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MATHEMATICAL INTERPRETATION OF EXPERIMENTAL RESEARCH RESULTS ON NONLINEAR OPTICAL MATERIAL PROPERTIES

The problem of mathematical interpretation of experimental research results concerning the influence of incorporated TiO_2 nanoparticles on the optical properties of the nonlinear optical material potassium dihydrogen phosphate has been formulated and solved, by using the computational physics methods. The mathematical model is reduced to a Fredholm integral equation of the first kind. A spline-iteration modification of the Landweber regularization method is suggested for solving the ill-posed problem. The results of computational experiments are compared with those of physical ones.

Keywords: incorporated TiO_2 nanoparticles, nonlinear optical material potassium dihydrogen phosphate, Fredholm integral equation, Landweber regularization method.

1. Introduction

This work is aimed at elucidating the concept of mathematical interpretation of experimental research results. The essence of the problem consists in that modern scientific data of experimental researches have to be studied more carefully, in our opinion, from the mathematical analysis viewpoint. This approach makes it possible to enrich the body of experimental information and to obtain results, whose physical meaning is deeper and more comprehensive. In this sense, a situation where the stage of physical interpretation is preceded by the stage of mathematical interpretation seems to be the best. When interpreting the results of physical measurements, there often arise problems that are called ill-posed (incorrectly formulated) in mathematics. Such problems are dealt, when the parameters of some external influences have to be determined by analyzing the regularities in physical phenomena invoked by those influences.

As a typical example, we may point to the experimental solution of the majority of spectrographic problems, when the measurements are aimed at finding a true energy distribution in the spectrum of the examined source, not distorted by a measurement device. The incorrectness of the problem in this physical situation follows from the origin of a mathematical model, which establishes relationships between true quantities and those observed with the help of real devices. Such a model is formulated in the form of a Fredholm integral equation.

It should be noted that the theory of integral equations and the practice of their application have been one of the central research objects for a lot of branches of mathematics within the last century. On the one hand, the integral equations turned out at the crossroad of many domains of abstract mathematics such as functional analysis, theory of functions, mathematical physics, algebra, computational mathematics, probability theory. On the other hand, their development was stimulated by needs of the model approach in numerous problems of physics, astrophysics, biophysics, mechanics, engineering, and other disciplines. Within the last 50 years, the main attention was paid to the development of regular methods for the solution of ill-posed problems. The latter include, first of all, the solution of Fredholm integral equations of the first kind. These equations, or their systems, arise in a considerable number of application tasks. A lot of problems can be reduced to them, e.g., the spectral composition of light radiation, processing of experimental data associated with the diagnostics of spherical or axially symmetric plasma formations, determination of a true distribution for the configurations of ternary stars, automatic regulation, research of the wave reflection from a plane interface, the problems of acoustics, kinematics, seismics, and electrodynamics, mathematical processing of images, and so on.

A specific feature of ill-posed problems consists in that small "input" errors give rise to the appearance of substantial "output" errors. However, modern mathematics takes advantage of the so-called "regularization" methods that allow the sensitivity of the result to small "input" errors to be substantially reduced (smoothed out). The application of such methods in order to interpret the results of physical measurements often makes it possible to obtain rather exact results even if an "imperfect" equipment was used. A detailed review of available results and a large bibliography can be found, for example, in books [1] and [2].

Here are some more remarks. Note first of all that, in the modern mathematical literature, integral equations are considered as a subset of operator equations. As operator equations, we may classed, for example, systems of algebraic equations. In this work, the construction of a mathematical model in the form of a Fredholm equation of the first kind is regarded as an operator equation of the first kind. Moreover, while solving the problems of giving a mathematical interpretation to the results of experimental researches, at least two approaches emerge. One of them is associated only with the elimination of the influence of imperfections in the experimental equipment on the measurement results. In other words, this approach includes the solution of the problems dealing with the reduction to the ideal equipment. The other approach in the mathematical interpretation is characterized by a necessity of obtaining the parameters of information that is supplied to the experimental system on the basis of the registered information. In this case, the inverse problem has to be solved. The problem examined in this work is an example of the latter approach.

2. Formulation of the Physical Problem

The main body of this work is devoted to the analysis of a test example illustrating the application of computational physics methods to the solution of the problem dealing with the mathematical interpretation of the results obtained in the course of experimental researches of the influence of incorporated TiO_2 nanoparticles on the optical properties of a nonlinear optical material, single crystalline matrices of potassium dihydrogen phosphate KH_2PO_4 (KDP). Owing to a unique combination of their physical properties, these materials find the wide application in modern nonlinear optics, optoelectronics, and photonics.

In the course of experiments, the angular distribution of the laser radiation intensity transmitted through a specimen (the scattering indicatrix) was measured. In other words, the distribution of the light intensity was registered. The indicatrix details contain the information on the crystal structure, the influence of nanoparticle clusters in the crystal on the laser radiation parameters, and some other properties [3].

The measurement channel of a laser installation included a G-5 goniometer and a CCD linear array (1024 pixels $25 \times 200\ \mu m^2$, the 12-bit digital resolution) with an attached wide-aperture focusing lens (the diameter $d = 0.96$ cm). The design features of the measurement channel result in that the intensity distributions observed at small angles differ substantially from their predicted true values. The wide aperture of the focusing lens distorts the data, in particular, at small measurement angles ($\theta \leqslant 2^\circ$). Since the researched specimens are weakly scattering, just this interval is the most attractive for researchers.

In order to explain the meaning of the mathematical interpretation of experimental researches at the basic level, let us first consider the experimental results obtained for the intensity distribution of laser radiation that freely propagates in air (experiment without a test specimen). Let us suppose that the discrete experimental data for the scattering indicatrix can be approximated by a continuous function (Fig. 1). One of the ultimate goals of discussed experimental researches is the determination of the influence of the incorporation of titanium dioxide nanoparticles on the parameters of a laser beam passed through a KDP crystal. It seems that the laser beam parameters could be determined directly using an installation with a fiber-optic (the fiber diameter $d = 410\ \mu$m) spectrophotometer, which allows rather an exact profile of the laser beam (Fig. 2) within the interval of about $(-1^\circ, +1^\circ)$ to be obtained. However, the difficulty consists in that those measurements consume much more resources in comparison with the former installation, so that every new set of data would demand an expensive equipment and a long laborious work.

While analyzing the results of measurements carried out with the help of a lens-equipped detector, there emerges an issue concerning the relation between the true (Gaussian) angular distribution of the intensity in the laser beam before the lens (Fig. 2) and the measured scattering indicatrix (Fig. 1). It is evident that it is impossible to establish a quantitative relationship between those distributions making no use of mathematical analysis methods. In other words, the following problem arises: How can the parameters of the curve in Fig. 2 be obtained from the experimental results depicted in Fig. 1?

