Stable Sequential Kuhn-Tucker Theorem in One-Dimensional Inverse Problems of Dielectric Reflectometry

Konstantin P. Gaikovich, Petr K. Gaikovich, and Mikhail I. Sumin*
Institute for Physics of Microstructures RAS, GSP-105, Nizhny Novgorod, Russia, 607680
** Nizhny Novgorod State University, Gagarin ave., 23, Nizhny Novgorod, Russia, 603950*
Tel: (7831) 462 3320, Fax: (7831) 462 3320, e-mail: m.sumin@mail.ru

ABSTRACT
In this paper, a new approach in the theory of nonlinear ill-posed problems is applied to the statement of one-dimensional inverse scattering problems. The first problem is the problem of reflectometry subsurface analysis of one-dimensional permittivity inhomogeneities. The second is the problem of the synthesis of multilayer dielectric structures with a desired reflection spectrum.
Keywords: nonlinear inverse scattering problems, dual regularization.

1. INTRODUCTION

Notwithstanding to multiple approaches that has been developed in various applications, nonlinear ill-posed inverse scattering problems have no rigorous solution by now. Only few of one-dimensional problems can be reduced to Gelfand-Levitan-Marchenko equation that is solved explicitly [1], but this theory is inapplicable to layered or absorbing media. Parameterization and model-based algorithms have no convergence, statistical regularization is typically inconsistent. Regularization algorithms based on the gradient minimization of discrepancy converge only in linear problems on compact sets of functions [2]. Tikhonov's method of generalized discrepancy is effective to linear problems for continuous functions [3], but, as applied iteratively to nonlinear problems, it also can be not enough effective. Some approaches have been worked out based on the electromagnetic perturbation theory, where inverse scattering problems have been formulated for non-linear integral equations and solved iteratively, as a sequence of linear Fredholm integral equations of the 1st kind, beginning with Born approximation (see, for example, in [4-7]). But in such nonlinear problems, corresponding algorithms demonstrated good results only in cases of low contrast inhomogeneities or if there is a good first guess. Results of the numerical study revealed serious limitations for large perturbations, when the Born approximation (first guess of iterative method) gives poor results.

In [5,8], a new method of dual regularization [9-12] based on the Lagrange approach in the general optimization theory has been proposed in application to inverse scattering problems, and corresponding algorithms have been studied in numerical simulation in application to problems of reflectometry analysis of diffuse inhomogeneities in multilayer periodic structures of X-ray optics by multifrequency reflection data. Here, this new method is considered from a more generous point of view and proposed to applications in multifrequency reflectometry subsurface diagnostics of one-dimensional inhomogeneities of permittivity and in the similar problem of synthesis of aperiodic structures with a desired refraction spectrum.

2. LAGRANGE APPROACH IN INVERSE PROBLEMS

In most of inverse problems of physical diagnostics [3] it is convenient to transform the initial problem formulated in terms of differential equations to the statement based on the solution of integral equations, typically integral equations of the 1-st kind (Fredholm or Volterra), and there are a number of effective solving methods, such as Tikhonov's method of generalized discrepancy, regularization on compact sets, and some others [2]. Whereas this reduction to integral equation is a proper way in linear problems, in considered non-linear problems, the transfer from the differential statement to its "integral analog" can be a new independent and, mostly, more complicated problem. To make such a transition, one has to use various approximations (for, example, Born approximation). At that, errors appear, and the initial physical model may be essentially distorted.

However, such inverse problems can be formulated as problems of conditional optimization with the equality-kind restriction in the space of feasible solutions X

$$f(x) \to \min, \; g(x) = p, \;\; x \in D \subset X, \tag{1}$$

where $f: X \to R$ is a functional to be minimized, $g: X \to H$ is an operator that links desired solutions $x \in X$ to their indirect manifestations p from the space H obtained from a physical experiment; $D \subset X$ is a set determined from *a priori* information about the desired solution. Considered here problems can also be formulated as (1); at that *X, H* are infinite-dimensional Hilbert spaces. These problems are problems of mathematical or nonlinear programming due to nonlinearity of the continuous operator *g*.

In the theory of conditional optimization, the classical Lagrange principal is mainly used for the solution of problems of mathematical programming that is the criteria of optimality known as Kuhn-Tucker theorem for problems of convex programming (*f* is a convex functional, *g* is a linear operator, *D* is a convex set). The main condition of Kuhn-Tucker theorem is the supposition of the existence of Kuhn-Tucker vector in the problem (1), *i.e.* of the vector $\lambda^* \in H$ that satisfies inequality

$$f(x^*) \le f(x) + L(x,\lambda^*), \forall x \in D, \tag{2}$$

where $x^* \in D$ is the solution of (1), $L(x,\lambda) \equiv f(x) + \langle \lambda, g(x) - p \rangle$ is the Lagrange functional.

