A Symbolic-Numerical Algorithm for the Computation of Matrix Elements in the Parametric Eigenvalue Problem

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Abstract—A symbolic-numerical algorithm for the computation of the matrix elements in the parametric eigenvalue problem to a prescribed accuracy is presented. A procedure for calculating the oblate angular spheroidal functions that depend on a parameter is discussed. This procedure also yields the corresponding eigenvalues and the matrix elements (integrals of the eigenfunctions multiplied by their derivatives with respect to the parameter). The efficiency of the algorithm is confirmed by the computation of the eigenvalues, eigenfunctions, and the matrix elements and by the comparison with the known data and the asymptotic expansions for small and large values of the parameter. The algorithm is implemented as a package of programs in Maple–Fortran and is used for the reduction of a singular two-dimensional boundary value problem for the elliptic second-order partial differential equation to a regular boundary value problem for a system of second-order ordinary differential equations using the Kantorovich method.

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1. INTRODUCTION

The calculation of the dynamics of electron states of hydrogen-like atoms in a magnetic field in atomic physics is reduced to a boundary value problem for an elliptic second-order partial differential equation in a two-dimensional region for fixed values of the magnetic number and parity [1]. Efficient algorithms for the numerical solution of this problem (see [2]) are based on its reduction to a system of ordinary differential equations by the Kantorovich method [3].It is quite natural to use the oblate angular spheroidal functions [4] as the basis for the expansion of the unknown solution. It was shown in [5, 6] that an efficient application of the Kantorovich method requires the development of a set of symbolic–numerical algorithms for computing the following quantities to a prescribed accuracy:

• oblate angular spheroidal functions on a bounded interval of the parameter values,

• derivatives with respect to the parameter of the angular functions and of the matrix elements (integrals of the eigenfunctions multiplied by their derivatives with respect to the parameter),

• asymptotics in the radial parameter of the eigenfunctions and of the matrix elements that appear as variable coefficients in the system of ordinary differential equations,

• asymptotics of the solutions to the system of ordinary differential equations for small and large values of the radial variable,

• solutions of the boundary value problem for the system of second-order ordinary differential equations.

In this paper, we consider the reduction of the two-dimensional problem to a system of ordinary differential equations using the Kantorovich method with respect to the parametric basis consisting of the oblate angular spheroidal functions.

The eigenvalue problem for an ordinary differential equation on a finite interval of the variation of the independent angular variable is reduced to an algebraic problem by expanding the unknown solution in terms of the associated Legendre polynomials with unknown coefficients depending on the parameter. A symbolic-numerical algorithm for generating and solving the eigenvalue problem and for calculating the eigenfunctions, their derivatives with respect to the parameter, and the corresponding matrix elements to a prescribed accuracy is described. This algorithm is implemented in the Maple–Fortran environment. As a part of this algorithm, a symbolic algorithm for finding the asymptotics of the oblate angular spheroidal functions, their derivatives, and matrix elements is described. The latter algorithm is implemented in Maple. The eigenvalue problem for a second-order ordinary differential equation on a finite interval of the variation of the independent variable is reduced to an algebraic problem by expanding the unknown solution in terms of the generalized Laguerre polynomials. The efficiency of the algorithm is confirmed by the computation of the asymptotics of the matrix elements and by the comparison with the corresponding numerical values of the

matrix elements on a discrete grid of the parameter values in a finite interval. In addition to the algorithms mentioned above, a special symbolic algorithm for finding solutions to the system of ordinary differential equations in the Kantorovich method for large values of the radial variable r is developed and implemented in Maple.

The preliminary results of the computations obtained by the proposed symbolic-numerical method for the discrete spectrum states of the two-dimensional problem were announced in [6]. In addition, we construct a special symbolic-numerical algorithm for finding asymptotics of the continuous spectrum solutions of the two-dimensional boundary value problem subject to the boundary condition of the third kind and compare the asymptotic values of the matrix elements with the corresponding numerical results, which completes the set of symbolic-numerical algorithms designed for reducing the singular boundary value problem for the second-order elliptic partial differential equation in a two-dimensional region to a regular boundary value problem for a system of second-order ordinary differential equations in the Kantorovich method.

The paper is organized as follows. In Section 2, the problem is stated and reduced to a system of ordinary differential equations subject to boundary conditions on a finite interval by the Kantorovich method. In Section 3, an algorithm reducing the parametric eigenvalue problem to an algebraic problem and an algorithm for its solution are described. In Section 4, we describe an algorithm for calculating the derivatives of the basis functions and of the matrix elements with respect to the parameter. Section 5 is devoted to the algorithm for calculating the asymptotics of the matrix elements. In Sections 6 and 7 we present an algorithm for finding asymptotics of the solutions to the system of ordinary differential equations in the Kantorovich method for large r. In conclusion, we discuss the main results and further applications of the proposed algorithms.

2. STATEMENT OF THE PROBLEM

The Schrödinger equation $\hat{\Psi}(r, \eta, \varphi) = \Psi(r, \eta)\exp(im\varphi)/\sqrt{2\pi}$ for the wave function of the hydrogen-like atom with the nucleus charge Z in the axially symmetric magnetic field $\vec{B} = (0, 0, B)$ written in the spherical coordinates (r, θ, ϕ) for a fixed value of the magnetic quantum number $m = 0, \pm 1, \ldots$ and a fixed z-parity $\sigma = \pm 1$ is reduced to the second-order elliptic partial differential equation

$$\left(-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{\hat{A}^{(0)}}{r^2} - \frac{2Z}{r} - \epsilon\right)\Psi(r, \eta) = 0 \qquad (1)$$

in the domain $\Omega = \{0 < r < \infty, -1 < \eta = \cos\theta < 1\}$. Here, $\epsilon = 2E$ is the doubled energy (in Rydbergs, 1 Ry = (1/2)

a.u.) of the state $|m\sigma\rangle$ for fixed values of m and σ, $\hat{A}^{(0)} = A^{(0)} + \gamma m r^2$, the operator $A^{(0)} \equiv A^{(0)}(p)$ corresponds to the operator of the quasi-angular equation for the oblate spheroidal functions

$$A^{(0)}(p) = -\frac{\partial}{\partial\eta}f(\eta)\frac{\partial}{\partial\eta} + \frac{m^2}{f(\eta)} + p^2 f(\eta), \qquad (2)$$

where $f(\eta) = 1 - \eta^2$, and the term with the parameter $p = \gamma r^2/2$ corresponds to the potential energy of interaction of the electron with the magnetic field in the infinite nucleus mass approximation in the atomic system of units ($\hbar = m_e = e = 1$). Here, $\gamma = B/B_0$ and $B_0 \cong 2.35 \times 10^9 G$ is a dimensionless parameter that characterizes the strength of the magnetic field B.

In each subspace of the Hilbert space $\mathbf{H}_{m\sigma}$, the wave functions $\Psi(r, \eta) \equiv \Psi^{m\sigma}(r, \eta)$ satisfy the following boundary conditions on the boundary of Ω:

$$\lim_{\eta \to \pm 1} f(\eta)\frac{\partial\Psi(r, \eta)}{\partial\eta} = 0, \text{ if } m = 0,$$

$$\Psi(r, \pm 1) = 0, \text{ if } m \neq 0,$$

$$\frac{\partial\Psi(r, 0)}{\partial\eta} = 0, \text{ if } \sigma = +1, \qquad (3)$$

$$\Psi(r, 0) = 0, \text{ if } \sigma = -1,$$

$$\lim_{r \to 0} r^2\frac{\partial\Psi(r, \eta)}{\partial r} = 0. \qquad (4)$$

For large $r = r_{max}$, the discrete spectrum wave functions $\epsilon \equiv \{\epsilon_i\}_{i=1}^{i_{max}}$ satisfy the boundary condition of the first kind

$$\lim_{r \to \infty} r^2\Psi(r, \eta) = 0 \longrightarrow \Psi(r_{max}, \eta) = 0, \qquad (5)$$

which is a consequence of the asymptotic behavior of the solution. Here, the approximate value of the energy $\epsilon \equiv \epsilon(r_{max})$ is the unknown eigenvalue $\epsilon_i \equiv \epsilon_i(r_{max})$ in problem (1)–(5) on the finite interval $0 \leq r \leq r_{max}$ ($r_{max} \gg 1$), and the normalization condition

$$\int_0^{r_{max}}\int_{-1}^{1} r^2|\Psi(r, \eta)|^2 dr d\eta = 1 \qquad (6)$$

is fulfilled.

