DETERMINATION OF PLASMA PARAMETERS FROM SHAPES OF ATOMIC SPECTRAL LINES

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Abstract. This paper is concerned with the possibility of determination the basic plasma parameters such as temperature and electron density by using 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 spectral lines. Special attention was dedicated to reliability of obtained parameters. The methods for verifying the validity of the theory predicted model function with real plasma conditions and for detecting the presence of other undesirable broadening mechanisms are given. The comparison with plasma parameters determined by using standard diagnostics methods is also presented.

1. 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 physical mechanisms leading to it. 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 case of astrophysical plasmas. In fact, the only way of performing 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 (Griem, 1968, 1974, 1997). 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 velocity the Doppler broadening has a Gaussian distribution. The third mechanism depends on the electric micro-fields 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 cases when interactions between the emitter and ion is negligible in comparison with the interaction emitter electron, is a symmetric Lorentz function. For neutral and ionized emitters for which the interaction between emitter and ion is not negligible, more convenient distribution is asymmetric $j_{A,R}(\lambda)$ profile (Griem, 1974). In the case of neutral atoms, an important role may play the resonant and Van der Waals broadening and it should at least be 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 effect of the line broadening in plasma has to account for the radiative transfer. The lines may be broadened by self-absorption and this effect is especially important in the cases of strong lines and high pressures. Self-absorption will have the effect of destroying and especially broadening the lines and will therefore produce an apparently large width. In some cases, in conditions of inverse population, if induced (stimulated) emission exceeds the absorption, it may even cause line narrowing. This radiation additionally influences the shape of the line profile. There is also a contribution of instrumental broadening, which is characteristic of spectral device used for observation, and it must be known and taken into account appropriately.

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, there is also a great need for reasonably accurate measurements under the well-defined plasma conditions. For most of these measured lines, the electron impact broadening should indeed be the dominant mechanism, except for very partially ionized gases. The state of the 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, (Alexiou, 1995, 1997, 2000; Griem and Ralchenko, 2000).

All the mentioned processes exert influence on the shape of the spectral lines. Usually, 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 so important for pressure broadening. 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 Lorentzian profile. The fit to Voigt profile is more appropriate, because it includes Doppler broadening in the main Lorentzian profile. This profile can be used if the shape of the measured line is symmetric, which is the case of ionized emitters, where it is possibly to neglect the interactions between the emitter and perturbation partical - ion. In the case of neutral and ionized emitters for which the interaction between the emitter and ion is not negligible, the line profile is asymmetric. In principle there is no fundamental difference between the ionized emitters. However, the quasistatic approximation is better satisfied for singly than multiply ionized emitters within a given isoelectronic sequence because the relevant energy spacings are smaller and the times contributing to the relevant integrals are longer (Alexiou, 1994). The most convenient fit in these cases is the fit to the so-called "K" function i.e. the convolution integral (Griem, 1974) of a Gaussian and a plasma broadened spectral line profile $j_{A,R}(\lambda)$. Besides the $j_{A,R}(\lambda)$ and Doppler widths, the important role in "K" profile is played by the static ion broadening parameter A and Debye shielding and ion-ion correlation parameter R.

It should be mentioned that besides the quasistatic treatment of ions there is also the dynamic treatment of the ions (Griem, 1974; Barnard *et al.,* 1974) existing. If strong collisions do not overlap in time, the theory is valid for the whole range of ion broadenings,

from quasistatic to impact broadening. In this way, two situations are possible. First, quasistatic and dynamic ion treatment at the same time, in this case the resulting line pofil is asymmetric. Also, in this case it is possible the distinguish electron impact width and ion width. Second, if ions are not quasistatic (Alexiou, 1996, 1997; Oks, 1999), there is always a part of ion width which just adds to the electron impact width, and in this case the resulting line pofil is symmetric function. Experimentally, in this case, one cannot distinguish between the electronic and ionic impact contributions, and care must be taken at interpreting the line broadening parameters.

In the above text the asymmetry of the lines refers to a quasistatic broadening, consequently the approach ignores a number of important factors which too may contribute to the asymmetry of the lines, such as the gradients, quadrupoles, shifts or some other effects.

When the experimentalist gets a line without an apriori knowledge of the plasma parameters, he would like to be able to separate them from the experimental spectrum. 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. In the case of neutral and ionized emitters for which broadening by ions are not negligible, the line profile is often asymmetric. The most appropriate theoretical model function in these cases is the K profile (2), i.e., the convolution integral of a Gaussian and a plasma broadened spectral line profile $j_{A,R}(\lambda)$.

