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ON THE ACCURACY OF THE LORENTZ AND DOPPLER BROADENING FROM A SPECTRAL LINE PROFILE[1)]

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Some plasma parameters can be determined from the spectral line profile measured by means of the Fabry-Perot interferometer. The shape of the line emmited from low temperature plasma is usually described by Voigt's function. In the paper presented we investigate a calculation of the Lorentz and Doppler broadening and their possible errors. Carrying out the deconvolution we apply the least squares method (the Marquardt-Levenberg algorithm). An apparatus function is approximated by a rational function. An influence of noise with a normal distribution on the calculation of those parameters is also tested.

I. INTRODUCTION

From the Doppler and Lorentz broadenings it is possible to determine the temperature of neutral particles and the discharge particle density. In case of low temperature plasma (the temperature of the neutral particles 2×10^4 K, the concentration of the discharged particles $< 10^{21}$ m^{-3}, it is necessary to use an equipment with a high resolution such as the Fabry-Perot interferometer (FPI) for their determination [1, 4].

The measured line is usually narrow and therefore we cannot neglect the apparatus function of the FPI. Due to the fact that the profile is measured with a certain error the evaluation of the mentioned parameters is not regular from the mathematical point of view [1]. It means that a relatively small error can cause a high error of the result. The calculation of the parameters represents a nonlinear problem [7], whose solving may be difficult. For this reason the completed programs (procedures) are often used for the calculation (substraction of the apparatus function) and sometimes little attention is devoted to the fact that such subroutines must be tested adequately to be right and suitable

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under different conditions. Little attention is also devoted to the evaluation of the computing method and so to the measuring one. With the increasing possibility of computing techniques such considerations have an essential importance. And finally, we mostly cannot verify with sufficient accuracy the value of the measured parameters by means of another independent method.

In our contribution we consider the line with the Voigt's profile and we determine the Lorentz and Doppler broadening. The apparatus function of the FPI is approximated by the rational function. The unknown parameters are found by means of the least squares method (LSM) using the Marquardt-Levenberg algorithm [7].

II. THEORY

The relation between the initial (theoretical) spectral line profile $J_v(\lambda)$ and the registered one can be described as a convolution of J with the apparatus function $g(y)$

$$I(\lambda) = \int_{-\infty}^{\infty} J_v(\lambda - y) g(y) \, dy, \tag{1}$$

where λ is the wavelength. The line shape is described by the convolution of a Gaussian with a Lorentzian (the so-called Voigt function)

$$J_v(aL, aD, \gamma) = \frac{1}{\sqrt{\pi \ln 2}} \frac{1}{aD} V(x, y), \tag{2}$$

where

$$V(x, y) = \frac{y}{\pi} \int_{-\infty}^{\infty} \frac{e^{-z^2}}{y^2 + (x - z)^2} dz. \tag{3}$$

New variables introduced are defined as follows

$$\gamma = 2d/\lambda, \quad x = \gamma\sqrt{\ln 2}/aD, \quad y = aL\sqrt{\ln 2}/aD. \tag{4}$$

The symbol d is the distance between the mirrors of the Fabry-Perot inteferometer and the broadening parameters of the Lorentz and Doppler mechanisms denoted by aL, aD, respectively. Both profiles measured are given by tabular values at a discrete set of points of $w = \gamma_i - \mathrm{INT}(\gamma_i)$. The apparatus function of the Fabry-Perot ideal interferometer (the interferometer with absolutely plane and absolutely parallel mirrors) can be expressed by means of the Airy function as follows:

$$I(w) = \frac{(1 - R)^2}{1 + R^2 - 2R\cos 2\pi w}, \tag{5}$$

where R is the reflexivity of mirrors. In case of the Voigt function (3) the spectral line profile registered by the ideal FPI has the form [1]

$$I(aL, aD, w) = \frac{1}{I_{max}(aL, aD)} \frac{1 - R}{1 + R} \left[1 + 2 \sum_{n=1}^{\infty} R_e^n \exp\left(-\frac{n^2 Q^2}{4} \right) \cos 2\pi n w \right], \tag{6}$$

where $Q = 2\pi aD/\sqrt{\ln 2}$, $R_e = R\exp(-2\pi aL)$.