For large $r = r_{max}$ and a fixed value of the energy ϵ, the continuous spectrum wave functions satisfy the boundary condition of the third kind

$$\frac{\partial\Psi(r, \eta)}{\partial r} - \mu\Psi(r, \eta) = 0, \qquad (7)$$

which is a consequence of the asymptotic behavior of the solution. It is a well-known fact (see [7]) that there exists a function $\mu \equiv \mu(r_{max}, \epsilon)$ such that Eq. (7) is satisfied for any finite r.

Following the approach proposed by Kantorovich, we represent the solution $\Psi_i^{m\sigma}(r, \eta)$ as the expansion in terms of the one-dimensional basis functions $\Phi_j(\eta; r) \equiv \Phi_j^{m\sigma}(\eta; r)$ for fixed m and σ:

$$\Psi_i^{m\sigma}(r, \eta) = \sum_{j=1}^{j_{max}} \Phi_j^{m\sigma}(\eta; r)\chi_j^{(i)}(r). \qquad (8)$$

For each fixed r, $\Phi_j(\eta; r)$ are solutions of the one-dimensional parametric eigenvalue problem

$$\hat{A}^{(0)}(r)\Phi_j(\eta; r) = E_j(r)\Phi_j(\eta; r),$$
$$\int_{-1}^{1} \Phi_i(\eta; r)\Phi_j(\eta; r)d\eta = \delta_{ij} \qquad (9)$$

subject to boundary condition (3), where $\Psi(r, \eta)$ is replaced by $\Phi_j(\eta; r)$. Here, $E_j(r)$ are the unknown eigenvalues for fixed m and σ and δ_{ij} is the Kronecker delta.

Substitute expansion (8) into Eqs. (1)–(7) with account for (9) to obtain the boundary value problem for the system of second-order ordinary differential equations for the unknown vector $\chi^{(i)}(r) = \{\chi_j^{(i)}(r)\}_{j=1}^{j_{max}}$

$$\left(-\mathbf{I}\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{\mathbf{U}(\mathbf{r})}{\mathbf{r}^2} + \mathbf{Q}(r)\frac{d}{dr}\right.$$
$$\left. + \frac{1}{r^2}\frac{dr^2\mathbf{Q}(r)}{dr}\right)\chi^{(i)}(r) = \epsilon_i\mathbf{I}\chi^{(i)}(r). \qquad (10)$$

Here, $\mathbf{I}$ is an identity matrix, and $\mathbf{U}(r)$ and $\mathbf{Q}(r)$ are j_{max}-by-j_{max} matrices

$$U_{ij}(r) = \frac{E_i(r) + E_j(r)}{2}\delta_{ij} - 2Zr\delta_{ij} + r^2 H_{ij}(r),$$

$$H_{ij}(r) = \int_{-1}^{1} \frac{\partial\Phi_i(\eta; r)}{\partial r}\frac{\partial\Phi_j(\eta; r)}{\partial r}d\eta, \qquad (11)$$

$$Q_{ij}(r) = -\int_{-1}^{1} \Phi_i(\eta; r)\frac{\partial\Phi_j(\eta; r)}{\partial r}d\eta.$$

The regular bounded solutions $\chi^{(i)}(r)$ satisfy the boundary conditions

$$\lim_{r \to 0} r^2\left(\frac{d\chi^{(i)}(r)}{dr} - \mathbf{Q}(r)\chi^{(i)}(r)\right) = 0. \qquad (12)$$

The discrete spectrum solutions $\epsilon \equiv \{\epsilon_i\}_{i=1}^{i_{max}}$ corresponding to the unknown eigenvalues ϵ_i satisfy the boundary conditions

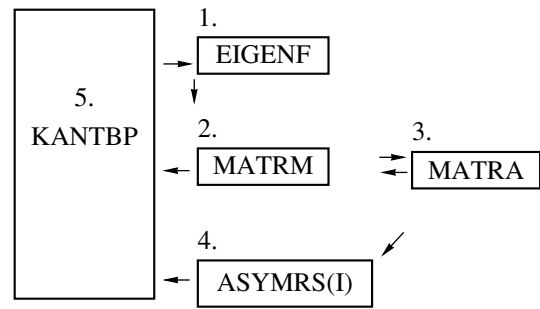$$\lim_{r \to \infty} r^2\chi^{(i)}(r) = 0 \longrightarrow \chi^{(i)}(r_{max}) = 0 \qquad (13)$$

Figure.

and the orthonormalization conditions

$$\int_{0}^{r_{max}} r^2(\chi^{(i)}(r))^T\chi^{(j)}(r)dr = \delta_{ij}. \qquad (14)$$

For the continuous spectrum, fixed values of the energy ϵ and the radial variable $r = r_{max}$, the bounded solutions $\chi(r) = \{\chi^{(i)}(r)\}_{i=1}^{N_o}$ $(N_o \leq j_{max})$ satisfy the boundary condition of the third kind with the matrix of unknown parameters $\Lambda = \{\delta_{ij}\mu_i\}_{i,j=1}^{N_o}$

$$\frac{d\chi^{(r)}}{dr} - \mathbf{Q}(r)\chi(r) = \chi(r)\Lambda, \qquad (15)$$

where N_o is the number of open channels.

Thus, to solve problem (1)–(7) in the framework of the Kantorovich method, we must solve the following problems.

(1) Reduce problem (9) to an algebraic problem and calculate the eigenvalues and eigenfunctions for the set of the parameter values in a bounded interval.

(2) Calculate matrix elements (11) that appear in the system of differential equations (10).

(3) Find the asymptotics of matrix elements (11).

(4) Find the asymptotics of the solution to system (10) and set up boundary conditions (15).

(5) Find a numerical solution of the boundary value problems for system (10) subject to the boundary conditions that were set up at step 4 and investigate the dependence of the convergence rate of expansion (8) on j_{max}.

To solve all these problems, we developed a package of symbolic-numerical computer algebra algorithms. Note that the algorithms for solving problems 3 and 4 are symbolic; for problem 5 they are numerical; and, for problems 1 and 2, a combination of symbolic and numerical procedures is used.

The structure of this package is depicted in the figure. The numbers in this figure denote the problem number; the name of the procedure is shown in the blocks; and the arrows show the functional dependences.

3. THE EIGENF ALGORITHM

Eigenfunctions (9) of the operator $\hat{A}^{(0)} = A^{(0)} + \gamma m r^2$ are also the eigenfunctions of the operator $A^{(0)} \equiv A^{(0)}(p)$ in (2) because their eigenvalues differ only in the constant shift $E_j(r) = \lambda_j(p) + \gamma m r^2$:

$$A^{(0)}(p)\Phi_j(\eta; p) = \lambda_j(p)\Phi_j(\eta; p). \quad (16)$$

For fixed $\sigma = \pm 1$ and $m \equiv |m|$, the unknown eigenfunctions—the oblate angular spheroidal functions—are sought in the form of the expansions

$$\Phi_j(\eta; r) = \sum_{s = (1-\sigma)/2}^{s_{max}} \tilde{P}_{m+s}^m(\eta)\tilde{c}_{sj}^{m\sigma}(r)$$

$$= \sum_{s = (1-\sigma)/2}^{s_{max}} P_{m+s}^m(\eta)c_{sj}^{m\sigma}(r) \quad (17)$$

[1] in the unnormalized Legendre polynomials $\tilde{P}_{m+s}^m(\eta)$ [4] and in the normalized Legendre polynomials $P_{m+s}^m(\eta)$ [8]:

$$A^{(0)}(0)P_{m+s}^m(\eta) = P_{m+s}^m(\eta)\lambda_s^{m\sigma}(0),$$

$$\lambda_s^{m\sigma}(0) = (s+m)(s+m+1), \quad (18)$$

$$s = 2(j-1) + (1-\sigma)/2,$$

$$\int_{-1}^{1} P_{m+s}^m(\eta)P_{m+s'}^m(\eta)d\eta = \delta_{ss'}. \quad (19)$$

