Journal of Russian Laser Research, Volume 26, Number 2, 2005

INVERSE PROBLEM METHOD IN LASER PHYSICS

A. I. Osipov, L. A. Shelepin, and S. L. Shelepin

P. N. Lebedev Physical Institute, Russian Academy of Sciences
Leninskii Pr. 53, Moscow 119991, Russia
e-mail: alex@shelepin.msk.ru

Abstract

Applications of the method of ill-posed inverse problems in laser physics are considered. Means of calculating the level cross sections of physical-chemical reactions with subsequent calculation of the reaction rate constants are developed. Mathematical and numerical aspects for the realization of ill-posed inverse problem are considered in detail using the concrete example of level cross sections of dissociation.

Keywords: active laser medium, ill-posed inverse problem, level cross section, rate constant.

1. Introduction

The analysis of processes proceeding in laser active media as well as under laser action on a substance is composed of the solution of the following problems:

1. Data origination on the events;
2. Analysis of the kinetics of processes in lasers;
3. Finding the relation of the medium's characteristics with the parameters of external actions.

The actual kinetic processes developing in laser media represent a complex of an abundance of events for separate atoms, molecules, ions, clusters, and radical ions. Their probabilities depend on the term structure of specific objects. Both the experiment and the theoretical models are the sources of information on the events. A summary of the theoretical data available (in item 1) is presented in handbook [1]. The range of substances discussed in this handbook is restricted by gases of a relatively simple composition, atoms, diatomic molecules as well as the simplest hydrocarbons, oxides, and some organic compounds. The description of the kinetic processes under various actions (items 2 and 3) are presented in detail, e.g., in monograph [2] and handbook [3].

Analysis of kinetic phenomena encounters a number of restrictions at present. This is primarily due to the lack of data on the probabilities of the events resulting from the complexity and even impossibility (in some energy ranges) of experiments. Theoretical calculation of the transition probabilities requires cumbersome and time-consuming quantum-mechanical calculations. By way of example, the calculations of the cross section of dissociation processes carried out in [4–6] necessitate knowledge of the potential surfaces and take plenty of time. In this connection, a qualitatively new approach is associated with the range of problems solved by the inverse problem method. This range of problems belongs to the so-called

Translated from a manuscript submitted February 9, 2005.

 1071-2836/05/2602-0116

ill-posed problems. The notion of the correct statement of the problems of mathematical physics was first coined by J. Hadamard [7, 8].

The solution of any qualitative problem usually consists of finding the "solution" z from the given "initial data" u, $z = R(u)$. These data will be considered as elements of the metric spaces Z and U, respectively. The metrics is usually determined by the statement of the problem.

The problem of finding the solution z from the space Z using " initial data" u from the space U is said to be correctly stated on the couple of metric spaces (Z, U) when the following requirements (conditions) are met:

1. There is a solution z from the space Z for any element $u \in U$;

2. The solution is uniquely determined;

3. The problem is stable on the spaces (Z, U).

J. Hadamard proceeded from the fact that any mathematical problem corresponding to the physical or technical one should be correct. Indeed, how can one physically interpret the solution if arbitrarily small variations in the initial data can cause profound variations in the solution? The problems that do not meet the listed correctness requirements are said to be ill-posed ones.

By way of explanation of the aforesaid we consider a system of two linear algebraic equations as a simple example,

$$x + 10y = 11,$$
$$10x + 101y = 111.$$

Its unique solution ($x = 1$, $y = 1$) can be easily found. With a little manipulation of the right-hand side of the first equation we have

$$x + 10y = 11.1,$$
$$10x + 101y = 111.$$

The solution now is as follows: $x = 11.1$, $y = 0$. Thus, a small variation in the initial data of the problem results in a drastic change of its solution.

The literally avalanche-like expansion of the circle of ill-posed problems of great practical consequence occurred from the middle of the 20th Century. Among them, in particular, are the solution of integral equations of the first kind to which belong the Fredholm and Volterra equations, the numerical summation of the Fourier series when the coefficients are known only approximately, the differentiation of the approximate functions, as well as a number of problems of linear programming and optimal control. The inverse problems arising in physics and engineering also belong to the ill-posed problems. The necessity of solving problems unstable with respect to the experimental errors often arises in the processing of data of physical experiments. The range of such problems is expanding steadily.

The development of the so-called regularization methods represented a certain breakthrough in the solution of ill-posed inverse problems. The seminal works in this field belong to A. N. Tikhonov [9–11]. The definition of the approximate solution of the ill-posed problem was formulated and the notions of regularization and the regularizing operator were introduced. The use of the regularization methods allowed one to solve practical problems from various fields of science. In particular, they were used in papers [12–14] to determine the cross sections of elementary reactions. However, application of the inverse problem method to issues of level kinetics were virtually not considered.

The present paper is devoted to applications of the inverse problem method in physical-chemical kinetics and laser physics. In this paper, the level cross sections are obtained and the level rate constants are calculated. These parameters are of fundamental importance for modeling of active laser media. In essence, application of the inverse problem method allows one to take a qualitative step to the problem of gaining data on the events. This method finds its application for calculations of characteristics of the events (interaction cross sections) with subsequent calculation of the reaction rate constants. These parameters are of significance in laser physics and physical gas dynamics, including the temperature range where exact measurements are impracticable.

This paper is subdivided into three parts. In Sec. 2, the general principles of solving ill-posed problems are considered. Section 3 is devoted to the analysis of a specific problem. A priori information is needed for its solution as opposed to the case of standard correct problems. Various directions of applications are discussed in Sec. 4.

2. General Principles of Solving Ill-posed Inverse Problems

Let us consider an ill-posed inverse problem

$$Az = u, \quad u \in U, \quad z \in Z. \tag{1}$$

Here, the operator A and the vector u on the right-hand side of the equation are the initial data. For the sake of simplicity we assume that the operator is specified exactly, while the right-hand side is known with some error δ. In this case, instead of the exact value u_E there is u_δ such that $\|u_E - u_\delta\| < \delta$. The element $z_\delta \in Z$ tending to the exact solution z_E with $\delta \to 0$ in the metrics Z is said to be an approximate solution.

The set of solutions $\{\tilde{z} : \tilde{z} \in Z, \|A\tilde{z} - u_\delta\| < \delta\}$ is referred to as commensurable in accuracy with the initial data. It is evident that the approximate stable solution is its member. However, such a class is too wide and among its members can be those that differ strongly. Because of this, the selection principle is needed to separate the solution stable to small variations. This principle should be based on the use of further a priori information on the solution. This information can be both quantitative (this results in quasi-solutions) and qualitative (e.g., the solution smoothness).

A number of difficulties associated with the incorrect formulation of the problem arises in the solution of the ill-conditioned systems of linear equations

$$\mathbf{Az} = \mathbf{u},$$

where $\mathbf{A}$ is the matrix with the elements $\mathbf{A}_{ij}$, $\mathbf{A} = \{\mathbf{A}_{ij}\}$, $\mathbf{z}$ is the sought vector with the coordinates $\mathbf{z}_j$, $\mathbf{z} = \{\mathbf{z}_j\}$, and $\mathbf{u}$ is the known vector with the coordinates $\mathbf{u}_i$, $\mathbf{u} = \{\mathbf{u}_i\}$. The determinant of degenerate systems is zero ($\det A = 0$) and the system has zero eigenvalues. For ill-conditioned systems of such a type the matrix A has eigenvalues close to zero. Since calculations are performed with a finite accuracy, this actually means that one cannot determine whether the given system of equations is a degenerate or ill-conditioned one. Thus, ill-conditioned and degenerate systems can be indistinguishable within the framework of the given accuracy.

Such systems do not comply not only with the requirement of stability of the well-behaved problem but virtually also the requirement of uniqueness of solution. Note that in some instances the finite difference approximation of operator equations in the form (1) leads to the systems of linear equations described.

In essence, the ill-conditioned system proves to be underdetermined, and the number of variables exceeds the number of linearly independent equations. Further a priori information on the solution is necessary to complete a definition of the system.

