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DETERMINATION OF THE TRUE TOTAL LINE INTENSITY AND THE TRUE HALFWIDTH OF THE LORENTZ COMPONENT FOR THE CLASS OF VOIGT PROFILES FROM GRAPHICAL ANALYSIS OF SPECTRUM

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The graphical determination of the true total line intensity and the true halfwidth of Lorentz component from optically thin Voigt type line profile was analysed. The corrections for total line intensity and Lorentz halfwidth, as well as the correction for continuum background intensity were calculated as the function of the arbitrary determined continuous background. The calculations were carried, for $a > 1.4$ where Voigt function could be well approximated with simple expansion. The assumption is that the halfwidth of Doppler component is known.

1. Introduction

The form of the observed spectral line profiles emitted from plasma is the result of several simultaneously acting line broadening mechanisms, beside instrumental broadening due to finite resolution of the system for spectral analysis.

Spectroscopical determination of the parameters of the plasma or emitting species throught the spectral line analysis assumes the measurements of the total line i tencities and the deconvolution of the observed line profiles in components.

Prior to the graphical profile analysis and deconvolution it is necessary to investigate possible artificial distortions of the profile. Inaccurately measured profiles could introduce significant errors in the determination of the total line intensities and line halfwidths.

Central part of the line may be self-absorbed. Many good experimental tests for optical thickness are available and furthermore it is possible to recover the true line profile in special cases, where optical depth is not too large[1].

In this work we assume that the lines are emitted from the optically thin plasma.

On the other hand, in practical analysis of the registered profiles, cutoff in the line wings is made in points where the background appears to become constant or where the overlaping with neighbouring lines takes place. In most cases this is only a few halfwidths far from the line centre. The remaining far wings intensities lost in this cutoff procedure may appreciable contribute to the total line intensity and therefore arbitary determined continuum background introduces distortion which may lead to significant errors. The corrections for graphically determined parameters where wing cutoff is applied could be obtained from the line profile theory. For the pure Lorentz profile is was already done[2].

The aim of this work is to discuss the influence of the arbitrary determined continuum background on the total line intensity and halfwidth and their corrections in general case where the absorption coefficient is given by the Voigt function. The separation of the registered Voigt profiles for $a > 1.4$ in Doppler and Lorentz components is undertaken as the function of arbitrary determined continuous background of the spectral line.

In a general case the instrumental profile is also given by the Voigt function[3]. If the independent measurement and the separation of this profile in Doppler and Lorentz components were made, it is possible to substract instrumental halfwidths from the corresponding total line Doppler and Lorentz components using the known relations.

Korb et al.[4] have discussed the error involved in the accurate determination of the equivalent width caused primarily by the indeterminancy of the zero absorptiton line. Meredith[5] have investigated numerically the error which arises from uncertainty in the determination of the 100 per cent transmitance and from the distortion of the line profile by the spectrometer and have constructed the families of correction curves which are applicable for the direct measurement method, which requires (1) that the two sets of measurements be made out to equal numbers of halfwidths from the line centre, and (2) that this distance extend to a region of small instrumental distortion.

2. *General remarks*

Let us suppose that the background intensity is determined incorrectly as shown in Fig. 1, so that measured line intensity equals zero at $|\Delta \lambda| = \Delta \lambda_B$, where $\Delta \lambda_B$ is the half base width. The aim of this paper is to find out the error introduced by this cutoff procedure and the way it can be corrected. It will be shown that the true total line intensity, I, and the true Lorentz half-halfwidth $\Delta \lambda_L$ can be expressed in terms of the measured quantities: the half base width $\Delta\lambda_B$, the apparent half-halfwidth $\Delta\lambda_V^*$ and known Doppler width $\Delta\lambda_D$ (we suppose that the temperature of the emitting species can be determined independently)*. The measured total line intensity I^* (shaded area in Fig. 1.) is than given by:

$$I^* = 2\int_0^{\Delta\lambda_B} P(\Delta\lambda)\,\mathrm{d}(\Delta\lambda) - 2\Delta\lambda_B P(\Delta\lambda_B) \tag{1}$$

where $P(\Delta\lambda)$ describes the symmterical line profile in the units of the wavelengths.

