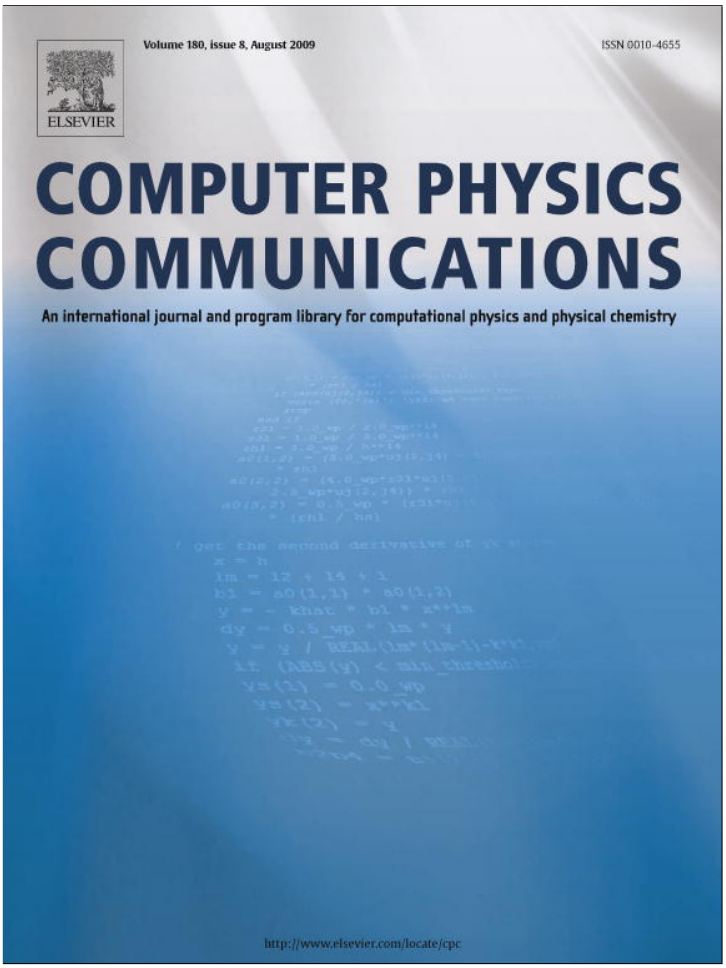

Computer Physics Communications 180 (2009) 1358–1375

Contents lists available at ScienceDirect

Computer Physics Communications

www.elsevier.com/locate/cpc

ODPEVP: A program for computing eigenvalues and eigenfunctions and their first derivatives with respect to the parameter of the parametric self-adjoined Sturm–Liouville problem ☆

O. Chuluunbaatar [a,*], A.A. Gusev [a], S.I. Vinitsky [a], A.G. Abrashkevich [b]

[a] Joint Institute for Nuclear Research, Dubna, 141980 Moscow region, Russia
[b] IBM Toronto Lab, 8200 Warden Avenue, Markham, ON L6G 1C7, Canada

ARTICLE INFO

Article history:
Received 7 January 2009
Accepted 21 April 2009
Available online 22 April 2009

PACS:
02.60.Lj
31.15.Ja
32.80.Fb

Keywords:
Eigenvalue problems
Kantorovich method
Finite element method
Ordinary differential equations
High-order accuracy approximations

ABSTRACT

A FORTRAN 77 program is presented for calculating with the given accuracy eigenvalues, eigenfunctions and their first derivatives with respect to the parameter of the parametric self-adjoined Sturm–Liouville problem with the parametric third type boundary conditions on the finite interval. The program calculates also potential matrix elements – integrals of the eigenfunctions multiplied by their first derivatives with respect to the parameter. Eigenvalues and matrix elements computed by the ODPEVP program can be used for solving the bound state and multi-channel scattering problems for a system of the coupled second-order ordinary differential equations with the help of the KANTBP programs [O. Chuluunbaatar, A.A. Gusev, A.G. Abrashkevich, A. Amaya-Tapia, M.S. Kaschiev, S.Y. Larsen, S.I. Vinitsky, Comput. Phys. Commun. 177 (2007) 649–675; O. Chuluunbaatar, A.A. Gusev, S.I. Vinitsky, A.G. Abrashkevich, Comput. Phys. Commun. 179 (2008) 685–693]. As a test desk, the program is applied to the calculation of the potential matrix elements for an integrable 2D-model of three identical particles on a line with pair zero-range potentials, a 3D-model of a hydrogen atom in a homogeneous magnetic field and a hydrogen atom on a three-dimensional sphere.

Program summary

Program title: ODPEVP
Catalogue identifier: AEDV_v1_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEDV_v1_0.html
Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland
Licensing provisions: Standard CPC license, http://cpc.cs.qub.ac.uk/licence/licence.html
No. of lines in distributed program, including test data, etc.: 3001
No. of bytes in distributed program, including test data, etc.: 24 195
Distribution format: tar.gz
Programming language: FORTRAN 77
Computer: Intel Xeon EM64T, Alpha 21264A, AMD Athlon MP, Pentium IV Xeon, Opteron 248, Intel Pentium IV
Operating system: OC Linux, Unix AIX 5.3, SunOS 5.8, Solaris, Windows XP
RAM: depends on

1. the number and order of finite elements;
2. the number of points; and
3. the number of eigenfunctions required.

Test run requires 4 MB
Classification: 2.1, 2.4
External routines: GAULEG [3]
Nature of problem: The three-dimensional boundary problem for the elliptic partial differential equation with an axial symmetry similar to the Schrödinger equation with the Coulomb and transverse oscillator potentials is reduced to the two-dimensional one. The latter finds wide applications in modeling

☆ This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

* Corresponding author.
E-mail address: chuka@jinr.ru (O. Chuluunbaatar).

0010-4655/$ – see front matter
doi:10.1016/j.cpc.2009.04.017

of photoionization and recombination of oppositively charged particles (positrons, antiprotons) in the magnet-optical trap [4], optical absorption in quantum wells [5], and channeling of likely charged particles in thin doped films [6,7] or neutral atoms and molecules in artificial waveguides or surfaces [8,9]. In the adiabatic approach [10] known in mathematics as Kantorovich method [11] the solution of the two-dimensional elliptic partial differential equation is expanded over basis functions with respect to the fast variable (for example, angular variable) and depended on the slow variable (for example, radial coordinate) as a parameter. An averaging of the problem by such a basis leads to a system of the second-order ordinary differential equations which contain potential matrix elements and the first-derivative coupling terms (see, e.g., [12,13,14]). The purpose of this paper is to present the finite element method procedure based on the use of high-order accuracy approximations for calculating eigenvalues, eigenfunctions and their first derivatives with respect to the parameter of the parametric self-adjoined Sturm–Liouville problem with the parametric third type boundary conditions on the finite interval. The program developed calculates potential matrix elements – integrals of the eigenfunctions multiplied by their derivatives with respect to the parameter. These matrix elements can be used for solving the bound state and multi-channel scattering problems for a system of the coupled second-order ordinary differential equations with the help of the KANTBP programs [1,2].

Solution method: The parametric self-adjoined Sturm–Liouville problem with the parametric third type boundary conditions is solved by the finite element method using high-order accuracy approximations [15]. The generalized algebraic eigenvalue problem $\mathbf{AF} = E\mathbf{BF}$ with respect to a pair of unknown $(E, \mathbf{F})$ arising after the replacement of the differential problem by the finite-element approximation is solved by the subspace iteration method using the SSPACE program [16]. First derivatives of the eigenfunctions with respect to the parameter which contained in potential matrix elements of the coupled system equations are obtained by solving the inhomogeneous algebraic equations. As a test desk, the program is applied to the calculation of the potential matrix elements for an integrable 2D-model of three identical particles on a line with pair zero-range potentials described in [1,17,18], a 3D-model of a hydrogen atom in a homogeneous magnetic field described in [14,19] and a hydrogen atom on a three-dimensional sphere [20].

Restrictions: The computer memory requirements depend on:

1. the number and order of finite elements;
2. the number of points; and
3. the number of eigenfunctions required.

Restrictions due to dimension sizes may be easily alleviated by altering PARAMETER statements (see sections below and listing for details). The user must also supply DOUBLE PRECISION functions POTCCL and POTCC1 for evaluating potential function $U(\rho, z)$ of Eq. (1) and its first derivative with respect to parameter ρ. The user should supply DOUBLE PRECISION functions F1FUNC and F2FUNC that evaluate functions $f_1(z)$ and $f_2(z)$ of Eq. (1). The user must also supply subroutine BOUNCF for evaluating the parametric third type boundary conditions.

Running time: The running time depends critically upon:

1. the number and order of finite elements;
2. the number of points on interval $[z_{\min}, z_{\max}]$; and
3. the number of eigenfunctions required.

The test run which accompanies this paper took 2 s with calculation of matrix potentials on the Intel Pentium IV 2.4 GHz.

References:

[1] O. Chuluunbaatar, A.A. Gusev, A.G. Abrashkevich, A. Amaya-Tapia, M.S. Kaschiev, S.Y. Larsen, S.I. Vinitsky, Comput. Phys. Comm. 177 (2007) 649–675
[2] O. Chuluunbaatar, A.A. Gusev, S.I. Vinitsky, A.G. Abrashkevich, Comput. Phys. Comm. 179 (2008) 685–693.
[3] W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes: The Art of Scientific Computing, Cambridge University Press, Cambridge, 1986.
[4] O. Chuluunbaatar, A.A. Gusev, S.I. Vinitsky, V.L. Derbov, L.A. Melnikov, V.V. Serov, Phys. Rev. A 77 (2008) 034702-1–4.
[5] E.M. Kazaryan, A.A. Kostanyan, H.A. Sarkisyan, Physica E 28 (2005) 423–430.
[6] Yu.N. Demkov, J.D. Meyer, Eur. Phys. J. B 42 (2004) 361–365.
[7] P.M. Krassovitskiy, N.Zh. Takibaev, Bull. Russian Acad. Sci. Phys. 70 (2006) 815–818.
[8] V.S. Melezhik, J.I. Kim, P. Schmelcher, Phys. Rev. A 76 (2007) 053611-1–15.
[9] F.M. Pen'kov, Phys. Rev. A 62 (2000) 044701-1–4.
[10] M. Born, X. Huang, Dynamical Theory of Crystal Lattices, The Clarendon Press, Oxford, England, 1954.
[11] L.V. Kantorovich, V.I. Krylov, Approximate Methods of Higher Analysis, Wiley, New York, 1964.
[12] U. Fano, Colloq. Int. C.N.R.S. 273 (1977) 127;
A.F. Starace, G.L. Webster, Phys. Rev. A 19 (1979) 1629–1640.
[13] C.V. Clark, K.T. Lu, A.F. Starace, in: H.G. Beyer, H. Kleinpoppen (eds.), Progress in Atomic Spectroscopy, Part C, Plenum, New York, 1984, pp. 247–320.
[14] O. Chuluunbaatar, A.A. Gusev, V.L. Derbov, M.S. Kaschiev, L.A. Melnikov, V.V. Serov, S.I. Vinitsky, J. Phys. A 40 (2007) 11485–11524.
[15] A.G. Abrashkevich, D.G. Abrashkevich, M.S. Kaschiev, I.V. Puzynin, Comput. Phys. Comm. 85 (1995) 40–64.
[16] K.J. Bathe, Finite Element Procedures in Engineering Analysis, Englewood Cliffs, Prentice-Hall, New York, 1982.

