Atomic spectral line free parameter deconvolution procedure

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We report an advanced numerical procedure for deconvolution of theoretical asymmetric convolution integral of a Gaussian and a plasma broadened spectral line profile $j_{A,R}(\lambda)$ for spectal lines. Our method determines all broadening parameters, self-consistently and directly from the line profile with minimal assumptions or prior knowledge. This method is useful for obtaining complete information on all plasma parameters directly from the recorded shape of a single line, which is very important in case no other diagnostic methods are available. The method is also convenient for determination of plasma parameters in the case of a symmetrical profile such as Voigt one.

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I. INTRODUCTION

The investigation of broadening of the spectral lines through different plasma parameters, which represent physical conditions and state of plasmas, helps us to understand the underlying physical mechanisms. Theoretical knowledge of physical mechanisms of broadening, based on plasma parameters, can be used for determining physical conditions and state of plasmas by analyzing the shapes of atomic spectral lines. That approach can be useful for determining parameters for laboratory plasmas as an independent method, but this is especially true in the case of astrophysical plasmas. In fact, the only diagnostic of astrophysical plasmas is the investigation of their radiation (spectral lines and continuum). The investigation of the spectral line shapes and parameters is very important because most of the information about celestial objects is acquired in that way.

In principle three different agents may contribute to the final width and shape of a spectral line: natural broadening, Doppler broadening, and interactions with neighboring particles [1–3]. The natural broadening is usually very small compared to the other contributions and has the well-known Lorentzian or dispersion distribution. Doppler broadening originates from the statistical velocity distribution of the emitting atoms, being directly dependent upon the plasma temperature. In the case of Maxwell distribution of velocities the Doppler broadening has a Gaussian distribution. The third mechanism depends on the electric microfields of neighboring particles and includes Stark, van der Waals, and resonant broadenings. This mechanism becomes important with the increase of the pressure and represents the so-called pressure broadening. The profile representing this broadening, in the case where electron broadening dominates, is a symmetric Lorentz function. For neutral and ionized emitters for which ion broadening is generally not negligible, a more convenient profile is the asymmetric $j_{A,R}(\lambda)$ profile, Ref. [2]. Resonant and van der Waals broadening may be important for neutral atom broadening and they should generally be at least estimated. This requires some independent measurements or estimation of neutral atom densities, in addition to the usual measurements of electron density and electron temperature.

One additional broadening factor in plasmas is radiative transfer, which is especially important for strong lines and high pressures. This effect broadens the lines and may therefore lead to an anomalously large width. In addition, line narrowing is possible in cases of population inversion. Finally instrumental broadening is another broadening mechanism.

Most measurements have been concerned with isolated lines of neutral atoms and of ions in low and intermediate charge states for a large number of elements. Besides this, there is also a great need for reasonably accurate measurements under well-defined plasma conditions. For most of these measured lines, the electron impact broadening should indeed be the dominant mechanism, except for only partially ionized gases. The state of art in impact line broadening theory today is well represented by the convergence of fully quantum mechanical and semiclassical calculations. This situation is well described in a number of papers dealing with impact broadening, Refs. [4–8].

All the above-mentioned processes have an influence on the shape of the spectral lines. In most cases, it is resonable to presume Doppler and Stark broadening (or any other kind of pressure broadening), as being statistically independent processes. In this case the electron collision is irrelevant regarding the Doppler broadening, but it is very important for pressure broadening. The corresponding profile contributions can be separately convolved to obtain the total shape of the line. In order to analyze the experimental data the first step is the fit to a Lorentzian profile. The fit to Voigt profile is more appropriate, because it includes Doppler broadening as well as the Lorentzian profile. This profile can be used if the shape of the measured line is symmetric, which is usually the case of ionized emitters, where it is normally possibly to neglect the interactions between the emitter and perturbing ions. In the case of neutral and ionized emitters for which broadening by ions is not negligible, the line profile is often asymmetric. In principle there is no fundamental difference between the singly and multiply ionized emitters. However, the quasistatic approximation for perturbing ions is better satisfied for singly than multiply ionized emitters within a given isoelectronic sequence because the relevant energy spacings are smaller and the widths are larger [9]. The most convenient fit in these cases is the fit to the so-called ''*K*'' function, i.e., the convolution integral (Ref. [2]) of a Gauss-

ian and a plasma broadened spectral line profile $j_{A,R}(\lambda)$. Besides the $j_{A,R}(\lambda)$ and Doppler widths, the static ion broadening parameter A, and Debye shielding and ion-ion correlation parameter R, play an important role in the K profile.

