Approximation of the shape of hydrogen H_β spectral line with Voigt profiles

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Abstract

Stark broadening of hydrogen H_β line and good theoretical connection between its Stark halfwidth and plasma electron density favor it as one of the most reliable tools in plasma diagnostics. Problems occur when the Stark halfwidth has to be extracted from the measured halfwidth. Since the Stark profile cannot be described with an analytical function, the halfwidth extraction requires a very complicated deconvolution procedure. Results of attempt to apply two Voigt profiles to describe the shape of plasma broadened H_β line are presented. Instead of Voigt function, pseudo Voigt is used in this work. Obtained results are applied to experimental profiles and presented in the paper.

Introduction

The spectroscopic methods for determination of plasma electron densities are widely applied for both laboratory and astrophysical plasmas. Some of them are based on the Stark broadening of neutral and ion spectral lines where the halfwidths (width at half of line intensity FWH) and shifts are connected to the plasma electron density number. The observed line profiles emitted from plasmas are always resulted by the mutual action of different broadening mechanisms. Usually Stark broadening is dominant, but other mechanisms, like van der Waals, resonance, Doppler and instrumental broadening, can also have considerable contributions. The result is a profile that is the convolution of profiles caused by different broadening mechanisms. When Stark, Doppler and instrumental broadening are dominant over others, the resulting profile is the convolution of Stark (Lorentz) profile and Gaussian profile (Doppler and instrumental). The main difficulty is to extract the pure Stark profile, or, at least, Stark width, in order to obtain the plasma electron density. The situation is particularly complicated in the case of hydrogen Balmer spectral lines, especially for the H_β line. Theoretical profiles (Kepple et al. 1968, Vidal et al. 1973, Touma et al. 2000) of this line cannot be given in analytical form but in form of approximation (Gigosos et al. 2003) which, consequently, makes analytical deconvolution impossible. Therefore,

number of papers considered the possibility to apply the Voigt function in the deconvolution procedure (Ortiz-Mora et al. 2020, Olivero et al. 1977, Temme 2010). It was shown in (Konjević et al. 2012) that the use of one Voigt function for approximation of plasma broadened profiles of H_β is not appropriate at low plasma electron densities (bellow Fine structure limit – $4 \cdot 10^{13}$ cm^{-3}) nor at higher values (above Fine structure limit). This is quite expectable since H_β at higher electron densities is strongly asymmetric with two peaks of different intensities and a dip between them.

Procedures and results

Assumption in this work is that the components of H_β are concentrated in two groups forming two "profiles" with maximums approximately corresponding to the peaks of H_β. Under this assumption two Pseudo Voigt (PV) functions (NIST 2022) are used to fit the experimental profiles. PV is a linear combination of a Gaussian curve $G(x)$ and a Lorentzian curve $L(x)$ (instead of their convolution, which gives the Voigt function):

$$V_p(x,w) = \eta \cdot L(x,w) + (1-\eta) \cdot G(x,w) \text{ with } 0 < \eta < 1 \quad (1)$$

where w is the full width at half of maximum (FWHM) of PV profile. There are several choices for the parameter η. The next expression is accurate to 1 % (Ida et al 2000, Thompson et al. 1987):

$$\eta = 1.36603 \cdot (w_L/w) - 0.47719 \cdot (w_L/w)^2 + 0.11116 \cdot (w_L/w)^3 \,. \quad (2)$$

FWHM w is given as:

$$w = (w_G^5 + 2.69269 \cdot w_G^4 w_L + 2.42843 \cdot w_G^3 w_L^2 + \\ +4.47163 \cdot w_G^2 w_L^3 + 0.07842 \cdot w_G w_L^4 + w_L^5)^{1/5} \quad (3)$$

