REGULARIZATION ALGORITHMS: APPLICATIONS

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1 Introduction

Beginning from 1966, we (together with A.V. Goneharzsky, A.S. Leonov and other members of the mathematical school headed by A.N. Tikhonov) proposed new approaches for solving linear and nonlinear ill-posed problems:

(a) on compact sets of bounded monotone functions (with further generalization on sets of convex and monotone convex functions);

(b) in Hilbert and reflexive Banach spaces including cases where the operator (linear or nonlinear) is specified with an error and there exist *a priori* constraints on the unknown solutions (generalized descrepancy principle, generalized discrepancy method etc).

For detailed explanation of the theory and the full list of references , see books [1]–[4]. In [1]–[2] it is possible to find fortran programs (with test examples) for solving linear ill-posed problems with and without *a priori* constraints including one and two-dimensional equations of convolution type.

Now these methods are very well known and used in theoretical investigations as well as in applications. Some applications from astrophysics and vibrational spectroscopy are described below.

2 Inverse Problems in Astrophysics

Astrophysics deals with immensely remote objects, such as stars and galaxies, whose properties can only be measured by those indirect manifestations which are observable from the Earth or from a spacecraft in Earth's orbit. Hence, inverse problems, the majority of which are ill-posed, must be solved in order to interpret observed data. We shall describe only some results from our experience with solving inverse problems in astrophysics, see [4]–[6], and for computer programs (in fortran), refer [6].

2.1 Wolf-Rayet Stars in Close Binary Systems

A wide range of important inverse problems in astrophysics are associated with the interpretation of the observed properties of close binary systems. The pioneering studies in this field were carried out by H. Russel, J. Merrill, Z. Kopal, A. Batten, D. Popper, V.P. Tsesevich, D. Ya. Martynov, A.M. Shul'berg, M.I. Lavrov, and V.A. Krat. The more important attributes of stars, such as their masses, radii, temperatures, and structure of atmospheres, can be successfully estimated by studying the motion and various interaction effects of gravitationally coupled binary star systems. Such a complete set of attributes cannot be obtained for a single star. Hence, it is very fortunate for the astrophysicist when a particular object is a close binary system.

Note that almost every other star in the Galaxy belongs to a binary or a multiple system. At present, more than 4000 eclipsing binary systems (i.e. systems whose orbital planes are oriented in such a way that,as seen from the Earth, the components eclipse each other twice each orbital period) are known. Close binary systems include various stellar objects: normal main sequence stars, supergiants, Wolf-Rayet stars, subdwarfs, subgiants, white dwafts, neutron stars, and, probably, black holes. A series of inverse problems can be formulated on the basis of the light curves and radial velocity curves of binary systems. When solved by standard regularization methods, various important attributes of stars and binary systems can be assessed. As a result, reliable conclusions concerning the nature and evolution of these stystems can be made.

Wolf-Rayet stars (WR-stars), which lie in the galaetic plane, were discovered by Wolf and Rayet more than a hundred years ago. At present, about 300 such stars are known. But why are those stars so remarkable among other hundred billion stars of the Galaxy and why do astronomers pay so much attention to them? In fact, the optical spectra of WR-stars are very peculiar because they simultaneously contain strong emission lines of hydrogen, atomic and ionized helium, nitrogen, carbon, and oxygen in various ionization states. For many of these lines to be excited, the temperature of matter or radiation must reach several hundred thousand degrees, while the visible continuum of WR-stars can be roughly described by blackbody radiation sources with mean temperatures of 10,000 to 20,000 degrees. This means that the matter in WR-stars is far from being in thermodynamic equilibrium. Moreover, the observations (and the analyses done on their basis) unambiguously indicate that WR-stars have anomalous chemical compositions. WR-stars, for example, contain far more helium than normal stars.

However, any decisive conclusion about WR-stars is very difficult whilst the observations only involved single stars. A WR-star itself (the core containing the main part of the mass) is hidden inside a thick atmosphere that expands radially with a velocity of several thousand kilometers per second. By contrast, when observing the Sun we see a sharp-edged disk. This is because the Sun's shell where the visible radiation is produced is 300 km thick; i.e. only about 10^{-4} of the Sun's radius. But the atmosphere of a WR-star stretches for many millions of kilometers and is much larger than the star's core, even though the mass of the atmosphere is only 10^{-9} of the total mass of the star.