It should be mentioned that ions are not necessarily quasistatic. Some old dynamical treatments of ions may be found in Refs. [2] and [10]. If ions are quasistatic, we generally get an asymmetric profile. As shown in Refs. [11], [5], and [12] in the general case (i.e., ion dynamics) there is always an impact ionic contribution, which simply adds to (and may not be distinguished from) the electron impact contribution. The relative importance of this impact ionic contribution diminishes with increasing density. We must emphasize that care must be taken in interpreting the line broadening parameters if ion impact is important, as we cannot experimentally distinguish between the electronic and ionic contributions.

In this paper the asymmetry of the lines refers to the asymmetry brought about by quasistatic broadening, consequently the approach ignores a number of important factors, which may also contribute to the asymmetry of the lines, such as the gradients, quadrupoles, shifts, or some other effects.

The absence of appropriate deconvoluting procedure for the most general theoretical K function, which completely describes the broadening of the atomic spectral lines, made us initiate this paper. When the experimentalist gets a line without an *a priori* knowledge of the plasma parameters, one would like to be able to extract them directly from the experimental spectrum. To this end we have devised a new deconvolution method.

II. THEORETICAL BACKGROUND

Traditional classification, according to the mathematical approximations introduced into a more general theory of line broadening, recognizes the quasistatic approximation first developed by Holtsmark, impact approximation first treated by Lorentz, and a number of intermediate approximations and computer simulations [3]. The corresponding line-shape functions have no simple analytic forms, with the exception of the impact approximation for isolated lines, i.e., lines that are not overlapping with other transitions in the same spectrum. In this impact approximation the profile of the line is Lorentzian and is given by

$$L(\lambda)=L_o+L_{\max}\frac{W_L^2}{4(\lambda-\lambda_o)^2+W_L^2}, \tag{2.1}$$

where L_o is the baseline (offset), $L_{\max}$ is maximum intensity (intensity for $\lambda=\lambda_o$), W_L full width at half-maximum (FWHM), i.e., the so-called half-width and λ_o the wavelength of the line center. Besides the Lorentz (impact), the Gaussian (Doppler) function is also important in plasma spectroscopy. In many cases, assuming the velocity distribution to be Maxwellian, i.e., the relevant isotropic velocity distribution to be Gaussian, the corresponding line-shape function has the Gaussian form

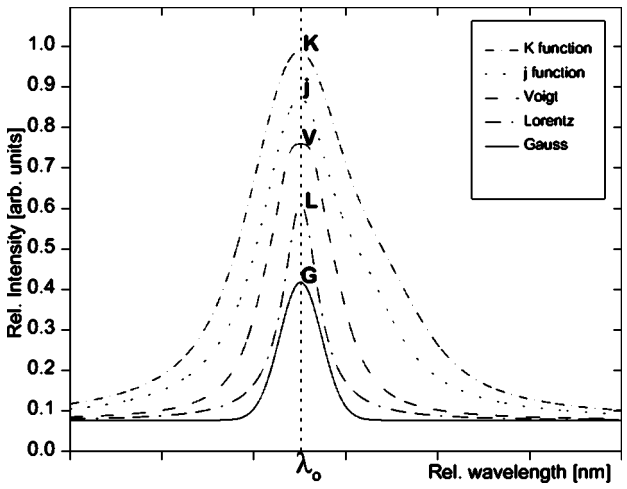

FIG. 1. Gauss (Doppler), Lorentz and $j_{A,R}$ (impact) profiles with equal half-widths (FWHM). Also shown are the Voigt and K profiles resulting from the convolution of Gauss and Lorentz, and Gauss and $j_{A,R}$, respectively.

$$G(\lambda)=G_o+G_{max}\exp\left(-\frac{4\ln 2(\lambda-\lambda_o)^2}{W_G^2}\right), \tag{2.2}$$

where G_o is the baseline (offset), G_{max} is the maximum intensity (intensity for $\lambda=\lambda_o$), and λ_o is the wavelength of the line center, with the Doppler full width at half-maximum given by

$$W_G=2\sqrt{\frac{2\ln 2\,kT}{m}}\frac{\lambda_o}{c}. \tag{2.3}$$

Here, T is the emitter equivalent kinetic temperature, m is its mass, and k and c are the Boltzmann constant and velocity of the light, respectively. The shape of this line is shown in Fig. 1, along with other considered line profiles.

It is well known that the intensity distribution of a spectral line broadened by two independent effects is expressed by the equation

$$f(\lambda)=\int_{-\infty}^{\infty}g(\lambda-\lambda_o-\lambda')h(\lambda')d\lambda'. \tag{2.4}$$

Here $g(\lambda')$ and $h(\lambda')$ are the profiles that can be used if only one of the broadening effects is present. All functions f, g, and h denote intensities, and λ' is given in either wavelength or frequency units.