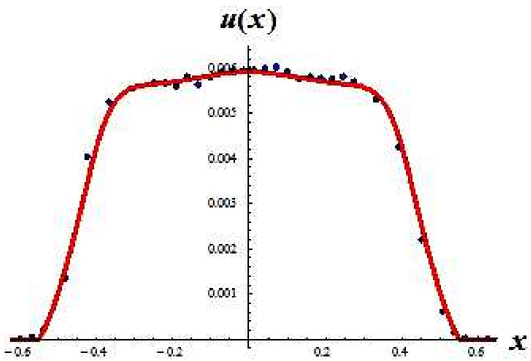

Fig. 1. Scattering indicatrix obtained with the use of a detector with a lens. $u(x)$ is the dimensionless power of laser radiation

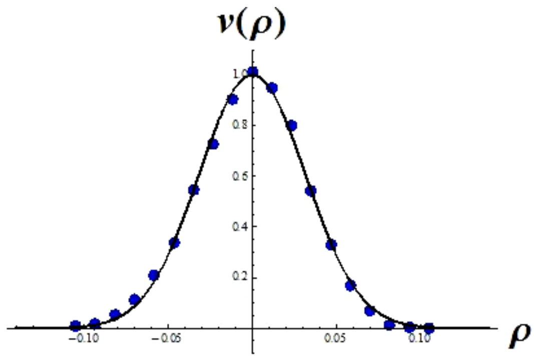

Fig. 2. Scattering indicatrix (profile of a laser beam) obtained on a high-precision installation with the use of a fiber-optic detector. $v(p)$ is the dimensionless intensity of laser radiation ($v(0) = 1$)

3. Mathematical Model for Measurement Channel of Laser Installation

The problem of mathematical interpretation of experimental research results is proposed to be solved using the method of computational physics [4]. This method includes several stages:

1) the development of a mathematical model for the measurement channel of the laser installation;

2) the verification of the mathematical model adequacy;

3) the determination of the main properties of the equations that compose the mathematical model;

4) the choice and/or the modification of the methods of solution of the inverse problem;

5) computational experiments;

6) the comparison between the results of computational and physical experiments;

7) the physical interpretation of the experimental research results.

The first two stages of the method were performed in work [3].

It will be recalled that, in the most general form, the mathematical modeling can be reduced to the construction of an operator A (of either mapping or transformation), which is interpreted as a formalization of the measurement process, when the element v (the curve in Fig. 2) is transformed into the element u (the curve in Fig. 1), i.e. $Av = u$. It should be emphasized that a physical implementation of the operator A is the measurement channel of the laser installation, namely, a G-5 goniometer, a CCD linear array, and a wide-aperture focusing lens. The formalization in this specific case is based on the assumption that the infinitesimal value of the registered radiation power can be approximated by the expression

$$\Delta u = v(P)G(O;P)\Delta S,$$

where $v(P)$ is the true radiation intensity scattered by the specimen, $G(O;P)$ is a function of the radiation transmission at the beam incidence point on the lens (it is determined by the ratio between the radiation power registered by the CCD linear array and the power of radiation incident on the lens), and ΔS is an element of the lens aperture area. Then, it is natural to evaluate the radiation power measured by the detector according to the expression

$$u(O) = \iint\limits_S v(P)G(O;P)dS, \quad (1)$$

where O is the point at the lens center.

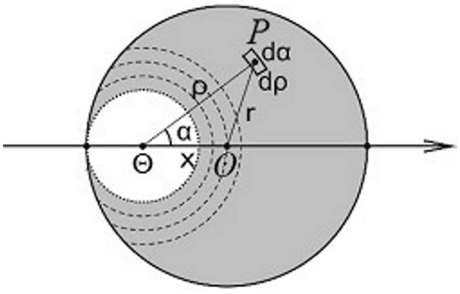

Fig. 3. Isointensity curves on the lens

Denoting the distance from the specimen to the lens as L and the rotation angle of the goniometer arm from the initial beam direction, when the beam center Θ coincides with the lens center O, as θ_0, we may accept the coordinate of the lens center to equal $x = L\sin\theta_0 \approx L\theta_0$, and, with an error not exceeding 0.1% ($L = 20$ cm, $|x| \leqslant 0.7$ cm), write the relation

$$r^2 = \rho^2 + x^2 - 2\,\rho\, x\cos\alpha,$$

where r is the polar radius of an arbitrary point of the lens aperture reckoned in the coordinate system with the origin at the lens center O ($r = |OP|$), ρ is the polar radius of this point with respect to the center Θ of the laser beam ($\rho = |\Theta P|$), and α is the corresponding polar angle. In this case, expression (1) acquires the form

$$u\,(x) = \iint\limits_S v(s,t)\tilde{G}(x;s,t)\,ds\,dt,\quad x \in [-a,a], (a \leqslant 0.7\text{ cm}), \tag{2}$$

where the coordinate origin coincides with the beam center Θ, x is the coordinate of lens center, and $s = \rho\cos\alpha$ and $t = \rho\sin\alpha$ are the coordinates of an arbitrary point of the lens aperture.

Owing to the isotropy of studied specimens, the intensity distribution is axially symmetric. Therefore, the isointensity curves are circles with the radius $\rho = L\sin\theta \approx L\theta$, so that relation (2) is expedient to be expressed in the polar coordinate system,

$$u(x) = \int\limits_{\rho_1(x)}^{\rho_2(x)} \rho v(\rho) \int\limits_{\alpha_1(x,\rho)}^{\alpha_2(x,\rho)} G(x;\rho,\alpha)d\rho d\alpha,\quad x \in [-a,a], \tag{3}$$

where $\alpha_1(x,\rho), \rho_1(x)$ and $\alpha_2(x,\rho), \rho_2(x)$ are the corresponding limiting values of $\alpha(x,\rho)$, $\rho(x)$ (Fig. 3). In addition, the radiation transmission function $\tilde{G}(x;s,t)$ at the point P of laser beam incidence on the lens is supposed to be a characteristic of the measurement process; it is equal to the ratio between the registered radiation power and the radiation power incident on the lens and depends on the distance to the lens center r:

$$\tilde{G}(x;s,t) = \hat{G}(r) = \hat{G}((\rho^2 + x^2 - 2\rho x\cos\alpha)^{1/2}) = G(x;\rho,\alpha). \tag{4}$$

The function $\hat{G}(r)$ can be determined directly, because the beam diameter ($\delta \approx 0.9$ mm) is much smaller than the lens size. In the analyzed example, the function $\hat{G}(r)$ was determined with the use of experimental data (Fig. 1) for the profile of a laser beam that freely propagates in air. They can be approximated by a continuous function, the form of which is close to the real transmission function, since $\delta \ll d$. It should be noted that, by definition, the shape of the function $\hat{G}(r)$ curve is completely similar to the scattering indicatrix (Fig. 1).

For the approximation of experimental values, the following set of functions was used: Gaussian, parabola, and "hat" [5]. Therefore, the sought function $\hat{G}(r)$ can approximately be written as follows:

$$\hat{G}(r) = \chi_1(R_1^2 - r^2)\Bigg(A\exp((r/r_A)^2) - (r/r_B)^2 - C\exp\left(-\frac{(r/r_C)^2}{1-(r/r_H)^2}\right)\chi_0(r_H^2 - r^2)\Bigg), \tag{5}$$

where $R_1 = 0.55089$ cm, $A = 2.223$, $C = 1.277$, $r_A = 0.5808$ cm, $r_B = 0.2357$ cm, $r_C = 0.3574$ cm, $r_H = 0.4711$ cm, and $\chi(s)$ is the Heaviside function:

$$\chi_1(s) = \begin{cases}1, & s \geqslant 0,\\ 0, & s < 0,\end{cases} \qquad \chi_0(s) = \begin{cases}1, & s > 0,\\ 0, & s \leqslant 0.\end{cases}$$

The corresponding relative root-mean-square approximation error amounts to 3.6%. Since the laser beam diameter does not equal zero, we used the value $R_1 = 0.5509$ cm ($R_1 > R$) in calculations. The function $G(x,\rho,\alpha)$ is symmetric (see Eq. (4)); therefore, the internal integral in Eq. (3) can be calculated as follows:

$$K_\rho(x,\rho) = \int\limits_0^{\alpha_2(x,\rho)} G(x,\rho,\alpha)d\alpha = \frac{1}{2}\int\limits_{\alpha_1(x,\rho)}^{\alpha_2(x,\rho)} G(x,\rho,\alpha)d\alpha.$$