Unfortunately, it is impossible to use both Lagrange principal and Kuhn-Tucker theorem in practice directly because they are unstable relative to data errors – and it is the consequence of the same instability of these problems themselves. However, it is possible to overcome this shortcoming on the base of the dual regularization approach [9-12] that is a formal procedure of Tikhonov stabilization of the solution of the problem of concave optimization dual to (1):

$$V(\lambda) \equiv \min_{x \in D} L(x,\lambda) \to \max, \lambda \in H \tag{3}$$

with the simultaneous parallel construction of minimizing sequence in the initial problem (1). The main condition of stability of so-called stable sequential Kuhn-Tucker theorem [11] for the problem (1) is the existence of the generalized Kuhn-Tucker vector $\lambda^* \in H$ that satisfy

$$f(x^*) \le L_c(x,\lambda^*), \forall x \in D, \tag{4}$$

where $L_c(x,\lambda) \equiv f(x) + \langle \lambda, g(x) - p \rangle + \mu(\|g(x) - p\| + \|g(x) - p\|^2)$ is the modified Lagrange functional, $\mu > 0$ is a penalty coefficient. It is possible to demonstrate that the existence of the generalized Kuhn-Tucker vector in the nonlinear problem (1) is its typical property. In cases, when there is no such vector, the penalty coefficient μ should approach infinity concordantly to data errors, so this method covers a broad region of possible applications. The applied here procedure of the minimizing, sequence construction that is included in the stable sequence Kuhn-Tucker theorem coincides, in fact, with the procedure of dual regularization itself [9-11].

3. ELECTRODYNAMICS OF MEDIA WITH ONE DIMENSIONAL PERMITTIVITY PROFILES

In a media with an inhomogeneous distribution of complex permittivity $\varepsilon(\mathbf{r}) = \varepsilon_i + \varepsilon_1(\mathbf{r})$ in a quite generous case of an inhomogeneity $\varepsilon_1(\mathbf{r})$ in a multilayer medium with permittivity ε_i in i^{th} –layer, the complex amplitudes of vectors of electrical and magnetic fields **E**, **H** [$\sim \exp(-i\omega t)$] are determined by the complex amplitude of the source electric current density $\mathbf{j}$ from Maxwell equations that, using formalism of Green functions, can be reduced to the nonlinear integral equation [6]:

$$\mathbf{E}(\mathbf{r}) = \mathbf{E_0}(\mathbf{r}) + \mathbf{E}_1(\mathbf{r}) = \mathbf{E_0}(\mathbf{r}) - \frac{i\omega}{4\pi}\int_V \ddot{\mathbf{G}}(\mathbf{r}',\mathbf{r})\varepsilon_1(\mathbf{r}')\mathbf{E}(\mathbf{r}')d\mathbf{r}', \tag{5}$$

$$\mathbf{E}_0(\mathbf{r}) = \int_V \mathbf{j}(\mathbf{r}')\ddot{\mathbf{G}}(x - x', y - y', z, z')d\mathbf{r}' \tag{6}$$

where the total electric field $\mathbf{E}(\mathbf{r})$ is expressed as the sum of probing field $\mathbf{E_0}(\mathbf{r})$ and scattered field $\mathbf{E}_1(\mathbf{r})$. Equation (5) is a Fredholm integral equation of the 2-nd kind for soling the direct problem – calculation of $\mathbf{E}(\mathbf{r})$ that can be expressed by Neumann series. The inverse scattering problem – to retrieve subsurface inhomogeneities $\varepsilon_1(\mathbf{r})$ by measurements of scattered field – can be solved beginning with Born approximation:

$$\mathbf{E}_1(\mathbf{r}) = -\frac{i\omega}{4\pi}\int_V \ddot{\mathbf{G}}(\mathbf{r}',\mathbf{r})\varepsilon_1(\mathbf{r}')\mathbf{E}_0(\mathbf{r}')d\mathbf{r}', \tag{7}$$

