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A simple algorithm for spectral line deconvolution

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Abstract

The objective of this work is to develop a numerical procedure to subtract the instrumental function from a measured spectral line profile. The measuring device (for example, a Fabry–Perot Interferometer) distorts the spectral line profile and the experimentally measured one is a convolution of this profile and the instrumental function. Restoring the spectral line profile is strongly affected by numerical instabilities and the problem has been overcome by using the Tikhonov regularization method. The approach is very simple and easy for programming and it is particularly useful for "noisy" experimental data. © 2001 Elsevier Science Ltd. All rights reserved.

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1. Introduction

The subtraction of the instrumental function from a measured spectral line profile plays an important role in low-temperature plasma diagnostics. A spectral line with frequency profile $z(\omega)$, passing through a measuring device with instrumental function $A(\omega)$, is recorded experimentally as $u(\omega)$. By definition, $u(\omega)$ is a convolution of the instrumental function and the spectral line profile:

$$\int_{-\infty}^{\infty} A(\omega-\omega')z(\omega') = u(\omega). \tag{1}$$

The instrumental function has a normalization $\int_{-\infty}^{\infty} A(\omega)\,\mathrm{d}\omega = 1$. There are no limitations regarding the experimental profile, but for convenience it is assumed to be $\int_{-\infty}^{\infty} u(\omega)\,\mathrm{d}\omega = 1$. The spectral line profile $z(\omega)$ may be a singe line or several closely lying lines, which may be poorly separated. Such a situation may occur, for example, if the spectral line belongs to

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element with rich isotope structure. The instrumental function will blur the distinction between these lines and the deconvolution becomes highly desirable.

To solve Eq. (1) can be a formidable task. The experimentally measured spectral line profile $u(\omega)$ is recorded with certain precision and the error associated with these kind of measurements often exceeds 5–10%. From mathematical point of view the solution of (1) is considered as *unstable*, which means that small changes in the right-hand side of (1) $u(\omega)$ potentially lead to huge changes in the solution $z(\omega)$. This is in fact a *multi-valued* solution, because $u(\omega)$ usually represents non-exact, "noisy" experimental data and variation of $u(\omega)$ within the limits of its uncertainty δ generates a family of solutions whose differences significantly exceed δ. It is not multi-valued if only we restrict the class of admissible solutions, using a priori information. The integral equation (1) is an ill-posed problem and can be treated by using the Tikhonov's regularization method [1–3]. The stability of Eq. (1) is of utmost concern and a whole class of different methods for a variety of situations has been developed. A summary of the most frequently used numerical techniques is given in a recent article [4].

2. Tikhonov's regularization method

2.1. Tikhonov's regularization method

The general algorithm for solving the inverse problem

$$A(\omega) * z(\omega) = u(\omega) \tag{2}$$

has been proposed by Tikhonov [1,2]. "A" is usually a linear operator acting on z. The regularization method aims to obtain a single-valued, though an approximate solution. Single-valued (stable) solution means that small variation of the right-hand side of Eq. (2) leads to comparable variation of the solution. The concept is to artificially add a stabilizing term to Eq. (2) in order to make it stable. This is achieved indirectly, by introducing the so-called smoothing function

$$\mathbf{M}^\alpha[z, u^\delta] = \rho^2(A * z, u^\delta) + \alpha\Omega[z].$$

Tikhonov proved, that the problem of getting a single-valued (stable) solution is equivalent to the problem of minimizing the smoothing function $\mathbf{M}^\alpha$

$$\min \mathbf{M}^\alpha[z^\alpha, u^\delta] \tag{3a}$$

with the restriction

$$\rho(A * z^\alpha, u^\delta) = \delta. \tag{3b}$$

The fundamental idea of Tikhonov's regularization method is that Eqs. (3) generate a stable (single-valued) solution and the uncertainty of this solution does not exceed the uncertainty of the right-hand side $u(\omega)$ [1–3]. Eq. (3a) introduces a new variable α, called regularization parameter, which must be determined from Eq. (3b). The right-hand side of (3b) is the uncertainty of $u(\omega)$, a good measure of which is the experimental error. The definition of $\rho(a, b) = \|a - b\|$ depends on the particular case and $\Omega[z]$ is the stabilizing operator. $z^\alpha(\omega)$ is the function, for which $\mathbf{M}^\alpha$ has minimum.