For the same reason, it is clear that $\alpha_1(x,\rho) = -\alpha_2(x,\rho)$. Using the relation for the triangle sides, the upper integration limit, $\alpha_2(x,\rho)$, can be found,

$$\alpha_2(x,\rho) = \begin{cases} \arccos\left(\frac{\rho^2+x^2-R_1^2}{2\,\rho\,x}\right), & \rho + x > R_1, \\ \pi, & \rho + x \leqslant R_1. \end{cases}$$

Now, we can calculate the internal integral in Eq. (4):

$$K(x,\rho) = \int\limits_0^{\alpha_2(x,\rho)} G(x,\rho,\alpha)d\alpha = \frac{1}{2}\int\limits_{\alpha_1(x,\rho)}^{\alpha_2(x,\rho)} G(x,\rho,\alpha)d\alpha.$$

Taking this expression into account (Fig. 4), the integral relation (3) can be rewritten in the form

$$u\,(x) = 2\int\limits_{\rho_1(x)}^{\rho_2(x)} \rho\, v(\rho)\, K_\rho(x,\rho)\, d\rho, \quad x \in [-a, a].$$

While determining the limits of integration $\rho_1(x)$ and $\rho_2(x)$, two possible variants of the lens arrangement with respect to the laser beam center have to be considered. In one of them, the beam center is located in a circle with the radius $R_1{:}x \leqslant R_1$ (Fig. 3). In the other, the beam center is beyond the circle, i.e. $x > R_1$.

In work [3], it was shown that the mathematical model for the measurement channel of laser installation is ultimately reduced to a Fredholm integral equation of the first kind,

$$u\,(x) = \int\limits_0^b K(x,\rho)\, v(\rho)\, d\rho, \quad x \in [-a, a], \tag{6}$$

where $K(x,\rho) = 2\rho K_\rho(x,\rho)$, and $b = 2R_1$. The free term $u\,(x)$ in Eq. (6) is supposed to be a given function in the real Hilbert space $L_2[-a,a]$, and the sought function $v(\rho)$ is an element of the real Hilbert space $L_2[0,b]$.

4. Verification of Mathematical Model Adequacy

To verify the reliability of the mathematical model for the measurement channel of the laser installation for optical diagnostics, we used the Fredholm first-kind integral equation (6) with the kernel $K(x,\rho) = 2\rho K_\rho(x,\rho)$ and the data describing a true intensity distribution in the scattered laser beam, $v(\rho)$. To obtain the intensity distribution function $v(\rho)$, an optical fiber with small aperture (the diameter $d = 410\ \mu$m) was used as a measurement channel. The theoretical values of the function $\bar{u}(x)$ were obtained by directly calculating integral (6). They were compared with the experimentally registered and approximated scattering indicatrix $u(x)$.

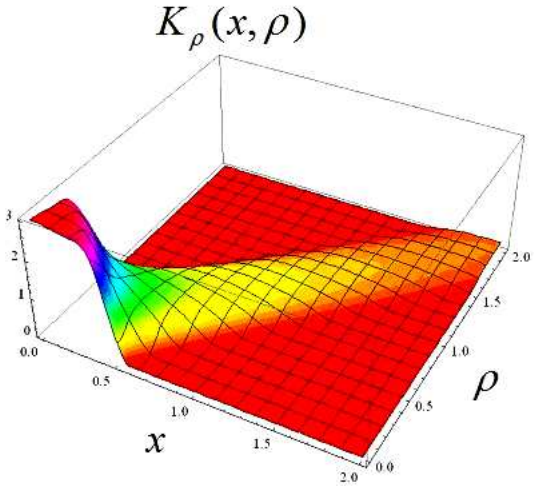

Fig. 4. Instrument function $K_\rho(x,\rho)$

A series of experiments were carried out, in which, in particular,

a) the scattering of the laser beam propagating in air (without a specimen) and

b) the scattering of the laser beam after its passage through a wafer of the KDP crystal with TiO_2 impurities were studied. In all series of measurements, laser beams had a Gaussian distribution of intensity,

$$v(\rho) = a_k \exp\left(-\left(\rho/\rho_k\right)^2\right), \quad k = 1, 2,$$

with $\rho_1 = 0.0447214$ cm and $\rho_2 = 0.0421182$ cm.

In Fig. 5, the solid curve demonstrates the plot of the function $\bar{u}\,(x)$ obtained with the use of formula (6) with the kernel $K(x,\rho) = 2\rho K_\rho(x,\rho)$ corresponding to this experiment and the function $v(\rho)$ at $k = 2$. The symbols in the figure correspond to experimental values of radiation power transmitted through the lens. The approximation error for the results obtained did not exceed 5%.

In Fig. 6, the theoretical dependences of the laser radiation intensity $\bar{u}\,(x)$ and the corresponding approximated analogs of the scattering indicatrix $u(x)$

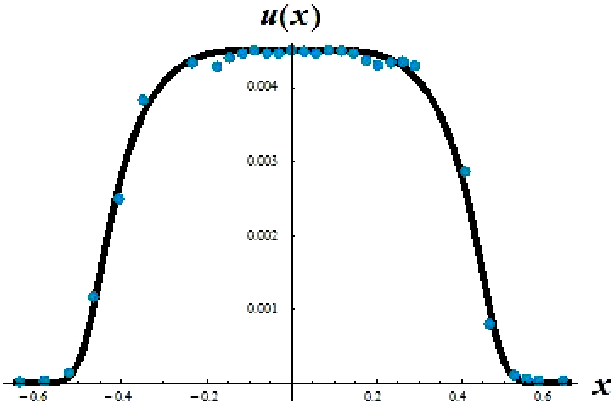

Fig. 5. Theoretical curve (formula (6)) for the distribution of radiation intensity at studying a KDP crystal with TiO_2. Disks correspond to the experimental data obtained with a detector and a lens

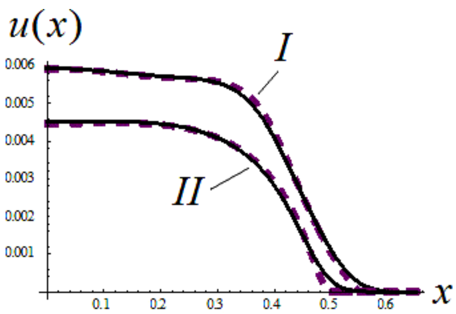

Fig. 6. Theoretical curves for the laser radiation intensity distributions and the scattering indicatrices (dashed curves): variants a (I) and b (II)

are exhibited. The upper curves correspond to the radiation intensity without a specimen, whereas the lower ones to the radiation intensity after the laser beam transmission through a wafer of the KDP crystal with TiO_2 impurities.

On the basis of the presented data, a conclusion can be drawn concerning the reliability of the mathematical model (6) for the description of the measurement channel of the laser installation created on the basis of a G-5 goniometer and a detector (a CCD linear array and a focusing lens) for the optical diagnostics of weakly scattering specimens.

5. Incorrectness of the Problem

The mathematical formulation of the problem concerning the mathematical interpretation of the experimental research results obtained for the influence of incorporated TiO_2 nanoparticles on the optical properties of the nonlinear optical material KDP is made as follows. The radiation power measured by the detector, $u(x)$, is connected with the true radiation intensity scattered by the specimen, $v(\rho)$, by means of the operator equation

$$u = Av, \quad u \in L_2[-a,a], \quad v \in L_2[0,b], \tag{7}$$

where A is the Hilbert–Schmidt operator [6], provided that the kernel $K(x,\rho)$ of Eq. (6) belongs to the space $L_2([-a,a]\times[0,b])$, i.e.

$$\int\limits_0^b \int\limits_{-a}^a (K(x,\rho))^2\, dx\, d\rho < \infty. \tag{8}$$

The research of the properties of Eq. (6) is reduced to the study of properties of the operator A.

