Spectral line deconvolution

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Abstract: *The main objective of this work is to develop a numerical procedure to restore the profile of spectral lines recorded by a measuring device. This device (for example a Fabry-Perot Interferometer) distorts the spectral line profile and the experimentally measured one is a convolution of the real profile and the instrumental function. Restoring the line profile is strongly affected by numerical instabilities. The numerical procedure overcomes the problem associated with these instabilities by using the Tikhonov regularization method. This procedure has been further extended to restore the Electron Energy Distribution Function (EEDF), recorded by probe measurements. The numerical code is simple: its essential part is a solution of a system of linear algebraic equations.*

Introduction

The spectral line profile $z(\omega)$, passing through a measuring device with instrumental function $A(\omega)$, is recorded experimentally as $u(\omega)$. There is a simple relation between them

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

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

To solve the integral equation (1) may 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 change in the right hand side of (1) may lead to huge deviation in the solution. This is in fact a *multivalued* solution, because $u(\omega)$ usually represents non-exact, "noisy" experimental data. It turns out to be single valued if only we restrict the class of admissible solution, using *a priori* information. The integral equation (1) is an ill-posed problem and can be treated by using the Tikhonov regularization method [1,2].

Tikhonov's regularization method

The general algorithm for solution of the inverse problem

(2) $$A(\omega) * z(\omega) = u(\omega),$$

has been proposed by Tikhonov [1,2]. The problem is particularly delicate if $u(\omega)$ represent non-exact, "noisy" data. The regularization method aims to obtain a stable, though an approximate solution, rather than getting an exact solution of (1). The concept is to add a smoothing operator to equation (1) in order to make it stable, but keeping the variation of the solution in certain limits. Tikhonov proved, that the problem is equivalent to minimization of the function

(3a) $$M^{\alpha}[z,u^{\delta}] = \rho^2(A * z, u^{\delta}) + \alpha\Omega[z],$$

provided that α meets the condition

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

δ is a measure of the "noise", or with other words, the experimental error, Ω is the smoothing operator, $\rho(x,y) = \|x-y\|$ and α is a parameter to be determined. Tikhonov also proved, that the error incorporated in $z^{\alpha}(\omega)$ does not exceed the "noise" of $u(\omega)$. Lets have n discrete (experimental) points $u_k = u(\omega_k)$, k=1…n. The integral in (1) is replaced by a sum for all k=1…n. Thus equation (1) reduces to a linear system of algebraic equations

(4) $$\sum_{k=1}^{n} A_{km} z_m = u_k.$$

Equation (4) is unstable and the Tikhonov's regularization method must be applied. Tikhonov suggests $\Omega[z] = \|z\|^2$ as appropriate smoothing operator. For discrete points $\|x\|^2 = \sum_{k=1}^{n} x_k^2$. Function M^{α} reaches minimum if $\frac{\partial}{\partial z} M^{\alpha}[z,u^{\delta}]_{z=z_{\alpha}} = 0$, which is equivalent to

(5a) $$A^T A z^{\alpha} + \alpha z^{\alpha} = A^T u^{\delta}.$$

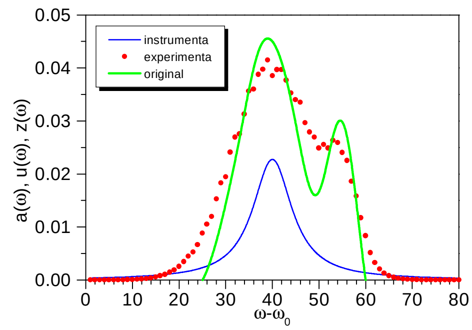
Equation (3b) readily reduces to

(5b) $$\sum_{m=1}^{n}\left(\sum_{k=1}^{n} A_{km} z_m^{\alpha} - u_k^{\delta}\right)^2 = \delta^2.$$

The parameter of regularization α is closely related and depends on the experimental error p through the parameter δ. The latter can be defined as $\delta = p\|u^{\delta}\|$. The desired solution z_k^{α}, k=1…n, and α are calculated simultaneously from (5a,b). Equation (4), multiplied by the transposed matrix A^T, is the same as (5) with the exception of the term αz^{α}. This is the concept of the regularization method: by adding α to all diagonal matrix elements $A^T A$, the linear system of algebraic equations (5a) becomes stable, but, instead of being zero, the left hand side of (5b) is equal to δ^2.

The real spectral line profile

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. The main objective of this work consists of reconstruction of the real profile of spectral line(s) by solving equation (1). The measuring device (the Fabry-Perot Interferometer) has a well-known instrumental function. The experimental function has been simulated, applying p=10% background "noise". Fig.1 illustrates the instrumental, "experimental" and deconvoluted (solution of Eq.4) functions.



Other applications

The plasma probe is widely used to measure the 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) [3].

Benefits from the research

The inverse problem is often met in applied mathematics, experimental and theoretical physics. The data acquisition is always accompanied by fluctuations in the data and the experimental results are to some extend "noisy". There are several areas of research, which can benefit from the present investigation:

1. *Atomic and molecular spectroscopy:* spectral line profile, Abel equation
2. *Plasma physics:* Boltzmann equation, Heat equation, nonlinear diffusion equation
3. *Applied mathematics*: some elliptic partial differential equations, nonlinear differential equations, integral equations

References

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