Whenever the Gaussian contribution of plasma broadening is not negligible one has to use a deconvolution procedure to determine the Stark width of the line. Where the electron impact broadening is the dominant mechanism, the contribution of ions to the line profile may be neglected, as is the case of the majority of the ionized atoms. The resulting profile has the Voigt form Ref. [13]. Then one is dealing with a Lorentzian distribution, the deconvolution from the Gaussian part being described in several papers [13–15].

In the case of a Voigt function, Eq. (2.4) is

$$V(\lambda)=V_o+V_{max}W_L^2 \times\int_{-\infty}^{\infty}\frac{\exp(-t^2)}{W_L^2+4[\lambda-(\lambda_o+(W_G/2\sqrt{\ln 2})t)]^2}dt, \tag{2.5}$$

where V_o is the baseline (offset) and $V_{\max}$ is the maximum of intensity (intensity for $\lambda=\lambda_o$).

However, in the case of nonhydrogenic atomic lines the ion broadening in most cases is not negligible and the line profiles are described by an asymmetric function. In the quasistatic ion approximation (Ref. [2]) the profile of an isolated spectral line emitted by a nonhydrogenic emitter is given by

$$j_{A,R}(\lambda)=j_o+j_{max}\int_0^{\infty}\frac{H_R(\beta)}{1+[2(\lambda-\lambda_o)/W_j-\alpha\beta^2]^2}d\beta, \tag{2.6}$$

where j_o is the baseline, j_{max} the maximum intensity, and $H_R(\beta)$ an electric microfield strength distribution function of normalized field strength $\beta=F/F_o$. F_o is the Holtsmark field strength. $A(\alpha=A^{4/3})$, the static ion broadening parameter is a measure of the relative importance of ion and electron broadenings and is given by Ref. [2]. R is the ratio of the mean distance between ions to the Debye radius, i.e., the Debye shielding parameter and W_j is the width (FWHM) of the j profile. The Debye shielding parameter for a singly ionized atom is given for singly charged perturbers by [2]

$$R=\sqrt[6]{\frac{36\pi e^6 N_e}{(kT_e)^3}}, \tag{2.7}$$

where N_e and T_e are the electron density and temperature, respectively. This parameter can be calculated, in the case of double and multiply ionized atoms (perturbers) from the equation for R, given in Ref. [2].

Electric microfield distributions in plasmas have been calculated by Hooper [16,17]. For the Holtsmark limit, i.e., for $R=0$, this function has the form

$$H_{R=0}(\beta)=H_o\beta\int_0^{\infty}x\sin(\beta x)\exp(-x^{3/2})dx, \tag{2.8}$$

where H_o is a normalization constant.

Finally, the convolution integral of both Gaussian and Stark broadening $j_{A,R}$ profiles, according to Eq. (2.4), is given by

$$K(\lambda)=K_o+K_{max}\int_{-\infty}^{\infty}\exp(-t^2)\left[\int_0^{\infty}\frac{H_R(\beta)}{1+[2(\lambda-\lambda_o-(W_G/2\sqrt{\ln 2})t)/W_j-\alpha\beta^2]^2}d\beta\right]dt. \tag{2.9}$$

Here K_o is the baseline (offset) and K_{max} is the maximum of intensity (intensity for $\lambda=\lambda_o$). The K function, i.e., the convolution integral (2.9) contains Voigt and Lorentz functions too. Namely, when the spectral line is symmetric, from the unified fitting procedure the parameter A comes out equal to zero. Thus, expression (2.9) reduces to Eq. (2.5). In this transformation use has been made of the fact that, the electric microfield distributions in plasmas were normalized to one. The derivation of the Lorentz function is not as evident as the derivation of the Voigt function. First, it yields from the unified fitting procedure, again, the parameter A equal to zero. Second, it derives from the assumption that the Gauss function does not have any influence on the final width of the spectral line. Hence, $W_G\to 0$, i.e., $t\to\infty$, which means that the Gauss function may be replaced with the delta function. Because of the delta function, the convolution integral (2.9) has a value different from zero only for $\lambda'=\lambda-\lambda_0$. Finally, all these transformations lead to the Lorentz function. In conclusion, it should be specified again, that the K function (2.9) in plasma broadening is represented as a general case of a spectral line profile. Thus, if there is a good fitting method, the fitting procedure will find which function represented the recorded spectral line and the parameters of that line.

For the evaluation of the influence of ion dynamic effects on the shape of nonhydrogenic atom lines we used the parameter

$$\sigma=\frac{4.03\times 10^{-7}W_j[\mathrm{nm}]}{(\lambda[\mathrm{nm}])^2}(N_e[\mathrm{m}^{-3}])^{2/3}\sqrt{\frac{\mu}{T_g[\mathrm{K}]}}, \tag{2.10}$$

where W_j is the electron FWHM at $N_e=10^{23}\,\mathrm{m}^{-3}$ and μ is the atom-ion perturber reduced mass in amu. The condition of validity for the ion dynamic correction is often expressed by

$$B=A^{1/3}\sigma<1. \tag{2.11}$$

The physical meaning of this condition is that all strong electron and ion collisions are separated in time, and have to be checked in all experimental conditions.