The convolution equation (6) for the probing field can be transformed in *k*-space over transversal co-ordinates:

$$\mathbf{E}_0(\kappa_x,\kappa_y,z) = 4\pi\int_{z'} \mathbf{j}(\kappa_x,\kappa_y,z')\ddot{\mathbf{G}}(\kappa_x,\kappa_y,z,z')dz', \tag{8}$$

where spectral components of Green tensors $\ddot{\mathbf{G}}(\kappa_x,\kappa_y,z,z')$ have been obtained explicitly for arbitrary multilayer media in [6]. In papers [6,7], have been considered various cases, when (7) can also be reduced to convolution equations over transversal co-ordinates, and then, using Fourier transform – to one dimensional integral Fredholm equations of the 1^{st} kind relative to $\varepsilon_1(\kappa_x,\kappa_y,z)$ that should be solved for each pair κ_x,κ_y. Then, finally, the inverse Fourier transform of obtained *k*-space distributions gives us desired solutions of initial 3D problems.

In cases of one-dimensional media, corresponding inverse problems are much simplified. Equation (5) in any case can be is reduced to one-dimensional integral equation in *k*-space:

$$\mathbf{E}(\kappa_x,\kappa_y,z)=\mathbf{E}_0(\kappa_x,\kappa_y,z)-\frac{i\omega}{4\pi}\int_{z'}\varepsilon_1(z')\ddot{\mathbf{g}}(\kappa_x,\kappa_y,z',z)\mathbf{E}(\kappa_x,\kappa_y,z')dz' \,. \quad (9)$$

However, the iterative solving of the inverse problem based on (9), as it was mention above, may lead to poor results in cases of strong inhomogeneities. So, to solve such inverse problems in frameworks of the dual regularization method, rewrite (9) as

$$\mathbf{E}^{\|,\perp}(\kappa_x,\kappa_y,z=0)=\mathbf{E}_0^{\|,\perp}(\kappa_x,\kappa_y,0)+R^{\|,\perp}[\varepsilon](\kappa_x,\kappa_y)\mathbf{E}_0^{\|,\perp}(\kappa_x,\kappa_y,0)\,. \quad (10)$$

Then, the statement of such inverse problems can be based on analysis of reflection coefficients at TH and TE polarizations of plane waves or of some functional of these coefficients that can be calculated from initial differential equations for any one-dimensional inhomogeneity. To retrieve the profile of permittivity inhomogeneities $\varepsilon_1(z)$, it is reasonable to use the frequency dependence of the informative part of reflection coefficients of a plane wave $\Delta r[\varepsilon_1](\omega)=R[\varepsilon](\omega)-R[\varepsilon_0](\omega)$, where ε_0 is a supposed permittivity of unperturbed (in general, multilayer) media. The solution is simplified, if the complex permittivity is determined by a single parameter of inhomogeneity, such as conductivity at low-frequency sounding of earth crust or a proper dimensionless coefficient *f* that determines permittivity in mixing formulas.

4. INVERSE PROBLEMS OF MEDIA DIAGNOSTICS AND OF SPECTRAL SYNTHESIS IN MULTILAYER STRUCTERES

4.1 Media diagnostics

In this statement, the problem of the medium diagnostics is formulated like this:

$$\Delta r[f](\omega)=\Delta r_0(\omega)\,, \quad (11)$$

where $\Delta r_0(\omega)$ - data of measurements. This problem is nonlinear and, to apply the dual regularization in nonlinear cases it is necessary to use modified Lagrange functions with added penalty terms – in the same way as it has been explained above. So, the modified Lagrange functional in (4) for our problem can be written as:

$$\begin{aligned}L_\mu[f](\boldsymbol{\lambda})=\|f\|^2+\int_{\Delta\omega}\left\langle\boldsymbol{\lambda}(\omega),\mathbf{\Delta r}[f](\omega)-\mathbf{\Delta r_0}(\omega)\right\rangle d\omega\\ +\mu\{\left(\int_{\Delta\omega}\left|\mathbf{\Delta r}[f](\omega)-\mathbf{\Delta r_0}(\omega)\right|^2 d\omega\right)^{1/2}+\left(\int_{\Delta\omega}\left|\mathbf{\Delta r}[f](\omega)-\mathbf{\Delta r_0}(\omega)\right|^2 d\omega\right)\},\end{aligned} \quad (12)$$