The regularization method conceptually poses the question as to whether the operator can be constructed, which gives the approximate but stable solution

$$z_\delta = R(u_\delta, \alpha)\,, \quad \alpha = \alpha(\delta), \tag{2}$$

such that

$$\|z_E - z_\delta\| \to 0, \quad \text{with} \quad \delta \to 0. \tag{3}$$

The operator $R(u_\delta, \alpha)$ acting from U to Z and dependent on the parameter α is referred to as the regularizing operator (or algorithm) and contains a priori information on the solution. One has also to determine some way or other the degree of insertion of this information into the system. Actually, a priori information should be enough to compensate the errors of the initial data. However, its too strong effect can distort the solution and move it away from the exact one.

The parameter α, named the regularization parameter, serves as a quantitative measure of insertion of a priori information. In the general case, α is the error function of the initial data δ with such values of α that the operator $R(u_\delta, \alpha)$ is the regularizing one.

In essence, the introduction of the parameter α allows one to construct some parametric family of well-posed problems, which passes into the original problem in the limiting case $\alpha \to 0$.

In the Tikhonov regularization method the original problem (1) is reduced to the problem of minimization of the functional

$$M^\alpha[z, u] = \|Az - u\|^2 + \alpha\Omega[z], \quad \Omega[z] = \|z\|^2, \tag{4}$$

where $\Omega[z]$ is the stabilizing functional or the stabilizer and α is the regularization parameter, which has to be selected by certain means. The functional $\Omega[z]$ contains a priori information on the solution character.

Problem (4) is actually a search problem of the conditional extremum of the functional $\Omega[z]$ under the condition $\|Az - u\| = \delta$. Therein lies the so-called variational principle [15]. The problem of finding the approximate solution is reduced to the variational problem on the minimization of the functional $\Omega[z]$ defined on $Z_1 \in Z$ on the set

$$Q = Z_1 \bigcap \{z : \|Az - u_\delta\| \le \delta\}. \tag{5}$$

The greatest lower bound of the functional $\Omega[z]$ (if it exists) is achieved on the element z_δ for which $\|Az - u_\delta\| = \delta$. The number $\|Az - u\|$ is often referred to as the discrepancy of the equation $Az = u$ on the element z. The element generated by $\Omega[z]$ is considered to be the result of application of some regularizing operator $R(u)$ to some vector on the right-hand side of the equation.

Thus, instead of the problem of minimization of the functional $\Omega[z]$ on the set Q one can seek the solution of the minimum problem of the functional $\Omega[z]$ on the set Z_1 under the condition that the following equality is met on the desired element z:

$$\|Az - u_\delta\| = \delta. \tag{6}$$

This is the classical problem of the calculus of variations on the constrained minimum. Solving it by the Lagrange's method of undetermined multipliers, we arrive at (4), where α has the meaning of the Lagrange's undetermined multiplier.

It should be noted that the problem of minimization of the functional $M^\alpha[z,u]$ possesses stability to small variations on the right-hand side u, whereas the original problem does not possesses the stability property. This stability can be achieved by narrowing the class of possible solutions due to the introduction of the functional $\Omega[z]$. Thus, it plays the stabilizing role. Because of this, it is said to be the stabilizing functional or the stabilizer.

Thus, the problem of finding the stable solution is reduced to the minimization problem of functional (4). However, in computational practice it will be more convenient to find the solution z_α by solving the Euler equation corresponding to the functional $M^\alpha[z,u]$. According to the theory of calculus of variations for functionals, the function z_α corresponds to the minimum of the functional $M^\alpha[z,u]$ provided that it satisfies to the equation

$$A^*A + \alpha Lz = A^*u,$$

called the Euler equation. Here, A^*A is the self-adjoint operator and $(Lz,z) = \|z\|^2 = \Omega[z]$. In some cases, such an equation can be solved much more easily as compared to the direct minimization of the functional $M^\alpha[z,u]$.

The nonnegative functional $\Omega[z]$ defined on the subset Z_1 of the set Z is the stabilizing one if

a) the element z_E belongs to the domain of its definition;

b) for any number $d > 0$ the set $Z_{1,d}$ of elements z from Z_1 for which $\Omega[z] \le d$ is compact on Z.

Depending on the type of information on the solution, the metrics of the norm $\|z\|^2$ of the stabilizing functional is chosen. By way of example, if the exact solution $z(s)$ is known to belong to the class of smooth functions, the sum of n derivatives is usually chosen with functional coefficients $q(s)$

$$\|z\|^2 = \int_a^b \left\{ \sum_n q_n(s) \left(\frac{d^n z}{ds^n} \right)^2 \right\} ds. \tag{7}$$

In the case where one has to find the solution closest to some profile (i.e., to some element z_0), instead of the norm $\|z\|^2$ the norm

$$\Omega[z] = \|z - z_0\|^2 \tag{8}$$

should be considered and so on.

The meaning of the regularization parameter α is clear from (4). At small α ($\alpha \sim 0$) the conditionality of system (4) is close to the ill-conditionality (1), while at large α system (4) is well-conditioned but its solution is far from the solution of the original inverse problem. Namely, the greater the regularization parameter, the smaller the contribution of information to the system under study as compared to the a priori one. It is apparent that in practice one has to choose intermediate α. The choice of the parameter α is the crucial issue in regularization theory.

As mentioned above, the regularization parameter α is generally a function of the initial data precision δ. However, it is generally difficult to find the regularization parameter α as a function of δ when considering specific problems. The number δ characterizing the error of initial information is known in practice. Because of this, the mechanism of matching of the choice of the parameter α to the known error of the right-hand side is necessary. It is required to find the regularization parameter α corresponding to the error δ from the allowed values. In other words, these values of the regularization parameter are those of the function $\alpha = \alpha(\delta)$ for which the operator $R(u_\delta, \alpha)$ is the regularization one. The choice

of the allowed value of the regularization parameter depends on the available information concerning approximate initial information. Various ways of finding such a value of α are described in the literature.

With the known error level of assignment of the right-hand side δ one should choose α from the discrepancy condition

$$\|Az_\delta^\alpha - u_\delta\|^2 = \delta^2. \tag{9}$$

The scheme of choosing the regularization parameter for the generalized discrepancy [16, 17] is of special interest in practice when both the right-hand side and the operator $\|A - A_h\| < h$ $(h \geq 0)$ are specified with an error. In this case, it is advisable to determine α as a root of the function

$$\rho_\eta^\alpha(z) = \|Az_\eta^\alpha - u_\delta\|^2 - (\delta + h\|z_\eta^\alpha\|)^2, \tag{10}$$

where η designates the set of error parameters of the operator and the right-hand side, $\eta = (h, \delta)$. The function $\rho_\eta^\alpha(z)$ is referred to as the generalized discrepancy.

In computational practice, the method of choosing the regularization parameter for the discrepancy (or the generalized discrepancy) is often realized in the following manner. The finite segment of the monotonic sequence of numbers $\alpha_0, \alpha_1, \ldots \alpha_n$, e.g., the segment of the geometric progression $\alpha_k = \alpha_0\, q^k$, $k = 0, 1, \ldots, n$, $q > 0$, is taken. For each value of α_n the element z^a is found, which minimizes the functional $M^\alpha[z, u]$, and the discrepancy $\|Az - u_\delta\|$ is calculated. Such number α_{k_0} is taken as a desired value α for which equality (9) [or (10) in the case of the generalized discrepancy] is fulfilled with a desired accuracy.

In some problems instead of the exact right-hand side u_e its approximation u_δ is available, whose error level δ is unknown. In this case, the approximations to z_E can also be found by minimization of the smoothing functional $M^\alpha[z, u]$. However, in this case the regularization parameter α cannot be found for the discrepancy. In these problems one can use the quasi-optimal value of α. The latter is defined as the value of α, which realizes

$$\inf_{\alpha>0} \left\| \alpha \frac{dz^\alpha}{d\alpha} \right\|_Z. \tag{11}$$

In the case where there are several such values, the minimum one is taken.

The case where the exact solution is a priori known to belong to some compact set should be considered separately. In such formulation, the selection of the solution can be performed without reliance on the error of the initial data δ, whose exact value is difficult to evaluate in some instances. The notion of the quasi-solution as an approximate solution of the ill-posed problem on the compact set was coined in [18–20]. The quasi-solution of Eq. (1) on the given compact set M of the space Z and with given $u_0 \in U$ is called the point $z_0 \in M$ for which $\|Az - u_0\|$ reaches its minimum on M. In these papers, a number of theorems on the existence, uniqueness, and continuous dependence of the quasi-solution on the right-hand side were also proved.