Using the relation (6) we can generate the profile. The applicability of the program can be tested choosing suitable values of R, aL, aD. The first example of such a test is shown in [3].

A straightforward calculation of the Voigt function (3) represents a relatively difficult task (it depends on the accuraxy and the speed of computation). Due to the importance of this function in plasma physics great numbers of approximations exist, which allow to make the calculation with the required accuracy in a reasonable time. As shown in [2, 8] the Voigt profile (3) can be obtained in the form of the real part of the complex probability function

$$w(z) = u(x, y) + \mathrm{i}v(x, y) = \frac{\mathrm{i}}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{z - t} dt \tag{7}$$

for the complex argument $z = x + \mathrm{i}y$. A comparison of several procedures is in [9]. In our case we use the algorithm presented in [10] (absolute error $< 10^{-7}$, relative error $< 10^{-6}$ excepting a high x and a small y). This approximation is suitable for most physical applications.

Computing the convolution (1) we can use several ways. As it is shown in [2] the rational function has advantageous properties. Approximating the apparatus function $g(y)$ by the m-term rational function

$$g(w) \approx \mathrm{Re} \sum_{k=1} \frac{\alpha_k + \mathrm{i}\beta_k}{w + x + \mathrm{i}y}, \tag{8}$$

where α_k, β_k, x_k, y_k are real coefficients (which are known or must be determined otherwise, e.g., by the LSM) we obtain directly for the registered profile

$$I(w) \approx \mathrm{Re} \sum_{k=1}^{m} (\beta_k - \mathrm{i}\alpha_k) w(z_k), \tag{9}$$

where $z_k = x_k' + \mathrm{i}y_k'$, $x_k' = (w - w_0 + x_k)\sqrt{\ln 2}/aD$, $y_k' = (aL + y)\sqrt{\ln 2}/aD$. The symbol w_0 denotes a centre of the line. Taking into account only a one-term rational function ($m = 1$) the equation (9) will be very simple

$$I(w) \approx \beta_k u(x, y) + \alpha_k v(x, y). \tag{10}$$

The theory of the LSM and its basic properties are summarized in [7, 8]. In the statistical analysis of experimental data not only the parameter values can be required and determined but also information on the statistical uncertainties of the parameter value. There is constructed an interval or a range of parameter value which will contain the "true" parameter with a given value of probability (it is usually 68.3%). In analogy with the linear case, we can estimate the error of the jth parameter as

$$\Delta_j = \sqrt{S_0/(Np)\,V_{jj}}, \tag{11}$$

where S is the sum of the residuals, N is the number of the measured values, p is the number of the computed parameters, V_{jj} is the diagonal element of the covariance matrix calculated from the inverse of the hessian [7, 8]. If the sum of residuals is a quadratic function of an unknown parameter (sufficiently near the minimum of this sum) the error Δ_j represents the standard deviation. All correlations between parameters are taken into account by this estimate if the hessian has converged during the minimization.

A certain suggestion on influence of the noise which is summed with the right signal can be obtained by means of the computer simulation. In our computer experiment we use "experimental" data generated as follows

$$I_i'(w_i) = \left(I(w_i) + \sigma\left(\sum_{i=1}^{12} C_i - 6\right)\right)/I_i(W_i), \tag{12}$$

where $I(w_i)$ is the value computed by (6), σ is the standard deviation, C_i are numbers with a uniform distribution. The relation (12) means that our data are weighted with the same relative error (the absolute errot has the Gauss distribution with the standard deviation σ).

III. RESULTS AND DISCUSSION

The aim and method of our study are described above. Here, we specify strictly the calculation. In all computations we have used relative units (see (4)).

A typical relation between the form of the apparatus function and the generated profiles (using (6)) is shown in Fig. 1. The comparison between the "experimental" and the fitted data in case of the apparatus function is in Fig. 2, 3, where both absolute differences (ΔI) and relative ones (ϱ_I) are plotted from the generated data (using Eq. 5). The relative error is related to the point where it is computed. Wee see from the figures that it is sufficient to make only a one-term approximation of the apparatus function. We obtain 4 coefficients in this case. We also tried a different number of fitted points, which had no further importance.