The summation in (17) is performed over even or odd integer s up to $s_{max} = 2(N_{max} - 1) + (1 - \sigma)/2$, where N_{max} is the number of terms in the expansion. The [1] unnormalized polynomials are related to the normalized ones by

$$\tilde{P}_{m+s}^m(\eta) = P_{m+s}^m(\eta)B_{sm},$$

$$B_{sm} = \sqrt{\frac{2(s+2m)!}{(2s+2m+1)s!}}. \quad (20)$$

The coefficients in expansions (17) satisfy the equations

$$\tilde{c}_{sj}^{m\sigma}(r) = c_{sj}^{m\sigma}(r)B_{sm}^{-1},$$

$$\sum_{s = (1-\sigma)/2}^{s_{max}} c_{sj}^{m\sigma}(r)c_{sj'}^{m\sigma}(r) = \delta_{jj'}. \quad (21)$$

The algebraic problems

$$\mathbf{A}^{(0)}\mathbf{c}_j = \lambda_j(r)\mathbf{c}_j, \quad (22)$$

$$\tilde{\mathbf{A}}^{(0)}\tilde{\mathbf{c}}_j = \tilde{\lambda}_j(r)\tilde{\mathbf{c}}_j \quad (23)$$

for finding the normalized eigenvalues $\mathbf{c}_j = \{c_{sj}^{m\sigma}(r)\}_{s = (1-\sigma)/2}^{s_{max}}$, the unnormalized eigenvalues $\tilde{\mathbf{c}}_j = $ [1] $\{\tilde{c}_{sj}^{m\sigma}(r)\}_{s = (1-\sigma)/2}^{s_{max}}$, and the corresponding eigenvectors $\lambda_j(r)$ and $\tilde{\lambda}_j(r) = \lambda_j(r)$ are determined by the symmetric three-diagonal matrix $\mathbf{A}^{(0)}$

$$A_{ss-2}^{(0)} = A_{s-2s}^{(0)} = -\frac{p^2}{(2s+2|m|-1)}$$

$$\times \sqrt{\frac{(s-1)s(s+2|m|-1)(s+2|m|)}{(2s+2|m|-3)(2s+2|m|+1)}}, \quad (24)$$

$$A_{ss}^{(0)} = (s+|m|)(s+|m|+1)$$

$$+ 2p^2\frac{(s^2+s+2s|m|+2m^2+|m|-1)}{(2s+2|m|-1)(2s+2|m|+3)}$$

and by the asymmetric three-diagonal matrix $\tilde{\mathbf{A}}^{(0)}$

$$\tilde{A}_{ss-2}^{(0)} = B_{sm}^{-1}A_{ss-2}^{(0)}B_{s-2m},$$

$$\tilde{A}_{s-2s}^{(0)} = B_{s-2m}^{-1}A_{s-2s}^{(0)}B_{sm}, \quad (25)$$

$$\tilde{A}_{ss}^{(0)} = A_{ss}^{(0)}.$$

Here, $A_{-2,0}^{(0)} = 0$ for $\sigma = +1$ and $A_{-1,1}^{(0)} = 0$ for $\sigma = -1$. Eigenvalue problems (22) and (23) generated in the symbolic-numerical algorithm EIGENF were solved using the built-in function *eigenvectors* in Maple or using the built-in function *Eigenvectors* in Mathematica. In addition, Mathematica includes the package *SpheroidalS1* for calculating the spheroidal functions using expansion (17) in terms of the unnormalized Leg- [1] endre polynomials $P_{m+s}^m(\eta)$ [9]. For large values of $s_{max} \sim 100$, to ensure the prescribed accuracy in the numerical solution of problem (22) with the symmetric matrix $\mathbf{A}^{(0)}$, the IMTQL2 procedure in the Fortran package EISPACL [10] was used. The choice of s_{max} for calculating the desired set of $j_{max} \sim 10$ solutions for the values of the parameter r in the interval $[0, r_{max}]$ was controlled by the fulfillment of orthogonality condition (21) up to the prescribed accuracy.

4. THE MATRM ALGORITHM

The characteristic set of matrix elements that must be calculated in applications has the form

$$Q_{ij}(r) = -I_{01;ij}, \quad \frac{\partial Q_{ij}(r)}{\partial r} = -I_{11;ij} - I_{02;ij},$$

$$H_{ij}(r) = I_{11;ij}, \quad \frac{\partial H_{ij}(r)}{\partial r} = I_{21;ij} + I_{12;ij}, \quad (26)$$

where $I_{kn;\,ij} \equiv I_{kn;\,ij}(r)$ are the basis integrals of the products of the derivatives (with respect to the parameter r) of the eigenfunctions:

$$I_{kn;\,ij} = \int\limits_{-1}^{1} \Phi_i^{(k)}(\eta;\,r)\Phi_j^{(n)}(\eta;\,r)d\eta. \qquad (27)$$

Here, the superscript in parentheses denotes the order of the derivatives:

$$\Phi_j^{(k)}(\eta;\,r) = \frac{\partial^k \Phi_j(\eta;\,r)}{\partial r^k}, \qquad (28)$$

$$\Phi_j^{(0)}(\eta;\,r) = \Phi_j(\eta;\,r).$$

Without loss of generality, we consider the derivatives with respect to the parameter r, which is related to the parameter p by Eq. (2).

For fixed values of the magnetic number m and the parity $\sigma = \pm 1$, the derivatives $\Phi_j^{(k)}(\eta;\,r)$ are represented as expansions in terms of an orthonormal basis, for example, in the associated Legendre polynomials:

$$\Phi_j^{(k)}(\eta;\,r) = \sum_{s=(1-\sigma)/2}^{s_{\max}} c_{sj}^{(k)} P_{m+s}^m(\eta). \qquad (29)$$

Here, the coefficients of the expansion

$$c_{sj}^{(k)} \equiv \frac{\partial^k c_{sj}(r)}{\partial r^k} \qquad (30)$$

are the derivatives with respect to the parameter of the components $c_{sj}^{(0)} \equiv c_{sj}(r)$ of the eigenvectors $\{\mathbf{c}_j^{(0)}\} \equiv \{c_{sj}(r)\}_{s=(1-\sigma)/2}^{s_{\max}}$ of the algebraic eigenvalue problem in $j_{\max}$ pairs of unknowns $\{\mathbf{c}^{(0)} \equiv \mathbf{c}_j^{(0)}, \lambda_j^{(0)} \equiv \lambda_j(r)\}_{j=1}^{j_{\max}}$

$$\mathbf{A}^{(0)}\mathbf{c}^{(0)} - \mathbf{c}^{(0)}\lambda^{(0)} = 0, \qquad (31)$$

$$(\mathbf{c}^{(0)})^T \mathbf{c}^{(0)} = \mathbf{I} \qquad (32)$$

with the symmetric matrix $\mathbf{A}^{(0)} \equiv \{A_{kl}^{(0)}(r)\}$ (see, e.g., (22)). To find the derivatives $\mathbf{c}^{(k)}$ and the derivatives

$$\lambda^{(k)} \equiv \lambda_j^{(k)} = \frac{\partial^k \lambda_j^{(0)}}{\partial r^k} \qquad (33)$$

of the eigenvalues $\lambda_j^{(0)} \equiv \lambda_j(r)$ of problem (31), we have the recurrent system of inhomogeneous algebraic equations

$$(\mathbf{A}^{(0)}\mathbf{c}^{(k)} - \mathbf{c}^{(k)}\lambda^{(0)})$$
$$+ (\mathbf{A}^{(k)}\mathbf{c}^{(0)} - \mathbf{c}^{(0)}\lambda^{(k)}) = \mathbf{b}_{(k)},$$
$$\mathbf{b}_{(k)} \equiv \sum_{n=1}^{k-1} \frac{k!(\mathbf{c}^{(k-n)}\lambda^{(n)} - \mathbf{A}^{(n)}\mathbf{c}^{(k-n)})}{n!(k-n)!} \qquad (34)$$

obtained by differentiating eigenvalue problem (31). Here,

$$\mathbf{A}^{(k)} \equiv \frac{\partial^k \mathbf{A}^{(0)}}{\partial r^k} \qquad (35)$$

is the derivative of the matrix $\mathbf{A} \equiv \mathbf{A}^{(0)}$.