2. THEORETICAL BACKGROUND

In the general case of non-hydrogenic 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 (Griem, 1974) the profile of an isolated spectral line emitted by a non-hydrogenic emitter is given by

$$j_{A,R}(\lambda) = j_0 + j_{\max} \int_0^\infty \frac{H_R(\beta)}{1 + [2(\lambda - \lambda_0)/W_j - \alpha\beta^2]^2} d\beta \tag{1}$$

where jo is the baseline, $j_{\max}$ maximum intensity, $H_R(\beta)$ an electric micro field strength distribution function of normalized field strength $\beta = F/F_0$. Fo is the Holtsmark field strength. $A(\alpha = A^{4/3})$ is the static ion broadening parameter as a measure of the relative importance of ion and electron broadenings. R is the ratio of the mean distance between ions to the Debye radius, i.e. the Debye shielding parameter and Wj is the width (FWHM) of the j profile. Electric micro field distributions in plasmas have been calculated by Hooper (1966, 1968).

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. The convolution integral of both Gaussian and Stark broadening $j_{A,R}(\lambda)$ profiles is given by

$$K(\lambda) = K_0 + K_{max} \int_{-\infty}^{+\infty} \exp(-t^2) \otimes$$

$$\left\{ \int_0^\infty \frac{H_R(\beta)}{1 + \left(2\dfrac{\lambda - \lambda_0 - \dfrac{W_G}{2\sqrt{\ln 2}} \cdot t}{W_e} - \alpha \cdot \beta^2\right)^2} \cdot d\beta \right\} \cdot dt \qquad (2)$$

where K_0 is the baseline, K_{max} the maximum intensity, and $H_R(\beta)$ an electric microfield strength distribution function (Hooper, 1966, 1968) of normalized field strength $\beta=F/F_0$. F_0 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 Griem (1974). R is the ratio of the mean distance between ions to the Debye radius, i.e., the Debye shielding parameter and Wj is the width (FWHM) of the j profile. λ_0 is actual position of the center of a line.

3. NUMERICAL PROCEDURE

The proposed function for various line shapes (2), is of the integral form and includes 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 methods of numerical integration to be applied. This procedure, combined with the simultaneous fitting of several free parameters, causes the deconvolution to be extremely difficult task and requires a number of computer supported mathematical techniques. Particular problems are the questions of convergence and reliability of deconvolution procedure, which are tightly connected with the quality of experimental data.

For the purpose of deconvolution iteration process we need to know the value of K function as a function of λ for every group of parameters (K_{max}, λo, Wj, W_G, R, A). The function $K(\lambda)$ is in integral form and we have to solve a triple integral in each step of iteration process of varying the above group of parameters. The first integral in the "K" function is the micro field strength distribution function $H_R(\beta)$, the second one is the $j_{A,R}(\lambda)$ function and the third is the convolution integral of a Gaussian and a plasma broadened spectral line profile $j_{A,R}(\lambda)$, denoted by $K(\lambda)$ - equation (2). All these integrals have no analytic solution and must be solved using the numerical integration.

The most difficult integral to deal with is the micro field strength distribution function, because this is a multidimensional integral. Straightforward manner would be the estimates of multidimensional integral by Monte Carlo method of integration. The numbers of random samples of points must be large in order to achieve satisfactory accuracy. That could be achieved at the cost in increased processor time. These reasons eliminate the Monte Carlo method of integration. The same reasons eliminate the Monte Carlo simulation method too. There are many theories developed for evaluating the micro field strength

distribution function. The best known are Holtsmark (1919), Baranger and Mozer (1959) and Hooper (1966, 1968) theories. Also developed was the phenomenological adjustable-parameter exponential method (APEX) (Iglesias, 1983, 1985), whose efficiency was demostrated by excellent agreement with computer simulations. The numerical evaluating of micro field strenght distribution function, as a function of β and R, in each step of iteration process, would impose a long processor time, and the method would be practically inapplicable. Instead, we have decided to solve the integral equation of micro field distribution in sufficient numbers of points (β, R), and after that we interpolated that two-dimensional surface by polynomial interpolation. In every iteration step, at varying parameters β, or R, we used previously hand determined interpolation polynomials for determining the value of micro field strength distribution in current points. For neutral and singly ionized atoms (emitters) there exists the tabular date-base in Hooper (1966, 1968). It should be noted, that this deconvolution procedure may involve any method of calculation of micro field strength distribution function depending on the kind and composition of analyzed plasmas.