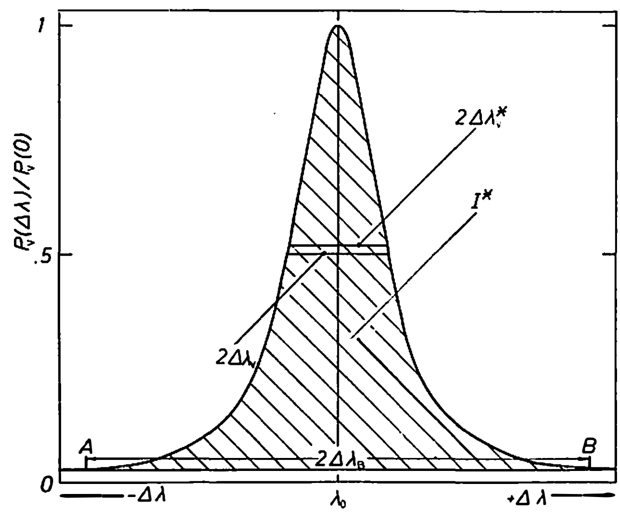

Fig. 1. Illustration of the correction for line intensity. The apparent Voigt half-width $2\Delta\lambda_V^*$ is always smaller then the true half-width $2\Delta\lambda_V$ due to incorrectly determined backgorund (base width $2\Delta\lambda_B$).

The normalised Voigt spectral line profil $P_V(\Delta\lambda)$ can be described as a convolution of pure Doppler (Gaussian) profile due to the thermal motion of the emitters and pure Lorentz dispersion profile:

$$P_D(\Delta\lambda) = \frac{1}{\sqrt{\pi}\,\Delta\lambda_D}\exp - (\Delta\lambda/\Delta\lambda_D)^2 \tag{2a}$$

$$P_L(\Delta\lambda) = \frac{1}{\pi\Delta\lambda_L}\left[1 + (\Delta\lambda/\Delta\lambda_L)^2\right]^{-1} \tag{2b}$$

with $\Delta\lambda = \lambda - \lambda_0 \cdot \Delta\lambda_D$ is Doppler width defined as $\Delta\lambda_D = (\lambda_0/c)\sqrt{2RT/\mu}$, where λ_0 is the wavelength of the line centre, c is the speed of light, R is a gas constant, T is temperatpre in K, μ is atomic weight of emitting species and $\Delta\lambda_L$ is half-half-

* Troughout the paper the notation is as follows: all the measured and uncorrected parameters are labeled with asterisk (*), and indices V, D and L are used to determine the Voigt, Doppler and Lorentz values, respectively.

width of the Lorentz profile. The resulting Voigt profile is usually expressed in terms of Voigt function $H(a, v)$[6]:

$$P_V(\Delta \lambda) = \frac{1}{\sqrt{\pi}\, \Delta \lambda_D} H(a, v) \tag{3}$$

where $H(a, v)$ is defined as:

$$H(a, v) = \frac{a}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-y^2}}{a^2 + (v - y)^2} dy \tag{4}$$

with $a = (\Delta \lambda_L / \Delta \lambda_D)$ and $v = (\Delta \lambda / \Delta \lambda_D)$.

3. *Correction formulae*

The integral in Eq. (4) can be solved by numerical methods[7] but in the case when the Lorentz broadening is dominant (e. g. the Stark broadening in the plasmas) the Voigt function can be approximated by following expansion[6]:

$$H(a, v) = \frac{a}{\sqrt{\pi}\,(a^2 + v^2)} \left[1 + \frac{3v^2 - a^2}{2\,(a^2 + v^2)^2} + \frac{15\, v^4 - 30\, a^2\, v^2 + 3a^4}{4\,(a^2 + v^2)^4} + \dots \right] \tag{5}$$

which is accurate up to 1% for values of $a > 1.4$.

Equation (5) can be transformed in the form which is more convenient for the purposes of our calculation:

$$H(a, x) = \frac{1}{\sqrt{\pi}\, a} \frac{1}{1 + x^2} \left[1 + \frac{1}{2\, a^2} \frac{3x^2 - 1}{(1 + x^2)^2} + \frac{15 x^4 - 30x^2 + 3}{4a^4\, (1 + x^2)^4} + \dots \right] \tag{6}$$

where we introduced a new dimensionless variable $x = v/a = \Delta \lambda / \Delta \lambda_L$.