where $\langle\cdot\rangle$ is a scalar product, $\boldsymbol{\lambda}=(\lambda_1,\lambda_2)$, $\mu>0$, and, to simplify above formulas, the complex-valued $\mathbf{\Delta r}$ is considered in (12) as a two-dimensional vector of its real and imaginary parts. The role of the parameter μ is that at large enough values the minimum of modified Lagrange function $L_\mu[f](\boldsymbol{\lambda})$ over $f(z)$ exists for any $\boldsymbol{\lambda}$. Then, following [9], we write the dual problem, regularized according Tikhonov [2] that is a problem of maximization of the concave functional in the Hilbert space $L_2^2(\omega_1,\omega_2)=L_2(\omega_1,\omega_2)\times L_2(\omega_1,\omega_2)$:

$$V_\mu^\alpha[f](\boldsymbol{\lambda})=\min_{f\in D}L_\mu[f](\boldsymbol{\lambda})-\alpha\|\boldsymbol{\lambda}\|^2\to\max_{\|\lambda\|\le\mu}, \quad (13)$$

where, maximum is found over $\boldsymbol{\lambda}$ from the set $\Lambda_\mu\equiv\{\boldsymbol{\lambda}=(\lambda_1,\lambda_2)\in L_2^2(\omega_1,\omega_2):\|\boldsymbol{\lambda}\|\le\mu\}$, $D=\{f\in L_2(z_n,0):|f(z)|\le 1\}$. At the maximization of the functional in (13), one can use an element of the supergradient of this functional that can be expressed explicitly.

The problem is complicated, if the power reflection coefficient is measured [4,5,8]. In this case, phase information is lost, and (11) can be written for $\Delta r[\varepsilon_1](\omega)=|R[\varepsilon](\omega)|^2-|R[\varepsilon_0](\omega)|^2$.

4.2 Synthesis of aperiodic multilayer structures with desired reflection spectra

The proposed method can also be applied in synthesis of multilayer structures with desired reflection properties. In this case the right side of (11) should be considered as an objective function. There are no data errors in this problem; however, the objective function may be unattainable. Such an approach can be applied in multilayer optics, for example, in development of X-ray mirrors with desired reflection spectra. The problem consists of the calculation of a vector **d** of layer's depths deviations from a properly chosen initial periodic multilayer structure of two materials. In the dual regularization approach, the corresponding algorithm can be expressed as:

$$\left|R[\mathbf{d}](\omega)\right|^2 = \left|R_0(\omega)\right|^2, \tag{14}$$

In this case $\Delta r[\mathbf{d}](\omega) = \left|R[\mathbf{d}](\omega)\right|^2 - \left|R[0](\omega)\right|^2$, and the problem is formulated as

$$\Delta r[\mathbf{d}](\omega) = \Delta r_0(\omega), \tag{15}$$

$$L_\mu[\mathbf{d}](\lambda) = \|\mathbf{d}\|^2 + \int_{\Delta\omega} \lambda(\omega)[\Delta r[\mathbf{d}](\omega) - \Delta r_{\mathbf{0}}(\omega)]d\omega$$

$$+\mu\left\{\left(\int_{\Delta\omega}\left|\Delta r[\mathbf{d}](\omega) - \Delta r_{\mathbf{0}}(\omega)\right|^2 d\omega\right)^{1/2} + \left(\int_{\Delta\omega}\left|\Delta r[\mathbf{d}](\omega) - \Delta r_{\mathbf{0}}(\omega)\right|^2 d\omega\right)\right\},$$

$$V_\mu^\alpha[\mathbf{d}](\lambda) = \min_{\mathbf{d}\in D} L_\mu[\mathbf{d}](\lambda) - \alpha \,\|\, \lambda \,\|^2 \to \max_{\|\lambda\|\le\mu}$$

where $\left|R_0(\omega)\right|^2$ is an objective function. This method can provide a better convergence to desired spectra in the synthesis multilayer mirrors in various spectral bands.

5. CONCLUSIONS

A new approach in the theory of nonlinear ill-posed problems based on Kuhn-Tucker theorem is applied to reflectometry inverse problems related to analysis of subsurface diagnostics of permittivity inhomogeneities by multifrequency reflection measurements and similar problems of synthesis of dielectric structures (multilayer aperiodic mirrors) with desired reflection spectra subsurface dielectric profiling and of electromagnetic. Based on the developed theory, solving algorithms have been worked out and tested in application to reflectometry diagnostics of diffuse inhomogeneities in periodic structures of X-ray optics and to synthesis of aperiodic mirrors with desired reflection spectra that demonstrate quite good results. Similar applications could be developed in different spectral bands – low-frequency sounding of earth crust, microwave ground-penetration radar diagnostics of subsurface permittivity profiles, and multilayer optics.

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