The situation is similar to looking at a lamp through a dense fog when the visible oreol seems to be much larger than the lamp itself. It is therefore not surprising that studies of single WR-stars, which are derived from observations of their total radiation show that the radii of WR-stars are 20–30 times bigger than the Sun's radius. In addition, their effective temperatures are much too low (30 000K) to excite line spectra. We have therefore to assume that the kinetic temperature of electrons in the atmosphere is very high (i.e. several hundred thousand degrees). The mechanism for such strong heating (one that occurs in the Sun's chromosphere and corona) is the dissipation of the energy of acoustic and magnetohydrodynamic waves emanating from the stars.

In 1964, Yagola, Goncharsky and A.M. Cherepashchuk commenced a study of WR-stars in eclipsing binary systems. The WR-stars are so immensely remote that no telescope from the Earth can resolve their disks. Nonetheless, observations taken during eclipses of binary systems containing WR-stars give us a unique possibility for depicting the star's disks in different colours. Thus continuous spectra can be built for the entire disk of a WR-star, and for its central and peripheral regions as well. When the partner of a binary system—a normal star from a spectral class O or B—eclipses the WR-star, the resultant light curve contains information about both; namely, the total luminosity of the WR-star and the brightness distribution over its disk. (The light curve is the plot of the star's radiation at a given wavelength or in a given wavelength range over time.)

We have proposed a new approach to the interpretation of the light curves of eclipsing binary systems on the basis of the modern regularization methods for ill–posed problems. Based on this efficient computer programs have been developed to solve these problems [6]. A natural *a priori* physical assumption is that the functions of interest are monotone and nonnegative. In addition, an extensive program of observations of all the known eclipsing binary systems containing WR-components has been undertaken (for more detail, see [6]).

Let us consider briefly the mathematical problem of interpreting the light curve of an eclipsing system containing a WR-star and a normal star from the spectral class O or B. The WR-star has an extended atmosphere, while its partner is an opaque star whose atmosphere is negligibly thin and its brightness distribution over the disk is determined by its spectral class. Both stars are spherical, travelling around their centre of mass in circular orbits. The light curve of the system depends on the angular position of the components in the orbital plane. It can be expressed as a function Δ of the distance between the components' disks in the plane perpendicular to the viewing line. The variations of light are completely determined by the mutual eclipses of the components. When the opaque star eclipses the WR-star, the measured light of the system is

$$l(\Delta) = L - \int\int_{S(\Delta)} I(\rho) d\sigma, \tag{1}$$

where L is the light when there is no eclipse in the system (it is constant if the system's radiation is not affected by reflection or tides), ρ is the polar radius of the WR-star's disk, $I(\rho)$ is the brightness distribution over the WR-component's disk under the assumption of spherical symmetry, $d\sigma$ is a surface element, and $S(\Delta)$ is the region of the eclipse overlap, which depends on the distance between the components.

If we recall that $dS = \rho(d\rho d\varphi)$ (φ being the polar angle on the WR-component's disk), the integration over φ transforms (1) into a one-dimensional Fredholm equation of first kind:

$$L - l(\Delta) = \int_0^r K(\Delta, \rho) I(\rho) d\rho, \tag{2}$$

where r is the radius of the WR-star. The expression for the kernel $K(\Delta, \rho)$ can be easily obtained. The equations describing the second minimum of the light curve and the eclipse of the normal component by the WR-star can be derived in a similar way. To do so, we take the brightness distribution over the normal component as known, and look for the absorption distribution over the WR-component's disk. Naturally, we have to assume that the brightness and absorption distributions we want are monotone and nonnegative. In addition, the radii of the components, and the angle i of the orbital plane to the plane perpendicular to the viewing line are unknowns. A complete description of the problem and the methods used to determine the unknown functions and geometrical parameters are given in [5]–[6]. Other problems concerning the interpretation of light curves for eclipsing binary systems are also presented there.

Figure 1 shows the brightness distributions $I_c(\xi)$ over the disk of the WR–star in the eclipsing system V444 Cygni. It can be seen, that although the total radius of the visible photosphere is 10 to 20 times that of the Sun and increases with the wavelength due to the strengthening role of free-free absorption, the radius of the central intensity peak in blue and ultraviolet (absorption is at a minimum in these spectral ranges because it only depends on light scattering by free electrons) is three times the radius of the Sun. It is natural to consider that the radius of the central peak is the radius of the WR-star itself (we call it the WR-core).