[17] O. Chuluunbaatar, A.A. Gusev, M.S. Kaschiev, V.A. Kaschieva, A. Amaya-Tapia, S.Y. Larsen, S.I. Vinitsky, J. Phys. B 39 (2006) 243–269.
[18] Yu.A. Kuperin, P.B. Kurasov, Yu.B. Melnikov, S.P. Merkuriev, Ann. Phys. 205 (1991) 330–361.
[19] O. Chuluunbaatar, A.A. Gusev, V.P. Gerdt, V.A. Rostovtsev, S.I. Vinitsky, A.G. Abrashkevich, M.S. Kaschiev, V.V. Serov, Comput. Phys. Comm. 178 (2008) 301–330.
[20] A.G. Abrashkevich, M.S. Kaschiev, S.I. Vinitsky, J. Comp. Phys. 163 (2000) 328–348.

1. Introduction

Mathematical models of physical processes such as photoionization and laser-stimulated recombination of hydrogen like atoms in a homogeneous magnetic field under influence of a laser field, axial channeling of the charged particles in thin films, and also excitation, de-excitation of wave-packet of a hydrogen atom in a homogeneous magnetic field under influence of the sequences with ultra-short laser pulses (so-called three-dimensional kicked hydrogen atom in a magnetic field) are subjects of recent studies [1–6].

Dynamics of these processes is described in a center of mass system by three-dimensional wave functions of stationary equations of Schrödinger type. We shall emphasize, that in a vicinity of the origin of a system of coordinates or the pair impact point the attractive or repulsive Coulomb potentials dominate while in asymptotic regions it is the oscillator potential in transversal variables. Similar problems arise in quantum well with a hydrogen like impurity in study of photoabsorbsion processes [7].

Mathematical models of these processes used in numerical studies to describe the dynamics of few-body systems are singular spectral, boundary and evolutionary problems for multi-dimensional equation of Schrödinger type in the coordinate space. We shall emphasize, that the presence of several interaction potentials between particles or particles with external fields leads to a division of the whole region to subregions where the relevant boundary problems are solved using the corresponding dominating potential. Hence a singular problem could be reduced to a regular one on a finite region by defining asymptotic boundary conditions with the help of an appropriate asymptotic decomposition of solutions on a border of the finite region in the form of conditions of the third type.

For solving a boundary problem in the complex region, in the framework of the projective method one has to construct basic functions with nonlinear parameters in one of the subregions or in each subregion. For the coordination of compound basic functions on borders of these regions it is necessary to use conditions of the third type. Hence the amount of nonlinear parameters in a variational functional essentially increases which requires significant computer resources to calculate them.

The multi-step Kantorovich method enables one to construct an economical algorithm for calculating of parametrical basic functions which take into account all features of complex regions and conditions of the coordination between them. The use of such basis allows us to lower the dimension of an initial boundary problem by reducing it to a system of ordinary differential equations with boundary conditions of the third type [8,9]. Discretization of boundary problems by the finite-element method (FEM) [10,11] results in sequences of parametrical algebraic problems for the numerical solution of which one needs to develop economical and efficient algorithms and programs.

In this work we present an ODPEVP program for calculating with a given accuracy eigenvalues, eigenfunctions and their first derivatives with respect to the parameter of the parametric self-adjoined Sturm–Liouville problem with the parametric third type boundary conditions on the finite interval. The program calculates also potential matrix elements – integrals of the eigenfunctions multiplied by their derivatives with respect to the parameter. Eigenvalues and matrix elements computed by the ODPEVP program can be used for solving the bound state and multi-channel scattering problems for a system of the coupled second-order ordinary differential equations with the help of the KANTBP programs [8,9].

The FEM is applied to construct numerical schemes for solving the corresponding boundary problem for parametric self-adjoined ordinary differential equations with an accuracy of order $O(h^{p+1})$ in grid step h [10,11]. The order of approximation, p, depends on the smoothness of the required solution.

As a benchmark, we present calculation with a given accuracy of eigenvalues, eigenfunctions and their first derivatives with respect to the parameter, corresponding matrix elements for Kantorovich reduction of an integrable 2D-model of three identical particles on a line with the pair zero-range potentials described in [8,12], a 3D-model of a hydrogen atom in a homogeneous magnetic field described in [1,14] and a hydrogen atom on a three-dimensional sphere [15,16]. The numeric results show that the program developed is very efficient and allows to obtain numerical solutions of the above problems with the required accuracy using very little computational resources.

The paper is organized as follows. In Section 2 we give a brief overview of the problem. The construction of the finite-element high-order schemes is discussed in Section 3. A description of the ODPEVP program is given in Section 4. Subroutine units are briefly described in Section 5. Test desk is discussed in Section 6.

2. Statement of the problem

Let us consider a boundary problem for a parametric self-adjoined second order ordinary differential equation

$$L(z;\rho)\psi(z;\rho) = \epsilon(\rho)\psi(z;\rho), \quad z \in [z_{\min}, z_{\max}],$$
$$L(z;\rho) \equiv -\frac{1}{f_1(z)}\frac{d}{dz}f_2(z)\frac{d}{dz} + U(\rho, z), \tag{1}$$

with parametric third type boundary conditions

$$l_1\big(\rho, \mu_1, \lambda_1(\rho), \psi(z;\rho)\big) \equiv \mu_1 f_2(z)\frac{d\psi(z;\rho)}{dz} + \lambda_1(\rho)\psi(z;\rho) = 0, \quad z = z_{\min}, \tag{2}$$

$$l_2\big(\rho, \mu_2, \lambda_2(\rho), \psi(z;\rho)\big) \equiv \mu_2 f_2(z)\frac{d\psi(z;\rho)}{dz} + \lambda_2(\rho)\psi(z;\rho) = 0, \quad z = z_{\max}. \tag{3}$$

Here ρ is a parameter, functions $f_1(z) > 0$, $f_2(z) > 0$ and $U(\rho, z)$ are continuous on finite interval $z \in (z_{\min}, z_{\max})$, and function $f_2(z)$ is differentiable by the variable on finite interval $z \in (z_{\min}, z_{\max})$. Also $U(\rho, z)$, $\lambda_1(\rho)$ and $\lambda_2(\rho)$ are differentiable by parameter ρ. If $\mu_j \lambda_j(\rho) \neq 0$, then $\mu_j = 1$. The normalization condition reads for eigenfunctions $\psi_i(z;\rho)$, $\psi_j(z;\rho)$

$$\int_{z_{\min}}^{z_{\max}} f_1(z)\psi_i(z;\rho)\psi_j(z;\rho)\,dz = \delta_{ij}, \tag{4}$$

where δ_{ij} is the Kronecker symbol, and $\epsilon_1(\rho) < \epsilon_2(\rho) < \cdots$.

The main goal of this paper is to develop an efficient numerical method that will allow one to calculate $\partial\psi_j(z;\rho)/\partial\rho$ with the same accuracy as was achieved for eigenfunctions of the boundary problem (1)–(3) and use it to compute potential matrix elements defined by formula

$$\begin{aligned} Q_{ij}(\rho) &= -\int_{z_{\min}}^{z_{\max}} f_1(z)\psi_i(z;\rho)\frac{\partial\psi_j(z;\rho)}{\partial\rho}\,dz, \\ H_{ij}(\rho) &= \int_{z_{\min}}^{z_{\max}} f_1(z)\frac{\partial\psi_i(z;\rho)}{\partial\rho}\frac{\partial\psi_j(z;\rho)}{\partial\rho}\,dz. \end{aligned} \tag{5}$$

The calculated eigenvalues and potential matrix elements can be used for solving the bound state and multi-channel scattering problems for a system of the coupled second-order ordinary differential equations with the help of the KANTBP programs [8,9].

Taking a derivative of the boundary problem (1)–(3) with respect to parameter ρ, we get that $\partial\psi_j(z;\rho)/\partial\rho$ can be obtained as a solution of the following boundary problem

$$\big(L(z;\rho) - \epsilon_j(\rho)\big)\frac{\partial\psi_j(z;\rho)}{\partial\rho} = -\left(\frac{\partial U(\rho,z)}{\partial\rho} - \frac{\partial\epsilon_j(\rho)}{\partial\rho}\right)\psi_j(z;\rho), \tag{6}$$

$$\frac{\partial l_1(\rho,\mu_1,\lambda_1(\rho),\psi_j(z_{\min};\rho))}{\partial\rho} = 0, \tag{7}$$

$$\frac{\partial l_2(\rho,\mu_2,\lambda_2(\rho),\psi_j(z_{\max};\rho))}{\partial\rho} = 0. \tag{8}$$