Let us consider an ill-posed inverse problem where the operator and the right-hand side are specified with the errors h and δ, respectively, $\eta = (h, \delta)$. Let the exact solution $z_E(s)$ be a priori known to be the function monotonic on the segment and bounded both above and below. We introduce into consideration a set $Z_C(\eta)$ of elements that satisfy the condition

$$\|Az_\eta^\alpha - u_\delta\| \leq h\|z_\eta^\alpha\| + \delta. \tag{12}$$

In this case, as is shown in [21], any member z_η from the set $Z_C(\eta)$ can be taken as an approximate solution with $z_\eta \to z_E(s)$ at $\eta \to 0$. In other words, z_η is a stable element. In the same book this result is generalized to the set of convex bounded functions.

The approaches to the solution of the ill-posed inverse problem on compact sets of special structure were considered in detail in [21–24]. The methods described are based on the iteration minimization of the discrepancy functional $\Phi(z) = \|A_h z - u_\delta\|$ on the set of elements $z \in M$.

The problem of finding an approximate solution can be solved by minimizing the functional $\Phi(z)$ on the set M. In this case, there is no need to find the minimum $\Phi(z)$ on this set. It is sufficient to find the member $z_\delta \in M$ such that $\Phi(z_\delta) \leq \delta$. Thus, to find the approximate solution on the set M, one has to construct the sequence $z_{(k)}$, which minimizes the functional $\Phi(z)$ on the closed bounded set.

An arbitrary member $z_1 \in M$ is taken as an initial point. Then, as the next step, one has to find the member $z_2 \in M$, which decreases the discrepancy

$$\|Az_2 - u_\delta\| < \|Az_1 - u_\delta\|.$$

The next point z_{n+1} can be chosen, e.g., on the basis of the direction of the discrepancy gradient $\|Az_n - u_\delta\|$ at the previous stage. Each iteration should be constructed in such a way that the iteration transformations leave the current point z_n within the boundaries of the compact set M.

In practice, it is better to use the conditional gradient method if the initial data u_δ is specified with poor accuracy (of the order of several percents). The detailed description of these methods can be found, e.g., in [25, 26].

3. Application of Inverse Problem Methods to Specific Issues of Laser Physics

The qualitative specific feature of the particular ill-posed inverse problems consists of the necessity of using an additional a priori information to select the necessary solution. By this feature these problems differ from well-behaved ones. By way of example, in the solution of a system of differential equations the specification of the initial and boundary conditions determines the solution uniquely. But each class of specific ill-posed inverse problems possesses its own peculiar features, since the insertion of a priori information should be based on the physical analysis of the system. Let us consider the specific features of application of inverse problem methods to the calculation of level cross sections of dissociation.

The rate constant of a chemical reaction with an arbitrary energy dependence of the process cross section is described by the following equation [1]:

$$K(T) = \left(\frac{8}{\pi\mu}\right)^{\frac{1}{2}} \left(\frac{1}{kT}\right)^{\frac{1}{2}} \int_0^\infty \mathcal{E} e^{-\frac{\mathcal{E}}{kT}} \sigma(\mathcal{E}) d\mathcal{E}, \tag{13}$$

where T is the gas temperature, $\mu = m_X \cdot m_Y/(m_X + m_Y)$ is the reduced mass of colliding particles X and Y, k is the Boltzmann constant, $\mathcal{E}$ is the relative energy of the colliding particles, and $\sigma(\mathcal{E})$ is the effective cross section. Relationship (13) was obtained under the assumption that the process cross section $\sigma(\mathcal{E})$ depends only on the energy of relative motion of colliding particles $\mathcal{E}$ and is independent of their internal energy (state). The Maxwellian distribution by the energy of relative motion of colliding particles $\mathcal{E}$ is assumed. The expression for $K(T)$ was obtained by Maxwellian averaging of the cross section over all possible molecular velocities [27].

The value of $K(T)$ corresponds to the Laplace transform $F(s)$ for the original $f(t) = t \cdot \sigma(t)$ with $t = \mathcal{E}$ and $s = 1/kT$,

$$K(T) = \frac{1}{kT}\left[\frac{8}{\pi\mu kT}\right]^{1/2} \cdot F(s), \quad F(s) = \int\limits_0^\infty f(t)\exp(-st)dt.$$

The determination of the characteristics of the elementary processes of physical-chemical reactions is a topical problem of contemporary kinetics. The effective reaction cross section $\sigma_v(\mathcal{E})$ is among the key characteristics. The cross section $\sigma_v(\mathcal{E})$ is that of elementary process with participation of the reacting molecule, which is on the vth vibrational level.

Let us assume that the reaction occurs in a medium where Boltzmann distribution of molecules by their vibrational energy occurs. In this case, to obtain the reaction rate constant $K(T)$ one has to average the cross sections $\sigma_v(\mathcal{E})$ not only by the Maxwellian velocity distribution but also by the Boltzmann distribution by the vibrational energy,

$$K(T) = \frac{1}{kT}\left(\frac{8}{\pi\mu kT}\right)^{1/2}\frac{1}{Q}\sum_{v=0}^{v*}\exp\left(-\frac{\mathcal{E}_v}{kT}\right)\int\limits_{D_0-\mathcal{E}_v}^{\infty}\mathcal{E}\exp\left(-\frac{\mathcal{E}}{kT}\right)\sigma_v(\mathcal{E})d\mathcal{E}. \tag{14}$$

Here, $\mathcal{E}_v$ is the energy of the vibrational level v, v^* is the last discrete level, Q is the vibrational statistical sum, and D_0 is the dissociation energy. The integration is performed with the variable lower limit $D_0-\mathcal{E}_v$, since the energy is assumed to be $\mathcal{E} < D_0 - \mathcal{E}_v$.

Introducing the level constants of the dissociation rate $K_v(T)$, expression (14) can be written as

$$K_v(T) = \frac{1}{kT}\left(\frac{8}{\pi\mu kT}\right)^{1/2}\frac{\exp(-\frac{\mathcal{E}_v}{kT})}{Q}\int\limits_{D_0-\mathcal{E}_v}^{\infty}\mathcal{E}\exp\left(-\frac{\mathcal{E}}{kT}\right)\sigma_v(\mathcal{E})d\mathcal{E}, \tag{15}$$

$$K(T) = \sum_{v=0}^{v^*}K_v(T). \tag{16}$$

Note that the value of $K(T)$ is determined experimentally [28–30] within the relatively narrow temperature range, while reliable experimental data on the values of $K(T)$ are lacking. Equation (15) is the input equation for determination of the level dissociation cross sections $\sigma_v(\mathcal{E})$.

Equation (15) by its structure is a first-kind Fredholm equation,

$$\int\limits_a^b \mathcal{K}(x,s)z(s)\,ds = u(x), \quad a \le s \le b, \quad c \le x \le d, \tag{17}$$

where $\mathcal{K}(x,s)$ is the kernel of the integral equation,

$$s \equiv \mathcal{E}, \quad x \equiv T,$$
$$z(s) \equiv \sigma_v(\mathcal{E}), \quad u(x) \equiv K_v(T),$$
$$\mathcal{K}(x,s) \equiv \mathcal{K}(T,\mathcal{E}) = \frac{1}{kT}\left(\frac{8}{\pi\mu kT}\right)^{1/2}\int\limits_{D_0-\mathcal{E}_v}^{\mathcal{E}^*}\exp\left(-\frac{\mathcal{E}}{kT}\right)d\mathcal{E},$$
$$D_0 - \mathcal{E}_v \le \mathcal{E} \le \mathcal{E}^*, \quad T_1 \le T \le T_2.$$

In going from (15) to (17) the upper limit of integration $\mathcal{E}^*$ is taken on the basis of the insensitivity of the results to its further increase. The right-hand side is considered on the temperature interval $[T_1, T_2]$ corresponding to the temperature range in which the experimental measurements for the rate constant are available.