Comparisons (absolute and relative differences) between the generated and fittead data are in Figs. 4, 5 for $R = 0.85$ and different values of aL and aD. Similar dependences are presented for $R = 0.95$ in Figs. 6, 7, 8, 9. For the ratio

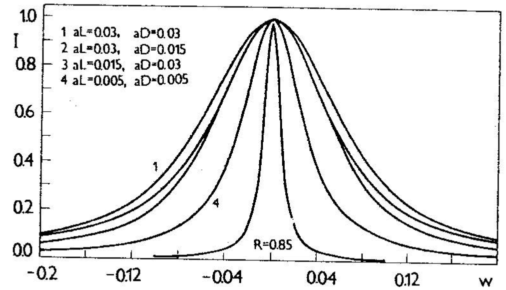

Fig. 1. A typical relation between the apparatus function and the generated profiles for $R = 0.85$ and various values of aL and aD.

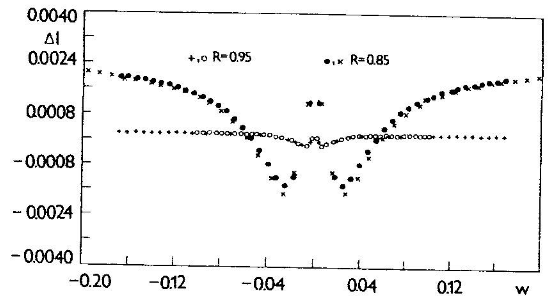

Fig. 2. Absolute differences between the generated apparatus function and its approximation by a one-term rational function (for a different value of R and a different number of used points).

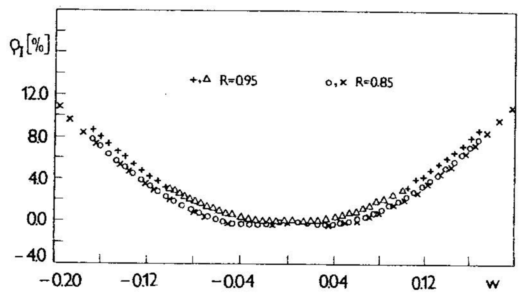

Fig. 3. Relative differences between the generated apparatus function and its approximation by a one-term rational function (for the same values as in Fig. 2).

of $aL/aD = 1$ these dependences are plotted specially in Fig. 8, 9. Besides the Lorentz and Doppler broadening we must evaluate the centre of the line and the so-called scalling factor, too.

We can see from the figures that the central part of the line is fitted very well. Towards the wings the relative error increases. A cause of this fact must be

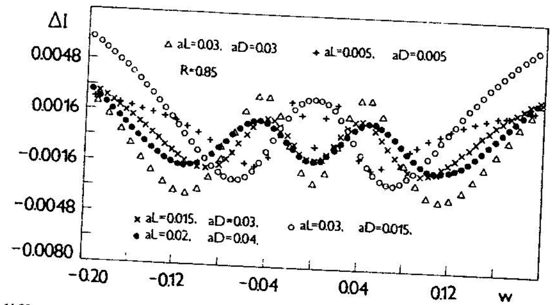

Fig. 4. Absolute differences between generated and fitted data for $R = 0.85$ and various values of aL and aD.

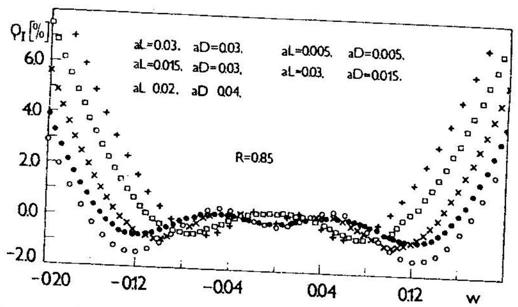

Fig. 5. Relative differences between generated and fitted data for the same values as in Fig. 4.