By the use of only first two members of expansion (6) (this step will be justified in section 4.) we obtained for the ratio of true total line intensity I to the measured line intensity I^* the following expresion:

$$\frac{I}{I^*} = \frac{\pi}{2} \left[\tan^{-1} x_B - \frac{x_B}{1 + x_B^2} - \frac{3}{2\, a^2} \frac{x_B^2}{(1 + x_B^2)^2} \right]^{-1} \tag{7}$$

where $x_B = \Delta \lambda_B / \Delta \lambda_L$ is yet unknown quantity.

The conection of the measured half-halfwidth $\Delta \lambda_V^*$ and the half base width $\Delta \lambda_B$ is given by the following relation (see Eq. (3) and Fig. 1.):

$$H(a, x_V^*) = \frac{1}{2}[H(a, 0) + H(a, x_B)] \tag{8}$$

where $x_V^* = \Delta \lambda_V^* / \Delta \lambda_L$, and $H(a, 0)$ is exactly given by:

$$H(a, 0) = e^{a^2}(1 - \mathrm{erf}\, a) \tag{9}$$

If we introduce the new parameters:

$$y = \frac{\Delta \lambda_L}{\Delta \lambda_V^*}, \quad a = \frac{\Delta \lambda_D}{\Delta \lambda_V^*}, \quad b = \frac{\Delta \lambda_B}{\Delta \lambda_V^*}, \tag{10}$$

all quantities appearing in Eq. (8) can be expressed as:

$$x_V^* = \frac{1}{y}, \quad a = \frac{y}{a}, \quad x_B = \frac{b}{y}. \tag{11}$$

The parameters a and b are given in terms of known $\Delta \lambda_D$ and experimentally determined quantities $\Delta \lambda_V^*$ and $\Delta \lambda_B$. The unknown y is then obtained by solving the Eq. (8).

The form of $H(a, 0)$ as given by Eq. (9) is not suitable for numerical calculation and following approximations, accurate up to 1%, should be used[8]:

$$H(a, 0) = \frac{1}{\sqrt{\pi}\, a}\left(1 - \frac{1}{2a^2} + \frac{3}{4a^4}\right), \text{ for } a \leq 0.35 \tag{9a}$$

$$H(a, 0) = 0.34802\, t - 0.09588\, t^2 + 0.74786\, t^3$$

$$t = (1 + 0.47047\, a)^{-1}, \text{ for } a \geq 0.35 \tag{9b}$$

The results are presented in Fig. 2. where the ratio I/I^* versus $\Delta \lambda_B / \Delta \lambda_V^*$ is shown with $\Delta \lambda_D / \Delta \lambda_V^*$ as a parameter. It can be seen that the correction for the measured total line intensity I^* is significant for all the values of $\Delta \lambda_B / \Delta \lambda_V^*$. Even cutoff at 100 half-halfwidths leaves approximately 2% residual intensity lost in the wings. The intensity correction weakly depends on paramter $\Delta \lambda_D \Delta / \lambda_V^*$.

Figure 3. shows the solution of Eq. (8) as the ratio $\Delta\lambda_L/\Delta\lambda_V^*$ versus $\Delta\lambda_B/\Delta\lambda_V^*$ with $\Delta\lambda_D/\Delta\lambda_V^*$ as the parameter. For $\Delta\lambda_B/\Delta\lambda_V^* > 20$ this ratio is practically constant but as $\Delta\lambda_B/\Delta\lambda_V^*$ tends to smaller values (the case frequently met in practical spectrum analysis) the ratio changes and becomes up to 10% higher. The dependence on the parameter $\Delta\lambda_D/\Delta\lambda_V^*$ in this region is of substantial importance.