From Ref. [10] a simple parametric expression was derived for the evaluation of the total full width for dynamic ions of isolated lines. When ion dynamics contributes to the linewidth, the total line width of the $K(\lambda)$ profile is well represented for neutral atoms by

$$W_t\approx W_j[1+1.75AD_J(1-0.75R)], \tag{2.12}$$

and for singly ionized atoms by

$$W_t\approx W_j[1+1.75AD_J(1-1.2R)], \tag{2.13}$$

where

$$D_J=\frac{1.36}{1.75(1-0.75R)}B^{-1/3},\quad B<\left(\frac{1.36}{1.75(1-0.75R)}\right)^3 \tag{2.14}$$

or

$$D_J=1,\quad B\geqslant\left(\frac{1.36}{1.75(1-0.75R)}\right)^3. \tag{2.15}$$

In the case $D_J=1$ the influence of ion dynamics is negligible and the line shape is treated using the quasistatic ion approximation. Expressions (2.12) and (2.13) are approximate total widths of a line, only when the influence of ion dynamics is not negligible. This is an approximate total width because of the used function $j(\lambda,A,R)$ instead of $j(\lambda,A,R,\sigma)$. Namely, Barnard *et al.* [10] presents a simple algorithm for generating the $j(\lambda,A,R,\sigma)$ profile obtained by fusing the electron and ion contributions. One can evaluate the ion dynamic correction to the FWHM by comparing the widths of the unified $j(\lambda,A,R,\sigma)$ to those of the $j(\lambda,A,R)$ profiles, for which ions are treated as quasistatic. In the region where Eq. (2.11) is satisfied, the difference between the two widths is due to ion motion. Differences between the widths computed form the $j(\lambda,A,R)$ and the actual widths of the $j(\lambda,A,R,\sigma)$ profiles are less than 1% for $B<1$, where the unified theory is valid.

Expressions (2.12) and (2.13) are valid only in the $R\leqslant 0.8$ and $0.05\leqslant A\leqslant 0.5$ domains. Reference [2] also discusses cases outside this range.

III. NUMERICAL PROCEDURE FOR DECONVOLUTION

The proposed functions for various line shapes, Eqs. (2.9) and (2.5), are of the integral form and include several parameters. Some of these parameters can be determined in separate experiments, but not all of them. Furthermore, it is impossible to find an analytical solution for the integrals and numerical methods must be used. This procedure, combined with the simultaneous fitting of a several free parameters, causes the deconvolution to be an extremely difficult task and requires a number of computer supported mathematical techniques. Particular problems are the questions of convergence and reliability of the deconvolution procedure, which are tightly connected with the quality of experimental data.

For deconvolution purposes we are looking to best fit the experimental profile in a six-dimensional parameter space $(K_{\max},\lambda_o,W_j,W_G,R,A)$. Furthermore function evaluations are expensive, as the computation of a triple integral is required. The first integral in the K function is the microfield strength distribution function $H_R(\beta)$, the second one is the $j_{A,R}(\lambda)$ function (2.6), and the third is the convolution integral of a Gaussian and a plasma broadened spectral line profile $j_{A,R}(\lambda)$, denoted by $K(\lambda)$, Eq. (2.9). All these integrals have no analytic solution and must be solved numerically.

The most difficult integral to deal with it is the microfield strength distribution function, because in general this involves a multidimensional integral over many ionic configurations. A straightforward Monte Carlo integration is too expensive and many methods have been developed for evaluating this microfield distribution, among which best known are the Holtsmark [18], Baranger-Mozer [19], and Hooper [16,17] methods. By far the fastest method is the APEX method [20,21], whose accuracy was demonstrated by its excellent agreement with computer simulations. However, APEX does not employ the R parameter and this would necessitate a modification of the standard j function. The solution adopted in the present paper is to solve the integral equation for the microfield distribution for a sufficient number of points (β,R) and use this interpolation table to evaluate the microfield distribution at the points needed for the integral evaluation by polynomial interpolation.

For the purpose of testing and demonstrating our deconvolution procedure we have decided to use a tabulated dataset of values of the microfield strength distribution function, evaluated by Hooper. The existing sets of data allowed us to use a fourth-order polynomial as the highest. Thus, in our case the interpolated microfield strength distribution function has the following form:

$$H_R(\beta)=a_\beta+b_\beta R+c_\beta R^2+d_\beta R^3+e_\beta R^4, \tag{3.1}$$

where a_β, b_β, c_β, d_β, and e_β are parameters that depend on normalized field strength β. The five interpolating polynomial parameters lead us to a system of five equations with five unknown parameters, and this system is not very difficult to handle.