Multiplying Eq. (6) from the left by eigenfunction $\psi_i(z;\rho)$ and integrating over the interval $z \in [z_{\min}, z_{\max}]$, we obtain

$$\begin{aligned} \int_{z_{\min}}^{z_{\max}} f_1(z)\psi_i(z;\rho)\big(L(z;\rho) - \epsilon_j(\rho)\big)\frac{\partial\psi_j(z;\rho)}{\partial\rho}\,dz &\equiv \big(\epsilon_i(\rho) - \epsilon_j(\rho)\big)\int_{z_{\min}}^{z_{\max}} f_1(z)\psi_i(z;\rho)\frac{\partial\psi_j(z;\rho)}{\partial\rho}\,dz + f_{ij}(\rho, z_{\min}, z_{\max}) \\ &= -\int_{z_{\min}}^{z_{\max}} f_1(z)\psi_i(z;\rho)\left(\frac{\partial U(\rho,z)}{\partial\rho} - \frac{\partial\epsilon_j(\rho)}{\partial\rho}\right)\psi_j(z;\rho)\,dz, \end{aligned} \tag{9}$$

where

$$f_{ij}(\rho, z_{\min}, z_{\max}) = \begin{cases} \frac{\partial\lambda_2(\rho)}{\partial\rho}\psi_i(z_{\max};\rho)\psi_j(z_{\max};\rho) - \frac{\partial\lambda_1(\rho)}{\partial\rho}\psi_i(z_{\min};\rho)\psi_j(z_{\min};\rho), & \text{if } \mu_1\lambda_1(\rho) \neq 0,\ \mu_2\lambda_2(\rho) \neq 0, \\ \frac{\partial\lambda_2(\rho)}{\partial\rho}\psi_i(z_{\max};\rho)\psi_j(z_{\max};\rho), & \text{if } \mu_1\lambda_1(\rho) = 0,\ \mu_2\lambda_2(\rho) \neq 0, \\ -\frac{\partial\lambda_1(\rho)}{\partial\rho}\psi_i(z_{\min};\rho)\psi_j(z_{\min};\rho), & \text{if } \mu_1\lambda_1(\rho) \neq 0,\ \mu_2\lambda_2(\rho) = 0, \\ 0, & \text{if } \mu_1\lambda_1(\rho) = 0,\ \mu_2\lambda_2(\rho) = 0. \end{cases} \tag{10}$$

From here we find

$$\frac{\partial\epsilon_j(\rho)}{\partial\rho} = \int_{z_{\min}}^{z_{\max}} f_1(z)\psi_j(z;\rho)\frac{\partial U(\rho,z)}{\partial\rho}\psi_j(z;\rho)\,dz + f_{jj}(\rho, z_{\min}, z_{\max}). \tag{11}$$

Now the problem (6)–(8) has a solution, but it is not unique. From the normalization condition (4) we obtain the required additional condition

$$\int_{z_{\min}}^{z_{\max}} f_1(z)\psi_j(z;\rho)\frac{\partial\psi_j(z;\rho)}{\partial\rho}\,dz = 0. \tag{12}$$

Thus, problem (6)–(8) with additional conditions (11), (12) has now a unique solution.

In the most of applications the following formulas

$$\begin{aligned} Q_{ij}(\rho) &= \frac{1}{\epsilon_i(\rho) - \epsilon_j(\rho)}\int_{z_{\min}}^{z_{\max}} f_1(z)\psi_i(z;\rho)\frac{\partial U(\rho,z)}{\partial\rho}\psi_j(z;\rho)\,dz + \frac{f_{ij}(\rho, z_{\min}, z_{\max})}{\epsilon_i(\rho) - \epsilon_j(\rho)}, \quad i \neq j, \\ Q_{ii}(\rho) &= 0, \end{aligned} \tag{13}$$

and

$$H_{ij}(\rho) = -\sum_{l=1} Q_{il}(\rho) Q_{lj}(\rho), \tag{14}$$

are usually used. Note that Eq. (14) has a rather slow convergence which means that in order to get a high level of accuracy one should include a sufficiently large number of terms in a sum over l. This circumstance can present a serious problem from the computational point of view, especially in regard to demands for required computational resources and computation time. An explicit example has been given in paper [15] and can be examined with the help of *Test III* benchmark.

The continuity of eigenfunction $\psi_j(z;\rho)$ with respect to parameter ρ is very important for calculations of the potential matrix elements (5) and their further applications for solution of a system of coupled differential equations as considered in [8]. Hence we required $\psi_j(z;\rho) > 0$ in the vicinity of the right boundary point $z = z_{\max}$.

3. High order approximations of the finite-element method

Let us consider a numerical algorithm for the calculation of the eigenfunctions $\psi(z;\rho)$ and their derivative with respect to the parameter ρ of the parametric boundary problem (1)–(3). Computational schemes of the high order of accuracy are derived from the Rayleigh–Ritz variational functional

$$\mathcal{R}(\psi,\epsilon) = \left\{ \int_{z_{\min}}^{z_{\max}} \left(f_2(z) \left(\frac{d\psi(z;\rho)}{dz} \right)^2 + f_1(z) U(\rho,z) \psi^2(z;\rho) \right) dz + g(\rho, z_{\min}, z_{\max}) \right\} \times \left\{ \int_{z_{\min}}^{z_{\max}} f_1(z) \psi^2(z;\rho)\, dz \right\}^{-1}, \tag{15}$$

on the basis of the FEM. Here

$$g(\rho, z_{\min}, z_{\max}) = \begin{cases} \lambda_2(\rho)\psi(z_{\max};\rho)\psi(z_{\max};\rho) - \lambda_1(\rho)\psi(z_{\min};\rho)\psi(z_{\min};\rho), & \text{if } \mu_1\lambda_1(\rho) \neq 0,\ \mu_2\lambda_2(\rho) \neq 0, \\ \lambda_2(\rho)\psi(z_{\max};\rho)\psi(z_{\max};\rho), & \text{if } \mu_1\lambda_1(\rho) = 0,\ \mu_2\lambda_2(\rho) \neq 0, \\ -\lambda_1(\rho)\psi(z_{\min};\rho)\psi(z_{\min};\rho), & \text{if } \mu_1\lambda_1(\rho) \neq 0,\ \mu_2\lambda_2(\rho) = 0, \\ 0, & \text{if } \mu_1\lambda_1(\rho) = 0,\ \mu_2\lambda_2(\rho) = 0. \end{cases} \tag{16}$$

The general idea of the FEM in one-dimensional space is to divide interval $[z_{\min}, z_{\max}]$ into many small domains called elements. The size of elements can be defined very freely so that physical properties can be taken into account.

The interval $\Delta = [z_{\min}, z_{\max}]$ is covered by a system of n subintervals $\Delta_j = [z_{j-1}, z_j]$ in such a way that $\Delta = \bigcup_{j=1}^{n} \Delta_j$. In each subinterval Δ_j the nodes

$$z_{j,r}^p = z_{j-1} + \frac{h_j}{p} r, \quad h_j = z_j - z_{j-1},\ r = \overline{0,p}, \tag{17}$$

and the Lagrange elements $\{\phi_{j,r}^p(z)\}_{r=0}^p$

$$\phi_{j,r}^p(z) = \prod_{i=0, i\neq r}^{p} \frac{(z - z_{j,i}^p)}{(z_{j,r}^p - z_{j,i}^p)} \tag{18}$$

are determined. By means of the Lagrange elements $\phi_{j,r}^p(z)$, we define a set of local functions $N_l(z)$ as follows:

$$N_l^p(z) = \begin{cases} \begin{cases} \phi_{1,0}^p(z), & z \in \Delta_1, \\ 0, & z \notin \Delta_1, \end{cases} & l = 0, \\ \begin{cases} \phi_{j,r}^p(z), & z \in \Delta_j, \\ 0, & z \notin \Delta_j, \end{cases} & l = r + p(j-1),\ r = \overline{1,p-1}, \\ \begin{cases} \phi_{j,p}^p(z), & z \in \Delta_j, \\ \phi_{j+1,0}^p(z), & z \in \Delta_{j+1}, \\ 0, & z \notin \Delta_j \cup \Delta_{j+1}, \end{cases} & l = jp,\ j = \overline{1,n-1}, \\ \begin{cases} \phi_{n,p}^p(z), & z \in \Delta_n, \\ 0, & z \notin \Delta_n, \end{cases} & l = np. \end{cases} \tag{19}$$

The functions $\{N_l^p(z)\}_{l=0}^L$, $L = np$, form a basis in the space of polynomials of the pth order. Now, each function $\psi(z;\rho)$ is approximated by a finite sum of local functions $N_l^p(z)$

$$\psi(z;\rho) = \sum_{l=0}^{L} \psi^l\left(z_{j,r}^p, \rho\right) N_l^p(z). \tag{20}$$

After substituting expansion (20) into the variational functional (15) and minimizing it [10,11] we obtain the generalized eigenvalue problem

$$\mathbf{A}^p \boldsymbol{\psi}^h = \epsilon^h \mathbf{B}^p \boldsymbol{\psi}^h, \qquad \mathbf{A}^p = \hat{\mathbf{A}}^p + \mathbf{M}. \tag{21}$$

Here $\mathbf{A}^p$ is the stiffness matrix; $\mathbf{B}^p$ is the mass matrix and positive definite; $\mathbf{M}$ is the diagonal matrix with zero elements, except the first and last elements that are equal $\lambda_2(\rho)$ (or zero) and $-\lambda_1(\rho)$ (or zero), respectively; $\boldsymbol{\psi}^h$ is the vector approximating solution on the finite-element grid; and ϵ^h is the corresponding eigenvalue. The matrices $\hat{\mathbf{A}}^p$ and $\mathbf{B}^p$ have the following form

$$\hat{\mathbf{A}}^p = \sum_{j=1}^{n} \mathbf{a}_j^p, \qquad \mathbf{B}^p = \sum_{j=1}^{n} \mathbf{b}_j^p, \tag{22}$$

where the local matrices $\mathbf{a}_j^p$ and $\mathbf{b}_j^p$ are calculated as

$$\begin{aligned}
\left(\mathbf{a}_j^p\right)^{qr} &= \int_{-1}^{+1} \left\{ f_2(z) \frac{4}{h_j^2} \frac{d\phi_{j,q}^p(z)}{dz} \frac{d\phi_{j,r}^p(z)}{dz} + f_1(z) U(\rho, z) \phi_{j,q}^p(z) \phi_{j,r}^p(z) \right\} \frac{h_j}{2}\, d\eta, \\
\left(\mathbf{b}_j^p\right)^{qr} &= \int_{-1}^{+1} f_1(z) \phi_{j,q}^p(z) \phi_{j,r}^p(z) \frac{h_j}{2}\, d\eta, \\
z &= z_{j-1} + 0.5 h_j (1+\eta), \quad q, r = \overline{0, p}.
\end{aligned} \tag{23}$$

Integrals (23) are evaluated using the Gaussian quadrature formulae

$$\begin{aligned}
\left(\mathbf{a}_j^p\right)^{qr} &= \sum_{g=0}^{p} \left\{ f_2(z_g) \frac{4}{h_j^2} \frac{d\phi_{j,q}^p(z_g)}{dz} \frac{d\phi_{j,r}^p(z_g)}{dz} + f_1(z_g) U(\rho, z_g) \phi_{j,q}^p(z_g) \phi_{j,r}^p(z_g) \right\} \frac{h_j}{2} w_g, \\
\left(\mathbf{b}_j^p\right)^{qr} &= \sum_{g=0}^{p} f_1(z_g) \phi_{j,q}^p(z_g) \phi_{j,r}^p(z_g) \frac{h_j}{2} w_g,
\end{aligned} \tag{24}$$

where $z_g = z_{j-1} + 0.5 h_j (1+\eta_g)$, η_g and w_g, $g = \overline{0, p}$ are the Gaussian nodes and weights.