Since $\lambda^{(0)}$ is an eigenvalue of problem (31), the system has a solution if and only if the right-hand side is orthogonal to the eigenfunction $\mathbf{c}^{(0)}$. Multiply (34) by $(\mathbf{c}^{(0)})^T$ and use normalization condition (32) to obtain the expression

$$\lambda^{(k)} = (\mathbf{c}^{(0)})^T \mathbf{A}^{(k)}\mathbf{c}^{(0)} - (\mathbf{c}^{(0)})^T \mathbf{b}_{(k)} \qquad (36)$$

for $\lambda^{(k)}$ and the system of linear algebraic inhomogeneous equations

$$\mathbf{K}\mathbf{c}^{(k)} \equiv \mathbf{A}^{(0)}\mathbf{c}^{(k)} - \mathbf{c}^{(k)}\lambda^{(0)} = \mathbf{b}^{(k)},$$
$$\mathbf{b}^{(k)} \equiv \sum_{n=1}^{k} \frac{k!(\mathbf{c}^{(k-n)}\lambda^{(n)} - \mathbf{A}^{(n)}\mathbf{c}^{(k-n)})}{n!(k-n)!}. \qquad (37)$$

Problem (37) has a solution, but it is not unique. Normalization condition (32) implies the additions condition

$$\sum_{n=0}^{k} \frac{k!}{n!(k-n)!}(\mathbf{c}^{(k-n)})^T \mathbf{c}^{(n)} = 0 \qquad (38)$$

that ensures the uniqueness of the solution to (37). Since $\lambda^{(0)}$ is an eigenvalue of problem (31), the matrix $\mathbf{K}$ is singular or almost singular in the case of a numerical solution.

The algorithm for solving (37) involves a sequence of three steps for each value of k.

Step 1. Calculation of the solutions $\mathbf{v}^{(k)}$ and $\mathbf{w}$ of two auxiliary systems of linear algebraic inhomogeneous equations

$$\overline{\mathbf{K}}\mathbf{v}^{(k)} = \overline{\mathbf{b}}^{(k)}, \quad \overline{\mathbf{K}}\mathbf{w} = \mathbf{d} \qquad (39)$$

2 with the nonsingular matrix $\overline{\mathbf{K}}$ and the right-hand sides $\overline{\mathbf{b}}^{(k)}$ and $\mathbf{d}$:

$$\overline{K}_{ss'} = \begin{cases} K_{ss'}, & (s-S)(s'-S) \neq 0, \\ \delta_{ss'}, & (s-S)(s'-S) = 0, \end{cases}$$

$$\overline{b}_s^{(k)} = \begin{cases} b_s^{(k)}, & s \neq S, \\ 0, & s = S, \end{cases} \tag{40}$$

$$d_s = \begin{cases} K_{sS}, & s \neq S, \\ 0, & s = S. \end{cases}$$

Here, S is the index of the component of the vector $\mathbf{c}^{(0)} \equiv \{\mathbf{c}_j^{(0)}\}$ with the maximal absolute value: $|\{c_{Sj}(r)\}| = \max_{(1-\sigma)/2 \le s \le s_{max}} |\{c_{sj}(r)\}|$.

Step 2. Calculation of the three auxiliary coefficients $\gamma_1^{(k)}$, γ_2, and $\gamma^{(k)}$

$$\gamma_1^{(k)} = (\mathbf{v}^{(k)})^T \mathbf{c}^{(0)}, \quad \gamma_2 = \mathbf{w}^T \mathbf{c}^{(0)},$$

$$\gamma^{(k)} = -\frac{\gamma_1^{(k)} - F_N^{(k)}}{(c_s^{(0)} - \gamma_2)} \tag{41}$$

using normalization condition (38)

$$F_N^{(k)} = -\sum_{n=1}^{k-1} \frac{k!(\mathbf{c}^{(k-n)})^T \mathbf{c}^{(n)}}{2n!(k-n)!}. \tag{42}$$

Step 3. Calculation of the vector $\mathbf{c}^{(k)}$

$$c_s^{(k)} = \begin{cases} v_s^{(k)} - \gamma^{(k)} w_s, & s \neq S, \\ \gamma^{(k)}, & s = S. \end{cases} \tag{43}$$

The set of vectors $\mathbf{c}^{(k)}$ produced by this algorithm is used to calculate the set of basis matrix elements (26)

$$I_{kn;\,ij} = (\mathbf{c}_i^{(k)})^T \mathbf{c}_j^{(n)}, \quad i, j = 1, \ldots, j_{max}. \tag{44}$$

Symbolic-numerical algorithm (36)–(44) is implemented as the program MATRM in the environment Maple–Fortran and in Mathematica (recall that the oblate angular spheroidal functions are included in the package *SpheroidalS1* in Mathematica [9]). For large $s_{max} \sim 100$, to ensure the prescribed accuracy in the numerical solution of system (39), the F07BEF procedure in the Fortran package NAG Fortran Library Routine Document [11] was used. The choice of s_{max} for calculating the desired set of $j_{max} \sim 10$ solutions for the values of the parameter r in the interval $[0, r_{max}]$ was controlled by the fulfillment of condition (38) up to the prescribed accuracy.

5. THE MATRA ALGORITHM

For small r, the values of the matrix elements E_j, $H_{jj'}$, and $Q_{jj'}$ are characterized by the quantum numbers $l = |m| + s = 2j - 2 + |m|$ for even states ($\sigma = +1$) and $l = |m| + s = 2j - 1 + |m|$ for odd states ($\sigma = -1$). They are represented by asymptotic series in powers of r for fixed j and j':

$$E_j(r) = E_j^{(0)} + E_j^{(2)} r^2 + \sum_{k=1}^{k_{max}/4} r^{4k} E_j^{(4k)},$$

$$H_{jj'}(r) = \sum_{k=1}^{k_{max}/4} r^{4k-2} H_{jj'}^{(4k-2)}, \tag{45}$$

$$Q_{jj'}(r) = \sum_{k=1}^{k_{max}/4} r^{4k-1} Q_{jj'}^{(4k-1)}.$$

The regular behavior of the matrix elements is consistent with boundary conditions (12) for the regular bounded solutions (10). To calculate the matrix elements, we used a modification of the algorithm described in the preceding section. In this modification, system (34) appearing at the kth step is solved analytically. The eigenvectors and the eigenfunctions are substituted in the form of the Taylor series

$$\mathbf{c}_j(r) = \sum_{k=0}^{k_{max}} \frac{\mathbf{c}_j^{(k)} r^k}{k!}, \quad \lambda_j(r) = \sum_{k=0}^{k_{max}} \frac{\lambda_j^{(k)} r^{(k)}}{k!} \tag{46}$$

with the initial conditions

$$c_{sj}^{(0)} = \delta_{sj}^{(0)}, \quad \lambda_j^{(0)} = (|m| + s)(|m| + s + 1). \tag{47}$$

Using this algorithm, which was implemented in Maple, we found the expansion coefficients of the matrix elements up to $k_{max} = 20$. Note that these asymptotic expansions have a finite radius of convergence because the parameter p has branch points in the complex plane [6, 12, 13].