Expression (3.1) is applicable for any emitter for which there is a date base of microfield strength distribution function. For neutral and singly ionized emitters there exists a tabular date base in the papers [16] and [17]. It should be noted, that this deconvolution procedure may involve any method of calculation of microfield strength distribution function depending on the kind and composition of analyzed plasmas.

The second integral in Eq. (2.9) is the $j_{A,R}(\lambda)$ and it is evaluated by trapezoidal quadrature. The third integral is evaluted by the Gauss-Hermite method with $\exp(-t^2)$ as a weight function. In this manner the number of terms in the numerical sum is reduced in comparison with other quadrature methods. The same method may be used in Eq. (2.5). It must be noted, that in cases where $(W_G>0.5W_j)$ in Eq. (2.9) or $(W_G>0.5W_L)$ in Eq. (2.5), which represent frequent physical situations in astrophysical plasmas [22], this method of integration is not applicable. Then, the integration must be done by classical quadrature methods, which greatly slow down the iteration process, but these methods are the only correct ones in these regions.

In general, the base line K_o in functions (2.9) and V_o in Eq. (2.5) is a function of wavelength. In many cases it is a nearly constant, or linear function, but in some cases it may have more complex dependence [23]. We have included in our procedure the fitting of background by a cubic polinomial, as independent step, in order to prepare experimental data for the main deconvolution procedure.

In this way, we have solved Eqs. (2.9) and (2.5) and now we can start with the fitting procedure itself. For Eq. (2.9), the fitting procedure will give the values for

W_G, W_j, λ_o, R, A, and $K_{\max}$. In the case of Voigt profiles (2.5), the fitting procedure will determine W_G, W_L, λ_o, and $V_{\max}$.

We are using the standard manner of defining the best fit: the sum of the squares of the deviations (chi-square) of the theoretical function from the experimental point should be at its minimum. In other words, we are seeking for the global minimum of the chi-square function, which is the hypersurface of N dimensions in a hyperspace of $N+1$ dimensions, where N is equal to a number of parameters for the appropriate theoretical function. N is equal to six for the K profile and four for the Voigt function.

The necessary condition for the minimum of chi-square sum is that the partial derivatives of the function are equal to zero. Therefore, in the case of the K profile we have a system of six nonlinear homogeneous equations with six parameters and in the case of Voigt profiles we have a system of four nonlinear homogenous equations with four parameters. We are seeking the numerical solutions of these systems by using the well-known Newton method of successive approximations. Kantorovich and Ostrowski [24,25] have investigated the conditions of convergence of the Newton method. In these cases we have two homogenous systems of algebraic and transcendental equations with real coefficients. The functions are defined and continuous, along with their partial derivatives of first and second orders. If the initial parameters lie in the domain sufficiently close to the true solutions of the system, the conditions for convergence are fulfilled.

The computer solution of this problem faces a number of numerical difficulties. Newton's method requires successive solutions of the inverse Jacobi matrices of the system of equations for each step, which are error prone due to roundoff errors. Moreover, the numerical partial derivatives in the Jacobi matrix are themselves subject to roundoff error. These roundoff errors are a destabilizing convergence, though the mathematical conditions for convergence are fulfilled. The algorithm was stabilized by reducing the iteration procedure to independent parameters only by neglecting the off-diagonal elements of the Jacobi matrix. This simplification alleviates the roundoff errors in the calculation of the inverse Jacobi matrix. Further stabilization of the iterative process may be achieved by weighing the off-diagonal elements of the inverse Jacobi matrix by real numbers in the range (0,1]. These modifications of Newton's method do not affect either the convergence or the uniqueness of the mathematical solution, but do affect somewhat the speed of convergence. In this way we were able to find numerical solutions for fitting functions with more than three free parameters, which is difficult for nonpolynomial fits.

This algorithm has shown great numerical stability, under variation of initial parameters. This has been demonstrated by fitting of about 100 of experimental data sets, for both K and Voigt profiles.

This sophisticated deconvolution method, which allows direct determination of all six parameters by fitting the theoretical K profile (2.9), on the experimental data, requires a sufficient number of experimental points per line, and small statistical errors. The upper limits for well conditioning of this method are a minimum twenty experimental points per line [the borderline is $(-3/2W_j+\lambda_o<\lambda<+3/2W_j+\lambda_o)$, where W_j is the FWHM], and the maximal statistical indeterminacy in intensity is 5% at every experimental point. Poor experimental measurements weaken the conditioning of the system of equations, and make this method inapplicable. This has been demonstrated by testing the sensitivity of the algorithm by generating random statistical noise with a Gaussian distribution in every point involved in theoretical profiles. In the case of a Voigt profile, where there are four parameters, the condition of applicability is more elastic.