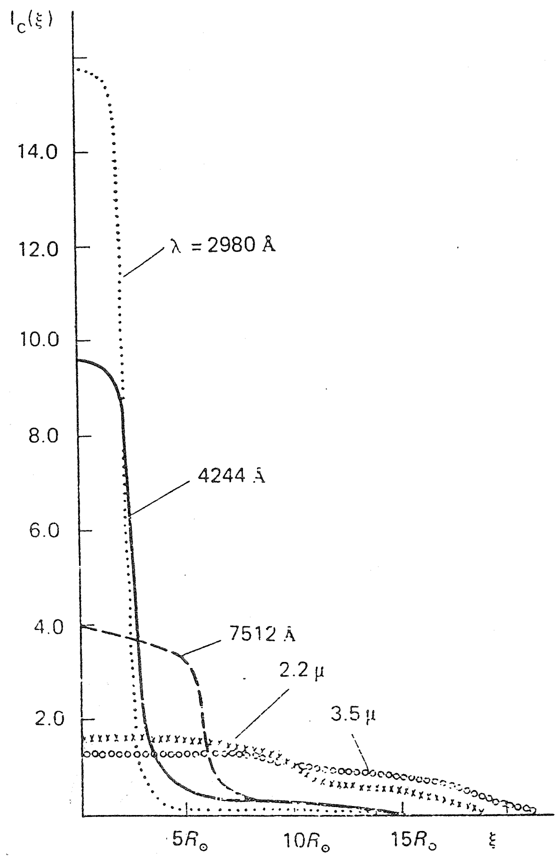

Figure 1. Distribution of brightness over the disc of a Wolf-Rayet star in ultraviolet ($\lambda = 2980$ Å), visible (λ from 4244 to 7512 Å), and infrared (λ from 2.2 to 3.5 μ) spectral ranges restored from the analysis of light curves in the binary eclipsing system V 444 Cygni. The central region of the star's disk are more blue and, therefore, more hot than periphery. The radius of the core of the Wolf-Rayet star is about $3R_\odot$, while that of the expanding atmosphere, whose mass is 10^{-9} of that of the core, is about $20R_\odot$.

Since brightness distributions over the WR-component's disk are obtained for different wavelengths, we can plot the spectra of the WR-core and that of the shell. Such spectra are presented in Figure 2. Although the radiation temperature of the WR-component's disk as a whole is 20 000 K, these spectra show that that of the WR-core is close to 100 000 K . The relatively low temperature of the disk as a whole is due to the low-temperature (700 K) recombination radiation of the extended atmosphere, which contributes 80% of the visible radiation. These results were recently verified by observations in infrared and in ultraviolet from the OAO–2 orbital station of USA.

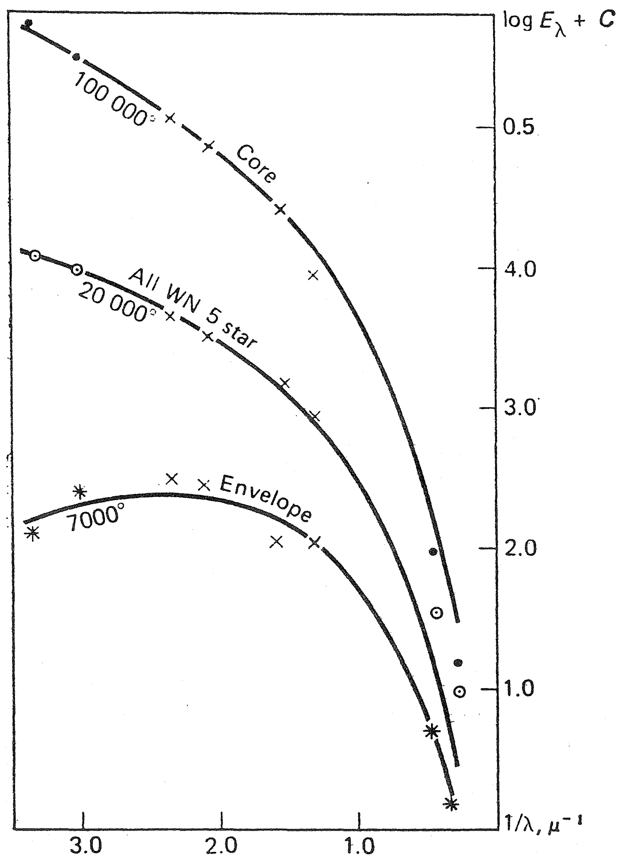

Figure 2. The observed spectra of continuum for different parts of the Wolf-Rayet star's disk obtainde from the data in Figure 1. Crosses correspond to the visible range, while asterisks, circles, and dots to new data on light curves of the system V 444 Cygni obtained in the ultra-

violet (J. Eaton, USA) and in infrared (L. Hartmann, USA) ranges. Solid lines are the spectra of black bodies with corresponding temperatures. The radiation temperature of the Wolf-Rayet star's core is close to $100,000\ K$, while that of the disk as a whole can be roughly described by black-body radiation with the temperature of $20,000\ K$.