The problem of striping the spectral line off the continuum could be inverted. According to results shown in Fig. 4. in the region $\Delta\lambda_B/\Delta\lambda_V^* < 20$, the wings may also appreciably affect the precise continuum height measurements and therefore the determination of continuum factors or the line to continuum temperature method. E. g. the intensity $P_V(\Delta\lambda_B)$ for $\Delta\lambda_B/\Delta\lambda_V^* = 10$ is still about 1% of the ma-

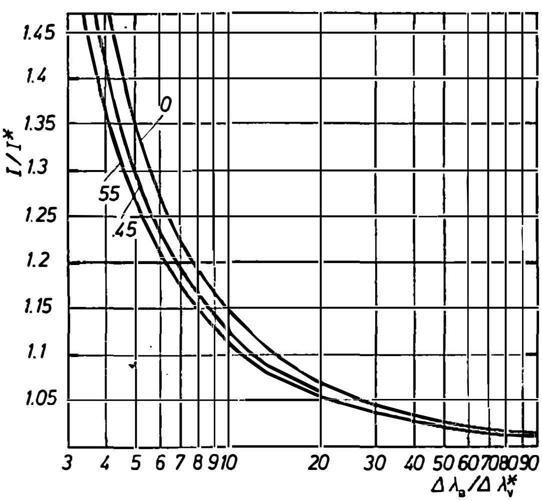

Fig. 2. Ratio of true total line intensity I to measured line intensity I^* versus the ratio of base half-vidth $\Delta\lambda_B$ to measured Voigt half-halfwidth $\Delta\lambda_V^*$ with $\Delta\lambda_D/\Delta\lambda_V^*$ as a parameter.

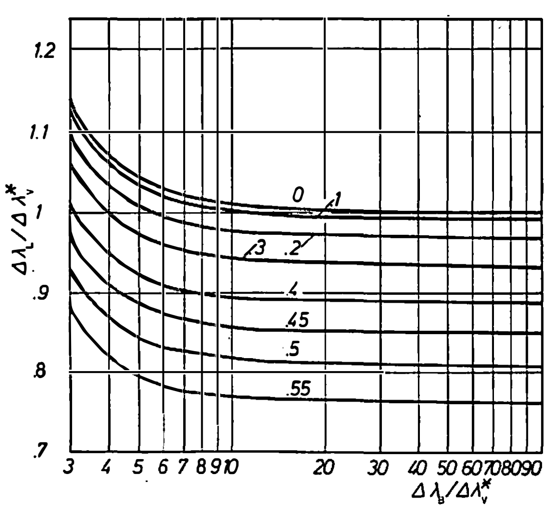

Fig. 3. Ratio of true Lorentz half-halfwidth $\Delta\lambda_L$ to measured Voigt half-halfwidth $\Delta\lambda_V^*$ versus the ratio of base halfwidth $\Delta\lambda_B$ to measured Voigt half-halfwidth $\Delta\lambda_V^*$ with $\Delta\lambda_D/\Delta\lambda_V^*$ as a parameter.

ximum intensity P_V (0) at the line centre (Fig. 4.) which may be quite significant compared to weak continuous background, which then appears much stronger than it actually is. For precise continuum intensity measurements one should therefore apply the wing formulae for correction.

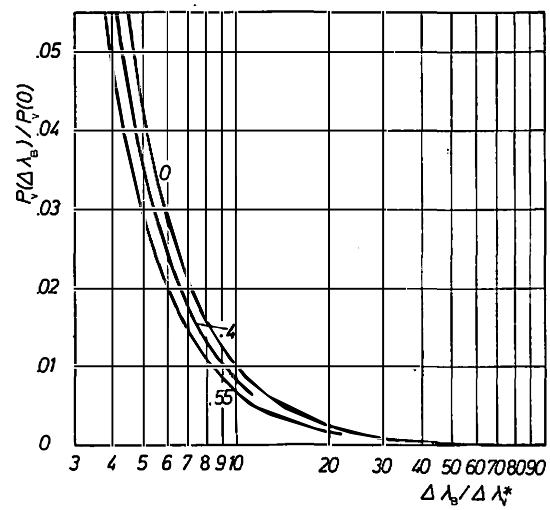

Fig. 4. Residual intensity $P_V(\Delta\lambda_B)$ normalized to the maximum intensity P_V (O) versus the ratio of base halfwidth $\Delta\lambda_B$ to measured Voigt half-halfwidth $\Delta\lambda_V^*$ with $\Delta\lambda_D/\Delta\lambda_V^*$ as ε parameter.