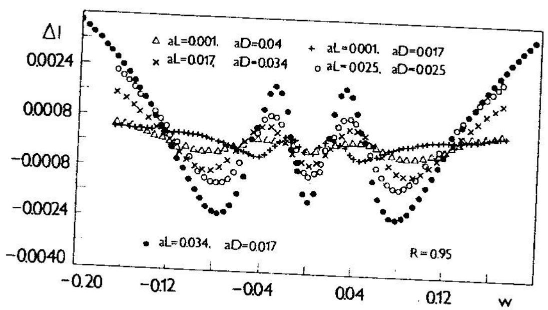

Fig. 6. Absolute differences between generated and fitted data for $R = 0.95$ and various values of aL and aD.

investigated. It means, for example, to use more terms in (8) or to try other ways of computation of the convolution integral (1). It would be also interesting to compare our procedure with the others which do not use the rational function and to find thus its position between them. In Tab. 1 ($R = 0.85$) and Tab. 2

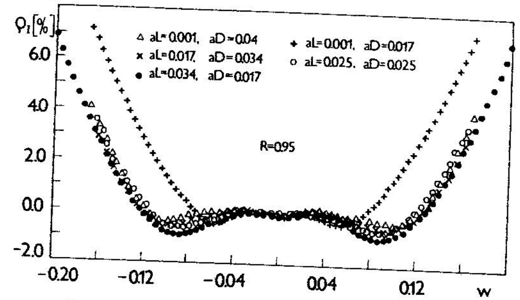

Fig. 7. Relative differences between generated and fitted data for the same values as in Fig. 6.

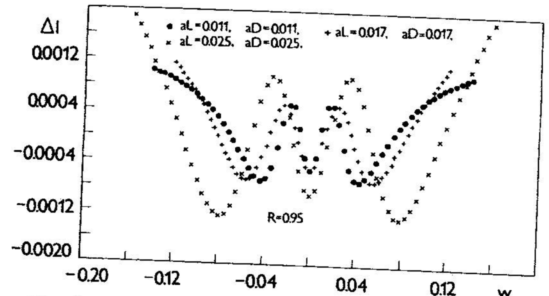

Fig. 8. Dependences as in Fig. 7 but for $aL/aD = 1$.

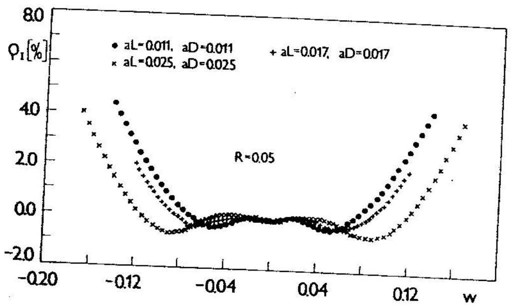

Fig. 9.

($R = 0.95$) there are presented results of our computations for several chosen values of aL and aD. The symbols $\hat{aL}$ and $\hat{aD}$ denote evaluated values, ΔaL, ΔaD their absolute error, respectively, using Eq. (11).

We also study the influence of noise (12) on the course of the calculation. The results are presented in Tabs. 3—6. The used method, as it follows from our simulation, is resistant to the noise and its influence may be characterized by (11). It means that the parameters are determined with less accuracy when the standard deviation increases.

Table 1 ($R = 0.85$)

aL	aD	aL	aD	ΔaL	ΔaD	S_0
0.011	0.050	0.0145	0.0475	0.0002	0.0002	1.89e-4
0.030	0.030	0.0350	0.0244	0.0004	0.0006	4.69e-4
0.040	0.040	0.0478	0.0324	0.0004	0.0006	5.81e-4
0.015	0.030	0.0173	0.0278	0.0001	0.0002	1.67e-4
0.030	0.015	0.0321	0.0127	0.0003	0.0008	6.97e-4
0.020	0.040	0.0234	0.0373	0.0001	0.0002	1.37e-4

Table 2 ($R = 0.95$)

aL	aD	aL	aD	ΔaL	ΔaD	S_0
0.017	0.017	0.0175	0.0165	0.00003	0.00004	2.10e-5
0.017	0.034	0.0181	0.0333	0.00006	0.00006	2.37e-5
0.011	0.011	0.0113	0.0107	0.00003	0.00004	2.12e-5
0.034	0.040	0.0375	0.0377	0.00011	0.00012	1.61e-4
0.025	0.025	0.0264	0.0238	0.00007	0.00009	7.50e-5
0.040	0.020	0.0433	0.0156	0.00020	0.00045	8.32e-4
0.034	0.017	0.0360	0.0144	0.00012	0.00026	2.86e-4
0.001	0.017	0.0011	0.0169	0.00001	0.00001	7.00e-6
0.001	0.039	0.0013	0.0338	0.00002	0.00001	6.80e-6
0.001	0.040	0.0014	0.0398	0.00001	0.00001	5.87e-6
0.017	0.001	0.0171	0.0015	0.00006	0.00059	1.51e-4
0.034	0.001	0.0344	0.0038	0.00016	0.00011	8.14e-4
0.040	0.001	0.0408	0.0012	0.00028	0.00554	7.97e-4