The second integral in (2) is the $j_{A,R}(\lambda)$ and it is evaluated by summation method. 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 comparation with the summation methods. It must be noted, that in cases where ($W_G > 0.5W_j$) in (2) which are frequent physical situations in astrophysical plasmas (Popović *et al.,* 1999), this method of integration is not applicable. Then, the integration must be performed by clasical summation methods, which greatly slow down the iteration process, but these methods are the only correct, in these regions.

In general, the base line Ko in function (2) is a function of wavelength. In many cases it is nearly constant, or linear function, but in some cases it may have more complex dependence (Glenzer *et al.,* 1992). We have included in our procedure the fitting of background by cubic polinomial, as independent step, in order to prepare experimental data for the main deconvolution procedure. In this way, we have solved the equation (2) and now we can start with fitting procedure itself. For the equation (2), the fitting procedure will give the values for W_G, W_j, λo, R, A and K_{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 points is at its minimum. In other words, we are seeking the global minimum of the Chi-Square function which is hyper-surface of N dimensions in a hyperspace of N+1 dimensions, where N is equal to a number of parameters for appropriate theoretical function. N is equal to six for the "K" profile (Milosavljević and Poparić, 2001).

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 "K" profile we have a system of six nonlinear homogeneous equations with six parameters.. We are seeking the numerical solutions of these systems by using the well-known Newton method of successive approximations. Ostrowski and Kantorovich (Demidovich, 1987) have investigated the conditions of convergence of 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 its partial derivatives of first and second orders. If the initial parameters lie in the domain sufficiently close to the expected solutions of the system, the conditions for convergence are fulfilled.

The seeking for the numerical solution of this problem by employing computer is accompanied by a number of numerical difficulties. The Newtons method requires

successive solving of the inverse Jacobi matrices of the system of equations for each step, which are error prone due to the errors of rounding. Moreover, the numerical partial derivatives in Jacobi matrix itself are sources of errors of rounding. These errors of rounding are destabilizing the convergence of solution of the system, although the all-mathematical conditions are fulfilled. The stabilization of iterative process may be achieved by weighting the non-diagonal elements of inverse Jacobi matrix by real numbers in the domain (0, 1] (Milosavljević and Poparić, 2001). We introduce the dynamic weighting of the off-diagonal Jacobian elements in the domain of (0,1]. During the iterative process, if the convergence of process becomes unstable, they are automatically adjusted by decreasing toward zero. The conditions of positive-definiteness of the weighted Jacobian matrix are always achieved by decreasing off-diagonal dynamic weighting parameters. For sufficiently small off-diagonal weighting parameters the weighted Jacobian matrix becomes diagonally dominant and positive-definite. The algorithm dynamically decreases weighting parameters until the condition for positive-definiteness is fulfilled. Also, when the convergence of process is stable, they can be increased in order to accelerate process. They are adjusted dynamically during the minimizing process. They are not fixed. In that manner, the stability of iterative process is achieved. So, our deconvolution method meets the condition of positive-definiteness and has no problems with stability and reproducibility (Milosavljević and Poparić, 2003). These modifications of Newton's method do not affect the conditions of convergence and uniqueness of mathematical solution, but do affect somewhat the speed of convergence. In this way we have contrived to give numerical solutions for fitting functions with more than three free parameters, which is difficult for non-polynomial fits.

This algorithm has shown a great stability in numerical sense, under variation of initial parameters. This has been demonstrated by fitting of about one hundred of experimental data sets, for "K" profile.

This sophisticated deconvolution method, which allows direct determining of all six parameters by fitting theoretical K-profile (2), on experimental data, requires sufficient number of experimental points per line, and small statistical errors. The upper limits of numerical conditionality of this method are a minimum twenty experimental points per line (the border of line is $(-3/2W_j+\lambda_o<\lambda<+3/2W_j+\lambda_o)$, where W_j (FWHM), and maximal statistical indeterminacy in intensity is 5% at every experimental point. Poor experimental measurements weaken the conditionality of the system of equations, and lead to non-applicability of this method. This has been concluded by testing the sensitivity of the algorithm by generating random statistical noise with Gaussian distribution in every point involved by theoretical profiles.