Thus, by solving an inverse problem related to the interpretation of the light curves of eclipsing binary stars we were able to separate the radiation of the WR-core from that of the extended atmosphere and to give estimates of the radius, temperature and luminosity of the WR-core. From the knowlege of the mass, radius, and temperature of a star, we can make conclusions about its nature and evolutionary history [5]–[6].

2.2 Neutron Stars and Black Holes in Binary Systems

According to our modern understanding [7], a star at the end of its evolution can become either a white dwarf (if its mass M is less than $1.4\ M_{\odot}$), or a neutron star (if $M > 1.4\ M_{\odot}$), or a black hole (if $M > 2\ M_{\odot}$).

White dwarfs were discovered at the beginning of the century and are now relatively well studied. Several thousand white dwarfs are known within 100 parsec from the Earth. The pressure inside such stars does not depend on temperature, but is determined by the quantum mechanically degenerated electron gas. Although the mass of a white dwarf is about $0.85\ M_{\odot}$, its radius is very small (of the order of the Earth's radius), hence the density is about one tonne per cubic centimeter. In his famous paper on this subject, which was published in 1931, Chandrasekhar, who was then 20 and who was later awarded the Nobel prize in 1983, showed that, as the mass of a white dwarf increases, the degeneration of the matter must become relativistic (i.e. the velocities of the electrons approach the speed of light). As a result, the decreased pressure of the electron gas cannot oppose gravity. Therefore, a white dwarf whose mass exceeds the Chandrasekhar limit (for a helium white dwarf this limit is about $1.4\ M_{\odot}$) must collapse.

The physical basis for the formation of neutron stars was formulated by Landau in the 1930's. A neutron star consists of degenerate neutron gas, its mass is about $1\ M_{\odot}$, its radius about 10 to 20 km, its density of the order of a billion tonnes per cubic centimeter. The radiopulsars, which were discovered in 1967, are in fact rapidly rotating (with the period of ≥ 1.5 ms), strongly magnetized (magnetic field strength $\simeq 10^{12}$ Gs) neutron stars. In 1972, X-ray pulsars were also discovered. They are rapidly rotating, strongly magnetized neutron stars but they are the components of close binary systems accreting matter supplied by normal star partners. At present, several hundred radiopulsars and several dozen X-ray pulsars are known.

Black holes are predicted by Einstein's theory of general relativity. It is now believed that the pressure of degenerate neutron matter in a neutron star with a mass greater than 2 $M_\odot$ (the Oppenheimer-Volkov limit) cannot oppose star's gravity, so the star must suffer a relativistic collapse, i.e. it implodes without limit to produce a black hole. The radius of a nonrotating black hole tends to $r_g = 2\ GM/c^2$, where $G = 6.67 \times 10^{-8}$ dyne $\cdot sm^2/g^2$ is the graviational constant, M is the star's mass, and c is the speed of light. The value r_g (gravitational radius) is about 6 km for $M = 2M_\odot$. In the local coordinates of the star, its radius reaches r_g in a finite time and then falls without limit. In the coordinate system of a remote observer, the radius of a star subjected to the relativistic collapse tends to r_g over an infinitely long time but it gets very close to r_g in the first few moments of collapse.

Neither light nor any other signal can leave the "surface" of a black hole because of its enormously strong gravity. The gravitational force is so strong that from the viewpoint of a remote observer time stops at radius r_g, hence the object is graviationally self-connected. For a nonrotating black hole, the radius r_g determines the event horizon, which cannot be overcome as seen by a remote observer. Therefore, no process occurring within a sphere of radius r_g is accessible for a remote observer.

It was shown by Zeldovich and Novikov and by Shklovsky that the accretion of matter from a normal star to a relativistic object in a close binary system will result in intense X-ray radiation. To clarify this, let us consider a system of a normal star and a relativistic object. If the radius of the normal star is large enough then the tidal effect of the relativistic object results in a distortion of the star's sphere. The star becomes pear-shaped and almost fills up the Roche lobe of the binary system. Hence, matter flows from the star's surface to the relativistic object, forming a rotating disk-shaped shell (accretion disk) in the vicinity of the relativistic object. The supernova explosion, which gave rise to the relativistic object in the system, may affect the roational axis of the normal star in such a way that it may not be perpendicular to the orbital plane, and therefore precesses slowly.

The friction between different layers of the disk decreases its angular momentum and makes the disk's matter fall into the central relativistic object. But the gravitational potential at the surface of a neutron star or a black hole is so strong that the inner layers of the disk will be accelerated to almost light speed. This heats the matter up to ten million degrees and powerful ($10^{36} - 10^{38} erg/s$) X-ray radiation will be emitted. This theory of disk accretion by neutron stars and black holes was developed by Shakura and Syunyaev, Novikov and Thorne, Pringle and Rees.