Table 3

σ	$R = 0.95$, $aL = 0.011$, $aD = 0.011$, $N = 59$				
	aL	aD	ΔaL	ΔaD	S_0
0.000	0.0113	0.0108	0.00003	0.00004	2.12e-5
0.001	0.0112	0.0108	0.00003	0.00005	3.18e-5
0.005	0.0111	0.0110	0.00002	0.00012	2.03e-4
0.010	0.0110	0.0113	0.00016	0.00022	7.09e-4
0.025	0.0106	0.0121	0.00039	0.00053	4.21e-3
0.050	0.0100	0.0131	0.00080	0.00103	1.64e-2
0.075	0.0096	0.0139	0.00124	0.00152	3.85e-2

Table 4

σ	$R = 0.95$, $aL = 0.025$, $aD = 0.025$, $N = 69$				
	aL	aD	ΔaL	ΔaD	S_0
0.000	0.0264	0.0238	0.00007	0.00009	7.50e-5
0.001	0.0264	0.0237	0.00008	0.00010	8.50e-5
0.005	0.0265	0.0235	0.00018	0.00024	4.87e-4
0.010	0.0267	0.0232	0.00035	0.00046	1.80e-3
0.025	0.0273	0.0222	0.00086	0.00117	1.11e-2
0.050	0.0282	0.0203	0.00168	0.00245	4.45e-2
0.075	0.0292	0.0182	0.00245	0.00390	1.00e-1

Table 5

σ	$R = 0.95$, $aL = 0.034$, $aD = 0.017$, $N = 79$				
	aL	aD	ΔaL	ΔaD	S_0
0.000	0.0360	0.0144	0.00012	0.00026	2.86e-4
0.001	0.0360	0.0143	0.00003	0.00027	2.93e-4
0.005	0.0361	0.0143	0.00019	0.00040	6.40e-4
0.010	0.0362	0.0143	0.00031	0.00067	1.80e-3
0.025	0.0360	0.0143	0.00075	0.00160	1.01e-2
0.050	0.0368	0.0141	0.00150	0.00330	3.99e-2
0.075	0.0372	0.0140	0.00230	0.00500	8.98e-2

Table 6

σ	$R = 0.95$, $aL = 0.034$, $aD = 0.40$, $N = 99$				
	aL	aD	ΔaL	ΔaD	S_0
0.000	0.0372	0.0377	0.00011	0.00012	1.61e-4
0.001	0.0372	0.0377	0.00011	0.00026	1.83e-4
0.005	0.0371	0.0377	0.00023	0.00026	7.34e-4
0.010	0.0371	0.0378	0.00042	0.00048	8.46e-3
0.050	0.0371	0.0378	0.00200	0.00230	5.80e-2
0.075	0.0372	0.0376	0.00300	0.00350	1.30e-1

IV. CONCLUSION

As it follows from the presented results the suggested method for the calculation of aL, aD is a suitable for application in hysics of low temperature plasma and is resistant to random noise. nevertheless, we find that even in case when very precise input data (without noise) are generated there appears a difference between the chosen parameters and the computed ones (several per cent). It is not clear if it is a characteristic of this method or if it depends on the suitability of the used numerical procedures. The solution of such questions has not been yet accomplished.

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О ТОЧНОСТИ ЛОРЕНЦЕВСКОГО И ДОППЛЕРОВСКОГО УШИРЕНИЯ ИЗ СПЕКТРАЛЬНОГО КОНТУРА

Некоторые параметры плазмы могут быть определены из спектральной линии, измеренной с помощью интерферометра Фабри-Церо. Формы линии излучения низкотемпературной плазмы принято описывать функцией Войта. В данной работе мы исследуем вычисление лоренцевского и доплеровского уширения и их возможные ошибки. Производя развертку, мы используем метод наименьших квадратов (алгоритм Маркварта-Левенберга). Аппаратная функция аппроксимирована рациональной функцией. Рассмотрено также влияние шума с нормальным распределением на вычисление вышеуказанных параметров.