Theorem 1. *The Hilbert–Schmidt operator A with the square-integrable kernel $K(x,\rho)$ is a compact linear operator in a Hilbert space with the norm satisfying the inequality*

$$||A|| \leqslant \left(\int\limits_0^b \int\limits_{-a}^a (K(x,\rho))^2\, dx\, d\rho\right)^{1/2} \tag{9}$$

(see work [6]).

Actually, instead of the exact data $K(x,\rho)$ and $u(x)$, we know only their approximations $\tilde{K}(x,\rho)$ and $u_\delta(x)$, for which

$$\int\limits_0^b \int\limits_{-a}^a \left(\tilde{K}(x,\rho)\right)^2 dx\, d\rho < \infty, \quad \|u - u_\delta\| \leqslant \delta. \tag{10}$$

Therefore, while carrying out computational experiments, the initial mathematical formulation (7) of the problem concerning the mathematical interpretation of experimental research results can undoubtedly be written in the form of an approximate operator equation with error level δ, h:

$$A_h v = u_\delta, \quad u_\delta \in L_2[-a,a], \quad v \in L_2[0,b], \tag{11}$$

where $\|u - u_\delta\| \leqslant \delta$ and $\|A - A_h\| \leqslant h$. In this case, the norm of the operator A_h satisfies the inequality

$$||A_h|| \leqslant \left(\int\limits_0^b \int\limits_{-a}^a \left(\tilde{K}(x,\rho)\right)^2 dx\, d\rho\right)^{1/2}. \tag{12}$$

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Hence, we may assert that Eq. (11) is an operator equation of the first kind, where $A_h \in \Lambda(V, U)$ is the linear compact operator from the Hilbert space $V = L_2[0, b]$ to the Hilbert space $U = L_2[-a, a]$, $u_\delta \in \in U$ is a given element, $v \in V$ is a sought element, and $\Lambda(V, U)$ is the space of all finite linear operators determined on V.

The compactness of the operator A_h is of principal importance from the viewpoint of choosing a method and constructing an algorithm for the solution of the first-kind operator equation (11), since the compact operator A_h in an infinite-dimensional space V has no finite inverse operator A_h^{-1} in the space U [6]. However, this means that a formal inversion of Eq. (11) or an attempt to find a solution of problem (11) in the form $v = A_h^{-1} u_\delta$ would not result in satisfactory results under real experimental conditions, because infinitesimally small variations in registered results associated with the experimental procedure would give rise to an arbitrarily large deviation in the reconstructed function $v(\rho)$. Therefore, the solution of problem (11) is unstable, and the problem itself is an Hadamard ill-posed one [7–10].

The problem

$$u = Av, \quad u \in U, \quad v \in V, \quad A \in \Lambda(V,\, U),$$

is called Hadamard well-posed if three conditions are satisfied:

1) the range of values of the operator A, Range(A), coincides with U, i.e. Range(A) $= U$ (solvability condition),

$$\text{for } \forall\, u \in U \quad \exists\, v \in V;$$

2) from the equality $Av_1 = Av_2$ for some $v_1, v_2 \in V$, it follows that $v_1 = v_2$ (uniqueness condition),

$$\text{for } \forall\, v_1, v_2 \in V : Av_1 = Av_2 \Rightarrow v_1 = v_2;$$

3) the inverse operator A^{-1} is continuous on U (stability condition),

$$\lim_{\substack{\delta\to 0\\ h\to 0}} \sup_{\substack{u_\delta : ||u-u_\delta||_U \leqslant \delta\\ A_h : ||A-A_h||_{V\to U} \leqslant h}} \inf_{v\in A^{-1}u} \left\| v - A_h^{-1} u_\delta \right\|_V = 0.$$

In the case where at least one of those conditions is violated, the problem is called ill-posed or, simply, incorrect. In the practice of experimental researches, this is the third condition that is violated most often. At the mathematical modeling, it can be formulated as follows: Insignificant variations in the input data (A, u) can give rise to arbitrarily large changes in the output data (v).

In order to overcome the incorrectness of the problem, let us introduce a regularizing operator $R_\alpha(\delta, h, A_h)$ [5], for which

$$\lim_{\substack{\delta\to 0\\ h\to 0}} \sup_{\substack{u_\delta : ||u-u_\delta||_U \leqslant \delta\\ A_h : ||A-A_h||_{V\to U} \leqslant h}} \inf_{v\in A^{-1}u} \|v - R_\alpha(\delta, h, A_h) u_\delta\|_V = 0,$$

where $A^{-1}u$ is the complete preimage of an element u, and α is the regularization parameter.

Now, after the mathematical model has been formulated and a conclusion about the reliability of the mathematical model (6) for the measurement channel of a laser installation for optical diagnostics of weakly scattering specimens created on the basis of a goniometer G-5 and the detector consisting of a CCD linear array and a focusing lens has been made, we proceed to the stage of the inverse problem solution, namely, the determination of the function $v(\rho)$ on the basis of the known $u(x)$ and $K(x, \rho)$. In the operator representation, this problem looks like Eq. (7) and is ill-posed.

In order to obtain an approximate solution of Eq. (11) in the framework of the specific problem under consideration, the iterative Landweber method was chosen (see Eq. (II.8)):

$$v_k = (E - \mu\, A_h^* A_h) v_{k-1} + \mu\, A_h^* u_\delta,$$
$$k = 1,\, 2, ...;\; (0 < \mu < 2/\, \|A_h\|^2),\; v_0 = 0.$$

Sound arguments in favor of this choice are the simplicity of the software code implementation of the method, as well as a high level of computation compatibility and a sufficient level of efficiency with respect to both the required iteration number and the approximate solution accuracy. The realization of the Landweber method needs in the initialization of the regularization parameter α determining the termination of the iterative process.

A physical feature of the problem is the condition

$$v(\rho) \geqslant 0, \quad \forall\, \rho \in (-\infty, \infty). \tag{13}$$

In this work, we propose an approach of the *a posteriori* determination of the iteration number k_*. It is based on the application of the smoothing functional (Tikhonov parametric functional, see Eq. (I.3))

$$\Phi_\alpha[v, u_\delta] = \|A\, v - u_\delta\|_U^2 + \alpha\, \Omega\, [v],$$

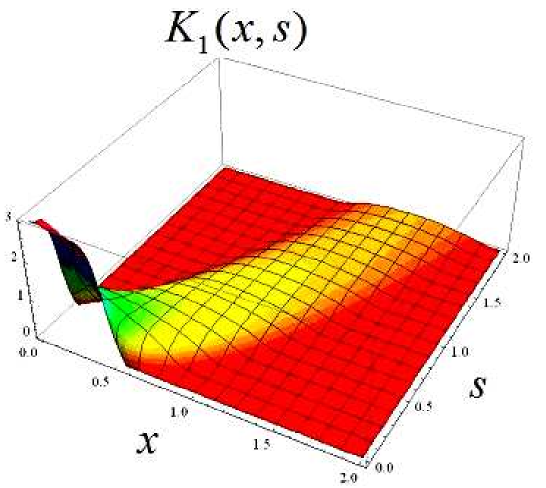

Fig. 7. Kernel of the integral equation (16)

where $\Omega[v]$ is the stabilizing functional, and α is the regularization parameter, together with the discrepancy principle (see Eq. (II.10))

$$\| Av_{k_*} - u_\delta\| \in [a_1\delta,\, a_2\delta].$$

Concerning the exact solution $v(\rho)$ of Eq. (6), the statement that this solution is continuous on $[0, b]$, has a continuous derivative, and is square-integrable on $[0, b]$ is valid *a priori*. Therefore, we may suppose that the space V is a Hilbert–Sobolev space: $V = W_2^1[0, b] = H^1[0, b]$. Under such a formulation, the stabilizing functional $\Omega\,[v]$ and the Tikhonov parametric functional $\Phi_\alpha[v, u_\delta]$ can be presented in the form (see Eq. (I.8))

$$\begin{aligned}
&\Omega\,[v] = \|v\|^2_{W_2^1},\\
&\Phi_\alpha[v, u_\delta] = \quad ||A_h\, v - u_\delta||^2_{L_2} + \alpha\,\|v\|^2_{W_2^1} =\\
&= \int\limits_{-a}^{a}\left[\int\limits_{0}^{b}\tilde{K}(x,\rho)v(\rho), d\rho - u_\delta\right]^2 d\,x+ \\
&+\alpha\int\limits_{0}^{b}\left[v^2(\rho) + [[v'(\rho)\right]^2]d\rho.
\end{aligned} \tag{14}$$