To calculate matrix elements (11) for large r in the form of a series in inverse powers of p without taking into account the exponentially small terms in the neighborhood $\eta \in D_1$ ($D_1 = [1 - \eta_1, 1]$), $\eta_1 = o(p^{1/2 - \epsilon})$ ($0 < \epsilon < 1/2$), the solution is sought in the form (see [14])

$$\Phi_j(y; p) = e^{-p(1-\eta)}(1-\eta^2)^{\frac{|m|}{2}} F_n(y), \tag{48}$$

where $y = 2p(1-\eta)$ and $n = j - 1$. The auxiliary function $F_n(y)$ is a solution of the eigenvalue problem

$$\left(y\frac{d^2}{dy^2} + (|m| + 1 - y)\frac{d}{dy} + \beta_n(p)\right) F_n(y)$$

$$= \frac{1}{4p}\left(y^2 \frac{d^2}{dy^2} + (2|m| + 2 - y)\right) y \frac{d}{dy} \tag{49}$$

$$+ (|m| + 1)(|m| - y)F_n(y)$$

for a fixed m with the corresponding spectral parameter

$$\beta_n(p) = -\frac{|m| + 1}{2} + \frac{\lambda_n}{4p} \qquad (50)$$

and with the additional normalization condition

$$\frac{1}{2p}\int_0^\infty \Phi_i(y; p)\Phi_j(y; p)dy = \delta_{ij}. \qquad (51)$$

Since Eq. (49) corresponds to the equation for the generalized Laguerre polynomials in the limit $p \longrightarrow \infty$, its solution is sought in the form of a series in inverse powers of p for $k_{max} > |m|$:

$$F_n(y) = \sqrt{2}p^{\frac{|m| + 1}{2}}\sum_{k=0}^{k_{max}}\left(\frac{1}{4p}\right)^k\sum_{s=-k}^{k}c_{s,n}^{(k)}L_{n+s}^{(|m|)}(y), \qquad (52)$$

$$\beta_n(p) = \beta_n^{(0)} + \sum_{k=1}^{k_{max}}\left(\frac{1}{4p}\right)^k\beta_n^{(k)}.$$

Here, $L_n^{(|m|)}(y)$ are the generalized Laguerre polynomials [4]

$$\langle n_l | n_r \rangle \equiv \int_0^\infty dy\, y^{|m|}e^{-y}L_{n_l}^{(|m|)}(y)L_{n_r}^{(|m|)}(y) \qquad (53)$$

$$= \frac{(n_l + |m|)!}{n_l!}\delta_{n_l n_r}.$$

The substitution of (52) in (49) yields an algebraic problem of type (34) and recurrences for finding the unknown coefficients $c_{s,n}^{(k)}$ and $\beta_n^{(k)}$ for $k \geq 1$ and $s \neq 0$:

$$sc_{s,n}^{(k)} = f_{s,n}^{(k)},$$

$$\begin{aligned}
f_{s,n}^{(k)} = &[(n + s + |m| + 1)(2n + 2s + |m| + 1) \\
&- (n + s + |m|)(|m| + 1)]c_{s,n}^{(k-1)} \\
&- (n + s + |m|)(n + s)c_{s-1,n}^{(k-1)} \\
&- (n + s + |m| + 1)(n + s + 1)c_{s+1,n}^{(k-1)} \\
&+ \sum_{k'=1}^{k-|s|}\beta_n^{(k')}c_{s,n}^{(k-k')}.
\end{aligned} \qquad (54)$$

The initial values are

$$\beta_n^{(0)} = n, \quad c_{0,n}^{(0)} = \sqrt{\frac{n!}{(n+|m|)!}}, \qquad (55)$$

and $c_{j,n}^{(i)} = 0$ for $|j| > i$. The unknown coefficients $c_{0,n}^{(k)}$ $(k \geq 1)$ are found from conditions (51) for each order

$1/(4p)$ with the additional integral $\langle n_l | y^a | n_r \rangle$ for $0 \leq a \leq |m|$. In terms of (48), the matrix elements are determined by the integrals

$$Q_{jj'}(r) = -\frac{1}{2p}\int_0^\infty dy\Phi_j(y; r)\partial\Phi_{j'}(y; r),$$

$$H_{jj'}(r) = \frac{1}{2p}\int_0^\infty dy\partial\Phi_j(y; r)\partial\Phi_{j'}(y; r), \qquad (56)$$

where

$$\partial\Phi_j(y; r) = \left(\frac{\partial}{\partial r} + \frac{2y}{r}\frac{\partial}{\partial y}\right)\Phi_j(y; r), \qquad (57)$$

and their asymptotic expansions in inverse powers of r without account for the exponentially small terms have the form

$$r^{-2}E_j(r) = E_j^{(0)} + \sum_{k=1}^{k_{max}}r^{-2k}E_j^{(2k)},$$

$$H_{jj'}(r) = \sum_{k=1}^{k_{max}}r^{-2k}H_{jj'}^{(2k)}, \qquad (58)$$

$$Q_{jj'}(r) = \sum_{k=1}^{k_{max}}r^{-2k+1}Q_{jj'}^{(2k-1)}.$$

In these formulas, the asymptotic quantum numbers n_l and n_r are related to j and j' as $n_l = j - 1$ and $n_r = j' - 1$.

The computations were performed using the MATRA algorithm described above implemented in Maple and Mathematica up to $k_{max} = 6$. Below, we present the first several coefficients:

$$E_j^{(0)} = \gamma(2n + m + |m| + 1),$$

$$E_j^{(2)} = -2n^2 - 2n|m| - 2n - |m| - 1,$$

$$\begin{aligned}
E_j^{(4)} = &(2\gamma)^{-1}(-4n^3 - 6n^2 - 4n - 1 - 2|m| \\
&- m^2 - 6n^2|m| - 2nm^2 - 6n|m|)
\end{aligned} \qquad (59)$$

and matrix elements for $n = \min(n_l, n_r)$:

$$Q_{jj'}^{(1)} = (n_r - n_l)\sqrt{n + 1}\sqrt{n + |m| + 1}\delta_{|n_l - n_r|, 1},$$

$$\begin{aligned}
Q_{jj'}^{(3)} = &(4\gamma)^{-1}(n_r - n_l)\sqrt{n + 1}\sqrt{n + |m| + 1} \\
&\times((2n + |m| + 2)\delta_{|n_l - n_r|, 1} \\
&+ \sqrt{n + 2}\sqrt{n + |m| + 2}\delta_{|n_l - n_r|, 2}),
\end{aligned}$$

$$\begin{aligned}
H_{jj'}^{(2)} = &(2n^2 + 2n + 2|m|n + |m| + 1)\delta_{|n_l - n_r|, 0} \\
&- \sqrt{n + 1}\sqrt{n + |m| + 1}
\end{aligned}$$

Table 1. Values of the partial sums $Q_{jj'}(r) = \sum_{k=1}^{k_{max}} r^{-2k+1} Q_{jj'}^{(2k-1)}$ depending on k_{max} for $\gamma = 1$, $m = 0$, $Z = 1$, and $r = 10$. The last row contains the corresponding numerical values (n.v.)

k_{max}	Q_{12}, 10^{-1}	Q_{23}, 10^{-1}	Q_{34}, 10^{-1}
1	1.000000	2.000000	3.000000
2	1.010000	2.040000	3.090000
3	1.010300	2.042550	3.098700
4	1.010310	2.042749	3.099744
5	1.010310	2.042766	3.099882
6	1.010310	2.042767	3.099901
n.v.	1.010310	2.042767	3.099904
k_{max}	Q_{13}, 10^{-3}	Q_{24}, 10^{-3}	Q_{14}, 10^{-5}
1	0	0	0
2	1.000000	3.000000	0
3	1.060000	3.300000	1.500000
4	1.064150	3.334050	1.710000
5	1.064465	3.338235	1.736288
6	1.064490	3.338777	1.739596
n.v.	1.064492	3.338861	1.740089

$$\times \sqrt{n+2}\sqrt{n+|m|+2}\,\delta_{|n_l-n_r|,\,2}, \tag{60}$$

$$H_{jj'}^{(4)} = \gamma^{-1}((2n+|m|+1)$$

$$\times (2n^2+2n+2|m|n+|m|+2)\delta_{|n_l-n_r|,\,0}$$

$$+ \sqrt{n+1}\sqrt{n+|m|+1}$$

$$\times ((n^2+2n+|m|n+|m|+2)\delta_{|n_l-n_r|,\,1}$$

$$- \sqrt{n+2}\sqrt{n+|m|+2}$$

$$\times [(2n+|m|+3)\delta_{|n_l-n_r|,\,2}$$

$$+ \sqrt{n+3}\sqrt{n+|m|+3}\,\delta_{|n_l-n_r|,\,3}])).$$

Tables 1 and 2 illustrate the convergence of the partial sums of asymptotic expansions (58) for the matrix elements to the corresponding numerical values (26) obtained using the MATRM algorithm described in Section 4 for $s_{max} = 200$. For large r, to achieve the prescribed accuracy in the calculation of matrix elements (26), the length of the vector s_{max} must be considerably increased. For this reason, for $r \geq r_0 > j_{max}/\sqrt{\gamma}$, the matrix elements were calculated by asymptotic formulas in the framework of the unified symbolic-numerical algorithm consisting of EIGENF, MATRM, and MATRA.