Let $\epsilon_j(\rho)$, $\psi_j(z;\rho) \in \mathcal{H}^2$ are the exact solution of (1)–(3) and ϵ_j^h, $\boldsymbol{\psi}_j^h \in \mathcal{H}^1$ are the numerical solution of (21). Then for $U(\rho, z) > 0$, $\lambda_1(\rho) \leqslant 0$ and $\lambda_2(\rho) \geqslant 0$ the following estimates are valid [10]

$$\left|\epsilon_j(\rho) - \epsilon_j^h\right| \leqslant c_1 h^{2p}, \quad \left\|\psi_j(z;\rho) - \boldsymbol{\psi}_j^h\right\|_0 \leqslant c_2 h^{p+1}, \quad c_1 > 0,\ c_2 > 0, \tag{25}$$

where $\|v(z;\rho)\|_0^2 = \int_{z_{\min}}^{z_{\max}} f_1(z) v^2(z;\rho)\, dz$, h the maximal step of the finite-element grid, p is the order of finite elements, j is the number of the corresponding eigensolution, and constants c_1 and c_2 do not depend on step h. It is necessary to mention that the second estimate of Eq. (25) is valid also for solution $\partial\psi_j(z;\rho)/\partial\rho$ of problem (6)–(8), (12). This fact guarantees the same accuracy for eigenfunctions and their derivatives within the present method.

In order to solve the generalized eigenvalue problem (21), the subspace iteration method [10,11] elaborated by Bathe [11] for the solution of large symmetric banded matrix eigenvalue problems has been chosen. This method uses a skyline storage mode, which stores components of the matrix column vectors within the banded region of the matrix, and is ideally suited for banded finite element matrices. The procedure chooses a vector subspace of the full solution space and iterates upon the successive solutions in the subspace (for details, see [11]). The iterations continue until the desired set of solutions in the iteration subspace converges to within the specified tolerance on the Rayleigh quotients for the eigenpairs. If matrix $\mathbf{A}^p$ in Eq. (21) is not positively defined, problem (21) is replaced by the following problem:

$$\tilde{\mathbf{A}}^p \boldsymbol{\phi}^h = \tilde{\epsilon}^h \mathbf{B}^p \boldsymbol{\phi}^h, \qquad \tilde{\mathbf{A}}^p = \mathbf{A}^p - \alpha \mathbf{B}^p. \tag{26}$$

The number α (the shift of the energy spectrum) is chosen in such a way that matrix $\tilde{\mathbf{A}}^p$ is positive. The eigenvector of problem (21) is the same, and $\epsilon^h = \tilde{\epsilon}^h + \alpha$.

3.1. Calculations of parametric derivative of the eigenfunctions, and matrix elements

The boundary problem (6)–(8) is reduced to the linear system of inhomogeneous algebraic equations

$$\mathbf{L} \frac{\partial \boldsymbol{\psi}^h}{\partial \rho} \equiv \left(\mathbf{A}^p - \epsilon^h \mathbf{B}^p\right) \frac{\partial \boldsymbol{\psi}^h}{\partial \rho} = b, \qquad b = -\left(\frac{\partial \mathbf{A}^p}{\partial \rho} - \frac{\partial \epsilon^h}{\partial \rho} \mathbf{B}^p \right) \boldsymbol{\psi}^h. \tag{27}$$

The normalization, orthogonalization and additional conditions are read as

$$\left(\boldsymbol{\psi}^h\right)^T \mathbf{B}^p \boldsymbol{\psi}^h = 1, \qquad \left(\frac{\partial \boldsymbol{\psi}^h}{\partial \rho} \right)^T \mathbf{B}^p \boldsymbol{\psi}^h = 0, \qquad \frac{\partial \epsilon^h}{\partial \rho} = \left(\boldsymbol{\psi}^h\right)^T \frac{\partial \mathbf{A}^p}{\partial \rho} \boldsymbol{\psi}^h. \tag{28}$$

From here, potential matrix elements Q_{ij}^h and H_{ij}^h have the form

$$Q_{ij}^h = -\left(\boldsymbol{\psi}_i^h\right)^T \mathbf{B}^p \frac{\partial \boldsymbol{\psi}_j^h}{\partial \rho}, \qquad H_{ij}^h = \left(\frac{\partial \boldsymbol{\psi}_i^h}{\partial \rho} \right)^T \mathbf{B}^p \frac{\partial \boldsymbol{\psi}_j^h}{\partial \rho}. \tag{29}$$

Since ϵ^h is an eigenvalue of (21), matrix $\mathbf{L}$ in Eq. (27) is degenerate. In this case the algorithm for solving Eq. (27) can be written in three steps as follows:

Step k1. Calculate solutions $\mathbf{v}$ and $\mathbf{w}$ of the auxiliary inhomogeneous systems of algebraic equations

$$\bar{\mathbf{L}}\mathbf{v} = \bar{\mathbf{b}}, \qquad \bar{\mathbf{L}}\mathbf{w} = \mathbf{d}, \tag{30}$$

with non-degenerate matrix $\bar{\mathbf{L}}$ and right-hand sides $\bar{\mathbf{b}}$ and $\mathbf{d}$

$$\bar{L}_{ss'} = \begin{cases} L_{ss'}, & (s-S)(s'-S) \neq 0, \\ \delta_{ss'}, & (s-S)(s'-S) = 0, \end{cases}$$
$$\bar{b}_s = \begin{cases} b_s, & s \neq S, \\ 0, & s = S, \end{cases} \qquad d_s = \begin{cases} L_{sS}, & s \neq S, \\ 0, & s = S, \end{cases} \tag{31}$$

where S is the number of the greatest absolute value element of vector $\mathbf{B}^p\boldsymbol{\psi}^h$.

Step k2. Evaluate coefficient γ

$$\gamma = -\frac{\gamma_1}{(\mathbf{D}_S - \gamma_2)}, \qquad \gamma_1 = \mathbf{v}^T\mathbf{B}^p\boldsymbol{\psi}^h, \qquad \gamma_2 = \mathbf{w}^T\mathbf{B}^p\boldsymbol{\psi}^h, \qquad \mathbf{D}_S = \left(\mathbf{B}^p\boldsymbol{\psi}^h\right)_S. \tag{32}$$

Step k3. Evaluate vector $\partial\boldsymbol{\psi}^h/\partial\rho$

$$\frac{\partial\psi_s^h}{\partial\rho} = \begin{cases} v_s - \gamma w_s, & s \neq S, \\ \gamma, & s = S. \end{cases} \tag{33}$$

From the consideration above it is evident, that the derivative computed has the same accuracy as the calculated eigenfunction.

Theorem. *Let $L(z;\rho)$ from (1) is bounded positively defined operator on space $\mathcal{H}^1$ with energy norm, and $\lambda_1(\rho) \leqslant 0$, $\lambda_2(\rho) \geqslant 0$. Also $\partial U(\rho,z)/\partial\rho$, $\partial\lambda_1(\rho)/\partial\rho$ and $\partial\lambda_2(\rho)/\partial\rho$ are bounded in each value of the real parameter ρ. Then for exact values of solutions, $\partial\epsilon_j(\rho)/\partial\rho$, $\partial\psi_j(z;\rho)/\partial\rho \in \mathcal{H}^2$, from (6)–(8), (11), (12) and potential matrix elements, $Q_{ij}(\rho)$, $H_{ij}(\rho)$, from (5), and corresponded numerical values, $\partial\epsilon_j^h/\partial\rho$, $\partial\boldsymbol{\psi}_j^h/\partial\rho \in \mathcal{H}^1$, from (27), (28) and Q_{ij}^h, H_{ij}^h, from (29) the following estimates are valid*:

$$\left|\frac{\partial\epsilon_j(\rho)}{\partial\rho} - \frac{\partial\epsilon_j^h}{\partial\rho}\right| \leqslant c_3h^{2p}, \qquad \left\|\frac{\partial\psi_j(z;\rho)}{\partial\rho} - \frac{\partial\boldsymbol{\psi}_j^h}{\partial\rho}\right\|_0 \leqslant c_4h^{p+1}, \qquad \left|Q_{ij}(\rho) - Q_{ij}^h\right| \leqslant c_5h^{2p}, \qquad \left|H_{ij}(\rho) - H_{ij}^h\right| \leqslant c_6h^{2p},$$

where h the maximal step of the finite-element grid; p is the order of finite elements; i, j are the number of the corresponding solutions; and constants c_3, c_4, c_5 and c_6 do not depend on step h.

Proof is straightforward following the scheme of proof of estimations (25) in accordance with [10].

3.2. Finding the lower bound for the lowest eigenvalue of the generalized eigenvalue problem

In general case it is impossible to define the lower bound for the lowest eigenvalue of Eq. (21), because the lowest eigenvalue $\epsilon_1(\rho)$ is depended on the parameter ρ. But, we can use the following algorithm to find the lower bound for the lowest eigenvalue $\epsilon_1(\rho)$:

Step 1. Calculate $\mathbf{LDL}^{\mathrm{T}}$ factorization of $\mathbf{A}^p - \alpha\mathbf{B}^p$.
Step 2. If some elements of the diagonal matrix $\mathbf{D}$ are less than zero then put $\alpha = \alpha - 1$ and go to **Step 3**, else go to **Step 5**.
Step 3. Calculate $\mathbf{LDL}^{\mathrm{T}}$ factorization of $\mathbf{A}^p - \alpha\mathbf{B}^p$.
Step 4. If some elements of the diagonal matrix $\mathbf{D}$ are less than zero then put $\alpha = \alpha - 1$ and go to **Step 3**, else put $\alpha = \alpha - 0.5$ and go to **Step 8**.
Step 5. Put $\alpha = \alpha + 1$ and calculate $\mathbf{LDL}^{\mathrm{T}}$ factorization of $\mathbf{A}^p - \alpha\mathbf{B}^p$.
Step 6. If all elements of the diagonal matrix $\mathbf{D}$ are greater than zero then put $\alpha = \alpha + 1$ and repeat **Step 5**.
Step 7. Put $\alpha = \alpha - 1.5$.
Step 8. End.

After using the above algorithm one should find the lower bound for the lowest eigenvalue, and always $\epsilon_1(\rho) - \alpha \leqslant 1.5$.