The number k_* is determined, e.g., from the condition that the functional $S_S(v_k, u_\delta) = |\Omega_S\,[v_k] - 1.0|$ has the extreme value on v_{k_*}:

$$v_{k_*} = \arg\,[\inf_k\ S_S[v_k, u_\delta]],$$

$$\Omega_S\,[v_k] = \frac{\|v_k\|^2_{W_2^1}}{\|\exp\,(-500.0\rho^2)\|^2_{W_2^1}}. \tag{15}$$

6. Computational Experiments

At the computational experiment stage, a new unknown function, $w(s) = v(\sqrt{s})$, is introduced, by making the substitution $s = \rho^2$. Then

$$\begin{aligned}
&u\,(x) = \int\limits_{0}^{b^2} w(s)\,K_1(x,s)\,ds,\\
&K_1(x,s) = K_\rho(x,\sqrt{s}).
\end{aligned} \tag{16}$$

In the absence of a specimen, the profile of the function $K_1(x, s)$ is shown in Fig. 7.

It should be emphasized that, while constructing the regularizing algorithm, only the following additional information was used:

$$w(s) \geqslant 0, \quad \forall\, s \in (-\infty, \infty).$$

The algorithm of the Landweber method is formulated as follows:

$$\begin{aligned}
&w_0(s) = \tilde{w}_0(s),\\
&w_m(s) = w^+_{m-1}(s) + \eta\,\big[F(s) -\\
&-\int\limits_{0}^{\alpha_s}\Re(s,t)\;w^+_{m-1}(t)\,dt\big],\; m = 1, 2, ...,\\
&w^+_m(s) = \,(w_m(s) + |w_m(s)|)/2,\\
&0 < \eta < 2/\,\|A_1^*A_1\|\,,\\
&F(s) = \int\limits_{0}^{\alpha_s} K_1(x,s)u_\delta(x)dx, \quad \alpha_s = a + R_1,\\
&\Re(t,s) = \Re(s,t) = \int\limits_{0}^{b^2} K_1(x,t)\,K_1(x,s)\,dx,\\
&||A_1^*A_1||^2 = \;||\Re(t,s)||^2 \leqslant \int\limits_{0}^{\alpha_s}\int\limits_{0}^{\alpha_s}\Re^2(t,s)\,dt\,ds.
\end{aligned} \tag{17}$$

A series of computational experiments was carried out, in which the quantities β_n, the multipliers in the arguments of Gaussian functions,

$$v_n(\rho) = a_n\exp\Big(-\left(\rho/\rho_n\right)^2\Big) = a_n\exp\left(-\beta_n\rho^2\right);$$

$$a_n = 1; \quad n = 1, 2,$$

were determined. Those functions simulate the intensity distributions in a laser beam in the cases where

a) the laser beam propagates without a specimen, and

b) the laser beam passed through a wafer of the KDP crystal with TiO_2 impurities.

To monitor the accuracy of solving the problem with the help of the regularizing Landweber algorithm (17),

1) the discrepancy functional $\|A_h\, w_k - w_\delta\|_{L_2}$,

2) the Tikhonov stabilizing functional $\Omega[w_k] = \|w_k\|^2_{L_2}$, and

3) the Sobolev stabilizing functional $\Omega[w_k] = \|w_k\|^2_{W_2^1}$

were used.

The exact values of *a posteriori* known multipliers in the arguments of exponential functions are

$$\bar{\beta}_1 = 500.0, \quad \bar{\beta}_2 = 563.717200778126.$$

In the both indicated calculation variants, the function

$$\tilde{w_0}(s) = \exp(-20.0s)$$

was taken as a zeroth-order approximation.

In Fig. 8, to illustrate the application of the Tikhonov stabilizator

$$\Omega_{\rm T}[w_k] = \frac{\|w_k\|^2_{L_2}}{\|\exp(-500.0s)\|^2_{L_2}},$$

the plot of the function $S_{\rm T}(k) = |\Omega_{\rm T}[w_k] - 1.0|$, $(k = \overline{26, 51})$ is shown.

The Sobolev stabilizator was also used in a similar way (Fig. 9):

$$\Omega_{\rm S}[w_k] = \frac{\|w_k\|^2_{W_2^1}}{\|\exp(-500.0\, s)\|^2_{W_2^1}},$$

$$S_{\rm S}(k) = |\Omega_{\rm S}[w_k] - 1.0|\,.(k = \overline{26, 51}\,).$$

The results of the computational experiment according to algorithm (17) are as follows:

$$\tilde{\beta}_1(k = 40) = 499.9999988285064,$$

$$\tilde{\beta}_2(k = 61) = 563.7172007781256.$$

A comparison of the values obtained for the coefficients in the exponential function arguments with the exact ones speaks for itself. In effect, we obtained asymptotically exact solutions of Eq. (7) or, in other words, normal solutions (I.7) of this equation:

$$v_n^\dagger(\rho) = \exp\left(-\bar{\beta}_n \rho^2\right), \quad n = 1, 2.$$

The errors $\Delta_n = \left|\bar{\beta}_n - \tilde{\beta}_n\right|$ can be interpreted as a result of the number rounding in the computer representation.

Of undoubted interest is the answer to the question about the error magnitude for the solution of Eq. (11) with an inexact right-hand side,

$$Av = u_\delta. \qquad (18)$$

When studying the influence of the error in the right-hand side of Eq. (18) on the solution $v(\rho)$, as the "output" function, we took a function that interpolates the experimental values of scattering indicatrix after the beam passage through the KDP crystal with TiO_2 impurities (Fig. 10). The corresponding mean-square approximation error equals $\delta = 0.051127$.