Remark. The sum of the coefficients $E_j^{(2)} + H_{jj}^{(2)} = 0$; i.e., for $r \gg 1$, the diagonal centrifugal potentials $\sim r^-$

^{2} vanish. To calculate the exponentially small terms in (58), one can use an additional expansion of the solution in the region $D_2 = [0, 1-\eta_2]$, $\eta_2 < \eta_1$, $\eta_2 = o(p^{-1/2-\varepsilon})$ following [14].

6. THE ASYMRS(1) ALGORITHM

Step 1. To solve system of radial equations (10) for large $r \geq r_{max}$, we change to the new vector function $\phi_{i_o}(r) = \{\phi_{ji_o}(r)\}_{j=1}^{j_{max}}$ defined by

$$\chi_{ji_o}(r) = \frac{\exp(w(r))\phi_{ji_o}(r)}{r\sqrt{2\pi p_{i_o}}}, \tag{61}$$

$$w(r) = ip_{i_o}r + \iota\zeta\ln(2p_{i_o}r) + \iota\delta_{i_o},$$

where p_{i_o} is the momentum in the channel $i_o \leq N_o$, ζ is the characteristic parameter, and $\delta_{i_o} \equiv \delta_{i_o}(\zeta)$ is the phase shift. The components $\phi_{ji_o}(r)$ satisfy the system of ordinary differential equations

$$\left(-\frac{d^2}{dr^2} - \left(2\iota p_{i_o} + \frac{2\iota\zeta}{r}\right)\frac{d}{dr}\right.$$

$$+ p_{i_o}^2 + H_{jj}(r) - \epsilon + \frac{2p_{i_o}\zeta - 2Z}{r}$$

$$\left. + \frac{E_j(r) + \iota\zeta + \zeta^2}{r^2}\right)\phi_{ji_o}(r) \tag{62}$$

$$= \sum_{j'=1, j'\neq j}^{j_{max}} \left(-2Q_{jj'}(r)\frac{d}{dr} - 2\iota p_{i_o}Q_{jj'}(r)\right.$$

$$\left. - H_{jj'}(r) - \frac{dQ_{jj'}(r)}{dr} - \frac{2\iota\zeta Q_{jj'}(r)}{r}\right)\phi_{j'i_o}(r)$$

for $r_{max} \leq r < \infty$.

Step 2. The asymptotics of the functions $\phi_{ji_o}(r)$ are sought as an expansion in inverse powers of r:

$$\phi_{ji_o}(r) = \sum_{k=0}^{k_{max}} \phi_{ji_o}^{(k)} r^{-k}. \tag{63}$$

Substituting expansion (63) into (62), we obtain the following system of recurrences for the unknown coefficients $\phi_{ji_o}^{(k)}$:

$$(p_{i_o}^2 - 2E + E_j^{(0)})\phi_{ji_o}^{(k)} = f_{ji_o}^{(k)},$$

$$f_{ji_o}^{(k)} = -(2p_{i_o}\zeta - 2Z + 2\iota p_{i_o}(k-1))\phi_{ji_o}^{(k-1)}$$

$$-(\zeta - 2\iota + \iota k)(\zeta - \iota + \iota k)\phi_{ji_o}^{(k-2)}$$

$$-\sum_{k'=1}^{k}(E_j^{(k')} + H_{jj}^{(k')})\phi_{ji_o}^{(k-k')} \qquad (64)$$

$$+\sum_{j'=1,\,j'\neq j}^{j_{max}}\sum_{k'=1}^{k}(-2\iota p_{i_o}Q_{jj'}^{(k')} - H_{jj'}^{(k')}$$

$$+ (2k - k' - 1 - 2\iota\zeta)Q_{jj'}^{(k'-1)})\phi_{j'i_o}^{(k-k')}.$$

Here, the indexes j_k ($k = 0, 1, \ldots, k_{max}$) range over the integers excluding i_o and j_{k+1}; i.e., $j_k = 1, 2, \ldots, j_{max}, j_k \neq i_o$, and $j_k \neq j_{k+1}$.

Step 3. The first three equations in (64), which contain the functions $\phi_{i_o i_o}^{(0)}$, $\phi_{j_o i_o}^{(0)}$, and $\phi_{i_o i_o}^{(1)}$ on their left-hand sides, imply the following initial conditions for recurrent procedure (64):

$$\phi_{i_o i_o}^{(0)} = \delta_{j_o i_o}, \quad p_{i_o} = \sqrt{2E - E_{i_o}^{(0)}}, \quad \zeta = \frac{Z}{p_{i_o}}. \quad (65)$$

Hence, we have $\delta_{i_o} = \arg\Gamma(1 - \iota\zeta)$.

Step 4. Substituting (65) in (64), we obtain the following recurrent set of algebraic equations for the unknown coefficients $\phi_{ji_o}^{(k)}$ for $k = 1, 2, \ldots, k_{max}$:

$$(E_j^{(0)} - E_{i_o}^{(0)})\phi_{ji_o}^{(k)} = f_{ji_o}^{(k)}. \quad (66)$$

System (66) is solved sequentially for $k = 1, 2, \ldots, k_{max}$:

$$\phi_{ji_o}^{(k)} = \frac{f_{ji_o}^{(k)}}{E_j^{(0)} - E_{i_o}^{(0)}}, \quad j \neq i_o, \qquad (67)$$

$$f_{i_o i_o}^{(k+1)} = 0 \longrightarrow \phi_{i_o i_o}^{(k)}.$$

The procedure ASYMRS(1) implemented as a sequence of Steps 1–4 in Maple yields expressions for the coefficients of the expansion of $\phi_{ji_o}^{(k)}$ up to $k_{max} = 5$, for example, for $j_{max} \geq i_o + k$ and $k = 0, 1, 2$, we have

$$\phi_{j_o i_o}^{(1)} = \frac{2\iota p_{i_o}Q_{j_1 i_o}^{(1)}}{E_{i_o}^{(0)} - E_{j_1}^{(0)}},$$

$$\phi_{i_o i_o}^{(1)} = \frac{\iota(Z^2 + \iota Z p_{i_o})}{2p_{i_o}^3} - \sum_{\substack{j_1 = \max(1, i_o - 1),\\ j_1 \neq i_o}}^{\min(j_{max}, i_o+1)} Q_{i_o j_1}^{(1)}\phi_{j_1 i_o}^{(1)}. \qquad (68)$$

It also yields explicit expressions for these coefficients when the asymptotics of matrix elements (58) found by the algorithm MATRA are substituted as the initial parameters:

Table 2. Values of the partial sums $H_{jj'}(r) = \sum_{k=1}^{k_{max}} r^{-2k}H_{jj'}^{(2k)}$ depending on k_{max} for $\gamma = 1$, $m = 0$, $Z = 1$, and $r = 10$. The last row contains the corresponding numerical values (n.v.)