4. Description of the program

Fig. 1 presents a flow diagram for the ODPEVP program. The function of each subroutine is described in Section 5. The ODPEVP program is called from the main routine (supplied by a user) which sets dimensions of the arrays and is responsible for the input data. In the present code each array declarator is written in terms of the symbolic names of constants. These constants are defined in the following PARAMETER statement in the main routine:

```
PARAMETER (MTOT=800000,MITOT=500000,NMESH1=5,NROOT1=6)
```

where

- MTOT is the dimension of the working DOUBLE PRECISION array TOT.
- MITOT is the dimension of the working INTEGER array ITOT.

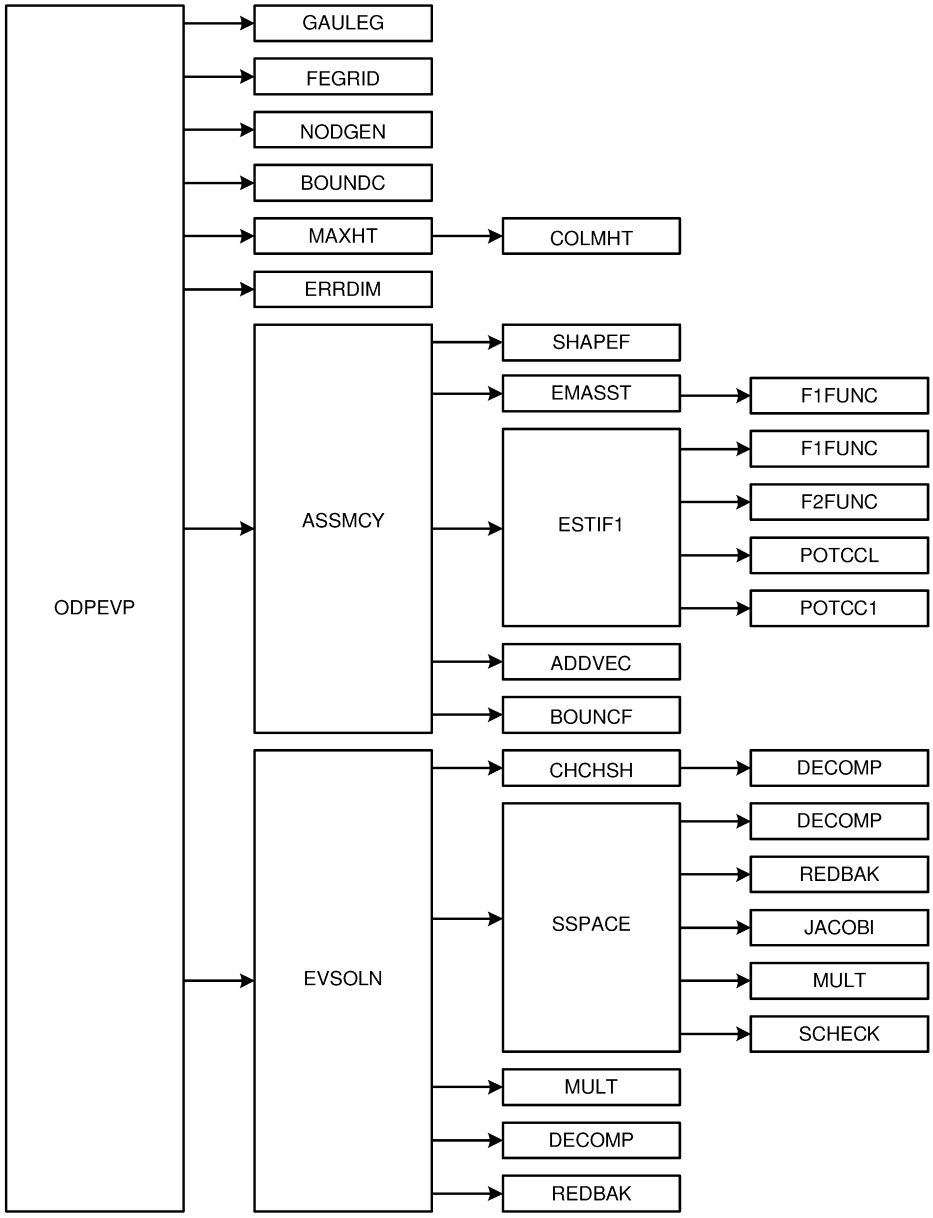

Fig. 1. Flow diagram of the ODPEVP program.

- NMESH1 is the dimension of the DOUBLE PRECISION array RMESH containing the information about the subdivision of the interval $[z_{\min}, z_{\max}]$ on subintervals and the number of elements on each one of them. NMESH1 is always odd and $\geqslant 3$.
- NROOT1 is the number of eigenvalues and eigenvectors required, and also the dimension of the DOUBLE PRECISION arrays HH, QQ, EIGV.

A more concrete assignment of these dimensions is discussed below. In order to change the dimensions in the code, all one has to do is to modify the single PARAMETER statement defined above in the main program unit.

The calling sequence for the subroutine ODPEVP is:

```
 CALL ODPEVP(TITLE,PARAM,HH,QQ,EIGV,NROOT,NPOL,RTOL,NITEM,
1            SHIFT,ICHK,IPRINT,IPRSTP,NMESH,RMESH,IBOUND,
2            FNOUT,IOUT,FMATR,IOUM,EVWFN,IOUF,TOT,ITOT,MTOT,
3            MITOT)
```

where the arguments have the following type and meaning:

- POTCCL is the name of the user-supplied DOUBLE PRECISION function which calculates the potential function $U(\rho, z)$ (PARAM $= \rho$, RG $= z$) and should be written as follows:

```
      FUNCTION POTCCL(PARAM,RG)
C . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
C .                                                           .
C .   P R O G R A M                                         .
C .                 TO CALCULATE THE PARAMETRIC POTENTIAL     .
C .                 FUNCTION AT POINTS RG AND PARAM           .
C .                                                           .
C . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
      IMPLICIT REAL*8 (A-H,O-Z)
      RETURN
      END
```

- POTCC1 is the name of the user-supplied DOUBLE PRECISION function which calculates first derivative of the potential function $U(\rho, z)$ with respect to the parameter ρ (PARAM $= \rho$, RG $= z$) and should be written as follows:

```
      FUNCTION POTCC1(PARAM,RG)
C . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
C .                                                           .
C .   P R O G R A M                                         .
C .                 TO CALCULATE FIRST DERIVATIVE OF PARAMETRIC  .
C                   POTENTIAL FUNCTION WITH RESPECT TO PARAMETER .
C .                 AT POINTS RG AND PARAM                    .
C .                                                           .
C . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
      IMPLICIT REAL*8 (A-H,O-Z)
      RETURN
      END
```

- F1FUNC is the name of the user-supplied DOUBLE PRECISION function which calculates the function $f_1(z)$ (RG $= z$) and should be written as follows:

```
      FUNCTION F1FUNC(RG)
C . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
C .                                                           .
C .   P R O G R A M                                         .
C .                 TO CALCULATE FUNCTION F1 AT POINT RG      .
C .                                                           .
C . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
      IMPLICIT REAL*8 (A-H,O-Z)
      RETURN
      END
```

- F2FUNC is the name of the user-supplied DOUBLE PRECISION function which calculates the function $f_2(z)$ (RG $= z$) and should be written as follows:

```
      FUNCTION F2FUNC(RG)
C . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
C .                                                           .
C .   P R O G R A M                                         .
C .                 TO CALCULATE FUNCTION F2 AT POINT RG      .
C .                                                           .
C . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
      IMPLICIT REAL*8 (A-H,O-Z)
      RETURN
      END
```

- BOUNCF is the name of the user-supplied subroutine which calculates the values $\lambda_1(\rho)$, $\lambda_2(\rho)$ and their first derivatives with respect to the parameter ρ (PARAM $= \rho$, DLMMN0 $= \lambda_1(\rho)$, DLMMX0 $= \lambda_2(\rho)$, DLMMN1 $= \partial\lambda_1(\rho)/\partial\rho$, DLMMX1 $= \partial\lambda_2(\rho)/\partial\rho$) and should be written as follows:

```
      SUBROUTINE BOUNCF(PARAM,DLMMN0,DLMMX0,DLMMN1,DLMMX1)
C . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
C .                                                           .
C .   P R O G R A M                                         .
C .                 TO CALCULATE DLMMN0, DLMMX0 AND THEIR     .
C .                 FIRST DERIVATIVES WITH RESPECT TO PARAMETER  .
C .                                                           .
C . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . .
      IMPLICIT REAL*8 (A-H,O-Z)
      RETURN
      END
```

The parameters PARAM, RG have the same meaning as described below and should not be changed by subroutine BOUNCF, and functions POTCCL, POTCC1, F1FUNC, F2FUNC.