4. PROBLEMS OF RELIABILITY OF OBTAINED PARAMETERS

The theoretically proposed model function for various line shapes Eq. (2), is of the integral form and includes several parameters. Some of these parameters can be determined in separate experiments, but not all of them. If one has experimentally obtained spectra, in principle one cans determine parameters which included in model function by solving the inverse problem. Because of complexity of theoretical model function and its integral form various numerical methods have to be used. In order to solve the inverse problem we are looking for the best fit or for parameters when the sum of the squares of the deviations of the theoretical function from the experimental point is at its minimum. In this minimization we vary through six-dimensional parameter space (K_{max}, λ_0, W_j, W_G, R, A). Actually, we

are seeking for the global minimum of the chi-square function, which is the hyper surface 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 in the case of the K profile. The advanced numerical method which enables the determination of all of six parameters proposed by theory model function was developed and presented by Milosavljević and Poparić (2001).

A great number of parameters and the complex topology of the hyper surface of the chi-square function, as a function of parameters, through the numerical method finds the global minimum, naturally intrude the question of reliability of such obtained parameters. A special problem is statistical noise, which leads to forming local minimums in the hyper surface of the chi-square function and its more complex topology. This problem can be overcome by determination of a confidence region for every concrete case. There are well-known methods for this kind of estimations (Press *et al.,* 1995).

The next problem is the cases when there is possibility of presence of other broadening mechanisms, such as radiative transfer, reabsorbtion, turbulence, ion dynamics and other broadening mechanism which are not included in theoretical model function. The parameters obtained by solving inverse problem in those cases do not have physical sense. A special care had to be dedicated to detection of these undesirable effects. There are methods for quantitative checking if some theoretical proposed model function appropriately fits some experimental data. Testing can be performed by estimation of convergence of the chi-square sum during decreasing the statistical noise. Non-zero limes value would show that proposed theoretical model function does not well describe the physical process, e.g. there is a presence of some additional effects, which had not been included in modeling.

Also, another testing can be performed by comparing of estimated mean value of chi-square sum and actual chi-square sum obtained from experimental set of data, at the same statistical noise level. So, it always can retrieve the presence of additional undesirable effects. Moreover, its magnitude can be estimated. Deconvolution procedure (Milosavljević and Poparić, 2001) does not enable to eliminate undesirable effects such as reabsorption, radiative transfer, ion dynamic (e.g. falling of quasistatic approximation), and other broadening mechanisms, but it is very important that their presence can always be discovered. If these effects are not negligible, the estimated parameters would not have a sense. But it is important that these effects can always be quantitatively detected and their importance can be quantitatively estimated by comparing with statistical noise level. In the cases where they are not negligible, additional diagnostic and modeling are needed.