Equation (17) is conveniently represented in the operator form

$$Az = u, \tag{18}$$

where A is the integral operator

$$A = \int_a^b \mathcal{K}(x, s)\, ds.$$

In the general case, the problem of solution of the first-kind Fredholm equation (17) [or (18)] is an ill-posed one [15]. Moreover, as indicated above, the rate constant $K(T)$ is the Laplace transform for the original function $\mathcal{E}\sigma(\mathcal{E})$. It is common knowledge that the inverse Laplace transform is unstable with respect to small variations in input data. Because of this, the inverse problem of determination of the cross sections $\sigma_v(\mathcal{E})$ belongs to the class of ill-posed inverse problems. One has to introduce further a priori information to solve such problems. The selection of the particular solution is determined by the physical requirements and is based on the analysis of the physical statement of the inverse problem. Such a treatment is specific for each class of problems.

From the physical standpoint, two types of cross sections have significance in the class of physical-chemical reactions under consideration. They are the bell-shaped cross sections with a maximum at the energy $\mathcal{E} = \mathcal{E}_{\max}$ and the monotonically increasing one having some finite bound $\sigma_{\max}$ with $\mathcal{E} \to \infty$. The availability of the maximum is attested by the Massey criterion (the rule of the adiabatic maximum according to which the cross section of inelastic interaction is maximum at the adiabaticity limit) [31]. On the other hand, the monotonically increasing cross sections flattening them out were obtained in a number of trajectory calculations [4–6]. Moreover, the cross section maximum cannot be above the gas-kinetic cross section σ_0. We perform calculations for both possible types of cross sections to prevent loss of generality and narrowing the range of possible solutions.

Thus, to determine the level cross sections of dissociation we have to solve ill-posed inverse problem (17) under the assumption that the cross section $\sigma_v(\mathcal{E})$ is a bounded nondecreasing function or a function with a single maximum. The cross section has a functional relationship with the relative energy of colliding particles $\mathcal{E}$.

In the case of a monotonically nondecreasing function, the cross section should satisfy the following conditions:

$$\begin{aligned} &\sigma_v(\mathcal{E}_1) \le \sigma_v(\mathcal{E}_2), \quad \mathcal{E}_1 < \mathcal{E}_2, \\ &0 \le \sigma_v(\mathcal{E}) \le \sigma_0, \end{aligned} \tag{19}$$

provided that the energy dependence of the cross section has a maximum,

$$\begin{aligned} &\sigma_v(\mathcal{E}_1) \le \sigma_v(\mathcal{E}_2), \quad \text{with} \quad \mathcal{E}_1 < \mathcal{E}_2 \le \mathcal{E}_{\max}, \\ &\sigma_v(\mathcal{E}_1) \ge \sigma_v(\mathcal{E}_2), \quad \text{with} \quad \mathcal{E}_{\max} \le \mathcal{E}_1 < \mathcal{E}_2, \\ &0 \le \sigma_v(\mathcal{E}) \le \sigma_0. \end{aligned} \tag{20}$$

Here, $\mathcal{E}_{\max}$ is the energy at which the cross section is maximum. We denote the set of monotonically nondecreasing functions meeting conditions (19) by G_1, while those meeting conditions (20) by B_1.

The sets G_1 and B_1 are the compacts in $L_p[a,b], p > 1$. This can be shown easily using the Helly theorem [32]. However, the application of iterative approaches minimizing successively the discrepancy functional $\Phi(z) = \|Az - u\|^2$ was found to be inefficient (the studies were carried out by the method of projections of the conjugate gradients [21]). Let us briefly consider the essence of this method by an example of the set G_1.

With finite difference approximation (18) the set G_1 passes into the convex one,

$$\left\{ z : \begin{array}{l} z_{i+1} - z_i \le 0, \quad i = 1, 2, \ldots, i_0 - 1, \\ 0 \le z_i \le C, \quad i = 1, 2, \ldots, i_0. \end{array} \right\} \tag{21}$$

The functional $\Phi(z) = \|Az - u\|^2$ passes into the quadratic function $\phi(z)$. Note that constraints (9) can be written in the form

$$\mathbf{Fz} \le \mathbf{g}, \tag{22}$$

where $\mathbf{F}$ is a matrix of size $m_0 \times i_0$, m_0 is the number of conditions that define the set, and $\mathbf{g}$ is the constraint vector of length m_0. Inequality (22) is intended to be the component-wise inequality. In the case where z is situated at the set boundary, one or several inequalities in (21) can become equalities.

Any function from the set G_1, e.g., $z(s)^{(k=0)} = 0$, is taken as an initial point at the step $k = 0$. Then the descent direction $p^{(k)}$,

$$p^{(k)} = -\operatorname{grad} \phi(z^{(k)}),$$

and the optimum step size a_k in this direction are calculated. The maximum step length $a_{\max}$ in this direction, i.e., such step length that leaves the solution within the set boundaries, is calculated. The minimum of two steps is chosen and the solution is "progressed" on this value in the direction $p^{(k)}$. If the maximum step length in the descent direction is nil, i.e., the solution is in the hyperplane of restrictions, further motion is carried out along the projection of $p^{(k)}$ on the hyperplane.

In spite of the fact that the method described is known for its efficiency, its application to the problem of determination of the level cross sections under consideration appears to be rather difficult. This is associated with the structure of the kernel $\mathcal{K}(T, \mathcal{E})$ of integral equation (17),

$$\mathcal{K}(T, \mathcal{E}) = \mathcal{E} \exp(-\mathcal{E}/kT).$$

The function experiences a surge and then strongly damps out exponentially. At large $\mathcal{E}$ the value of Az is rather small as compared to that at small $\mathcal{E}$.

As a result, the efficient way of decreasing the discrepancy functional $\Phi(z) = \|Az - u\|^2$ is the variation of the solution z only in the region of small $\mathcal{E}$. However, the variation should not remove the function beyond the boundaries of G_1, i.e., it should remain a monotonic one. This leads to the dependence of the result and the output value of discrepancy $\|Az - u\|^2$ on the choice of the initial point $z(s)^{(k=0)}$, since the tail portion of the solution is actually unchanged with the integration.

There is another problem in the search for solutions belonging to the set B_1. The point $\mathcal{E}_{\max}$ where the solution reaches its maximum is not known in advance. Nevertheless, it is required in the method to describe the set of restrictions in the form (21–22).

Thus, from the above discussion follows the poor applicability of the gradient methods to the solution of the problem under consideration. This is due to the form of the kernel $\mathcal{K}(T, \mathcal{E})$ of integral equation (17) and the form of sets to which the solution $\sigma(\mathcal{E})$ can belong. The way out should be sought for in the application of regularizing algorithms.

For the numerical solution one has to construct a finite difference approximation of Eq. (18), i.e., to determine the matrix of the operator A and the column of the right-hand side u. We enter the analytical meshes $\{s_j\}_{j=1}^{j_0}$ and $\{x_i\}_{i=1}^{i_0}$ in the segments $[a,b]$ and $[c,d]$ with the steps h_s and h_x, respectively. Using Simpson's numerical integration technique for the integral operator

$$A = \int_a^b \mathcal{K}(x,s)\,ds,$$

we write the corresponding matrix $\mathbf{A}$ of the size $i_0 \times j_0$ as

$$\begin{aligned}
\mathbf{A}_{i,j} &= 2\cdot\mathcal{K}(x_i,s_j)\frac{h_s}{3}, \quad j=3,5,\ldots,j_0-1, \quad i=1,2,\ldots,i_0,\\
\mathbf{A}_{i,j} &= 4\cdot\mathcal{K}(x_i,s_j)\frac{h_s}{3}, \quad j=2,4,\ldots,j_0-1, \quad i=1,2,\ldots,i_0,\\
\mathbf{A}_{i,1} &= \mathcal{K}(x_i,a)\frac{h_s}{3}, \quad i=1,2,\ldots,i_0,\\
\mathbf{A}_{i,j_0} &= \mathcal{K}(x_i,b)\frac{h_s}{3}, \quad i=1,2,\ldots,i_0.
\end{aligned} \tag{23}$$

Let us introduce the column vector $\mathbf{u}_i$ as the values of the function on the mesh $\{x_i\}_{i=1}^{i_0}$,

$$\mathbf{u}_i = u(x_i), \quad i=1,2,\ldots,i_0.$$

We obtain the finite difference analog of Eq. (18) to determine the vector of solution $\mathbf{z}_j$,

$$\mathbf{A}_{ij}\mathbf{z}_j = \mathbf{u}_i.$$

It will be recalled that in the Tikhonov regularization technique instead of the solution of the initial problem (18) the problem of minimization of the functional

$$M^\alpha[z,u] = \|Az-u\|^2 + \alpha\|z\|^2$$

is posed. This problem in turn is equivalent to the solution of the Euler equation

$$A^*A + \alpha Cz = A^*u, \tag{24}$$

where (z,Cz) approximates the norm $\|z\|^2$.