Input data

TITLE	CHARACTER	title of the run to be printed on the output listing. The title should be no longer than 70 characters.
PARAM	REAL*8	value of the parameter ρ.
HH	REAL*8	array HH of dimension NROOT × NROOT containing values of the potential matrix $\mathbf{H}(\rho)$.
QQ	REAL*8	array QQ of dimension NROOT × NROOT containing values of the potential matrix $\mathbf{Q}(\rho)$.
EIGV	REAL*8	array EIGV of dimension NROOT containing values of the calculated eigenvalues $\epsilon_j(\rho)$.
NROOT	INTEGER	number of eigenvalues and eigenvectors required.
NPOL	INTEGER	order of finite-element shape functions (interpolating Lagrange polynomials). Usually set to 6.
RTOL	REAL*8	convergence tolerance on eigenvalues (1.D–06 or smaller).
NITEM	INTEGER	maximum number of iterations permitted (usually set to 16).
SHIFT	REAL*8	contains the lower bound of lowest eigenvalue.
ICHK	INTEGER	key parameter. If ICHK $\neq 0$ the SHIFT is determined automatically by the program with help of the algorithm 3.2.
IPRINT	INTEGER	level of print: = 0 – minimal level of print. The initial data, short information about the numerical scheme parameters, main flags and keys, and eigenvalues calculated are printed out; = 1 – eigenfunctions calculated are printed out with step IPRSTP additionally; = 2 – information about nodal point distribution is printed out; = 3 – global matrices $\mathbf{A}^p$ and $\mathbf{B}^p$ are printed out additionally; = 4 – the highest level of print. The local stiffness and mass matrices together with all current information about the course of the subspace iteration method solution of the generalized eigenvalue problem are printed out.
IPRSTP	INTEGER	step with which eigenfunctions are printed out.
NMESH	INTEGER	dimension of array RMESH. NMESH always should be odd and $\geqslant 3$.
RMESH	REAL*8	array RMESH contains information about subdivision of interval $[z_{\min}, z_{\max}]$ of variable z on subintervals. The whole interval $[z_{\min}, z_{\max}]$ is divided as follows: RMESH(1) $= z_{\min}$, RMESH(NMESH) $= z_{\max}$, and the values of RMESH(I) set the number of elements for each subinterval [RMESH(I-1), RMESH(I+1)], where I = 2, 4, …, NMESH - 1.
IBOUND	INTEGER	parameter defining the type of boundary conditions set in the boundary points $z = z_{\min}$ and $z = z_{\max}$: = 1 – the Dirichlet–Dirichlet boundary conditions: $\psi(z_{\min};\rho) = 0$, $\psi(z_{\max};\rho) = 0$; = 2 – the Dirichlet–Neumann boundary conditions: $\psi(z_{\min};\rho) = 0$, $\lim_{z\to z_{\max}} f_2(z)\frac{d\psi(z;\rho)}{dz} = 0$; = 3 – the Neumann–Dirichlet boundary conditions: $\lim_{z\to z_{\min}} f_2(z)\frac{d\psi(z;\rho)}{dz} = 0$, $\psi(z_{\max};\rho) = 0$; = 4 – the Neumann–Neumann boundary conditions: $\lim_{z\to z_{\min}} f_2(z)\frac{d\psi(z;\rho)}{dz} = 0$, $\lim_{z\to z_{\max}} f_2(z)\frac{d\psi(z;\rho)}{dz} = 0$. If $\mu_1\lambda_1(\rho) \neq 0$ the value of IBOUND equals 3 or 4. If $\mu_2\lambda_2(\rho) \neq 0$ the value of IBOUND equals 2 or 4.
FNOUT	CHARACTER	name of the output file (up to 55 characters) for printing out the results of the calculation. It is system specific and may include a complete path to the file location.
IOUT	INTEGER	number of the output logical device for printing out the results of the calculation (usually set to 7).
FMATR	CHARACTER	name of the scratch file (up to 55 characters) for storing calculated matrices.
IOUM	INTEGER	number of the logical device for storing calculated matrices.
EVWFN	CHARACTER	name of the output file (up to 55 characters) for storing the results of the calculation, namely, the eigenvalues and eigenfunctions, their first derivatives with respect to the parameter, and finite-element grid points. It is used only if IOUF > 0.
IOUF	INTEGER	number of the logical device for storing data into file EVWFN.
TOT	REAL*8	working vector of the DOUBLE PRECISION type.
ITOT	INTEGER	working vector of the INTEGER type.
MTOT	INTEGER	dimension of the DOUBLE PRECISION working array ITOT. The last address ILAST of array TOT is calculated and then compared with the given value of MTOT. If ILAST > MTOT the message about an error is printed and the execution of the program is aborted. In the last case, in order to carry out the required calculation it is necessary to increase the dimension MTOT of array TOT to the quantity ILAST taken from the message.
MITOT	INTEGER	dimension of the INTEGER working array ITOT. The last address ILAST of array ITOT is calculated and then compared with the given value of MITOT. If ILAST > MITOT the message about an error is printed and the execution of the program is aborted. In the last case, in order to carry out the required calculation it is necessary to increase the dimension MITOT of array ITOT to the quantity ILAST taken from the message.

Output data

The results of the calculation of eigenvalues and eigenfunctions are written using unformatted segmented records into file EVWFN, according to the following operator:

```
      WRITE(IOUF) NN,NROOT,NGRID,(EIGV(I),I=1,NROOT),
     1                           (BUP(I),I=1,NROOT),
     2                           (XGRID(I),I=1,NGRID),
     3                           ((R(I,J),I=1,NN),J=1,NROOT),
     4                           ((DR(I,J),I=1,NN),J=1,NROOT)
```

In the above, parameters presented in the WRITE statement have the following meaning:

- NGRID is the number of finite-element grid points.
- NN is the number of nodes of eigenfunctions.
- NROOT is the number of eigenvalues.
- Arrays EIGV and BUP contain the eigenvalues calculated and their first derivative with respect to the parameter ρ.
- Array XGRID contains the values of the finite-element grid points.
- Arrays R and DR contain NROOT eigenfunctions each per NN elements and their first derivative with respect to parameter ρ.

5. Description of subprogram units

A flow diagram for the ODPEVP program is presented in Fig. 1. The function of each subroutine is briefly described below. Additional details may be found in COMMENT cards within the program.

- Subroutine ADDVEC [8] assembles the element stiffness and mass matrices and the first derivative of stiffness matrix with respect to parameter ρ into the corresponding global vector using a compact storage form.
- Subroutine ASSMCY controls the calculation of element stiffness and mass matrices, the first derivative of stiffness matrix with respect to parameter ρ, and assembles them into the corresponding global matrices.
- User-supplied subroutine BOUNCF calculates $\lambda_1(\rho)$, $\lambda_2(\rho)$ and their first derivatives with respect to the parameter ρ.
- Subroutine BOUNDC [8] sets the Dirichlet or Neumann boundary conditions.
- Subroutine COLMHT [8] calculates column heights in banded matrix.
- Subroutine CHCHSH calculates the lower bound of lowest eigenvalue.
- Subroutine DECOMP [11] calculates $\mathbf{LDL}^{\mathrm{T}}$ factorization of stiffness matrix. This factorization is used in subroutine REDBAK [11] to reduce and back-substitute the iteration vectors.
- Subroutine EMASST calculates an element mass matrix.
- Subroutine ERRDIM prints error messages when high-speed storage requested by a user is exceeded and stops the execution of program ODPEVP.
- Subroutine ESTIF1 calculates the local on element stiffness matrix and its first derivative with respect to the parameter ρ.
- Subroutine EVSOLN prepares all input data for the SSPACE program, prints out the calculated eigenfunctions and first derivative with respect to the parameter ρ, and writes them into the file EVWFN, if necessary. Also calculates the potential matrices $\mathbf{H}(\rho)$ and $\mathbf{Q}(\rho)$.
- User-supplied DOUBLE PRECISION function F1FUNC calculates the function $f_1(z)$.
- User-supplied DOUBLE PRECISION function F2FUNC calculates the function $f_2(z)$.
- Subroutine FEGRID [8] calculates nodal points for the finite-element grid.
- Subroutine GAULEG [17] calculates nodes and weights of the Gauss–Legendre quadrature.
- Subroutine GAUSSJ [17] calculates linear equation solution by the Gauss–Jordan matrix inversion method.
- Subroutine JACOBI [11] solves the generalized eigenproblem in subspace using the generalized Jacobi iteration.
- Subroutine MAXHT [8] calculates addresses of diagonal elements in banded matrix.
- Subroutine MULT [11] evaluates a product of the two vectors stored in compact form.
- Subroutine NODGEN [8] generates a nodal point distribution for the finite-element grid.
- User-supplied DOUBLE PRECISION function POTCCL calculates the potential function $U(\rho, z)$.
- User-supplied DOUBLE PRECISION function POTCC1 calculates the first derivative of potential function $U(\rho, z)$ with respect to parameter ρ.
- Subroutine SCHECK [11] evaluates shift for Sturm sequence check (called only if SHIFT $= 0$).
- Subroutine SHAPEF [8] calculates shape functions of the given order and their derivatives with respect to the master element coordinate η at a specified value of z.
- Subroutine SSPACE [11] finds the smallest eigenvalues and the corresponding eigenvectors in the generalized eigenproblem using the subspace iteration method [11]. We have added to this program the possibility of finding the eigensolutions closest to the energy spectrum shift given and also the possibility of using the previously calculated eigenvectors as the starting vectors for inverse iterations. The list of arguments for this program is adequately commented in the routine; so, the interested reader is referred to the program listing for further details. Warning messages will be issued if the requested accuracy RTOL is not obtained after NITEM iterations or if the stiffness matrix $\mathbf{A}^p$ is not positively defined.

6. Test deck

6.1. Test I

We consider a boundary problem for the angular oblate spheroidal functions [18] with respect to a variable $-1 < \eta = \cos\theta < 1$ in the form [1,14]:

$$-\frac{d}{d\eta}\left(1-\eta^2\right)\frac{d\Phi_j(\eta;r)}{\partial\eta}+\left(\frac{m^2}{1-\eta^2}+\frac{\gamma^2 r^4}{4}\left(1-\eta^2\right)\right)\Phi_j(\eta;r)=\lambda_j(r)\Phi_j(\eta;r), \tag{34}$$

with boundary conditions

$$\begin{aligned}&\lim_{\eta\to\pm1}\left(1-\eta^2\right)\frac{d\Phi_j(\eta;r)}{d\eta}=0, \quad \text{if } m=0, \quad \text{and}\\ &\Phi_j(\pm1;r)=0, \quad \text{if } m\neq 0,\end{aligned} \tag{35}$$

where $m = 0, \pm 1, \ldots$ is the magnetic quantum number, $\gamma = B/B_0$, $B_0 \cong 2.35 \times 10^5$ T is a dimensionless parameter which determines the field strength B. The boundary problem (34), (35) has even and odd eigenfunctions.

We test only the even eigenfunctions with boundary conditions in variable $0 \leqslant \eta \leqslant 1$ at $m = 0$ and $\gamma = 1$

$$\left.\frac{d\Phi_j(\eta; r)}{d\eta}\right|_{\eta=0} = 0, \qquad \lim_{\eta\to 1}\left(1-\eta^2\right)\frac{d\Phi_j(\eta; r)}{d\eta} = 0. \tag{36}$$

Here $\lambda_1(\rho) = \lambda_2(\rho) = 0$.

