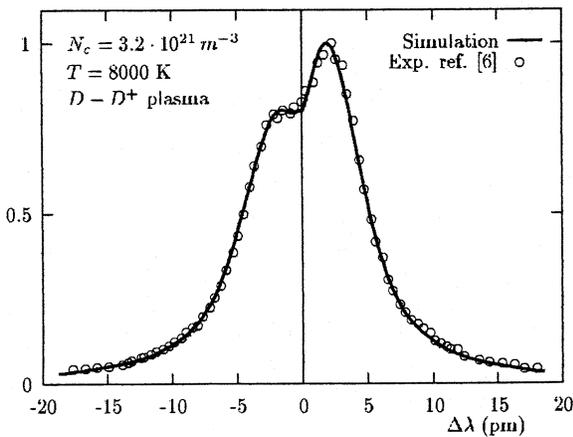


Figure 3: Two-photon polarization spectrum of the $1s \rightarrow 2s$ Lyman- α transition. Comparison of experiment and simulation.

The obtained results have allowed us to make tables of complete line profiles for plasma diagnosis. In Fig. 4 the dependence of the full width at half maximum (FWHM) of the studied transition is shown as a function of the electron density and the temperature of the plasma. The smooth dependence of $\Delta\lambda_{1/2}$ with temperature for the emission profiles allows us to obtain the density of perturbers from direct measurements of the line width.

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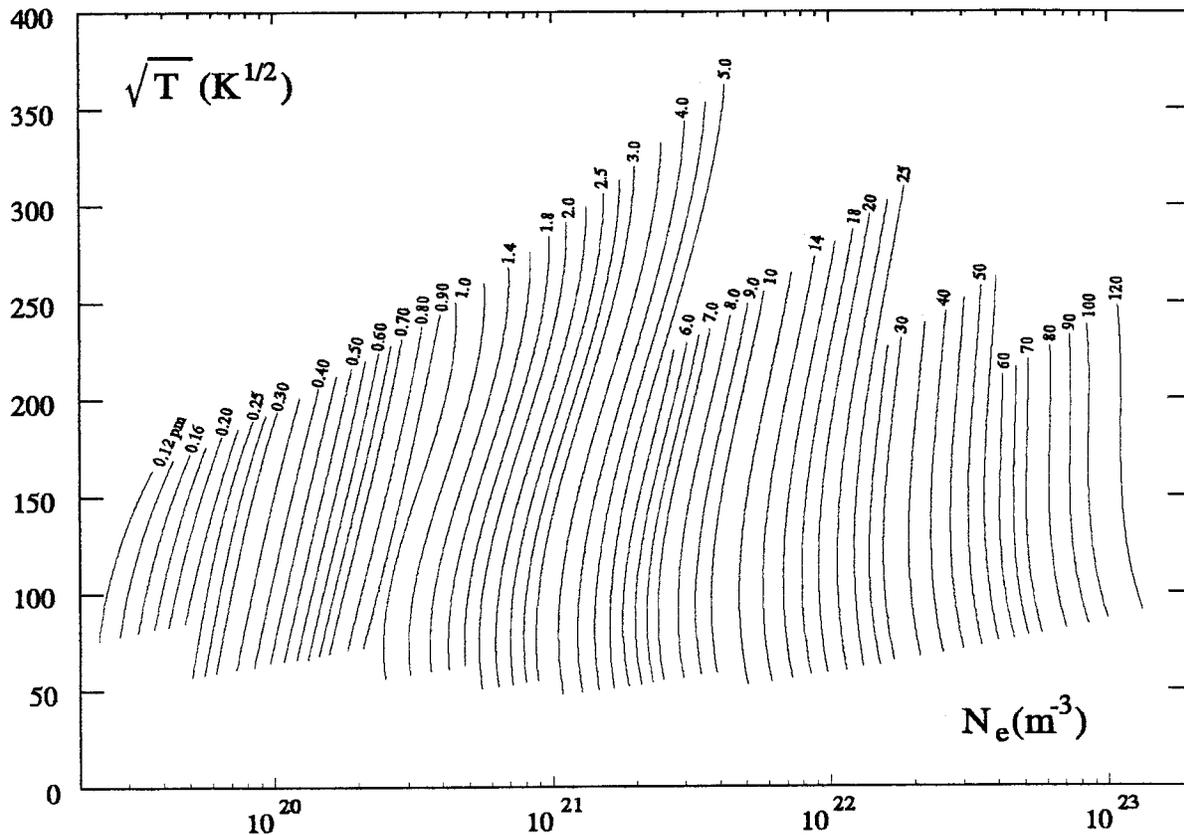


Figure 4: Curves of constant Stark width in a H-H+ plasma ($\mu = 0.5$). The numbers close to the lines show the full width at half maximum (in pm) for the transition $n = 1 \rightarrow n = 2$ that can be measured with polarization spectroscopy by two photon absorption.

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