4. *Discussion and conclusion*

All calculated quantities, the true total line intensity, the true Lorentz half-halfwidth and the continuum intensity correction are expressed in the terms of experimentally determined quantities, the apparent Voigt half-halfwidth, the halfwidth of the base line and the Doppler width.

Evaluating the Eq. (7) of section 3., we started from Eq. (6), retaining only the first two members of the expansion. We have investigated the error introduced by neglecting the higher members of the expansion (6). The first member by itself describes the pure Lorentz profile. Figure 5. shows the change of measured intensity I^* (as follows from the first two members of Eq. (6)) relative to the value calculated for pure Lorentz profile I_L^* (full line) and the same for the case when the third member of the expansion (6) is included (dashed line). The two curves practically coincide, and for $a > 1.4$ thay canot be distinguished. It is therefore justified to remain only the first two members of the expansion (6).

From Figs. 5. and 2. one can conclude that for the total line intensity corrections only, the supposition of pure Lorentz profile may be sufficient in the case when $a > 1.4$. It is of course the consequence of the fact that the Voigt profile is practically Lorentzian in the far wings. It is easy to show that in the case of pure

Doppler profile ($a = 0$) the similar correction would be always less than 1% in the region of interest. One can conclude that the correction for the total line intensity rapidly grows up for $0 < a \leqslant 1.4$.

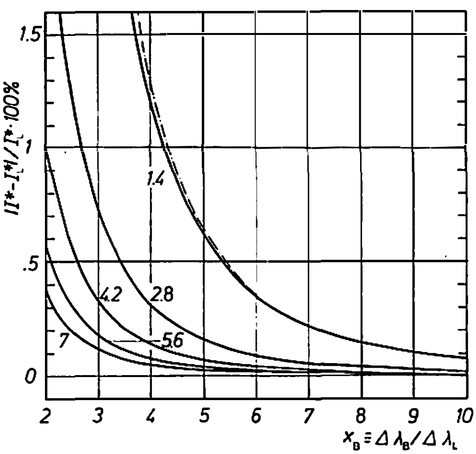

Fig. 5. Change of measured intensity I^* relative to the value obtained for pure Lorentz profile I_L^* versus the ratio x_B of base halfwidth $\Delta\lambda_B$ and the true Lorentz half-halfwidth $\Delta\lambda_L$ with $a = \Delta\lambda_L/\Delta\lambda_D$ as a parameter: a) I^* calculated from the first two members of Eq. (6) (full line); b) the third member of expansion (6) is included (dashed line).

For determination of the Lorentz component (Lorentz halfwidth) from the Voigt profile or the residual background intensity (Figs. 3. and 4.) one should start from the corrected Lorentz profile, Eq. (6). From Fig. 3. one can see that the correction factor $\Delta\lambda_L/\Delta\lambda_V^*$ changes for about 10% from the limiting value $\Delta\lambda_L/\Delta\lambda_V$ ($\Delta\lambda_B$ tends then to infinity) and in that limit coincide with the values obtained by Davies and Vaugham[9]. (It should be noticed that the results in Ref. (9) are expressed in terms of Doppler halfwidth $\Delta\lambda_D^{1/2}$ which should not be confused with Doppler width $\Delta\lambda_D$!). On the other hand the uncertainty in the positioning the correction curve for $a > 0.55$ causes the relative error of the same order of magnitude. Hence, the correction for Lorentz half-halwidth may become meaningless for $a < 1.4$.

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ODREĐIVANJE PRAVOG UKUPNOG INTENZITETA LINIJE I PRAVE POLUŠIRINE LORENTZOVE KOMPONENTE ZA KLASU VOIGTOVIH PROFILA GRAFIČKOM ANALIZOM SPEKTRA

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Prikazano je grafičko određivanje pravog ukupnog intenziteta i prave poluširine Lorentzove komponente optički tankog linijskog profila Voigtovog tipa. Izračunate su popravke za ukupni intenzitet linije i Lorentzovu poluširinu, kao i korekcija intenziteta kontinuumske pozadine, kao funkcije proizvoljno određene kontinuumske pozadine. Računi su provedeni za $a > 1.4$ gdje se Voigtova funkcija može dobro aproksimirati jednostavnim razvojem. Pretpostavljeno je da je poluširina Dopplerove komponente poznata.