The following values of numerical parameters and characters have been used in the test run via the supplied input file MAGNET.INP

```
&PARAMS TITLE='  PARAMETRIC DIFFERENTIAL EQUATION I    ',
        PARAM=11.51962D0,NROOT=6,NPOL=4,RTOL=1.D-13,NITEM=100,
        SHIFT=-10.D0,ICHK=1,IPRINT=2,IPRSTP=400,IBOUND=4,
        NMESH=3,RMESH=0.D0,400.D0,1.D0,
        FNOUT='MAGNET.LPR',IOUT=7,FMATR='MAGNET.MAT',IOUM=11,
        EVWFN='MAGNET.WFN',IOUF=0
&END
```

Remark. To compare calculated potential matrix elements $\mathbf{H}(\rho)$, $\mathbf{Q}(\rho)$ with the results in [14] the user should recalculate diagonal matrix elements $H_{ii}(\rho)$ by the formula

$$H_{ii}(\rho) = H_{ii}(\rho) + \frac{\epsilon_i(\rho)}{\rho^2} - \frac{2}{\rho}. \tag{37}$$

6.2. Test II

We consider a boundary problem

$$-\frac{\partial^2\psi_j(\theta; \rho)}{\partial\theta^2} = \epsilon_j(\rho)\psi_j(\theta; \rho), \tag{38}$$

with boundary conditions in angular variable $-\pi/6 \leqslant \theta \leqslant \pi/6$

$$\frac{\partial\psi_j(\theta; \rho)}{\partial\theta} - \rho c\bar{\kappa}\psi_j(\theta; \rho) = 0, \quad \theta = -\frac{\pi}{6}, \tag{39}$$

$$\frac{\partial\psi_j(\theta; \rho)}{\partial\theta} + \rho c\bar{\kappa}\psi_j(\theta; \rho) = 0, \quad \theta = \frac{\pi}{6}. \tag{40}$$

The boundary problem (38)–(40) has exact even and odd eigenfunctions, and also analytical potential matrix elements $\mathbf{H}(\rho)$, $\mathbf{Q}(\rho)$ [8,12, 13].

We test only even eigenfunctions with the boundary conditions in angular variable $-\pi/6 \leqslant \theta \leqslant 0$ at $c = -1$ and $\bar{\kappa} = \pi/6$

$$\frac{\partial\psi_j(\theta; \rho)}{\partial\theta} - \rho c\bar{\kappa}\psi_j(\theta; \rho) = 0, \quad \theta = -\frac{\pi}{6}, \tag{41}$$

$$\frac{\partial\psi_j(\theta; \rho)}{\partial\theta} = 0, \quad \theta = 0. \tag{42}$$

Here $\lambda_1(\rho) = -\rho c\bar{\kappa}$ and $\lambda_2(\rho) = 0$.

The following values of numerical parameters and characters have been used in the test run via the supplied input file 3DELTA.INP

```
&PARAMS TITLE='  PARAMETRIC DIFFERENTIAL EQUATION II   ',
        PARAM=2.00469D0,NROOT=6,NPOL=4,RTOL=1.D-13,NITEM=100,
        SHIFT=-10.D0,ICHK=1,IPRINT=2,IPRSTP=400,IBOUND=4,
        NMESH=3,RMESH=-0.5235987755982989D0,800.D0,0.D0,
        FNOUT='3DELTA.LPR',IOUT=8,FMATR='3DELTA.MAT',IOUM=12,
        EVWFN='3DELTA.WFN',IOUF=0
&END
```

Remark. To compare calculated potential matrix elements $\mathbf{H}(\rho)$, $\mathbf{Q}(\rho)$ with results in [8] the user should recalculate diagonal matrix elements $H_{ii}(\rho)$ by the formula

$$H_{ii}(\rho) = H_{ii}(\rho) + \frac{\epsilon_i(\rho)}{\rho^2}. \tag{43}$$

6.3. Test III

Consider the following eigenvalue problem of hydrogen atom on a three-dimensional sphere

$$\left(-\frac{1}{\sin^2(\alpha)}\frac{d}{d\alpha}\sin^2(\alpha)\frac{d}{d\alpha} - 2r\cot(\alpha)\right)\psi(\alpha; r) = E(r)\psi(\alpha; r), \tag{44}$$

$$\lim_{\alpha\to 0}\sin^2(\alpha)\frac{d\psi(\alpha; r)}{d\alpha} = 0, \qquad \lim_{\alpha\to\pi}\sin^2(\alpha)\frac{d\psi(\alpha; r)}{d\alpha} = 0. \tag{45}$$

Problem (44) has an analytical solution

$$E_n(r) = -r^2\left(\frac{1}{n^2} - \frac{n^2-1}{r^2}\right), \quad n = 1, 2, \ldots \tag{46}$$

with eigenfunctions $\psi_n(\alpha; r)$ which are the radial functions of a hydrogen atom on a three-dimensional sphere [15,16]

$$\psi_n(\alpha, r) = C_n(r)\,\mathrm{Re}\left\{\exp\left(-\imath\alpha(n-1-\imath\sigma)\right){}_2F_1\left(-n+1, 1+\imath\sigma, 2, 1-\exp(2\imath\alpha)\right)\right\},$$
$$C_n(r) = \frac{2\sqrt{\sigma(n^2+\sigma^2)}}{\sqrt{1-\exp(-2\pi\sigma)}}, \quad \sigma = \frac{r}{n}, \tag{47}$$

where ${}_2F_1$ is a full hypergeometric function [18].

The following values of numerical parameters and characters have been used in the test run via the supplied input file HYDRON.INP

```
&PARAMS TITLE='  PARAMETRIC DIFFERENTIAL EQUATION III ',
        PARAM=8.D0,NROOT=6,NPOL=4,RTOL=1.D-13,NITEM=100,
        SHIFT=-10.D0,ICHK=1,IPRINT=2,IPRSTP=400,IBOUND=4,
        NMESH=3,RMESH=0.D0,400.D0,3.141592653589793D0,
        FNOUT='ABRASH.LPR',IOUT=7,FMATR='ABRASH.MAT',IOUM=11,
        EVWFN='ABRASH.WFN',IOUF=0
&END
```


Acknowledgements

The authors thank Profs. V.P. Gerdt, V.V. Pupyshev, I.V. Puzynin and S.L. Yakovlev for useful discussions. O.C., A.A.G. and S.I.V. acknowledge financial support from the Bulgarian Foundation for Scientific Investigations, RFBR Grants Nos. 08-01-00604 and 07-01-00660, and the theme 09-6-1060-2005/2010 "Mathematical support of experimental and theoretical studies conducted by JINR".

Appendix A. Test run output

```
 PROBLEM:   PARAMETRIC DIFFERENTIAL EQUATION I
 ********

              C O N T R O L   I N F O R M A T I O N
              -------------------------------------

    NUMBER OF ENERGY LEVELS REQUIRED. . . . . (NROOT ) =      6
    NUMBER OF FINITE ELEMENTS . . . . . . . . (NELEM ) =    400
    NUMBER OF GRID POINTS . . . . . . . . . . (NGRID ) =   1601
    ORDER  OF SHAPE FUNCTIONS . . . . . . . . (NPOL  ) =      4
    ORDER  OF GAUSS-LEGENDRE QUADRATURE . . . (NGQ   ) =      5
    NUMBER OF SUBSPACE ITERATION VECTORS. . . (NC    ) =     12
    BOUNDARY CONDITION CODE . . . . . . . . . (IBOUND) =      4
    SHIFT OF DOUBLE ENERGY SPECTRUM . . . . . (SHIFT ) =   -10.0000
    CONVERGENCE TOLERANCE . . . . . . . . . . (RTOL  ) =   0.100000E-12
    VALUE OF PARAMETER. . . . . . . . . . . . (PARAM ) =    11.5196

   SUBDIVISION OF RHO-REGION ON THE FINITE-ELEMENT GROUPS:
   ******************************************************

  NO OF  NUMBER OF  BEGIN OF  LENGTH OF    GRID     END OF
  GROUP  ELEMENTS   INTERVAL   ELEMENT     STEP    INTERVAL
  -----  --------   --------   -------     ----    --------
    1       400      0.00000   0.00250   0.000625      1.000

    LAST ADDRESS OF ARRAY ITOT USED =       8807


              T O T A L   S Y S T E M   D A T A
              ---------------------------------

    TOTAL NUMBER OF ALGEBRAIC EQUATIONS. . . . (NN ) =     1601
    TOTAL NUMBER OF MATRIX ELEMENTS. . . . . . (NWK) =     5601
    MAXIMUM HALF BANDWIDTH . . . . . . . . . . (MK ) =        5
    MEAN    HALF BANDWIDTH . . . . . . . . . . (MMK) =        3


    LAST ADDRESS OF ARRAY TOT USED =      12999
```

```
     LAST ADDRESS OF ARRAY TOT USED =      45256


 THERE ARE    0 ROOTS LOWER THEN SHIFT
 CONVERGENCE REACHED FOR RTOL 0.1000E-12
 I T E R A T I O N   N U M B E R   27
 RELATIVE TOLERANCE REACHED ON EIGENVALUES
  0.1686E-17 0.1446E-15 0.0000E+00 0.0000E+00 0.0000E+00 0.4431E-13
```

ROOT NUMBER	EIGENVALUE	DERIVATIVE
1	131.6978190423784	23.03991454532688
2	393.0465776953899	69.12818558702216
3	650.2504800146933	115.2433376999127
4	903.2033485769872	161.4069643663601
5	1151.789459036675	207.6445825421709
6	1395.882038049846	253.9865811918269

R — EIGENFUNCTION

R						
0.0000	-.22274964D-23	0.89303396D-24	0.22239605D-22	-.11106591D-19	0.30880481D-16	-.11249627D-13
0.2500	0.44557304D-20	-.70037339D-18	0.52788096D-16	-.25638041D-14	0.90742591D-13	-.26726604D-11
0.5000	0.59893375D-13	-.51378822D-11	0.21053777D-09	-.54780510D-08	0.10146586D-06	-.14226801D-05
0.7500	0.82047136D-06	-.29630640D-04	0.49284800D-03	-.49838295D-02	0.34023245D-01	-.16430949D+00
1.0000	0.11475799D+02	0.11386247D+02	0.11293729D+02	0.11197966D+02	0.11098636D+02	0.10995357D+02

R — ITS DERIVATIVE

R						
0.0000	0.79313330D-24	0.16717921D-23	-.25982994D-21	0.24924824D-19	-.14107815D-16	0.49670201D-14
0.2500	-.38454263D-19	0.58658153D-17	-.43241464D-15	0.20512551D-13	-.70340668D-12	0.18688340D-10
0.5000	-.33974850D-12	0.28224816D-10	-.11170940D-08	0.27985656D-07	-.49719792D-06	0.66503536D-05
0.7500	-.22911857D-05	0.77342703D-04	-.11888254D-02	0.10935688D-01	-.66359810D-01	0.27458239D+00
1.0000	0.10038777D+01	0.10121499D+01	0.10212586D+01	0.10313304D+01	0.10425178D+01	0.10550076D+01

P O T E N T I A L M A T R I C E S H(I,J) A N D Q(I,J):