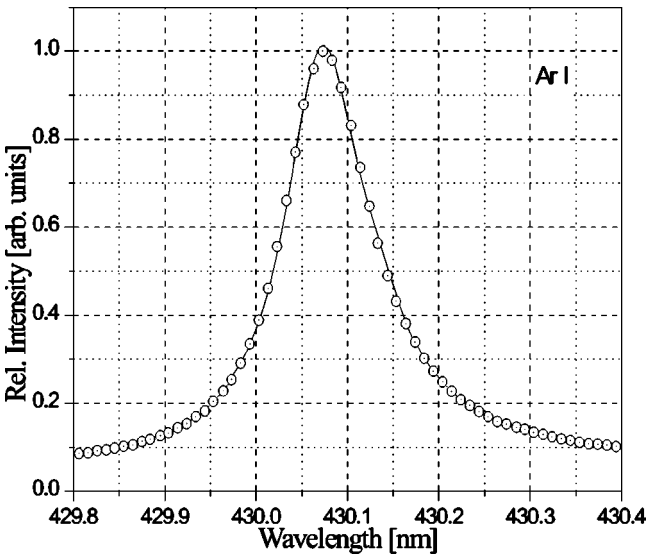

FIG. 2. Our fit of Ar I 430.01 nm line profile. The circles are digitized from the data of Hahn and Woltz [26]. The horizontal axis is shifted slightly by an offset in the wavelength calibration of the monochromator, according to Ref. [26].

IV. APPLICATION OF THE METHOD, BENCHMARKING, AND DISCUSSION

The principal objective of this study was the analysis of asymmetric isolated spectral lines having minimal overlap with the neighboring lines, under the conditions of optimum plasma source stability. The algorithm is demonstrated by fitting experimental data taken from Ref. [26], and analyzing the Ar I 430.01 nm spectral line. Hahn and Woltz [26] used this argon line to illustrate an asymmetric theoretical fit and a Lorentzian fit to the experimental data. For that purpose they had to fix R and W_G, i.e., $R=0.52$ and $W_G=0.0058$ nm, respectively. They have obtained for the total width of the line $W_t=0.105$ nm and for ion broadening parameter $A=0.137$. We have treated the same spectral line with our free parameters fitting procedure, by using K profile (2.9). The result is shown in Fig. 2.

The deviation of the asymmetric theoretical fit from the experimental points is very small. Since the fit is performed without predetermined parameters, we have obtained from the fitting procedure $W_G=0.00582$ nm, $R=0.505$, and $A=0.145$, and for the total width of the line, $W_t=0.107$ nm. All these values are in very good agreement with the data of Hahn and Woltz. According to their results [26] for Argon

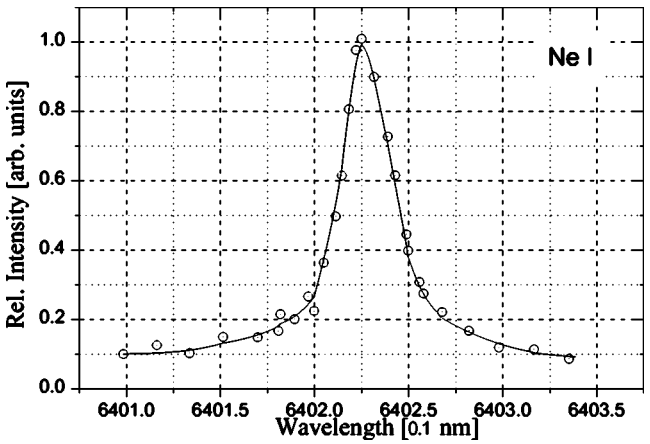

FIG. 3. Our fit of Ne I 640.22 nm line profile. The circles are digitized points from data in Ref. [28].

''blue'' lines, their plasma parameters are $0.623\times10^{23}\mathrm{m}^{-3}$ for the electron density and 11 900 K for the electron temperature. They have determined the electron density from the width of the hydrogen H_β line by the Vidal-Cooper-Smith Stark broadening theory. They determined the temperature by applying the conservation and equlibrium equations for local thermodynamic equlibrium plasmas. For determining their plasma parameters we used Eqs. (2.3) and (2.7). Our calculated values are 0.61×10^{23} m^{-3} for electron density and 12 500 K for electron temperature. The difference between our calculated and their measured plasma parameters shows that each line ''senses'' plasma conditions differently. This slight discrepancy is however within experimental uncertainty. We have applied the method to Hahn and Woltz's measured spectral line and obtained the same parameters as they did, *without* any prior knowlede or assumption of the plasma parameters.