We formalize the boundary conditions for the cross sections belonging to the compact sets under consideration. The type of cross sections, which belongs to the compact set B_1, should satisfy the following boundary conditions:

$$\begin{aligned}
z(a) &= 0,\\
z(b) &= 0, \quad z'(b) = 0.
\end{aligned} \tag{25}$$

The cross sections belonging to the set G_1 satisfy the boundary conditions

$$\begin{aligned}
z(a) &= 0,\\
z'(b) &= 0.
\end{aligned} \tag{26}$$

Conditions (25) on the numerical mesh $\{s_j\}_{j=1}^{j_0}$ with the step h_s take the form

$$\mathbf{z}_1 = z(a) = 0,$$
$$\mathbf{z}_{j_0} = z(b) = 0,$$
$$(\mathbf{z}_{j_0} - \mathbf{z}_{j_0-1})/h_s = z'(b) = 0.$$

This is neither more nor less than the system of linear equations

$$\mathbf{F}_{j_0 n}\mathbf{z}_{j_0} = \mathbf{g}_n,$$

where $\mathbf{F}$ is the matrix of the size $j_0 \times m_1$, $\mathbf{g}_{m_1}$ is the column, and m_1 is the number of boundary conditions. The rows $\mathbf{F}$ represent the coefficients in the quantization of derivatives, while the columns correspond to the mesh in z. The rows of the vector g are the values of the boundary conditions,

$$\mathbf{F} = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 \\ 0 & 0 & 0 & \dots & -1 & 1 \end{pmatrix}, \qquad \mathbf{g} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

Similar reasoning is true in the case of boundary conditions for $z \in G_1$. It should be noted that not only the conditions at the boundaries but also any condition of the form $z^{(n)}(s_j) = u_0$, where u_0 is the number, can be written in the same way.

To account for the specified conditions in the system, we write the matrix $\mathbf{F}$ below the matrix $\mathbf{A}$ and the column $\mathbf{g}$ below the column $\mathbf{u}$. We obtain the matrix $\tilde{\mathbf{A}}$ with the size $[i_0 + n] \times j_0$ and the column $\tilde{\mathbf{u}}_{i_0+n}$. In what follows we shall use the extended matrices $\tilde{\mathbf{A}}$ and $\tilde{\mathbf{u}}$ instead of $\mathbf{A}$ and $\mathbf{u}$.

The matrix $\mathbf{A}$ of the integral operator A is ill-conditioned because of the specific features of the structure of the kernel $\mathcal{K}(x, s)$ discussed above. The introduction of the boundary conditions improves the conditionality of the matrix $\mathbf{A}$. Being a system of linearly independent equations they somewhat redefine the system and actually fix some points of the solution. However, this information is inadequate to obtain a stable solution.

The stable solution can be obtained under the assumption that the cross section $\sigma(\mathcal{E})_v$ sought belongs to the class of smooth functions. Physically, this supposition does not restrict the general formulation of the problem. This means mathematically that the solution $z(s)$ is continuous on $[a, b]$ and has quadratically integrable derivatives. For this reason we choose the space metric of the norm $\|z\|^2$ in the form

$$\|z\|^2 = \int_a^b \left\{ \sum_n q_n(s) \left(\frac{d^n z}{ds^n} \right)^2 \right\} ds, \tag{27}$$

where $q_n(s)$ is the factor function of the nth order derivative. This is the stabilizer of the nth order of smoothness first considered in [11]. In the course of numerical experiments performed it appears that $n = 3$ is an optimum for the solution of the present problem. In this case,

$$\|z\|^2 = \int_a^b \{[q_0(s)z(s)]^2 + [q_1(s)z'(s)]^2 + [q_2(s)z''(s)]^2 + [q_3(s)z'''(s)]^2\}\, ds. \tag{28}$$

For the numerical approximation of the stabilizing functional we use the rectangular formulas,

$$\int_a^b [q_0(s)z(s)]^2\,ds \approx \sum_{j=1}^{j_0}(q_{0j}z_j)^2 h_s, \tag{29}$$

$$\int_a^b [q_1(s)z'(s)]^2\,ds \approx \sum_{j=2}^{j_0}(q_{1j}z_j - q_{1j-1}z_{j-1})^2/h_s, \tag{30}$$

$$\int_a^b [q_2(s)z''(s)]^2\,ds \approx \sum_{j=3}^{j_0}(q_{2j}z_j - 2q_{2j-1}z_{j-1} + q_{2j-2}z_{j-2})^2/(h_s)^2, \tag{31}$$

$$\int_a^b [q_3(s)z'''(s)]^2\,ds \approx \sum_{j=4}^{j_0}(q_{3j}z_j - 3q_{3j-1}z_{j-1} + 3q_{3j-2}z_{j-2} - q_{3j-3}z_{j-3})^2/(h_s)^3. \tag{32}$$

To obtain the regularized solution stable to small variations of the right-hand side of equation, one has to solve Euler equation (24) within the framework of the Tikhonov regularization technique,

$$A^*A + \alpha Cz = A^*u.$$

We write it in the matrix form. With consideration for the aforesaid for the problem discussed, this equation takes the form

$$[\tilde{\mathbf{A}}^E\tilde{\mathbf{A}} + \alpha(\mathbf{C}_0^E\mathbf{C}_0 + \mathbf{C}_1^E\mathbf{C}_1 + \mathbf{C}_2^E\mathbf{C}_2 + \mathbf{C}_3^E\mathbf{C}_3)]\mathbf{z} = \tilde{\mathbf{A}}^E\tilde{\mathbf{u}}. \tag{33}$$

Here, the matrix $\tilde{\mathbf{A}}$ and the vector $\tilde{\mathbf{u}}$ are written with consideration for the boundary conditions and $(z, \mathbf{C}_n^E\mathbf{C}_n z)$ approximates the integral

$$\int_a^b [q_n(s)z^{(n)}(s)]^2\,ds.$$

When solving system (33) one has to determine the functional parameters

$$q_0(s),\ q_1(s),\ q_2(s),\ q_3(s).$$

The choice of the functional dependence of the parameters $q_n(s)$ depends on the set (B_1 or G_1) on which this problem is solved. As a result of the numerical experiments carried out it was found that for the search for solutions belonging to the set G_1 one should take in most cases the following parameters: $q_0(s) = 0$, $q_1(s) = s$ or 0, $q_2(s) = s^2$, and $q_3(s) = 0$. For the solution of the equation in the function class B_1 these parameters are $q_0(s) = 0.1$, $q_1(s) = q_2(s) = 0$, and $q_3(s) = (as + b)^2$, where a and b are the numbers.

As already mentioned above, the choice procedure for the regularization parameter α has a significant place in the regularization technique. Using it, a single stable solution having an acceptable accuracy is selected from the family of solutions of system (33).

The parameter α does not need to be correlated with the error of the right-hand side δ in our case, since the solution belongs to the compact. The smaller the discrepancy

$$\|Az^\alpha - u\|,$$

the closer the corresponding solution z^α to the exact one when the latter is a priori known to belong to the compact set [21]. It should be noted that the precision of experimental data for $K(T)$ is usually estimated at 25–30%; however, its exact value is unknown in some instances.

Let us formulate the algorithm of choice of the optimum value of the regularization parameter. For the sake of definiteness, the solution $\sigma_v(\mathcal{E})$ will be considered to belong to the set G_1 (in the case $\sigma_v(\mathcal{E}) \in B_1$ similar reasoning is true).