k_{max}	$H_{11}, 10^{-2}$	$H_{22}, 10^{-2}$	$H_{33}, 10^{-1}$
1	1.000000	5.000000	1.300000
2	1.020000	5.180000	1.370000
3	1.020800	5.193400	1.377580
4	1.020838	5.194606	1.378565
5	1.020840	5.194726	1.378706
6	1.020840	5.194738	1.378728
n.v.	1.020840	5.194740	1.378732
k_{max}	$H_{21}, 10^{-4}$	$H_{32}, 10^{-3}$	$H_{43}, 10^{-3}$
1	0	0	0
2	2.000000	1.000000	3.000000
3	2.160000	1.124000	3.504000
4	2.173700	1.140390	3.593310
5	2.174956	1.142691	3.610054
6	2.175078	1.143029	3.613336
n.v.	2.175092	1.143090	3.614180
k_{max}	$H_3, 10^{-2}$	$H_{42}, 10^{-2}$	$H_{41}, 10^{-4}$
1	−2.000000	−6.000000	0
2	−2.060000	−6.300000	−6.000000
3	−2.063100	−6.326100	−6.600000
4	−2.063280	−6.328740	−6.663300
5	−2.063289	−6.329018	−6.670482
6	−2.063289	−6.329045	−6.671343
n.v.	−2.063289	−6.329047	−6.671464

$$\phi_{i_o-1 i_o}^{(1)} = \iota\frac{p_{i_o}\sqrt{i_o-1}\sqrt{i_o+|m|-1}}{\gamma},$$

$$\phi_{i_o i_o}^{(1)} = \left[\iota\frac{Z^2}{2p_{i_o}^3} - \frac{Z}{2p_{i_o}^2}\right] - \iota\frac{p_{i_o}(2i_o+|m|-1)}{\gamma}, \qquad (69)$$

$$\phi_{i_o+1 i_o}^{(1)} = \iota\frac{p_{i_o}\sqrt{i_o}\sqrt{i_o+|m|}}{\gamma}.$$

Remark. If the scaled variable $\hat{r} = r\sqrt{\gamma}$, the effective charge $\hat{Z} = Z/\sqrt{\gamma}$, and the scaled momentum $\hat{p}_{i_o} = p_{i_o}/\sqrt{\gamma}$ are used, we may set $\gamma = 1$. Expansion (61) holds true for $\hat{r}_{;max} \gg \max(\hat{Z}^2/(2\hat{p}_{i_o}^2), (2i_o + |m| - 1)/\hat{p}_{i_o})$. The choice of a new value of r_{max} for the constructed expansions of the linearly independent solu-

tions for $p_{i_o} > 0$ is controlled by the fulfillment of the condition

$$\mathbf{Wr}(\mathbf{Q}(r); \boldsymbol{\chi}^*(r), \boldsymbol{\chi}(r)) = \frac{\iota}{\pi}\mathbf{I}_{oo} \qquad (70)$$

up to the prescribed accuracy. Here, $\mathbf{I}_{oo}$ is the N_o-by-N_o identity matrix, and the Wronskian $\mathbf{Wr}(\bullet; \boldsymbol{\chi}^*(r), \boldsymbol{\chi}(r))$ is determined by the relation

$$\mathbf{Wr}(\bullet; \boldsymbol{\chi}^*, \boldsymbol{\chi}) = r^2\Big[(\boldsymbol{\chi}^*)^T\Big(\frac{d\boldsymbol{\chi}}{dr} - \bullet\boldsymbol{\chi}\Big) \\ -\Big(\frac{d\boldsymbol{\chi}^*}{dr} - \bullet\boldsymbol{\chi}^*\Big)^T\boldsymbol{\chi}\Big]. \qquad (71)$$

The asymptotics thus obtained are used to set up boundary conditions (15) that must be satisfied by the bounded solutions to system (10).

7. THE ASYMRS(2) ALGORITHM

Step 1. Using initial conditions (65) obtained at Step 3 of the algorithm ASYMRS(1), we seek the solutions $\boldsymbol{\chi}_{i_o}(r)$ to system of radial equations (10) for large $r_{\max} \leq r < \infty$ in the form of the expansion

$$\chi_{ji_o}(r) = R(r)\phi_{ji_o}(r) + \frac{dR(r)}{dr}\psi_{ji_o}(r), \qquad (72)$$

in the solutions $R(r) \equiv R(p_{i_o}, r)$ to the ordinary differential equation

$$\Big(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + p_{i_o}^2 + \frac{2Z}{r}\Big)R(p_{i_o}, r) = 0, \qquad (73)$$

where $R(p_{i_o}, r) = \iota F(p_{i_o}, r) + G(p_{i_o}, r)$ is the sum composed of the regular $F(p_{i_o}, r)$ and the irregular $G(p_{i_o}, r)$ Coulomb functions (see [4]). The substitution of (72) in Eq. (10) with account for (73) yields the system of two coupled ordinary differential equations for the pair of unknown functions $\phi_{ji_o}(r)$ and $\psi_{ji_o}(r)$:

$$\Big(-\frac{d^2}{dr^2} - \frac{2}{r}\frac{d}{dr} + p_{i_o}^2 + H_{jj}(r) \\ -\epsilon + \frac{E_j(r)}{r^2}\Big)\phi_{ji_o}(r) \\ +\Big(\Big(2p_{i_o}^2 + \frac{4Z}{r}\Big)\frac{d}{dr} - \frac{2Z}{r^2}\Big)\psi_{ji_o}(r) \\ = -\sum_{j'=1, j'\neq j}^{j_{\max}}\Big(H_{jj'}(r) + Q_{jj'}(r)\frac{d}{dr} \qquad (74)$$

$$+\frac{1}{r^2}\frac{dr^2 Q_{jj'}(r)}{dr}\Big)\phi_{j'i_o}(r) \\ +\Big(2p_{i_o}^2 + \frac{4Z}{r}\Big)\sum_{j'=1, j'\neq j}^{j_{\max}}Q_{jj'}(r)\psi_{j'i_o}(r),$$

$$\Big(-\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + p_{i_o}^2 + H_{jj}(r) - \epsilon \\ +\frac{E_j(r) - 2}{r^2}\Big)\psi_{ji_o}(r) - 2\frac{d\phi_{ji_o}(r)}{dr} \\ = -\sum_{j'=1, j'\neq j}^{j_{\max}}\Big(H_{jj'}(r) + Q_{jj'}(r)\frac{d}{dr} \qquad (75) \\ +\frac{1}{r^2}\frac{r^2 Q_{jj'}(r)}{dr} - \frac{4Q_{jj'}(r)}{r}\Big)\psi_{j'i_o}(r) \\ -2\sum_{j'=1, j'\neq j}^{j_{\max}}Q_{jj'}(r)\phi_{j'i_o}(r).$$

Step 2. The asymptotics of the functions $\phi_{ji_o}(r)$ and $\psi_{ji_o}(r)$ are sought as expansions in inverse powers of r:

$$\phi_{ji_o}(r) = \sum_{k=0}^{k_{\max}}\phi_{ji_o}^{(k)}r^{-k}, \\ \psi_{ji_o}(r) = \sum_{k=0}^{k_{\max}}\psi_{ji_o}^{(k)}r^{-k}. \qquad (76)$$

Substituting expansion (76) into (74) and (75), we obtain the following system of recurrences for the unknown coefficients $\phi_{ji_o}^{(k)}$ and $\psi_{ji_o}^{(k)}$:

$$(p_{i_o}^2 - 2E + E_j^{(0)})\phi_{ji_0}^{(k)} = f_{ji_o}^{(k)}, \\ f_{ji_o}^{(k)} = 2p_{i_o}^2(k-1)\psi_{ji_o}^{(k-1)} + (k-2) \\ \times(k-3)\phi_{ji_o}^{(k-2)} + 2Z(2k-3)\psi_{ji_o}^{(k-2)} \\ -\sum_{k'=1}^{k}(E_j^{(k')} + H_{jj}^{(k')})\phi_{ji_o}^{(k-k')} \qquad (77) \\ +\sum_{j'=1, j'\neq j}^{j_{\max}}\sum_{k'=1}^{k}[((2k-k'-3)Q_{jj'}^{(k'-1)} - H_{jj'}^{(k')})\phi_{j'i_o}^{(k-k')} \\ +(2p_{i_o}^2 Q_{jj'}^{(k')} + 4ZQ_{jj'}^{(k'-1)})\psi_{j'i_o}^{(k-k')}], \\ (p_{i_o}^2 - 2E + E_j^{(0)})\psi_{ji_o}^{(k)} = g_{ji_o}^{(k)},$$

$$g_{ji_o}^{(k)} = -2(k-1)\phi_{ji_o}^{(k-1)} + k(k-1)\psi_{ji_o}^{(k-2)}$$

$$- \sum_{k'=1}^{j_{max}} (E_j^{(k')} + H_{jj}^{(k')})\psi_{ji_o}^{(k-k')} \qquad (78)$$

$$+ \sum_{j'=1, j'\neq j}^{j_{max}} \sum_{k'=1}^{k} [((2k-k'+1)Q_{jj'}^{(k'-1)}$$

$$- H_{jj'}^{(k')})\psi_{ji_o}^{(k-k')} - 2Q_{jj'}^{(k')}\phi_{j'i_o}^{(k-k')}].$$

Here, the indexes j_k ($k = 0, 1, \ldots, k_{max}$) range over the integers excluding i_o and j_{k+1}; i.e., $j_k = 1, 2, \ldots, j_{max}, j_k \neq i_o$, and $j_k \neq j_{k+1}$.