We have also used other lines to test our deconvolution-fitting procedure. For this, we chose one neon line for which results have been presented in Ref. [27]. The shape of this line was obtained from Ref. [28]. We have chosen this line for two reasons. First, the authors of Ref. [27] used the Voigt function for fitting to the experimental profile, and second, the asymmetry of this line is higher than the line of Hahn and Woltz. The Voigt function yields the wrong distribution for fitting on neutral spectral lines. Therefore it is not possible to compare all our fitting parameters with theirs, for example, *A* parameters. They fix the W_G at the value 0.0191 nm and using the standard fitting procedure described in Ref. [14], they got the Stark width, $W_t=0.0223$ nm. Their experimental points and our fitting curve is presented in Fig. 3.

The deviation of the asymmetric theoretical fit from the experimental points for this line is not small as in the case of Hahn and Woltz's line, but relatively is not large either. Since our fit is performed without predetermined parameters, we have obtained from fitting procedure $W_G=0.01777$ nm, $R=0.3510$, and $A=0.185$, and for the total width of the line, $W_t=0.0272$ nm. Our value for W_G shows a resonable agreement with the value of Purić *et al.* The authors have presented plasma parameters for this line, too. Their plasma paramers are 31 400 K electron temperature and $0.92\times10^{23}\mathrm{m}^{-3}$ for electron density. We have calculated the same parameters according to our fitting parameters of the neon line. Our calculated values are 30 000 K for electron temperature and $0.95\times10^{23}\,\mathrm{m}^{-3}$ for electron density. Here, we should point out that their plasma parameters are obtained from independent measurements. The electron density in the Ref. [27] was determined by the laser interferometry at a single wavelength (He-Ne laser 632.8 nm line) and from the H_β profile. For determining the electron temperature they used the Boltzmann slope of several Ne II lines. We determined these plasma parameters solely from their recorded neon spectra lines. For this neon line theoretical values by Griem are given in Ref. [2]. The ratio between the measured value and Griem's result is 0.78 for this line, according to the results of Ref. [27]. On the other hand, the ratio between the calculated value from our deconvoluting-fitting procedure and Griem's theoretical value, for the same neon line, is 0.95. This discrepancy is attributable to the use of a wrong distribution function for fitting of neutral lines in Ref. [27].

This comparison has demonstrated a big advantage of our method, as compared to earlier ones. Our fitting procedure can provide all plasma parameters. This is particularly important for astrophysical studies.

Up to now, to the authors' knowledge, all existing deconvolution procedures, Refs. [26,29–31] require at least one of parameters to be known and fixed during the fitting. For the Voigt and *K* convolution integrals it is necessary to fix W_G or W_G and *R*, as in Refs. [26,29–31]. In Ref. [29] and Ref. [31] the fitting procedure is performed by the convolution integral of a Gaussian and a plasma broadened spectral line profile $j_{A,R}(\lambda)$, for isolated spectral lines, but with the use of a fixed value for the ion broadening parameter *A*. A simple method for estimating *A* is described in Ref. [32]. For the full evaluation of the ion-broadening parameter *A* one can use the formula given in Ref. [2]. In our deconvolution procedure of atomic spectral line profile all plasma parameters are free, including W_G, *R*, and *A*, and they can be determined directly from the fitting procedure itself.

It should be noted that to apply this deconvolution and fitting method some assumptions or prior knowledge about plasmas condition are necessary. Accordingly, for each emitter ionization stage one needs to know the electric microfield distribution, in order to fit the ''K'' function. In the case of quasistatic or quasistatic and dynamic broadenig, our fitting procedure gives the electron impact width, static ion broadening parameter and, finally dynamic ion broadening parameter, respectivly. But, if ions are dynamic, it is not possible, as already discussed, to distinguish the electronic and ionic impact widths, and the method gives the total impact width.

We have also tested our fitting procedure with the Voigt and *K* convolution integral using our experimental data. For the Voigt function we have used our data published in Refs. [33–38]. The *K* convolution integral is used for the analysis of our new data on neutral rare gases. We have tested more than one hundred asymetric spectral lines, recorded under reproducibile plasma conditions. By comparing different spectral lines obtained under the same plasma conditions, we tested the stability of our deconvolution procedure. The obtained parameters, which are tied to plasma conditions, such

as T_e and N_e, are independent from the analyzed lines. Our calculated values of temperature from each spectral line and values obtained by the Boltzmann and Saha equations are in very good agreement, within $\pm 7\%$. The electron density calculated from each spectral line shows even better agreement with the values measured by interferometry, the agreement being within $\pm 5\%$.