We choose possible values of α in the form of a decreasing geometric progression

$$\alpha_{k+1} = \alpha_k \cdot \varrho,$$
$$\varrho < 1, \quad k = 1, 2, \ldots, k_0.$$

The progression factor ϱ and the number k_0 are chosen experimentally. Solving the system of linear equations (33) for each value of α_k with fixed parameters $q_n(s)$, we obtain the family of solutions

$$\Sigma_v = \{\sigma_v^{(\alpha_k)}(\mathcal{E})\}.$$

Only solutions belonging to the compact set on which the problem is considered have to be selected from the set Σ_v. In the case where some solution $\sigma_v^{\alpha_k}(\mathcal{E})$ does not meet conditions (19), it is removed from the set Σ_v. If the set Σ_v becomes empty as a result of such a selection, one has to alter the parameters $q_n(s)$.

The last step is the selection of the solution z_s^α that provides the minimum discrepancy

$$z_s^\alpha : \|Az_s^\alpha - u\| = \min$$

from Σ_v, which is a subset of G_1. If the discrepancy value is adequate, the function $z_s^\alpha(s)$ is taken as an approximate solution of Eq. (17). Otherwise one should change the parameters $q_n(s)$ and repeat the solution pattern.

As already mentioned above, the values of $K_v(T)$ are unknown from the experiment. As the simplest zero approximation $K_v(T)$ may be thought of as the same,

$$K_v^{(0)}(T) = \gamma K(T). \tag{34}$$

¿From equality (16) follows the normality condition

$$\gamma = 1/(v^* + 1).$$

Taking the value of $K_v^{(0)}(T)$ as input data and solving inverse problem (15) for each vibrational level v of the molecule, we obtain the set of level cross sections of the reaction in the zero approximation $\sigma_v^{(0)}(\mathcal{E})$.

It is obvious that the level cross sections found within the simplest approximation (34) need to be refined. We introduce the factor $\zeta(v)$, which depends on the level number v in such a way that

$$K_v^{(1)}(T) = \zeta(v)\gamma K(T). \tag{35}$$

For the function $\zeta(v)$ the equality

$$\sum_{v=0}^{v^*} \zeta(v) = \frac{1}{\gamma} = \frac{1}{v^*+1} \tag{36}$$

stemming from Eqs. (16) and (35) holds good.

Since $\zeta(v)$ is independent of $\mathcal{E}$, the problem of finding $K_v^{(1)}(T)$ is reduced to that of determining the refined cross section $\sigma_v^{(1)}(\mathcal{E})$ in terms of the already known one $\sigma_v^{(0)}(\mathcal{E})$,

$$\sigma_v^{(1)}(\mathcal{E}) = \zeta(v)\,\sigma_v^{(0)}(\mathcal{E}). \tag{37}$$

Besides Eq. (36) the following conditions for $\zeta(v)$ are taken:

$$\zeta(0) = 0, \tag{38}$$

$$\zeta(v^*) = \sigma_c / \max\left(\sigma_{v^*}^{(0)}(\mathcal{E})\right), \tag{39}$$

$$\zeta(v) \geq 0, \tag{40}$$

$$\zeta(v+1)\sigma_{v+1}(\varepsilon) > \zeta(v)\sigma_v(\varepsilon). \tag{41}$$

The choice of condition (38) is substantiated by the results of solution of the dynamic problem on the molecule dissociation upon a collision with an atom. These results show that the dissociation rate from the zeroth level is virtually nil [4–6, 33, 34]. Condition (39) determines the maximum possible reaction cross section and σ_c is the gas-kinetic cross section. Condition (41) is confirmed by trajectory calculations [4–6, 33].

In the general case, Eq. (36) has infinitely many solutions. However, using the system of conditions described above one can significantly narrow the class of possible solutions. Moreover, the conditions imposed are found to be sufficient to obtain an approximate solution in the class of smooth functions using the regularization technique. The regularization functional with parameters $q_0(s) = q_1(s) = q_2(s) = 0$ and $q_3(s) = 1$ was used when solving the system of equations (36).

The value of $\zeta\,(v)$ found allows one to calculate the refined cross sections $\sigma_v^{(1)}(\mathcal{E})$,

$$\sigma_v^{(1)} = \zeta(v)\,\sigma_v^{(0)}. \tag{42}$$

The cross sections are valid at all temperatures, since they depend only on the relative energy of colliding particles and the number of the level.

Figures 1 and 2 present the calculated cross sections $\sigma_v^{(1)}$ for the dissociation reaction $O_2 + O_2 \rightarrow O + O + O_2$. The experimental value of $K(T)$ was taken from [28]. The first-approximation function $\zeta(v)$ is shown in Fig. 3. Figure 1 shows the cross sections of the bell-shaped type, while Fig. 2 represents the monotonically increasing ones. In the range of moderate energies they give nearly the same results. However, the calculations [4–6] suggest that the second variant is preferred. The consideration carried out gives an indication of the fundamental importance of the physical analysis in the technique of inverse problems.

4. Directions of Applications

Ill-posed problems presently find applications in a wide circle of problems concerning many branches of physics. With the help of this part of mathematics a considerable advance has already been made

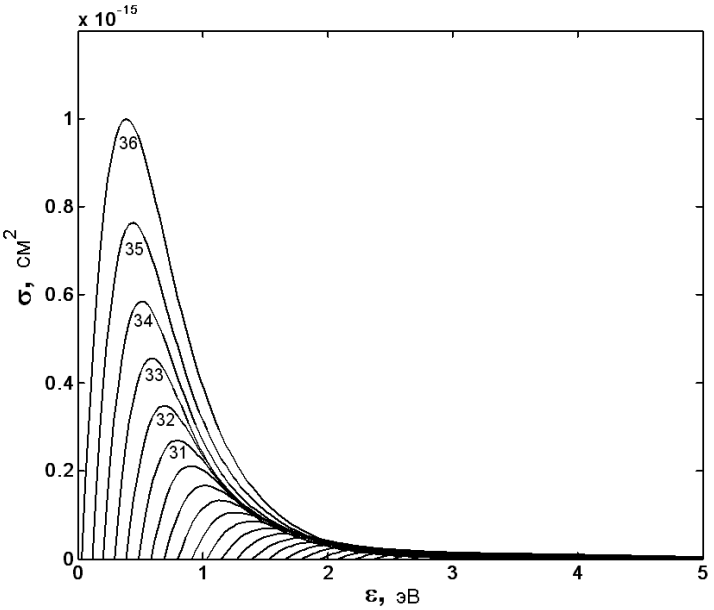

Fig. 1. Level cross sections of the reaction $O_2 + O_2 \rightarrow O + O + O_2$.

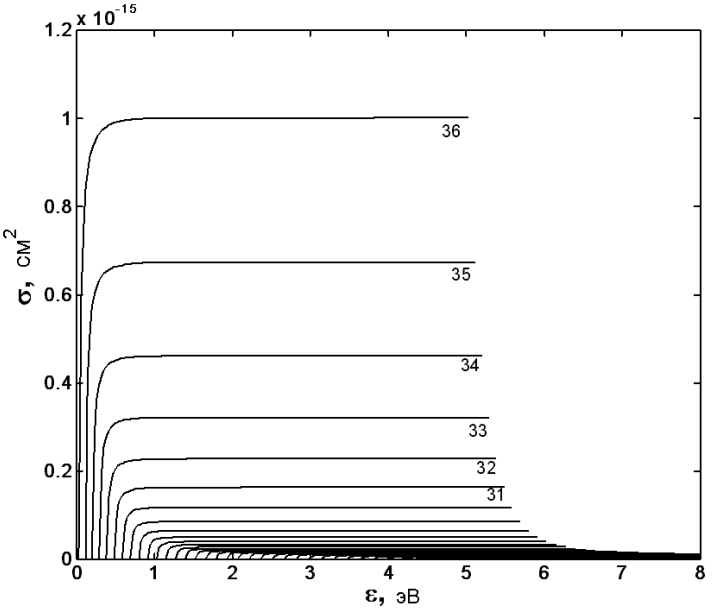

Fig. 2. Level cross sections of the reaction $O_2 + O_2 \rightarrow O + O + O_2$.