Recent observations from orbital laboratories have shown up thousands of compact X-ray sources, the majority of them being accreting neutron stars and, possibly, black holes in close binary systems. The powers, spectra, and variabilities of X-ray radiation of the sources contain very valuable information about the relativistic objects. At the same time, the relativistic objects can be effectively investigated on the basis of optical (photometric, spectral, and polarization) measurements of X-ray binary systems.

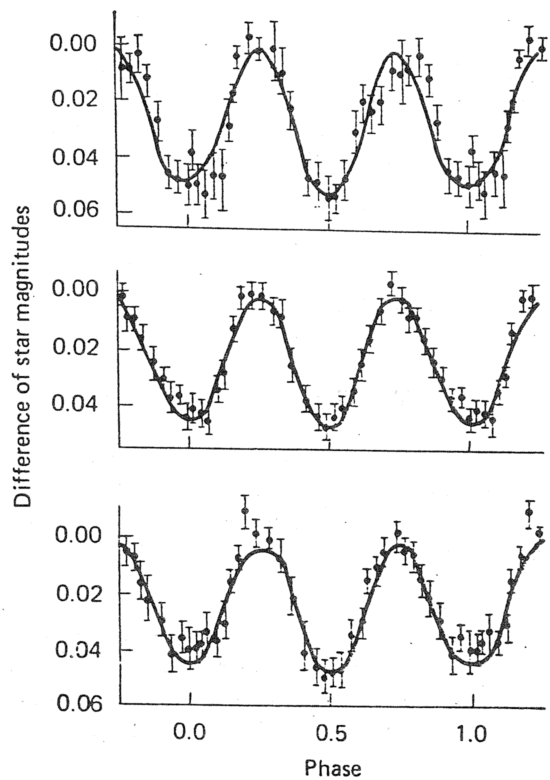

Figure 3. Observed (dots) and theoretical (solid lines) light curves for the X-ray binary system Cygni $X-1$. The lower limit of the mass of the X-ray source at a distance of more than two kilometers from the system is 7 $M_{\odot}$. Hence, the object Cygni $X-1$ can be considered as the first candidate for black holes.

It has been shown that the main causes of the optical variability of X-ray binary systems are the effect of the ellipsoidal shape of the optical star in systems with

OB-supergiants and the effect of reflection or, more strictly, the heating of the optical star's surface by the powerful X-ray radiation of the accreting relativistic object. The amplitude of the optical variability connected with the ellipsoidal shape of the normal star and its tidal deformation in the graviational field of the relativistic object depends on the ratio $q = m_x/m_v$ (where m_x and m_v are the masses of the X-ray and optical components), on the angle i between the normal to the orbital plane and the viewing line, and on the degree μ to which the Roche lobe is filled.

We have developed algorithms to solve the inverse problems related to interpretation of optical light curves of X-ray binary systems within the framework of a parametric model. These algorithms determine both the values of the parameters and to indicate the confidence intervals for these values [6].

Various kinds of X-ray binary systems were observed in an extensive program. In particular, the telescopes of the Mount Stromlo and Siding Spring observatories of the Australian National University were used by Chezepashchuk to investigate the binary systems of the Southern Hemisphere. Very significant results were obtained by analysing the observatory data by the new method.

The observed and theoretical light curves for the X-ray binary system Cygni X-1 are shown in Figure 3. These curves are seen to be in good agreement. Thus, on the basis of information received from a distance of more than two kiloparsecs, the mass of the relativistic object was estimated as $m_x > 7\ M_\odot$. This is far above the upper limit of mass for a neutron star, and convincingly indicates that the X-ray source of Cygni X-1 system is a black hole.

Note that the Cygni X-1 system is unique, since similar treatments of the data from many other X-ray sources (e.g. HD 153919, HZ Her, HD 77581) yield mass values not greater than $2\ M_\odot$ (characteristic of neutron stars). In addition, the optical characteristics of the accreting disks in X-ray binary systems have been studied, and agree with the theory of disk accretion of matter by relativistic objects.

The developed method was used to interpret light curves for other binary stars (for example SS 433, see [6]).

2.3 Determination of Structure and Dynamic Characteristics of Accreting Disks in Nova and Nova-like Stars

A nova or nova-like star is now known in fact to be a binary system, consisting of a red dwarf and a degenerate white dwarf surrounded with an accreting disk [8]. In order to understand the mechanism underlying explosions of nova and nova-like stars, we must study the structure of accreting disks at the different phases of flare activity of a binary system. In order to interpret the light curves of the stars, complex algorithms have been developed which restore the structure of an accreting disk from observations of optical eclipses [6]. It was found that a flare from a nova-like star can be related to changes in the parameters of the accreting disk, because the disk's radius, surface brightness and luminosity rise considerably during a flare.