The Tikhonov's regularization method is applied to solve Eq. (1), keeping in mind that the right-hand side of (1) is actually a set of discrete experimental values. Let us have n discrete values $u_k = u(\omega_k)$, $k = 1 \dots n$. The integral can be easily handled, if for all $k = 1 \dots n$ it is replaced by a sum. Thus (1) reduces to a linear system of algebraic equations

$$\hat{A}\vec{z} = \vec{u}^{\,\delta}. \tag{4}$$

Eq. (4) is conveniently written in vector form. Vector $\vec{u}^{\,\delta}$ comprises the set of experimental data u_k, $k = 1 \dots n$. Analogously, $\vec{z}$ comprises the set of discrete values z_k, $k = 1 \dots n$. Written explicitly, Eq. (4) reads $\sum_{m=1}^{n} A_{km} z_m = u_k$ with matrix elements A_{km} defined as

$$A_{km} = A(\omega_k - \omega_m)\Delta\omega_m, \quad \Delta\omega_m = \begin{cases} (\omega_2 - \omega_1)/2, & m = 1, \\ (\omega_{m+1} - \omega_{m-1})/2, & 2 \leqslant m \leqslant n-1, \\ (\omega_n - \omega_{n-1})/2, & m = n, \end{cases}$$

where $\Delta\omega_m$ are the integration coefficients. The center of the instrumental function is assumed to be at $\omega = 0$. Unfortunately, Eq. (4) is an ill-posed problem, remedy for which is the Tikhonov's regularization method. Function ρ must be explicitly defined. For matrix operator, $\rho^2(A * z^\alpha, u^\delta) \equiv \|\hat{A}\vec{z}^{\,\alpha} - \vec{u}^{\,\delta}\|^2$. A simple and efficient stabilizing operator $\Omega[z] = \|\vec{z}\|^2 = \sum_{k=1}^{n} z_k^2$ has been suggested by Tikhonov. With this choice of ρ and Ω the smoothing operator $\mathbf{M}^\alpha$ can be constructed:

$$\mathbf{M}^\alpha[\vec{z}, \vec{u}^{\,\delta}] = \|\hat{A}\vec{z} - \vec{u}^{\,\delta}\|^2 + \alpha\|\vec{z}\|^2. \tag{5}$$

The solution is vector $\vec{z}^{\,\alpha}$, for which $\mathbf{M}^\alpha$ reaches minimum. The most straightforward approach to minimize $\mathbf{M}^\alpha$ is to set the derivative of $\mathbf{M}^\alpha$ zero:

$$\frac{\partial}{\partial\vec{z}}\mathbf{M}^\alpha[\vec{z}, \vec{u}^{\,\delta}]_{\vec{z}=\vec{z}^{\,\alpha}} = 0,$$

which leads to $\hat{A}^{\mathrm{T}}\hat{A}\vec{z}^{\,\alpha} - \hat{A}^{\mathrm{T}}\vec{u}^{\,\delta} + \alpha\vec{z}^{\,\alpha} = 0$ [3]. With a little rearrangement, it takes form,

$$(\hat{A}^{\mathrm{T}}\hat{A} + \alpha\hat{\mathrm{I}})\vec{z}^{\,\alpha} = \hat{A}^{\mathrm{T}}\vec{u}^{\,\delta}, \tag{6a}$$

where $\hat{\mathrm{I}}$ is the unity matrix. Eq. (3b) readily reduces to

$$\|\hat{A}\vec{z}^{\,\alpha} - \vec{u}^{\,\delta}\| = \delta. \tag{6b}$$

Eqs. (6) are written in vector form. Written explicitly, (6a) and (6b) read $\sum_{m=1}^{n} B_{km} z_m^\alpha = \mathrm{v}_k$ and $\sqrt{\sum_{k=1}^{n}\sum_{m=1}^{n}(A_{km}z_m^\alpha - u_k^\delta)^2} = \delta$, respectively. Eq. (6a) is a system of linear algebraic equations with matrix $\hat{B} = \hat{A}^{\mathrm{T}}\hat{A} + \alpha\hat{\mathrm{I}}$. Matrix B is composed of matrix A multiplied by its transpose matrix A^{T}, plus α added to each diagonal element. The right-hand side of (6a) is a one-dimensional vector $\vec{\mathrm{v}} = \hat{A}^{\mathrm{T}}\vec{u}^{\,\delta}$, i.e. $\mathrm{v}_k = \sum_{m=1}^{n} A_{mk}u_m$. Both the solution z_k^α, $k = 1 \dots n$, and the regularization parameter α are calculated from (6a,b).