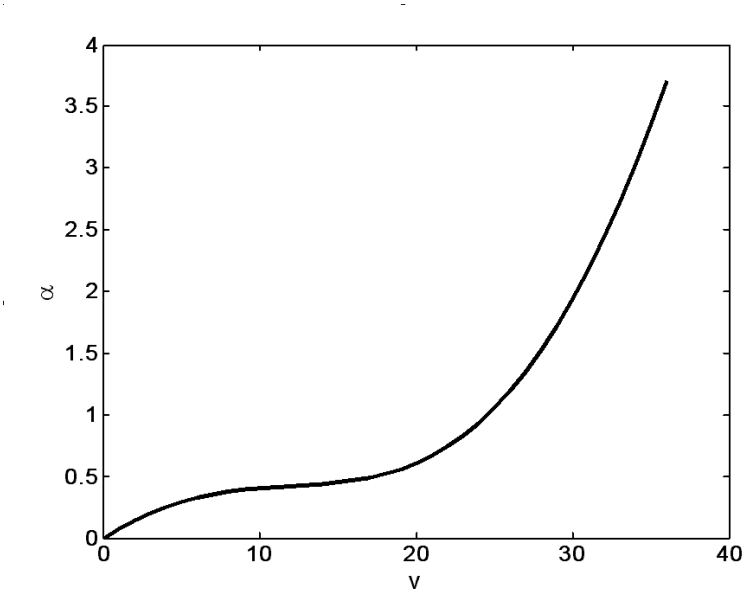

Fig. 3. First-approximation function $\zeta(v)$ for the reaction $O_2 + O_2 \rightarrow O + O + O_2$.

in computer-aided tomography, geophysics, mineral exploration, geoacoustics, acoustic probing of the ocean, and ecology.

As mentioned in the Introduction, the present paper is devoted to applications of the inverse problem methods to the branch of physical-chemical kinetics and laser physics. The design and creation of laser systems are based to a large extent on the kinetic models of active media. Under powerful radiation, laser, and electric discharge action significant disturbances of the thermal equilibrium occur in the chemically reacting gas. The Boltzmann distribution of molecules throughout the vibrational levels is also disturbed because of the energy pumping and chemical reactions of exchange and dissociation. In the calculations of the level kinetics (determination of the populations of individual molecule levels) one has to know the coefficients in the corresponding equations, i.e., the level reaction rate constants. The modeling of such systems can be based on the known level cross sections of the process. Using them, it is possible to calculate the level rate constant under the given thermally non-equilibrium conditions. The level kinetics is of great practical importance for the determination of the medium characteristics in the case of significant disturbances of the equilibrium (for instance, in gas lasers).

An important aspect of application of the theory of inverse problems is the analysis of non-Markov processes. The interaction is virtually never instantaneous and to a varying degree depends on the prehistory. The theory of non-Markov processes is presently developed, which analyzes this circle of phenomena. In some instances the dependence of the state $P(t)$ on the past is described by a Fredholm integro-differential equation of the first kind,

$$\frac{\partial P}{\partial t} = \int_0^\tau \Lambda\, Q[P(t-\tau)]d\tau,$$

where Q is a nonlinear function and Λ is the kernel of equation.

Along with the nonlocality in time is considered the multidimensional Fredholm equation, which describes both the spatial and temporal nonlocality [35]. The processes with memory in the nonequilibrium thermodynamics are considered in [36–38]. The corresponding effects are observed at low temperatures when the substance is irradiated with an ultrashort pulse in shock waves and dispersive systems.

Ill-posed problems are also extensively used in the theory of liquid state of the substance. If an ordinary Newtonian liquid is described by differential equations, for non-Newtonian liquids the relationship between the stress $\Pi(t)$ and the strain rate γ (fluidity) has the integrated form,

$$\Pi(t) = -\int \eta(t-s)\,\gamma(s)\,ds.$$

Here, η is the function of viscous memory. The stress is determined not only by the current value of the strain rate but also is the linear functional of the prehistory of variation of the strain rate. This approach is characteristic of the rheology (the set of investigation techniques of flow and strain in actual media). Notice that all liquids are in principle viscoelastic ones, since the attenuation of fluctuations occurs in a finite time. Because of this, any liquid can be generally considered as a non-Markov system.

In [39] the Boltzmann equation for a dense gas was generalized to the case of durable atomic collisions when, in particular, the hydrogen bonds can be formed between the molecules.

The non-Markov equations arise when the hysteresis processes are described. Thus for the electric current i in electric circuits with a hysteresis we have [40]

$$\frac{di}{dt} = \int F(\tau)\,i(t-\tau)\,d\tau + f(\tau),$$

where F is the integral kernel and f is some specified function.

In [41] is considered the generalization of the classical model "predator-victim," which takes into account the dependence on the living conditions in the past when the fertility of predators depends on their alimentation for some time preceding the occurrence of posterity.

The non-Markov approach is also applicable for the analysis of the spread of epidemiological processes (in particular, flue and respiratory diseases), and for cardiology and neuropsychology problems [42–44].

In recent years the number of papers devoted to the treatment of experimental data using the solution of ill-posed problems has grown rapidly. Actually, in many cases one has no way of acting directly on the object under study. The conclusions on the nature of the objects studied are made on the basis of the analysis of indirect information, which is contained in the characteristics measured. In other words one is led to judge from the consequences of some processes the causes that give rise to them, i.e., to solve inverse problems. In the general case the treatment of experimental data can be understood as a problem of finding the function $z(s)$ by the function $u(x)$ obtained from the observations,

$$u(x) = A[x, z(s)].$$

Here, A is some operator, which relates $z(s)$ to $u(x)$. In many cases the inverse problem of treatment of experimental data leads to a Fredholm integral equation of the first kind.

The elimination of instrumental distortions is an example of the ill-posed inverse problem. The so-called dynamic measurements result in instrumental distortions. In these measurements it is required to find the functional dependence between the physical quantities rather than a single simple value of one of them. When the measuring equipment is linear (which is the case for virtually all actual measuring

devices), the perfect relationship between $z(s) \equiv f_{\text{inp}}(t)$ and $u(x) \equiv f_{\text{out}}(\tau)$ is given by the formula

$$f_{\text{out}}(\tau) = \int_{-\infty}^{+\infty} f_{\text{inp}}(t)\, g(\tau - t)\, dt,$$

where f_{out} and f_{inp} are the output and input signals, respectively, and g is the instrument function of the device. The instrument function of the device corresponds to its response to the δ-pulse fed to its input. In some cases such distortions cannot be ignored (e.g., when they are due to the sluggishness of the device). A priori information on the signal to be regenerated is needed to solve this ill-posed inverse problem.

In [45,46] is considered the application of the technique of solving ill-posed inverse problems in the field of gravimetry of mineral resources. Since the sources of an abnormal gravitational field lie at a definite depth beneath the Earth surface, the field in the vicinity of them is accessible for direct measurement. The problem of determination of this field and hence of the structure of the sources from observational data on the Earth surface is reduced to the solution of a Fredholm integral equation of the first kind.

A considerable body of work is devoted to the solution of ill-posed problems in meteorology and hydrology [47–50]. In [47] is evaluated the emission of greenhouse gas (methane) to the atmosphere from the district of St. Petersburg and its suburbs. In the experiment was used the effect of accumulation of methane in the intermixing layer of atmosphere under the conditions of temperature inversion. In this case, the calculations are also reduced to the solution of a Fredholm equation of the first kind.

In [51], on the basis of the inverse problem method is considered the construction of the particle size distribution function from the data of the indicatrix of scattering of laser radiation. The problem of reconstruction of the diffuse image also results in a Fredholm integral equation of the first kind [46].

5. Conclusions

Thus, the general scheme of using the method of ill-posed inverse problems discussed suggests the broad potential of its practical application in laser physics. This is evidenced, in particular, by the example of calculation of the level cross sections of physical-chemical reactions. By way of example, the approach presented allows one to reduce significantly the calculating time of the cross sections of dissociation processes as compared to quasiclassical calculations [4–6].

The level cross sections obtained can be applied later on to determine the reaction rate in nonequilibrium systems with distribution functions of any kind.

The program suite on the basis of the MATLAB was created for the numerical implementation of the algorithm proposed. It was used to calculate the effective level cross sections of dissociation of the atmospheric gases [52, 53] and other systems.

Acknowledgments

This work was supported in part by the Russian Foundation for Basic Research (Grant No. 03-01-00436).