As a result of calculations, we obtained the following value of multiplier in the exponential function argument: $\tilde{\tilde{\beta}}_2\,(k = 31) = 556.412$. The rela-

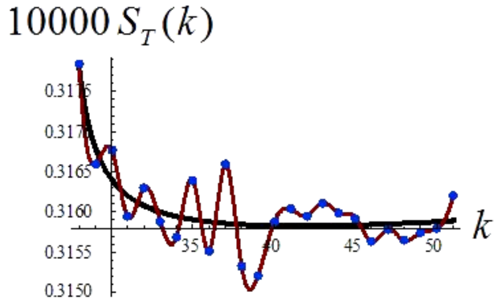

Fig. 8. Plot of the function $S_{\rm T}(k) = |\Omega_{\rm T}[w_k] - 1.0|$

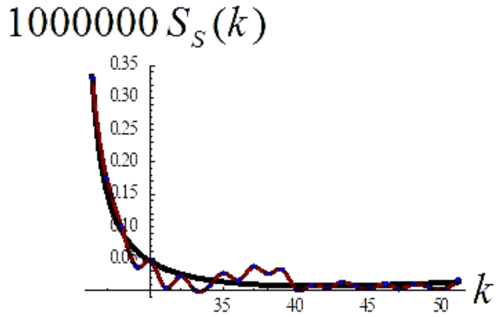

Fig. 9. Plot of the function $S_{\rm S}(k) = |\Omega_{\rm S}[w_k] - 1.0|$

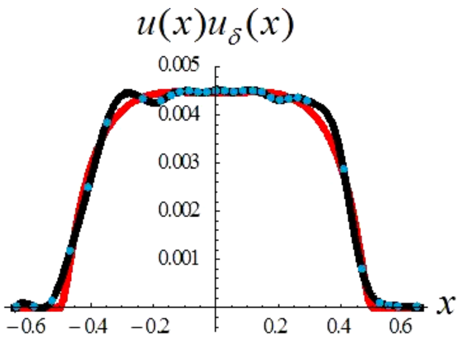

Fig. 10. Exact, $u(x)$, and approximate, $u_\delta(x)$, functions of the scattering indicatrix

tive mean-square approximation error for the function $\tilde{\tilde{v}}_2(\rho)$ equals 0.00925329, which is by a factor of 5.5 less than the approximation error of the function u_δ.

7. Conclusions

A mathematical model in the form of a Fredholm integral equation of the first kind for the measurement channel of the experimental laser installation has been formulated for the mathematical interpretation of experimental research results concerning the influence of TiO_2 nanoparticles on the optical properties of a nonlinear optical material. The verification of the adequacy of the mathematical model confirmed its reliability to an accuracy of nine significant digits. The theory of spline-iterative methods of computational physics for the solution of the problem of mathematical interpretation of experimental research results is developed, and a spline-iterative modification of the Landweber regularization method is elaborated.

The parameters of a laser beam obtained experimentally on the installation with a fiber optical spectrophotometer are confirmed by computational experiments. The mathematical interpretation of the experimental results revealed the self-focusing of a laser beam owing to the presence of TiO_2 impurities.

The solution of the problem concerning the mathematical interpretation of experimental research results can be regarded as the creation of a virtual high-precision experimental equipment. This approach makes it possible to obtain essentially significant physical results, which is impossible with the use of available facilities.

APPENDIX I

Let us consult the fundamentals of the mathematical analysis of modern scientific data concerning experimental researches in general physics. While carrying out experimental researches in laser physics, nonlinear optics, and quantum optics, instead of exact problem data A and u, only their approximation with the error levels δ and h are known:

$$||u - u_\delta|| \leqslant \delta, \quad ||A - A_h|| \leqslant h,$$

i.e. instead of the exact operator equation,

$$u = A\,v, \quad u \in U, \quad v \in V, \quad A \in \Lambda(V,\, U), \tag{I.1}$$

the approximate operator equation

$$A_h v = u_\delta, \quad u_\delta \in U, \quad A_{\,h} \in \Lambda(V,\, U). \tag{I.2}$$

is solved.

The constructive solution of the problem consists in the approximation of the normal solution of Eq. (I.1), i.e. the solution of Eq. (I.1) with the minimum norm in the space V,

$$v^\dagger \in \mathrm{Range}(A^\dagger) = \overline{\mathrm{Range}(A^*)} = \mathrm{Ker}(A)^\perp,$$

by the approximate solution of Eq. (I.2). Here, $A^\dagger$ is a linear operator pseudo-inverse to the operator A, i.e.

$$A^\dagger : \mathrm{Range}(A) \oplus \mathrm{Range}(A)^\perp \to V, \mathrm{Range}(A^\dagger) =$$
$$= \overline{\mathrm{Range}(A^*)} = \mathrm{Ker}(A)^\perp.$$

The operator $A^\dagger$ is continuous, if $\mathrm{Range}(A) = \overline{\mathrm{Range}(A)}$. The following statement is valid [8]: the normal solution $v^\dagger = A^\dagger u (u \in \mathrm{Range}(A) \oplus \mathrm{Range}(A)^\perp)$ is the unique solution of the equation $A^*Av = A^*u$ $(v \in \overline{\mathrm{Range}(A^*)})$.

As a rule, the mathematical models of type (I.1) in experimental researches of laser physics, nonlinear optics, and quantum optics have the property $\mathrm{Range}(A) \neq \overline{\mathrm{Range}(A)}$ (e.g., if A is a linear compact operator), i.e. solving the operator equation $Av = u$ is an ill-posed problem. The problem of stable approximation to the exact solution of Eq. (I.1) at imperfect input data $u_\delta \in U$, $A_h \in \Lambda(V, U)$, $\|u - u_\delta\| \leqslant \delta$, $\|A - A_h\| \leqslant h$ with known δ and h can be solved, only by using one of the regularization methods. Among them, a key role is played by the method, the theoretical basis of which was created by A.N. Tikhonov. According to this method, in order to solve Eq. (I.2), a smoothing functional (Tikhonov parametric functional) is introduced [7]:

$$\Phi_\alpha[v, u_\delta] = \quad ||A_h v - u_\delta||_U^2 + \alpha\Omega[v], \tag{I.3}$$

where $\Omega\,[v]$ is the stabilizing functional (the stabilizator; as a rule, $\Omega\,[v] = \|v\|_V^2$), $0 < \alpha < 1$ is the regularization parameter, and $\|A_h v - u_\delta\|_U^2$ is a discrepancy of Eq. (I.2) on the element v.

An element v_α is determined, on which functional (I.3) has a minimum, i.e.

$$\Phi_\alpha[v_\alpha, u_\delta] = \inf_{v \in V} \Phi_\alpha[v, u_\delta]. \tag{I.4}$$

If $\Omega\,[v] = \|v\|_V^2$ in the Tikhonov functional (I.3), the Euler equation has rather a simple form,

$$\alpha\, v_\alpha + A_h^* A_h v_\alpha = A_h^* u_\delta. \tag{I.5}$$

In addition,

$$v_\alpha = (\alpha E + A_h^* A_h)^{-1} A_h^* u_\delta = R_\alpha u_\delta, \qquad (I.6)$$

where $R_\alpha = (\alpha E + A_h^* A_h)^{-1} A_h^*$. If $(\delta, h) \to 0$. Then, according to the definition of regularization operator, there must be $\alpha \to \to 0$. Therefore,

$$v^\dagger = \lim_{\alpha \to 0} (\alpha E + A^* A)^{-1} A^* u \qquad (I.7)$$

should be taken as a solution of problem (I.4), if $\Omega[v] = \|v\|_V^2$.

Solution (I.7) is a normal one, i.e., if v and A are exact, the normal solution of all solutions of the equation

$$A\,v = u, \quad v \in V, \quad u \in U$$

is selected in the Tikhonov method. Formula (I.7) can be rewritten in a different form:

$$v^\dagger = A^\dagger u,$$

where $A^\dagger = \lim_{\alpha \to 0} (\alpha E + A^* A)^{-1} A^*$ is the operator pseudo-inverse to the operator A. If $\delta \neq 0$ and/or $h \neq 0$, the method brings about a solution v_α, which is an approximation to the normal solution $v^\dagger$. The following statement is valid for the approximation and regularization properties of R_α [11].