2.4 Mapping of the Distributions of Chemical Elements Over the Surface of the Peculiar Ap-stars

The Galaxy contains many stars in spectral class A whose atmospheres have chemical element contents several hundred (or even thousand) times larger than those of normal stars. The profiles of the absorption lines in the spectra of these stars are quite variable, which indicates that the chemical composition anomalies are localized at certain places on the star's surface, while the periodicity of the variations seems to be related to the rotations of the stars. The inverse problem of determining the local profiles of the absorption lines from the observed integral profiles was first formulated by Khokhlova (for a detailed bibliography, see [9]). To solve this problem, algorithms based on regularization methods were developed [6].

Let us briefly consider the mathematical formulation of this problem. We assume that the temporal variability of the profiles of the absorption lines is due to inhomogeneous distributions of the chemical element responsible for the absorption lines over the star's surface. We can thus write an equation for the local profiles of the absorption lines at each point of the visible surface of a star in terms of the integral profiles observed in different phases.

The profile of a line, which must be observed in the spectrum, averaged over the star's disk in the rotation phase ωt (ω is the angular velocity, t is time), can be written as

$$R(\lambda, \omega t) = 1 - \frac{\int\int_{\cos\theta>0} I\,[M, \theta, \lambda + \Delta\lambda_D(M)] \cos\theta dS_M}{\int\int_{\cos\theta>0} I_{\text{ cont}}\ (M, \theta) \cos\theta dS_M}, \tag{3}$$

where λ is the wavelength, M is a point on the star's surface, dS_M is a surface element on the sphere, θ is the angle between the normal to the star's surface at M and the viewing line (the domain of integration is the observed surface of the star, $\cos\theta > 0$), the phase ωt appears in the right-hand side in an implicit form through $\Delta\lambda_D(M)$ and $\theta, I(M, \theta, \lambda + \Delta\lambda_D(M))$ is the local intensity at M at a wavelength displaced by the Doppler shift $\Delta\lambda_D(M)$ (this shift is due to the star's rotation and depends on its orientation with respect to the observer), and $I_{\text{cont}}(M, \theta)$ is the intensity of the continuum at the point M.

We can rewrite (3) as

$$R(\lambda, \omega t) = \frac{\int\int_{\cos\theta>0} I_{\text{cont}}(M,\theta) R(M,\theta,\lambda + \Delta\lambda_D(M)) \cos\theta dS_M}{\int\int_{\cos\theta>0} I_{\text{cont}}(M,\theta)\cos\theta dS_M}, \tag{4}$$

where

$$R(M,\theta,\lambda) = 1 - \frac{I(M,\theta,\lambda)}{I_{\text{cont}}(M,\theta)} \tag{5}$$

is the depth of the local profile of the spectral line, this depth depending on θ and M; $I_{\text{cont}}(\theta, M)$ is the continuum intensity which we take to be independent of λ because the measured wavelength range is rather narrow and of M because the physical conditions on the star's surface are homogeneous. The dependence $I_{\text{cont}}(\theta)$ is defined by the limb darkening and we assume it is known for spectral class of the star. Hence, the local profile of the absorption line $R(M,\theta,\lambda)$ for a given M and θ can be approximated by a function $R_\tau(\lambda)$ belonging to a set of functions that depend on a parameter τ, the set being chosen on the basis of physical reasons. The problem of finding the distribution $\tau(M)$ (or, in other words, the local profile of the absorption line) can be reduced to a nonlinear integral equation of the first kind. To solve this equation, a regularizing algorithm was applied in which the Tikhonov functional was minimized by the method of conjugated gradients, and the regularization parameters was chosen on the basis of the alternative discrepancy principle [6].

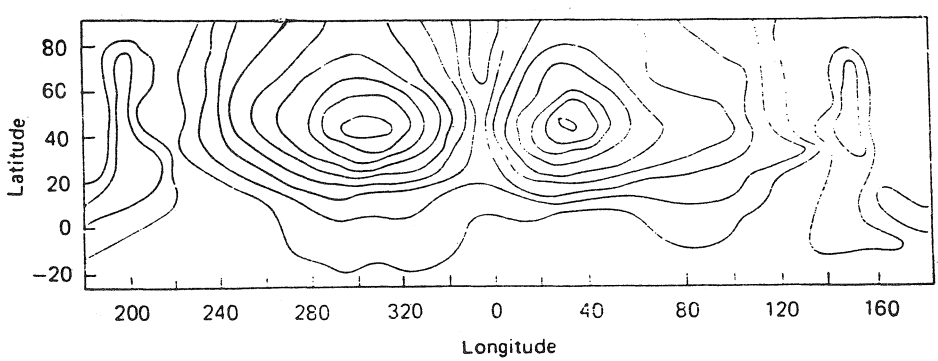

Figure 4. Distribution of silicon concentration over the surface of the peculiar Ap-star CU Virgo as obtained when solving the inverse problem on interpreting the variable profiles of the absorption line Si II $\lambda = 3862\mathring{A}$. Two spots where the silicon content is about $1,000$ times the normal level.