The fitting parameters should be I_1, w_{S1}, w_{G1}, l_{01} I_2, w_{S2},w_{G2} and l_{02} where I is used for intensity, w_L=w_S for Stark (Lorentz) width, w_G for Gaussian width and l_0 for peak positions. Fitting even one Voigt profile with all three parameters free, leads to overestimation of the Gaussian part (Konjević et al. 2012, also our experience). Fixing one of the parameters provide much better results (Konjević et al. 2012, our experience). Fortunately, in number of cases, the instrumental profile is Gaussian, resulting in instrumental width w_{Ins}. The plasma gas temperature can be measured in an independent way or can be estimated with a reasonably small error. Based on this fact, the Doppler width w_D, which is also Gaussian, can be calculated. The Gaussian width is $w_G = (w_{Ins}^2 + w_D^2)^{1/2}$ and can be considered as a known parameter. Secondly, the assumption is that both PV profiles have the same width w_S. This assumption is made because there is no reason why two fitting profiles would have different widths, since they are the subject of the same

electrical microfield. Now, the fitting parameters are I_1, I_2, l_{01}, l_{02} and w_S. The fitting code was written using *Mathematica*® package. This procedure was applied to more than 30 H_β line profiles recorded from plasmas of a wall stabilized arc (lower electron densities) and a T-tube (higher electron densities). The covered electron density range was $(1.3\text{-}76)\cdot 10^{16}$ cm-^{3} which is considerably more than one magnitude. Two examples of H_β line profiles, for low and high electron density, are presented in Figs. 1 and 2.

Reproducing the asymmetry and especially the dip of H_β has been always the problem in fitting procedures but, most of all, for theoretical calculations and modeling also. It can be seen from the presented figures that the fitted curves describe the profiles and the wings well, however the agreement in the center is not so good. If one is not interested to analyze the central part particularly, the rest of the fit is very useful for other considerations. Primarily, this fit enables the determination of the pure Stark width (because one of the fitting parameters is the Stark width) and, consequently, the extraction of the Gaussian part (if Stark, Doppler and instrumental broadenings are dominant). This is important if accurate Stark width is needed. Obtained results for other experimental H_β line profiles, used in this work, gave similar results, even at the highest plasma electron densities when the blue wing is considerably influenced by H_γ radiation.

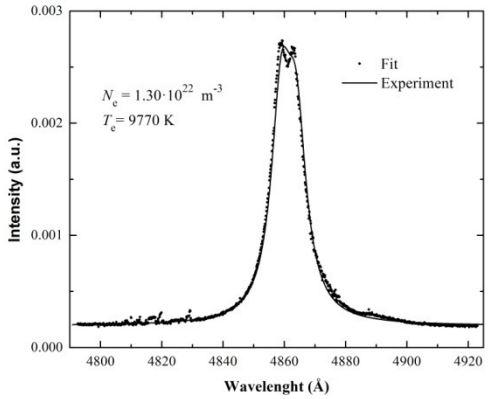

Figure 1. Experimental (wall stabilized arc) and fitted profiles at lower electron density.

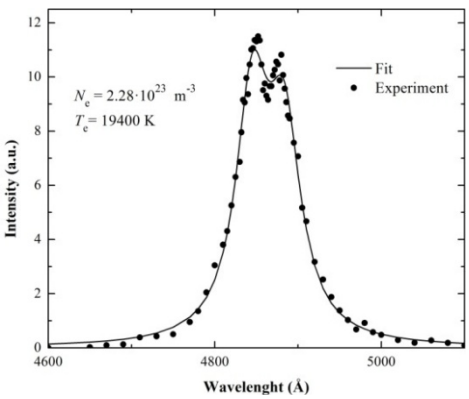

Figure 2. Experimental (T-tube) and fitted profiles at higher electron density.

Conclusions

In this work the Pseudo Voigt function was applied to fit experimental H_β spectral line in a wide range of plasma electron density values. The described method of fitting the H_β line profile enables to extract Stark halfwidth of the profile and gives the possibility for a more precise determination of the electron density.

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