References

1. G. G. Chernyi and S. A. Losev (Eds.), *Physical-Chemical Processes in Gas Dynamics* [in Russian], Vol. 1, *The Dynamics of the Physical-Chemical Processes in Gas and Plasma*, Moscow State University Press, Moscow (1995).
2. B. F. Gordiets, A. I. Osipov, and L. A. Shelepin, *Kinetical Processes in Gases and Molecular Lasers* [in Russian], Nauka, Moscow (1980).
3. G. G. Chernyi and S. A. Losev (Eds.), *Physical-Chemical Processes in Gas Dynamics* [in Russian], Vol. 2, *Physical-Chemical Kinetics and Thermodynamics*, Moscow State University Press, Moscow (1995).
4. F. Esposito and M. Capitelli, *Chem. Phys. Lett.*, **302**, 49 (1999).
5. F. Esposito and M. Capitelli, *Chem. Phys. Lett.*, **303**, 636 (1999).
6. F. Esposito and M. Capitelli, *Chem. Phys. Lett.*, **364**, 180 (2002).
7. J. Hadamard, "Sur les problemes aux derivees partielles et leur signification physique," *Bull. Univ. Princeton*, **13**, 49 (1902).
8. J. Hadamard, *Le probleme de Caucy et les equations aux derivees partielles lineaires hyperboliques*, Hermann, Paris (1932).
9. A. N. Tikhonov, *Dokl. Akad. Nauk SSSR*, **39**, 195 (1943).
10. A. N. Tikhonov, *Dokl. Akad. Nauk SSSR*, **151**, 501 (1963).
11. A. N. Tikhonov, *Dokl. Akad. Nauk SSSR*, **153**, 49 (1963).
12. A. M. Gubanov, E. K. Eroshenkov, O. A. Malkin, and L. S. Polak, *Kinetika i Kataliz*, **13**, 33 (1972).
13. A. S. Biryukov, V. K. Konyukhov, A. I. Lukovnikov, and R. I. Serikov, *Zh. Éksp. Teor. Fiz.*, **66**, 1248 (1974).
14. Y. A. Kulagin, R. I. Serikov, I. V. Simanovskii, and L. A. Shelepin, *J. Russ. Laser Res.*, **20**, 560 (1999).
15. A. N. Tikhonov and V. Ya. Arsenin, *Solutions of Ill-Posed Problems*, Halsted Press, New York (1977).
16. A. N. Tikhonov, A. V. Goncharskii, V. V. Stepanov, and A. G. Yagola, *Regularizing Algorithms and A Priori Information* [in Russian], Nauka, Moscow (1983).
17. A. V. Goncharskii, A. S. Leonov, and A. G. Yagola, *Zh. Vych. Mat. i Mat. Fiz.*, **12**, 1592 (1972).
18. V. K. Ivanov, *Izv. Vuzov. Matematika*, No. 2, 96 (1958).
19. V. K. Ivanov, *Dokl. Akad. Nauk SSSR*, **142**, 997 (1962).
20. V. K. Ivanov, *Dokl. Akad. Nauk SSSR*, **145**, 270 (1962).
21. A. N. Tikhonov, A. V. Goncharskii, V. V. Stepanov, and A. G. Yagola, *Numerical Methods of Solution of Ill-Posed Problems* [in Russian], Nauka, Moscow (1990).
22. A. V. Goncharskii and V. V. Stepanov, *Dokl. Akad. Nauk SSSR*, **245**, 1296 (1979).
23. A. V. Goncharskii and V. V. Stepanov, *Vestn. MGU*, Ser. 15, No. 3, 12 (1980).
24. A. V. Goncharskii and A. G. Yagola, *Dokl. Akad. Nauk SSSR*, **184**, 771 (1969).
25. F. P. Vasil'ev, *Methods of Solution of Extremum Problems* [in Russian], Nauka, Moscow (1981).
26. B. N. Pshenichnyi and Yu. M. Danilin, *Numerical Methods in Extremum Problems* [in Russian], Nauka, Moscow (1975).
27. J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids*, Wiley, New York (1954).
28. L. Jerig, K. Thielen, and P. Roth, *AIAA J.*, **29**, 1136 (1990).

29. L. B. Ibragimova, G. D. Smekhov, and O. P. Shatalov, *Mekh. Zhidk. i Gazov*, No. 1, 181 (1999).
30. O. E. Krivonosova, S. A. Losev, V. P. Nalivaiko, et al., "Advisable Data on the Rate Constants of Chemical Reactions between the Molecules Consisting of N and O Atoms", in: B. M. Smirnov (Ed.), *Chemistry of Plasma: Collection of Papers.* [in Russian], Issue 14, Energoatomizdat, Moscow (1987), p. 3.
31. M. S. Massey, *Rept. Progr. Phys.*, **12**, 248 (1949).
32. A. N. Kolmogorov and S. V. Fomin, *Elements of the Theory of Functions and Functional Analysis*, Vol. 1, Graylock Press, Rochester, New York (1957) and Vol. 2, Graylock Press, Albany, New York (1961).
33. S. V. Kulikov, A. L. Smirnov, and O. N. Ternovaya, *Zh. Khim. Fiz.*, No. 12, 53 (2000).
34. S. O. Macheret and I. V. Adamovich, *J. Chem. Phys.*, **113**, 7351 (2000).
35. C. Itzykson and J. B. Zuber, *Introduction to Quantum Field Theory*, McGraw-Hill, New York, (1980).
36. W. A. Day, *The Thermodynamics of Simple Materials with Fading Memory*, Springer-Verlag, New York (1972).
37. N. Petrov and I. Brankov, *Modern Problems of Thermodynamics* [in Russian], Mir, Moscow (1986).
38. S. L. Sobolev, *Usp. Fiz. Nauk*, **161**, 5 (1991).
39. V. I. Korobko, *The Golden Proportion and Problems of Harmony of the Systems* [in Russian], Publishers of the Association of Building Institutes, Moscow (1997).
40. E. M. Soroko, *Structural Harmony of the Systems* [in Russian], Nauka i Tekhnika, Minsk (1984).
41. V. I. Korobko, *The Golden Proportion Principle in the Vegetable World. The Strategy of Life under the Conditions of the Planetary Econical Crisis* [in Russian], Vol. 2, Gumanistika, St. Petersburg (2002).
42. R. M. Yulmetuev, S. A. Demin, N. A. Emelyanova, et al., *Physica* A, **331**, 300 (2004).
43. R. M. Yulmetuev, P. Haggi, and F. M. Gafarov, *Phys. Rev.* E, **62**, 6178 (2000).
44. R. M. Yulmetuev, P. Haggi, and F. M. Gafarov, *Phys. Rev.* E, **64**, 432 (2001).
45. A. N. Tikhonov and V. B. Glasko, *Zh. Vych. Mat. i Mat. Fiz.*, **5**, 463 (1965).
46. A. B. Vasil'eva and A. N. Tikhonov, *Integral Equations* [in Russian], Moscow State University Press, Moscow (1989).
47. A. V. Zinchenko, N. N. Paramonova, V. I. Privalov, and A. I. Reshetnikov, *Meteorolog. i Gidrolog.*, No. 5, 35 (2001).
48. V. A. Borzilov, N. V. Klepikova, et.al., *Complex of Mathematical Models of Atmospheric Propagation and Deposition of Radionuclides. Radiation Aspects of the Chenobyl' Accident* [in Russian], Gidrometeoizdat, St. Petersburg (1993), P. 82–86.
49. V. F. Raputa and A. I. Krylova, *Meteorol. Gidrol.*, No. 3, 49 (1995).
50. D. E. Haas-Laursen, D. E. Hartley, and R. G. Prinn, *J. Geophys. Res.*, **101**, 22823 (1996).
51. Yu. A. Kulagin, R. I. Serikov, I. V. Simanovskii and L. A. Shelepin, *Application of the Method of Direct and Inverse Problems for the Calculation of Particle Size Distribution Function* [in Russian], Preprint No. 46 of the P. N. Lebedev Physical Institute, Moscow (1999).
52. A. I. Osipov and S. L. Shelepin, *Vestn. Mosk. Univ. Ser. 3. Fiz. Astron.*, No. 5, 37 (2003).
53. A. I. Osipov and S. L. Shelepin, *Vestn. Mosk. Univ. Ser. 3. Fiz. Astron.*, No. 6, 64 (2004).