Further insight into the Tikhonov's regularization method can be achieved by comparing Eqs. (4) and (6). If the linear system of algebraic equations (4) is multiplied by the transposed matrix $\hat{A}^{\mathrm{T}}$, one gets

$$\hat{A}^{\mathrm{T}}\hat{A}\vec{z} = \hat{A}^{\mathrm{T}}\vec{u}^{\,\delta}. \tag{7}$$

The only difference between (6a), derived from the regularization method, and (7), is that α has been added to the matrix diagonal elements of (6a). This is the concept of the regularization method: by adding α to all diagonal matrix elements $A^T A$, the system of linear algebraic equations (6a) becomes stable (single-valued). But since the term $\alpha\vec{z}^{\alpha}$, resulting from the smoothing operator Ω, has been added to Eq. (6a), the norm of the error $\|\hat{A}\vec{z}^{\alpha} - \vec{u}^{\delta}\|$ is no longer zero (see Eq. (6b)). In contrast, $\|\hat{A}\vec{z} - \vec{u}^{\delta}\|$ is exactly zero for Eq. (7). Obviously, Eq. (6a) (slightly) differs from the originally derived equation (7) and solving (6a) will provide a solution $z^{\alpha}(\omega)$, different than the solution $z(\omega)$ of Eq. (7). But due to the constraint (6b), Eq. (6a) generates a solution $z^{\alpha}(\omega)$, whose error does not exceed the error δ of $u(\omega)$. Thus, the Tikhonov's regularization method provides an *approximate*, but *single-valued* solution, which depends on α through the parameter δ. Note that in the limiting case $\alpha \to 0$, Eq. (6a) approaches (7).

2.2. Numerical procedure

The numerical procedure starts with an appropriate choice of α. The matrix elements of B are calculated according to $\hat{B} = \hat{A}^T\hat{A} + \alpha\hat{I}$ and the system of linear algebraic equations (6a) is solved. The solution z_k^{α} is obtained and the left-hand side of (6b) is calculated:

$$\varphi(\alpha) = \sqrt{\sum_{k=1}^{n}\sum_{m=1}^{n}(A_{km}z_m^{\alpha} - u_k^{\delta})^2}. \tag{8}$$

If $|\varphi(\alpha) - \delta| \leqslant \varepsilon$, the numerical procedure stops and z_k^{α} is the solution. If not, another value for α is chosen and the aforementioned steps are repeated until (6b) is fulfilled. Fortunately, $\varphi(\alpha)$ is a monotonic function of α [1,2] (Fig. 1) and the equation $\varphi(\alpha) - \delta = 0$ can be solved without problems.

The numerical procedure described needs δ as an input parameter. By definition, δ is the uncertainty with which $u(\omega)$ is known. Its value depends on the particular situation, but the experimental data $u(\omega)$ often suggests the choice of δ. For example, if the experimental error ε_{exp} is equal for all ω, one may simply put $\delta = \varepsilon_{\text{exp}}\|\vec{u}\| = \varepsilon_{\text{exp}}\sqrt{\sum_{k=1}^{n} u_k^2}$. If ε_{exp} depends on ω, one may set as ε_{exp} the experimental error at the center of the experimental spectral line profile,

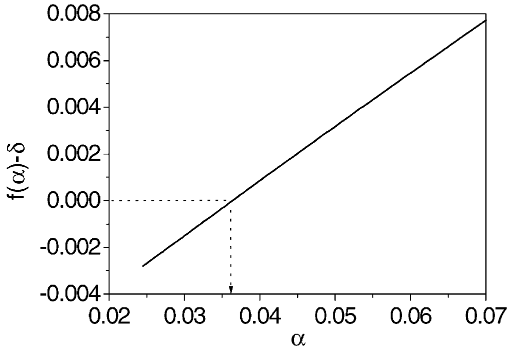

Fig. 1. A typical dependence of $\varphi(\alpha) - \delta$.

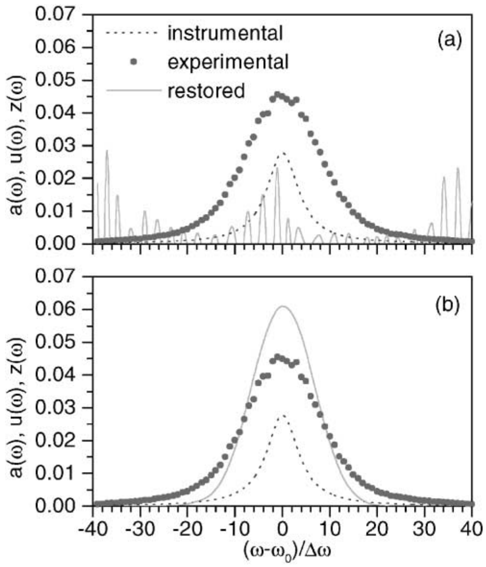

Fig. 2. A simulation of instrumental and "experimental" functions and the solution of Eqs. (7a), and Eqs. (6b).

since the values there are among the largest and give the major contribution to the uncertainty of the experimental data. The initial choice of α is easy, since the parameter of regularization α is closely related and depends on the experimental error δ. One may start with initial guess $\alpha = \delta$.