Step 3. The first two equations in system (77), (78), which contain the functions $\phi_{i_oi_o}^{(0)}$, $\phi_{j_0i_o}^{(0)}$, and $\psi_{i_oi_o}^{(0)}$, $\psi_{j_0i_o}^{(0)}$ on their left-hand sides, respectively, imply the following initial conditions for recurrent procedure (77), (78):

$$\phi_{j_0i_o}^{(0)} = \delta_{j_0i_o}, \quad \psi_{j_0i_o}^{(0)} = 0, \quad p_{i_o}^2 = 2E - E_{i_o}^{(0)}. \quad (79)$$

Step 4. Substituting (79) in (77) and (78), we obtain the following recurrent set of uncoupled algebraic equations for the unknown coefficients $\phi_{ji_o}^{(k)}$ and $\psi_{ji_o}^{(k)}$ for $k = 1, 2, \ldots, k_{max}$:

$$(E_j^{(0)} - E_{i_o}^{(0)})\phi_{ji_o}^{(k)} = f_{ji_o}^{(k)},$$
$$(E_j^{(0)} - E_{i_o}^{(0)})\psi_{ji_o}^{(k)} = g_{ji_o}^{(k)}. \qquad (80)$$

System (80) is solved sequentially for $k = 1, 2, \ldots, k_{max}$:

$$\phi_{ji_o}^{(k)} = \frac{f_{ji_o}^{(k)}}{E_j^{(0)} - E_{i_o}^{(0)}}, \quad j \neq i_o,$$

$$f_{i_oi_o}^{(k+1)} = 0 \longrightarrow \phi_{i_oi_o}^{(k)},$$

$$\psi_{ji_o}^{(k)} = \frac{g_{ji_o}^{(k)}}{E_j^{(0)} - E_{i_o}^{(0)}}, \quad j \neq i_o, \qquad (81)$$

$$g_{i_oi_o}^{(k+1)} = 0 \longrightarrow \psi_{i_oi_o}^{(k)}.$$

The procedure ASYMRS(2) implemented as a sequence of Steps 1–4 in Maple yields expressions for the coefficients of the expansion of $\phi_{ji_o}^{(k)}$ and $\psi_{ji_o}^{(k)}$ up to $k_{max} = 5$; for example, for $j_{max} \geq i_o + k$ and $k = 0, 1, 2$, we have

$$\phi_{j_1i_o}^{(1)} = 0,$$

$$\phi_{i_oi_o}^{(1)} = 0,$$

$$\psi_{j_1i_o}^{(1)} = \frac{2Q_{j_1i_o}^{(1)}}{E_{i_o}^{(0)} - E_{j_1}^{(0)}}, \qquad (82)$$

$$\psi_{i_oi_o}^{(1)} = -\sum_{j_0 = \max(1, i_o-1), j_0 \neq i_o}^{\min(j_{max}, i_o+1)} Q_{i_oj_0}^{(1)}\psi_{j_0i_o}^{(1)}.$$

It also yields explicit expressions for these coefficients when the asymptotics of matrix elements (58) found by the algorithm MATRA are substituted as the initial parameters:

$$\phi_{i_o-1i_o}^{(1)} = 0, \quad \psi_{i_o-1i_o}^{(1)} = \frac{\sqrt{i_o-1}\sqrt{i_o+|m|-1}}{\gamma},$$

$$\phi_{i_oi_o}^{(1)} = 0, \quad \psi_{i_oi_o}^{(1)} = -\frac{2i_o+|m|-1}{\gamma}, \qquad (83)$$

$$\phi_{i_o+1i_o}^{(1)} = 0, \quad \psi_{i_o+1i_o}^{(1)} = \frac{\sqrt{i_o}\sqrt{i_o+|m|}}{\gamma}.$$

Remark. In each kth order, recurrences (77) and (78) include implicitly only the factor Z/p_{i_o}, and recurrences (64) explicitly include the factor $(Z/p_{i_o})^2$. Expansion (72) holds for $\hat{r}_{max} \gg \max(\hat{Z}/\hat{p}_{i_o}, (2i_o + |m| - 1))$. As a result, for small $\hat{p}_{i_o}$ or for large values of the effective charge $\hat{Z}$ (i.e., for large values of the parameter $|\zeta| = |\hat{Z}/\hat{p}_{i_o}| \gg 1$), expansion (72) can be used more efficiently than expansion (61) for smaller values of $\hat{r}_{max}$; recall that (61) holds when $\hat{r}_{max}|\zeta|$ is considerably greater than $\hat{r}_{max}$ (because $|\zeta| \gg 1$).

8. CONCLUSIONS

A set of functionally connected symbolic-numerical algorithms EIGENF, MATRM, MATRA, and ASYMRS(I) (I = 1, 2) is developed that reduce the singular boundary value problem for a second-order elliptic partial differential equation in a two-dimensional region to a regular boundary value problem for a system of ordinary differential equations in the Kantorovich method.

A comparison of the asymptotic and numerical values of the matrix elements (integrals of the oblate angular spheroidal functions and their derivatives with respect to the parameter) is performed that demonstrates the scope and the efficiency of the symbolic algorithm MATRA and of the combined symbolic-numerical algorithms EIGENF and MATRM. When the matrix elements are calculated, the number of terms

s_{max} in expansion (17) increases with r. For this reason, the continuation of the numerical values of the matrix elements from the bounded interval of the parameter variation $0 < r \leq r_{max}$ to the entire plane as $r_{max} \longrightarrow \infty$ using the asymptotic algorithm MATRA makes it possible to considerably save computer resources. The results coincide with the computations performed using the finite element method [2] up to 10 significant digits. The analytical expressions for the matrix elements obtained by MATRA are also used as the initial parameters for the algorithm ASYMRS(I) (I = 1, 2), which calculates the asymptotics of the solutions to the system of radial equations required for solving the boundary value problem subject to the boundary conditions of the third kind. A description of the algorithm KANTBP for the numerical solution of the system of second-order ordinary differential equations (10)–(15) by the finite volume method will be given in subsequent papers.

The approach developed in this paper provides a convenient tool not only for the description of the formation and ionization of hydrogen-like atoms in magnetic traps [5] and the calculation of the wave function of hydrogen-like atoms [6] or the quantum point in a strong magnetic field [15], but also provides means for the analysis of accuracy and the rate of convergence of the representation of the solution to be found. For example, using the algorithm MATRM for calculating high-order derivatives of the matrix elements with respect to the parameter up to a prescribed accuracy, one can construct efficient operator approximations for the system of radial equations. Such approximations enable one to analyze the convergence of the sum rules over the spectrum of the parametric problem and obtain upper and lower bounds on the solution to be found [16]. In combination with the algorithm for the unitary decomposition of the evolution operator [17], this approach seems to be promising for computer simulation of Zeeman states in variable electric fields [18–20] and for the simulation of the behavior of ions in trapped models of quantum computers [21].

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SPELL: 1. unnormalized, 2. nonsingular