Theorem 2. *Let $v^\dagger \in V$ be a normal solution of Eq. (I.1). In the framework of method (I.6), if $\alpha(\delta, h) \to 0$ and $\lim_{\delta,h \to 0} \frac{h^2+\delta^2}{\alpha(\delta,h)} = 0$, then $\lim_{\delta,h\to 0} \left\|v_{\alpha(\delta,h)} - v^\dagger\right\| = 0$.*

The space that is used most often in applied calculations is the Hilbert space $L_2\,(G)$. It consists of the classes of functions that are equivalent among themselves and are Lebesgue square integrable, i.e. the integral $\int_G |u|^2(x)dx$ is definite and finite [6]. The scalar product on the space $L_2\,(G)$ of real functions is given by the equality

$$(u, v) = \int_G u(x)\, v(x)\, dx.$$

In optics problems, where unknown functions are rather smooth, Sobolev spaces are widely used [12]. The Sobolev space $W_p^k\,(G)$ is a functional space that includes functions from the Lebesgue space $L_p\,(G)$. These functions have generalized derivatives up to a given order, which also belong to $L_p\,(G)\,(G \subset R^n)$. In other words, $W_p^k\,(G)$ is a space of functions $u = u(x) = u(x_1, x_2, ..., x_n))$ determined on a set $G \subset R^n$, for which the p-th power of their absolute value and their generalized derivatives up to the k-th order inclusive are integrable. Sobolev spaces are Banach ones at $1 \leqslant p \leqslant \infty$ and Hilbert ones at $p = 2$ (in the latter case, they are denoted, as a rule, as $H_k\,(\Omega)$). The norm of the function $u \in W_p^k\,(\Omega)$ is introduced by the formula

$$\|u\|_{W_p^k G)} = \left(\sum_{0 \leqslant |\sigma| \leqslant k} \int_G |D^\sigma u|^p \right)^{1/p} =$$

$$= \sum_{0 \leqslant |\sigma| \leqslant k} ||D^\sigma u||_{L_p(G)} (1 \leqslant p < \infty), \qquad (I.8)$$

where $\sigma = (\sigma_1, \sigma_2, ..., \sigma_n)$ is a multiindex, and

$$D^\sigma u = \frac{\partial^{|\sigma|} u}{\partial\, x_1^{\sigma_1} \partial\, x_2^{\sigma_2} ... \partial\, x_n^{\sigma_n}}$$

is the partial derivative of the order $|\sigma| = \sum_{m=1}^{n} \sigma_m$ $(D^{(0)} u = u)$. The scalar product in $H_k\,(\Omega)$ is defined by the expression

$$(u, v) = \sum_{0 \leqslant |\sigma| \leqslant k} (D^\sigma u, D^\sigma v).$$

Sobolev spaces have a fundamental value in the theory and practice of numerical methods, variational problems, the theory of partial differential equations, theory of functions, approximation theory, control theory, and many other domains of mathematical analysis and its appendices.

APPENDIX II

As a rule, there are several methods to solve that of another complicated problem. This remark fully concerns an ill-posed problem. In this case, it is expedient to refer to the important class of regularizing algorithms proposed by A.V. Bakushinsky [11]. The idea of the approach consists in the construction of a parametric family of functions $\mathrm{G} = \{g_\alpha(\lambda), \alpha \in (0, 1)\}$ that are Borel-measurable on the half-axis $[0, \infty)$ and satisfy, at $\forall \upsilon \in [0, \upsilon_*]$, the conditions

$$\sup_{0 \leqslant \lambda < \infty} \lambda^\upsilon |1 - \lambda g_\alpha(\lambda)| \leqslant \chi_\upsilon\, \alpha^\upsilon, \qquad (II.1)$$

$$\sup_{0 \leqslant \lambda < \infty} \sqrt{\lambda} |g_\alpha(\lambda)| \leqslant \chi_* \alpha^{-1/2}, \qquad (II.2)$$

where υ_*, χ_υ, and χ_* are positive constants independent of α. The system of functions G is called generating for the regularization method,

$$R = R_\alpha = g_\alpha(A_h^* A_h)\, A_h^*, \quad g_\alpha \in \mathrm{G}. \qquad (II.3)$$

The parameter υ_* of the function g_α is called the qualification of the method R_α, and the parameter $\alpha = \alpha(\delta, h)$ the regularization parameter. Regularizators (II.3) make it possible to reach the optimum order of accuracy on the classes of equations (I.1) with source-representable solutions. While studying the problem of constructing optimum methods to solve the ill-posed equation (I.1), a central-symmetric set M is introduced into consideration; in the theory of ill-posed problems, it looks like [13]

$$\mathrm{M}_{\upsilon,\rho}(A) := \{z : z = |A|^\upsilon w, \ ||w||_V \leqslant \rho\},$$

where $\upsilon > 0$, $\rho > 0$, and $|A| = (A^* A)^{1/2}$.

The elements of the set $\mathrm{M}_{\upsilon,\rho}(A)$ are called source-representable. It is known that, if Eq. (I.1) has a source-representable solution $v^\dagger \in \mathrm{M}_{\upsilon,\rho}(A)$, then $v^\dagger$ is the smallest one in the metric of V. In addition, the relation $\overline{\mathrm{Range}(|A|^\upsilon)} = = \overline{\mathrm{Range}(A^*)}$ takes place for $\forall \upsilon > 0$, i.e. the elements $|A|^\upsilon w$ form an everywhere dense set in the subspace $\mathrm{Ker}(A)^\perp$, to which the normal solution of Eq. (I.1) belongs.

The regularizator set

$$\mathrm{R}_0 = \{g_\alpha(A_h^* A_h) A_h^*, g_\alpha \in \mathrm{G}\} \subset \mathrm{R}$$

includes the majority of known regularization methods [14]:

1. Tikhonov regularizator

$R_\alpha = (\alpha E + A_h^* A_h)^{-1} A_h^*$

is an element of set R_0 with the generating function

$g_\alpha(\lambda) = (\alpha + \lambda)^{-1}$

and the parameters $\chi_* = 1/2$ and $\chi_\upsilon = \upsilon^\upsilon(1-\upsilon)^{(1-\upsilon)}$. The qualification of Tikhonov method is $\upsilon_* = 1$.

2. Generalized Tikhonov regularizator

$$R_\alpha = (\alpha^{q+1} E + (A_h^* A_h)^{q+1})^{-1} (A_h^* A_h)^q A_h^* \in \mathrm{R}_0, \tag{II.4}$$

at $q \geqslant -1/2$. Regularizator (II.4) is generated by the function

$g_\alpha(\lambda) = \lambda^q (\alpha^{q+1} + \lambda^{q+1})^{-1}$

at $\upsilon_* = q + 1$.

3. Non-stationary iterative scheme of the Tikhonov method. First, $v_0 = 0$ is put. The elements v_k $(k = 1, 2, ...)$ are determined in turn as solutions of the equations

$$\alpha_k v_k + A_h^* A_h v_k = \alpha_k v_{k-1} + A_h^* u_\delta \ (0 < \alpha_k < \alpha_{k-1}, \tag{II.5}$$

e.g., $\alpha_k = q^k$, where $0 < q < 1$. Method (II.5) is generated by the function

$$g_\alpha(\lambda) = \frac{1}{\lambda}\left(1 - \prod_{i=1}^{k} \frac{\alpha_i}{\alpha_i + \lambda}\right), \quad \lambda \neq 0,$$

and satisfies conditions (II.1) and (II.2) for $\chi_\upsilon = O(\upsilon^\upsilon)$ at $0 < \upsilon \leqslant 1$, and for $\chi_\upsilon = O(c^{\upsilon^\upsilon})$ at $1 < \upsilon$. The qualification of the method is $\upsilon_* = \infty$.