5. APLLICATION AND COMPARISONS WITH STANDARD DIAGNOSTICS METHODS

The plasma parameters were determined using standard diagnostics methods. Thus, the electron temperature was determined from the ratios of the relative line intensities of spectral lines helium, argon and krypton, respectively with an estimated error of ±10%, assuming the existence of the LTE. The electron density decay was measured using a well-known single wavelength He-Ne laser interferometer technique for the 632.8 nm transition with an estimated error of ±9%. Temporal evolution of electron temperatures and electron densities are presented in Figs. (1-3).
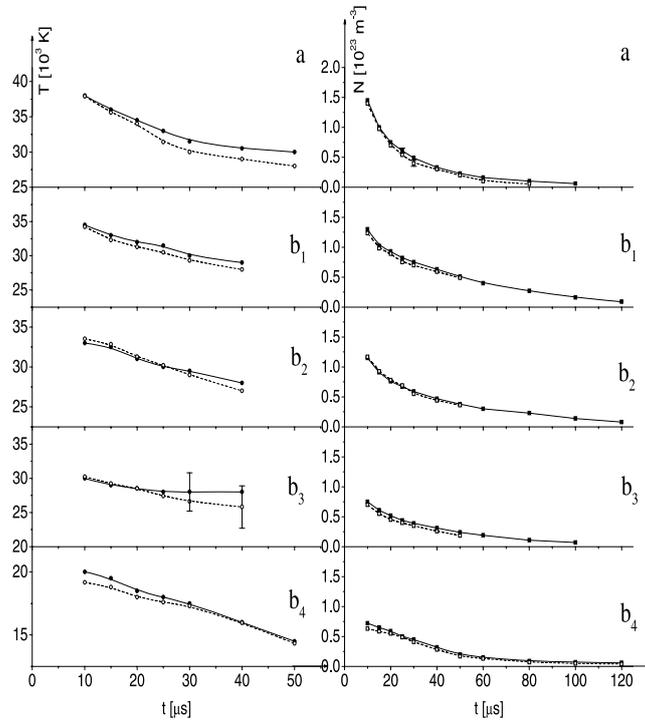
Fig. 1: Electron temperature (T) and density (N) decays for He I 706.52 nm. Full lines represent measured data using independent experimental techniques and dashed lines represent plasma parameters obtained using our line deconvolution procedure in various plasmas (Milosavljevic and Djeniže, 2003a). Error bars, indicated only in the case of the greatest disagreement (T in b_3), represent estimated accuracies of the measurements ($\pm 10\%$) and deconvolutions ($\pm 12\%$)
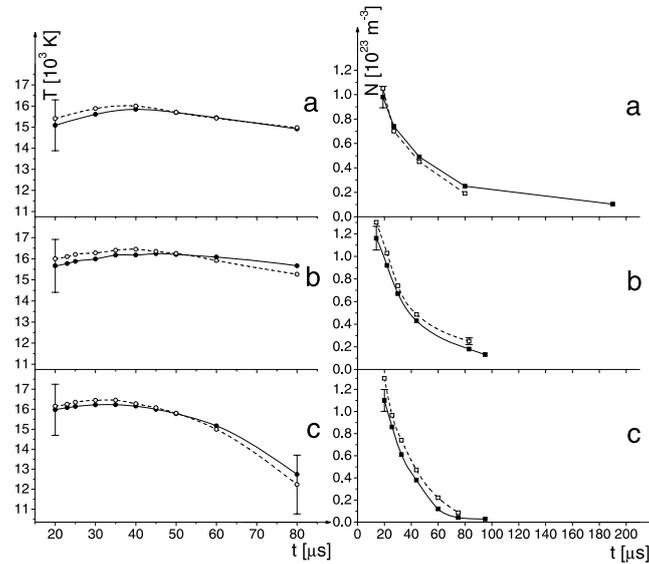
Fig. 2: Electron temperature (T) and density (N) decays for 5 lines of Ar I. Full lines represent measured data using independent experimental techniques and dashed lines represent plasma parameters obtained using our line deconvolution procedure in various plasmas (Milosavljevic and Djeniže, 2003b). Error bars, indicated only in the case of the greatest disagreement, represent estimated accuracies of the measurements (±10%) and deconvolutions (±12%)
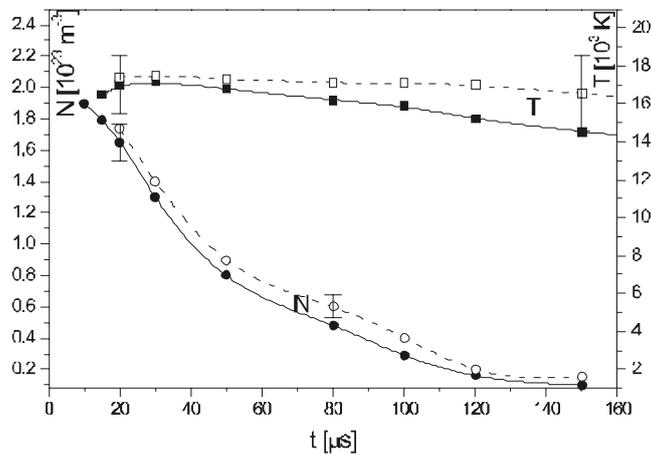
Fig. 3: Electron temperature (T) and density (N) decays for 20 lines of Kr I. Full lines represent measured data using independent experimental techniques and dashed lines represent plasma parameters obtained using our line deconvolution procedure in various plasmas (Milosavljevic et al., 2003). Error bars, indicated only in the case of the greatest disagreement, represent estimated accuracies of the measurements (±10%) and deconvolutions (±12%).

As can be seen from Figs. (1-3) there is a good agreement between the plasma parameters which were determined using standard diagnostics methods and parameters obtained by deconvolution method over a wide range of temperature and electron density. It shows first that, the proposed model function well describes the broadening of spectral lines over this range of plasma parameters, and second, that the deconvolution procedure is numerically stable and gives reliable plasma parameters.

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