V. SUMMARY

We have developed a free parameter deconvolution procedure for atomic spectral line profiles. This method gives complete information on the plasma parameters from a single recorded spectral line. The method determines all broadening plasma parameters self-consistenly and directly from the shape of spectral lines without any assumptions or prior knowledge. All one needs to know is the instrumental width of the spectrometer. This procedure can be applied to laboratory plasmas as an independent method for determining plasma parameters. On the other hand, in case of astrophysical plasmas, where no other diagnostic method is available, this method can be very useful.

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[1] H.R. Griem, Phys. Rev. **165**, 258 (1968).
[2] H.R. Griem, *Spectral Line Broadening by Plasmas* (Academic, New York, 1974).
[3] H.R. Griem, *Principles of Plasma Spectroscopy* (Cambridge University Press, Cambridge, England, 1997).
[4] S. Alexiou, Phys. Rev. Lett. **75**, 3406 (1995).
[5] S. Alexiou *et al.*, J. Quant. Spectrosc. Radiat. Transf. **58**, 399 (1997).
[6] S. Alexiou *et al.*, J. Quant. Spectrosc. Radiat. Transf. **65**, 15 (2000).
[7] S. Alexiou and R.W. Lee, *15th International Conference of Spectral Line Shapes*, edited by J. Seidel (AIP, New York, in press).
[8] H.R. Griem and Yu.V. Ralchenko, J. Quant. Spectrosc. Radiat. Transf. **65**, 287 (2000).
[9] S. Alexiou, Phys. Rev. A **49**, 106 (1994).
[10] J. Barnard, J. Cooper, and E.W. Smith, J. Quant. Spectrosc. Radiat. Transf. **14**, 1025 (1974).
[11] S. Alexiou, Phys. Rev. Lett. **76**, 1836 (1996).
[12] E. Oks, Phys. Rev. E **60**, R2480 (1999).
[13] H.C. van de Hulst and J.J.M. Reesinck, Astrophys. J. **106**, 121 (1947).
[14] J.T. Davies and J.M. Vaughan, Astrophys. J. **137**, 1302 (1963).
[15] R.F. de Vries, Rijnhuizen Report 65-26, Jutphaas, Nederland, 1965.
[16] C.F. Hooper, Jr., Phys. Rev. **149**, 77 (1966).
[17] C.F. Hooper, Jr., Phys. Rev. **165**, 215 (1968).
[18] J. Holtsmark, Ann. Phys. (Leipzig) **58**, 577 (1919).
[19] M. Baranger and B. Mozer, Phys. Rev. **115**, 521 (1959).
[20] C. Iglesias *et al.*, Phys. Rev. A **28**, 1667 (1983).
[21] C. Iglesias *et al.*, Phys. Rev. A **31**, 1698 (1985).
[22] L.C. Popović, M.S. Dimitrijević, and D. Tankosić, A&A Supp. Ser. **139**, 617 (1999).
[23] S. Glenzer, N.I. Uzelac, and H.J. Kunze, Phys. Rev. A **45**, 8795 (1992).
[24] L.V. Kantorovich, ''On Newton's Method,'' Trudy Matematicheskogo Instituta im. V. A. Steklova AN SSSR, v. XXVIII. M. L., 1949.
[25] B.P. Demidovich and I.A. Maron, *Computational Mathematics* (Mir, Moscow, 1987).
[26] D.T. Hahn and A. L. Woltz, Phys. Rev. A **42**, 1450 (1990).
[27] J. Purić, A. Srećković, S. Djeniže, J. Labat, and Lj. Ćirković, Phys. Lett. A **126**, 280 (1988).
[28] A. Srećković [private comunications about Ref. [27] (2000)].
[29] L.A. Woltz, J. Quant. Spectrosc. Radiat. Transf. **36**, 547 (1986).
[30] W.J. Douglas, L.W. Wiese, and A.L. Woltz, Phys. Rev. A **34**, 450 (1986).
[31] Z. Mijatović, R. Kobilarov, B.T. Vujčić, D. Nikolić, and N. Konjević, J. Quant. Spectrosc. Radiat. Transf. **50**, 329 (1993).
[32] S.A. Freudenstein and J. Cooper, Astrophys. J. **224**, 1079 (1978).
[33] S. Djeniže, V. Milosavljević, and A. Srećković, J. Quant. Spectrosc. Radiat. Transf. **59**, 71 (1998).
[34] V. Milosavljević and S. Djeniže, A&A Supp. Ser. **128**, 197 (1998).
[35] S. Djeniže and V. Milosavljević, A&A Supp. Ser. **131**, 355 (1998).
[36] V. Milosavljević, R. Konjević, and S. Djeniže, A&A Supp. Ser. **135**, 565 (1999).
[37] V. Milosavljević, S. Djeniže, M.S. Dimitrijević, and L.Č. Popović, Phys. Rev. E **62**, 4137 (2000).
[38] V. Milosavljević, M. S. Dimitrijević, and S. Djeniže, Astrophys. J. (to be published).