4. Implicit iterative scheme (the Fakeev–Lardy method). First, $v_0 = 0$ is put. The elements v_k are determined in turn from the equation

$$\begin{aligned} &\mu v_k + A_h^* A_h v_k = \mu\, v_{k-1} + A_h^* u_\delta, \\ &k = 1, 2, ...; \quad (0 < \mu = \mathrm{const}). \end{aligned} \tag{II.6}$$

The iterative method (II.6) turns out a regulizing one (Eq. (II.3)) if

$$g_\alpha(\lambda) = \frac{1}{\lambda}\left(1 - \left(\frac{\mu}{\mu + \lambda}\right)^{1/\alpha}\right), \quad \lambda \neq 0, \quad 1/\alpha = k = 1, 2, \ldots .$$

Conditions (II.1) and (II.2) are satisfied at $\chi_* = \mu^{-1/2}$, $\chi_\upsilon = (\upsilon \ \mu)^\upsilon$, and $k \geqslant \upsilon$. The qualification of the method is $\upsilon_* = \infty$.

5. Asymptotic regularization method. The generating function of this method looks like

$$g_t(\lambda) = \int_0^t e^{-(t-s)\lambda} ds = \frac{1}{\lambda}(1 - e^{-t\lambda}).$$

Therefore, $1 - \lambda g_t(\lambda) = e^{-t\lambda}$, and the approximate solution is determined by the formula

$$v_t = (E - A_h^* A_h g_t(A_h^* A_h)) v_0 + g_t(A_h^* A_h))\ A_h^* u_\delta, \tag{II.7}$$

for arbitrary $t = \alpha^{-1}$. Conditions (II.1) and (II.2) are satisfied at $\chi_* = 0.6382$ and $\chi_\upsilon = (\upsilon e)^\upsilon$. The qualification of the method is $\upsilon_* = \infty$.

6. Explicit iterative scheme (the Landweber method). First, $v_0 = 0$ is put. The elements v_k are determined in turn from the equation

$$\begin{aligned} &v_k = (E - \mu A_h^* A_h)\, v_{k-1} + \mu\, A_h^* u_\delta, \\ &k = 1, 2, ... \quad (0 < \mu < 2/||A_h||^2). \end{aligned} \tag{II.8}$$

The iterative method (II.8) is generated by the function

$$g_\alpha(\lambda) = \frac{1}{\lambda}\left(1 - (1 - \mu\lambda)^{1/\alpha}\right), \quad \lambda \neq 0,$$

where the regularization parameter α is such that the quantity $1/\alpha$ accepts only integer values: $1/\alpha = k = 1, 2, \ldots$. Conditions (II.1) and (II.2) are satisfied at $\chi_* = \mu^{1/2}$ and $\chi_\upsilon = (\upsilon/(\mu e))^\upsilon$. The qualification of the method is $\upsilon_* = \infty$.

The main result of the theory of ill-posed problems concerning the calculation of exact estimates for the approximations of Eq. (I.2) can be formulated as follows. For Eq. (I.2) with the approximately given operator A_h and the approximately given right-hand side u_δ, the order of convergence to the source-representable normal solution $v^\dagger \in \mathrm{M}_{\upsilon,\rho}(A)$ does not exceed $\frac{\upsilon}{\upsilon+1}$ for $\forall \nu > 0$, i.e. $\|v^\dagger - R_\alpha u_\delta\| = O\left((\delta + h)^{\upsilon/(\upsilon+1)}\right)$. The optimal order of accuracy at the indicated assumptions *a priori* provides the choice of a regularization parameter that satisfies the condition $\alpha = c(\delta + h)^{2/(\upsilon+1)}$, $c = \mathrm{const} > 0$.

If the information on the exact value of parameter υ, which determines the set $\mathrm{M}_{\upsilon,\rho}(A)$, is absent, the value of regularization parameter at the practical solution of problem (I.2) is determined directly in the course of solution, i.e. the *a posteriori* choice of α is made. One of the most effective and widespread methods of the *a posteriori* choice of a regularization parameter in the course of solution of Eq. (I.2) using the Tikhonov method (I.6) (in the case $A = A_h$ and $h = 0$) is called the discrepancy principle. It was proposed and substantiated by V.A. Morozov [15]. According to it, the parameter α is selected according to the condition

$$||\, A\, v_\alpha - u_\delta|| = \delta, \tag{II.9}$$

where $v_\alpha = (\alpha E + A^* A)^{-1} A^* u_\delta$. In practice, α is selected so that the functional $\|A\, v_\alpha - u_\delta\|$ should satisfy the condition

$$||\, A\, v_\alpha - u_\delta|| \in [a_1 \delta, a_2 \delta], \tag{II.10}$$

where a_1 and a_2 are certain numbers given beforehand $(1 < a_1 < a_2)$.

In the case where the operator A_h is given inexactly, Goncharsky *et al.* [16, 17] proposed a generalized discrepancy principle. According to it, there must be

$$||\, A_h v_\alpha - u_\delta|| \in [a_1(\delta + ||v_\alpha||\, h), a_2(\delta + ||v_\alpha||\, h)]. \tag{II.11}$$

It is known [13, 14] that the regularizing algorithms (II.3) that satisfy conditions (II.1) and (II.2), together with Morozov's discrepancy principle (II.10) or the generalized discrepancy principle (II.11), allow the solution of problem (I.2) to be determined with the optimal order of accuracy on the set $\mathrm{M}_{\upsilon,\rho}(A)$ for every υ satisfying the condition $0 < \upsilon < (2\upsilon_* - 1)$.

To solve problem (I.2), M. Defriese and C. De Mol [18] combined the Landweber iterative method and the *a posteriori* choice of a regularization parameter α (the iteration number $1/\alpha = k_*$). The essence of the stopping rule is as follows: the iterative process (I.6) is continued, if

$$||A_h\ v_k - u_\delta|| > \frac{2\delta}{2\delta - \mu||A_h||^2}, \quad \text{(II.12)}$$

or terminated, if the inequality

$$||A_h\ v_{k_*} - u_\delta|| \leqslant \frac{2\delta}{2\delta - \mu||A_h||^2} \quad \text{(II.13)}$$

is obeyed for the first time. The resulting v_{k_*} is accepted as an approximate solution of Eq. (I.2).

A specific feature of principles (II.9), (II.11), and (II.13), as well as many others, is the fact that the error magnitude δ of the right-hand side u_δ in Eq. (I.2) is contained in the explicit form. However, in a lot of scientific experimental researches, owing to their uniqueness, the determination of the error δ is very often rather subjective, as well as the choice of the quantities a_1 and a_2 in Eq. (II.10) or (II.11). This problem is especially relevant under the condition of a unique experiment.

Along with the problem of finding the error δ, a considerable fraction of the subjective approach is inherent to a situation where that or another regularization method is selected. An important role in this case is played by the presence of the *a priori* or *a posteriori* information concerning the solution of the problem [8], as well as the experience in carrying out computational experiments.

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МАТЕМАТИЧНА ІНТЕРПРЕТАЦІЯ РЕЗУЛЬТАТІВ ЕКСПЕРИМЕНТАЛЬНИХ ДОСЛІДЖЕНЬ ВЛАСТИВОСТЕЙ НЕЛІНІЙНО-ОПТИЧНОГО МАТЕРІАЛУ

Р е з ю м е

Із використанням методів обчислювальної фізики формулюється та розв'язується проблема математичної інтерпретації результатів експериментальних досліджень впливу інкорпорованих наночастинок TiO_2 на оптичні властивості нелінійно-оптичного матеріалу KDP. Математична модель представляється у вигляді інтегрального рівняння Фредгольма першого роду. Пропонується сплайн-ітераційна модифікація методу регуляризації Ландвебера розв'язання некоректно поставленої задачі. Результати проведених обчислювальних експериментів порівнюються з апостеріорі відомими даними фізичних експериментів.