2.3. Advantages and limitations of the numerical approach

The main advantage of applying the Tikhonov's regularization method is that a single-valued solution is guaranteed. Otherwise, "noisy" experimental data would "blow up" the solution if Eq. (4) or (7) are solved (Fig. 2). Raw experimental data may be readily used; there is no need to smooth or approximate these data. The experimental data need not be equidistant. The matrix B is symmetric and positively defined; a good advantage when solving a system of linear algebraic equations. The solution is usually smooth in spite of the "noisy" character of the experimental data. Deconvolution with 1000 experimental points can easily be performed on a regular PC. There are few limitations regarding the experimental points. One of them is that at both ends they must be much smaller compared to the maximal value.

3. Results and discussions

The Fabry–Perot Interferometry is a very good tool for plasma diagnostics. The spectral line profiles provide information about the electron density, electron and gas temperature. Fortunately, the Fabry–Perot Interferometer has a well-known instrumental function. Fig. 2a illustrates simulated instrumental and "experimental" functions as well as the solution of Eq. (7). Without

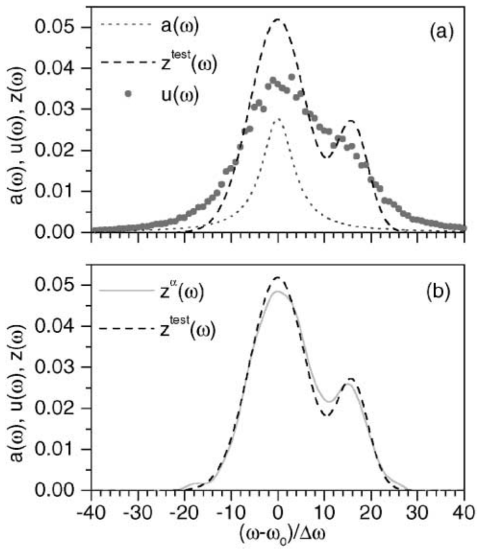

Fig. 3. A simulation of instrumental: (a) test and noisy "experimental" functions and; (b) comparison of the test function with the deconvoluted function.

applying the Tikhonov's regularization method the solution of (7) is practically meaningless. One can compare this solution with the solution of Eqs. (6) (Fig. 2b), when the Tikhonov's regularization method has been applied.

Fig. 3 displays a test of the numerical procedure. A spectral line, which consists of two overlapping components, has been chosen as a test profile (Fig. 3, dashed line). To simulate the experimental function, a convolution with an appropriately chosen instrumental function (dotted line) has been performed and a background "noise" of $p_{\exp} = 10\%$ has been additionally applied (each value has been multiplied by a random number between $1 - p_{\exp}$ and $1 + p_{\exp}$). The simulated experimental points are equidistant with difference between them $\Delta\omega$. The result is illustrated in Fig. 3a with full circles. The two spectral line components are hard to distinguish and the deconvolution is a real challenge. Fig. 3b shows a comparison of the deconvoluted function obtained by solving Eqs. (6) with $\delta = 0.10\varepsilon_{\exp}\sqrt{\sum_{k=1}^{n} u_k^2}$ and the test function. The spectral line components are now clearly visible. The minor difference between the test function and the deconvoluted one is due to the background noise applied to the experimental function. Apart from that, the deconvolution has been successful.

4. Other applications

The plasma probe is widely used to measure the electron energy distribution function (EEDF). From the experimentally measured high-energy part of the EEDF in the late afterglow the rate coefficient for superelastic collisions, hemiionization, Penning ionization, etc. can be determined. But the modulating voltage tends to broaden the EEDF and the real EEDF can be calculated by solving an inverse problem similar to (1), which has been demonstrated in [5]. The technique can be applied to other problems, which can be reduced to Eq. (1).

5. Conclusions

A numerical technique to subtract the instrumental function from "noisy" experimental data has been developed by using the Tikhonov's regularization method. The technique has been tested; a deconvolution has been performed and the test spectral line profile has been successfully restored. The numerical technique is simple; its essential part is a solution of a system of linear algebraic equations. There are very few limitations regarding the spectral line profile and the technique works in most practical cases.

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