When treated by a regularization method, spectroscopic observations, made both in the USSR and abroad, have led to rather interesting results. For example, Fig. 4 shows the reconstructed distribution of the equivalent widths of the silicon lines over the surface of the Ap-star CU Virgo. It can be seen that this star has two spots where the silicon content is about 1000 times the normal level. If the maps of chemical elements are compared with the distributions of magnetic field, we should obtain valuable information about the mechanisms resulting in the observed anomalies.

For some other inverse problems in astrophysics, the reader may refer to [6]. For example, the reconstruction of the strip-distribution of radio-brightness over a source, with errors in the antenna directivity diagrams being taken into account, is also an inverse problem, we have studied. This investigation resulted in the development of the theory of ill-posed problems with approximately specified operators [1]–[3].

According to our calculations, the regularization methods applied to radioastronomical observations with the 3% errors can improve the resolving power of a telescope by a factor of two to three without increasing the telescope's diameter [6]. Also, the regularizing algorithms are very useful in spectroscopy where the resolving power of a spectrometer can be significantly improved due to corrections of observed line profiles to the instrumental profile.

To conclude, we should note that the regularization methods for ill-posed problems resulted in a series of new promising branches in astrophysics. We believe that processing of astrophysical data without usage of modern mathematical methods and large computers is now as impossible as observations without a telescope.

3 Inverse Problems in Vibrational Spectroscopy

Now we consider inverse problems of vibrational spectroscopy, which consist of determining the parameters of force field of a molecule from experimentally measured data (mainly obtained from analysis of the vibrational spectra of the molecules). For detailed explanation and the full list of references, the reader may refer to our books [10]–[11] and the main publications in English [12]–[14].

The concept of the force field of a molecule arose from a consideration of it as a quantum–mechanical system consisting of point nuclei and electrons, where the masses of the nuclei and the electrons are quite different. In this connection, we can introduce a small parameter ξ, equal to the ratio of the mass of the electron to the sum of the masses of the nuclei of the molecule, and we can use the adiabatic theory of perturbations, based on expansion of all terms of Schrödinger's equation for the molecule in powers $\xi^{1/4}$. The second-order equations of perturbation theory enable one to speak of the motion of the nuclei in certain effective force field $U(q_1, \ldots, q_n)$, produced by the electron subsystem of the molecule (here $q_1, \ldots, q_4$ are the relative coordinates of the nuclei).

The force field plays an important role in determining the properties of the molecule. In particular, the equilibrium geometrical configuration of the nuclei of the atomes of the molecule (if it exists) $q^0 = (q_1^0, \ldots, q_n^0)$ satisfies the relations

$$\left(\frac{\partial U}{\partial q_i}\right)|_{q^0} = 0, \quad i = 1, 2, \ldots, n, \tag{6}$$

while the properties connected with small vibrations of the molecule are determined by the matrix of the force constants F with $F = (F_{ij})_{i,j=1,2,\ldots,n}$, where

$$F_{ij} = \left(\frac{\partial^2 U}{\partial q_i \partial q_j}\right)|_{q^0}. \tag{7}$$

Since we will henceforth use experimental data on the vibrational motion of the molecule, we will formulate the problem of determining the matix F, assuming a specified equilibrium configuration q^0. The number of generalized coordinates characterizing the configuration of N nuclei should be $n = 3N - 6$ ($3N - 5$ for a linear molecule). If $n > 3N - 6$,then the the coordinates will not be independent. Their introduction is justified by the convenience of taking into account the symmetry of the molecules and the interpretation of the results.

The frequencies of the vibrational spectra are the main form of the experimental data on the vibrations of the molecules. They are connected with the matrix of the force constants F by the eigenvalue problem

$$GFL = L\Lambda, \tag{8}$$

where Λ is a diagonal matrix consisting of the square of the frequencies of the normal vibrations of the molecule, $\Lambda = \mathrm{diag}\{w_1^2, \ldots, w_n^2\}$, and G is the matrix of the kinetic energy in the momentum representation, which depends only on the masses of the nuclei and their equilibrium configuration, which we assume to be known (possibly with some error), L is the matrix of the eigenvectors.

Within the approximation considered, the force field of the molecule is independent of the nuclear masses, and hence for the spectra of m isotopic varieties of the molecule, instead of (8) we use the system

$$G_i F L_i = L_i \Lambda_i, \quad \tau = 1, 2, \ldots, m, \tag{9}$$

where the subscript i indicates the isotopic variety.

Coriolis constants, which characterize the vibrational-rotational interaction in the molecule, the mean square amplitudes of the vibrations of the internuclear distances, which the methods of gas electron diffraction enable one to determine, and some other measured quantities (in particular, the constants of centrifugal distortion) are dependent on the matrix F (in terms of the eigenfrequencies and the eigenvectors, which are functions of the elements of this matrix).

The set of equations (8), (9) and others (or some of these, depending on the available experimental data) will be considered as a single nonlinear operator equation

$$Az = u, \quad z \in Z, \quad u \in U. \tag{10}$$

We represent the set of experimental data by a vector of a finite-dimensional space U. We also introduce a vector z of the finite-dimenisonal space Z, consisting either of the elements of the matrix F or of quantities, by means of which this matrix can be parametrized. Then the operator A places in correspondence with the real symmetric matrix F (or the vector z) the set of eigenvalues of problems (8) or (9), the Coriolis constants, the mean amplitudes etc. Sometimes the a priori constraints on the elements of the matrix F are also known.

We now arrive at the following formulation of the inverse problem.

Problem I. Suppose we are given equation (10) with $z \in D \subseteq Z$, and $u \in U$, where Z and U are finite-dimensional spaces, $\mathcal{D}$ is a closed set of a priori constraints of the problem, and A is a nonlinear continuous operator in $\mathcal{D}$. It is required to find an approximate solution of equation (10), if instead of A and u, we are given their approximations A_h and u_δ such that $\|u_\delta - u\| \leq \delta$, $\|A_h z - Az\| \leq \phi[h, z]$ for all $z \in \mathcal{D}$. Here $\phi[h, z]$ is a known continuous functional which approaches zero as $h \to 0$ uniformly for all $z \in \mathcal{D} \cap \bar{S}(0, R)$, where $\bar{S}(0, R)$ is a closed sphere with centre at $z = 0$ and with radius R.

The error in specifying the operator A involves an error in determining the equilibrium configuration of the molecule, the parameters of which can be found experimentally. The form of the functional ϕ may be specified.

Note that Problem I in general satisfies none of the following conditions for the wellposedness of the problem: (i) solvability, (ii) uniqueness of the solution; and (3) stability.

A difficulty arises in assuming a solution of Problem I. We now consider the problem of finding a normal pseudosolution of Problem I.

Problem II. It is required to obtain

$$\inf \|z - z^0\| \; z \in \{z : z \in \mathcal{D}, \; \|Az - u\| = \mu\}, \text{ where } \mu = \inf_{z \in \mathcal{D}} \|Az - u\|. \tag{11}$$

The element $z^0 \in Z$ should be specified from *a priori* considerations about the solution, using both approximate quantum-mechanical calculations, and other ideas (for example the transferability of the force constants to similar fragments of the molecules).

It is obvious, in the case when a solution of Problem I exists and is unique that its normal pseudosolution is identical with the solution itself.

Taking all the above into account, we formulate the following problem.

Problem III. Suppose we are given equation (10) and the above conditions are satisfied. It is required to obtain approximations $z_\eta \in \mathcal{D}$ to the solution $\bar{z}$ of Problem II from the approximate data $(A_h, u_\delta, h, \delta)$ in such a way that

$$\lim_{h,\delta \to 0} z_\eta = \bar{z}. \tag{12}$$

The algorithm for finding z_η is based on Tikhonov regularization.

Numerical methods for solving Problem III, based on the generalized discrepancy principle and their variants, were proposed in [12]. On the basis of the above algorithms, we compiled a package of programs for processing spectroscopic data on a computer. It includes a unit for reading information, a unit for preparing additional data, a unit for solving the inverse problem, a unit for solving the direct problem, and a program dispatcher. For the results related to force fields calculations for some molecules, see [13]–[14].

4 Inverse Problems in Electronic Microscopy

There is not sufficient space to describe in details the interesting problems arising in electon microscopy data processing such as image restoration and different tomography problems. For details, see book [15] and articles [16]–[17]. All the numerical methods used were based on the generalized discrepancy method for linear and nonlinear problems including two-dimensional intergral equations of convolution type and three-dimensional integral equations which are of convolution type in two variables. These problems provide very good examples of the use of regularization methods for "nondestructive testing".

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