H-MATRIX AT THE PARAMETER = 11.51962

0.7653D-02	0.1209D-03	-.1543D-01	-.3686D-03	-.9037D-05	-.2528D-06
0.1209D-03	0.3876D-01	0.6268D-03	-.4704D-01	-.1537D-02	-.4837D-04
-.1543D-01	0.6268D-03	0.1023D+00	0.1953D-02	-.9569D-01	-.4014D-02
-.3686D-03	-.4704D-01	0.1953D-02	0.2000D+00	0.4612D-02	-.1623D+00
-.9037D-05	-.1537D-02	-.9569D-01	0.4612D-02	0.3339D+00	0.9217D-02
-.2528D-06	-.4837D-04	-.4014D-02	-.1623D+00	0.9217D-02	0.5064D+00

Q-MATRIX AT THE PARAMETER = 11.51962

-.1605D-16	0.8748D-01	0.6854D-03	0.8256D-05	0.1360D-06	0.2879D-08
-.8748D-01	-.4770D-16	0.1764D+00	0.2124D-02	0.3501D-04	0.7408D-06
-.6854D-03	-.1764D+00	0.2472D-16	0.2668D+00	0.4396D-02	0.9302D-04
-.8256D-05	-.2124D-02	-.2668D+00	-.9237D-16	0.3589D+00	0.7592D-02
-.1360D-06	-.3501D-04	-.4396D-02	-.3589D+00	-.6072D-17	0.4528D+00
-.2879D-08	-.7408D-06	-.9302D-04	-.7592D-02	-.4528D+00	0.6072D-17

```
 PROBLEM:   PARAMETRIC DIFFERENTIAL EQUATION II
 ********
```

```
               C O N T R O L   I N F O R M A T I O N
               -------------------------------------

     NUMBER OF ENERGY LEVELS REQUIRED. . . . (NROOT ) =      6
     NUMBER OF FINITE ELEMENTS . . . . . . . (NELEM ) =    800
     NUMBER OF GRID POINTS . . . . . . . . . (NGRID ) =   3201
     ORDER  OF SHAPE FUNCTIONS . . . . . . . (NPOL  ) =      4
     ORDER  OF GAUSS-LEGENDRE QUADRATURE . . . (NGQ   ) =      5
     NUMBER OF SUBSPACE ITERATION VECTORS. . . (NC    ) =     12
     BOUNDARY CONDITION CODE . . . . . . . . . (IBOUND) =      4
     SHIFT OF DOUBLE ENERGY SPECTRUM . . . . . (SHIFT ) =   -10.0000
     CONVERGENCE TOLERANCE . . . . . . . . . . (RTOL  ) =   0.100000E-12
     VALUE OF PARAMETER. . . . . . . . . . . . (PARAM ) =    2.00469


    SUBDIVISION OF RHO-REGION ON THE FINITE-ELEMENT GROUPS:
    ******************************************************

   NO OF  NUMBER OF  BEGIN OF  LENGTH OF    GRID     END OF
   GROUP  ELEMENTS   INTERVAL   ELEMENT     STEP    INTERVAL
   -----  --------   --------   -------     ----    --------
     1       800     -0.52360   0.00065   0.000164      0.000

     LAST ADDRESS OF ARRAY ITOT USED =      17607



               T O T A L   S Y S T E M   D A T A
               ---------------------------------

     TOTAL NUMBER OF ALGEBRAIC EQUATIONS. . . (NN ) =     3201
     TOTAL NUMBER OF MATRIX ELEMENTS. . . . . (NWK) =    11201
     MAXIMUM HALF BANDWIDTH . . . . . . . . . (MK ) =        5
     MEAN    HALF BANDWIDTH . . . . . . . . . (MMK) =        3


     LAST ADDRESS OF ARRAY TOT USED =      25799


     LAST ADDRESS OF ARRAY TOT USED =      90056

 THERE ARE    0 ROOTS LOWER THEN SHIFT
 CONVERGENCE REACHED FOR RTOL 0.1000E-12
 I T E R A T I O N   N U M B E R   15
 RELATIVE TOLERANCE REACHED ON EIGENVALUES
  0.0000E+00 0.5566E-14 0.3655E-14 0.3198E-14 0.9938E-15 0.5152E-13


*******************************************************************************

    R O O T   N U M B E R     E I G E N V A L U E         D E R I V A T I V E
   ----------------------   ---------------------       --------------------
             1                 -2.431524951096452       -1.458429440168202
             2                  31.91272127947840       -2.058234364971463
             3                  139.9725288836021       -2.012985124428196
             4                  319.9826816386258       -2.005659513377144
             5                  571.9861743548753       -2.003162124194071
             6                  895.9877805734652       -2.002017513522787

*******************************************************************************



        R              E I G E N F U N C T I O N
        -        ---------------------------------------

    -0.5236  0.16689503D+01 -.19826593D+01 0.19607443D+01 -.19571733D+01 0.19559545D+01 -.19553956D+01
    -0.4581  0.15627942D+01 -.17155517D+01 0.12800672D+01 -.65642720D+00 -.75119469D-01 0.80383895D+00
    -0.3927  0.14729301D+01 -.12165809D+01 -.13054335D+00 0.14458929D+01 -.19567782D+01 0.13466777D+01
    -0.3272  0.13984212D+01 -.55318460D+00 -.14667141D+01 0.17826097D+01 0.53663216D-01 -.18236288D+01
    -0.2618  0.13384908D+01 0.18497661D+00 -.19665197D+01 -.57447142D-01 0.19573666D+01 0.34289891D-01
    -0.1963  0.12925140D+01 0.89813754D+00 -.13449558D+01 -.18273543D+01 -.32200511D-01 0.17976623D+01
```

```
    -0.1309  0.12600115D+01 0.14899118D+01 0.43542857D-01 -.13658495D+01 -.19577197D+01 -.13955940D+01
    -0.0654  0.12406446D+01 0.18803190D+01 0.14072121D+01 0.76351636D+00 0.10733934D-01 -.74082992D+00
     0.0000  0.12342113D+01 0.20165941D+01 0.19684461D+01 0.19605399D+01 0.19578374D+01 0.19565974D+01

*******************************************************************************


        R             I T S   D E R I V A T I V E
        -        --------------------------------------

    -0.5236  0.16035732D+00 0.13094179D-02 -.60773212D-03 0.28686209D-03 -.16445461D-03 0.10614584D-03
    -0.4581  0.97967070D-01 0.59195008D-01 -.53622333D-01 0.46414585D-01 -.37602731D-01 0.27780685D-01
    -0.3927  0.46378558D-01 0.94296735D-01 -.66092299D-01 0.31427873D-01 -.65965486D-03 -.17886629D-01
    -0.3272  0.44915769D-02 0.10617026D+00 -.41890927D-01 -.12163048D-01 0.26868776D-01 -.87796247D-02
    -0.2618  -.28596841D-01 0.98927509D-01 -.52229874D-02 -.28852708D-01 0.12484460D-02 0.17146546D-01
    -0.1963  -.53606702D-01 0.79908343D-01 0.19110488D-01 -.10698146D-01 -.16125139D-01 -.40659005D-02
    -0.1309  -.71086469D-01 0.57828797D-01 0.22073763D-01 0.81688981D-02 -.16017773D-02 -.67842197D-02
    -0.0654  -.81421778D-01 0.40772504D-01 0.12788962D-01 0.78289098D-02 0.53756919D-02 0.35489858D-02
     0.0000  -.84841577D-01 0.34408945D-01 0.71690953D-02 0.30895655D-02 0.17195639D-02 0.10951726D-02

*******************************************************************************


          P O T E N T I A L   M A T R I C E S   H(I,J) A N D   Q(I,J):

     H-MATRIX AT THE PARAMETER =     2.00469
  0.2735D-02  -.2851D-03  -.8665D-03  0.4535D-03  -.2682D-03  0.1755D-03
  -.2851D-03  0.2976D-02  -.7163D-03  0.1031D-03  -.3044D-04  0.1246D-04
  -.8665D-03  -.7163D-03  0.6601D-03  -.2510D-03  0.4426D-04  -.1478D-04
  0.4535D-03  0.1031D-03  -.2510D-03  0.2870D-03  -.1270D-03  0.2453D-04
  -.2682D-03  -.3044D-04  0.4426D-04  -.1270D-03  0.1602D-03  -.7659D-04
  0.1755D-03  0.1246D-04  -.1478D-04  0.2453D-04  -.7659D-04  0.1022D-03

     Q-MATRIX AT THE PARAMETER =     2.00469
  -.3050D-15  -.5045D-01  0.1203D-01  -.5305D-02  0.2976D-02  -.1902D-02
  0.5045D-01  0.8823D-17  -.1884D-01  0.7053D-02  -.3760D-02  0.2349D-02
  -.1203D-01  0.1884D-01  0.3037D-17  -.1116D-01  0.4648D-02  -.2655D-02
  0.5305D-02  -.7053D-02  0.1116D-01  -.1669D-17  -.7954D-02  0.3479D-02
  -.2976D-02  0.3760D-02  -.4648D-02  0.7954D-02  0.1934D-17  -.6181D-02
  0.1902D-02  -.2349D-02  0.2655D-02  -.3479D-02  0.6181D-02  0.1714D-17


 PROBLEM:   PARAMETRIC DIFFERENTIAL EQUATION III
 ********


               C O N T R O L   I N F O R M A T I O N
               ------------------------------------

     NUMBER OF ENERGY LEVELS REQUIRED. . . . . (NROOT ) =      6
     NUMBER OF FINITE ELEMENTS . . . . . . . . (NELEM ) =    400
     NUMBER OF GRID POINTS . . . . . . . . . . (NGRID ) =   1601
     ORDER  OF SHAPE FUNCTIONS . . . . . . . . (NPOL  ) =      4
     ORDER  OF GAUSS-LEGENDRE QUADRATURE . . . (NGQ   ) =      5
     NUMBER OF SUBSPACE ITERATION VECTORS. . . (NC    ) =     12
     BOUNDARY CONDITION CODE . . . . . . . . . (IBOUND) =      4
     SHIFT OF DOUBLE ENERGY SPECTRUM . . . . . (SHIFT ) =   -10.0000
     CONVERGENCE TOLERANCE . . . . . . . . . . (RTOL  ) =   0.100000E-12
     VALUE OF PARAMETER. . . . . . . . . . . . (PARAM ) =    8.00000

    SUBDIVISION OF RHO-REGION ON THE FINITE-ELEMENT GROUPS:
    ******************************************************

   NO OF  NUMBER OF  BEGIN OF  LENGTH OF    GRID     END OF
   GROUP  ELEMENTS   INTERVAL   ELEMENT     STEP    INTERVAL
   -----  --------   --------   -------     ----    --------
     1       400      0.00000   0.00785   0.001963      3.142

     LAST ADDRESS OF ARRAY ITOT USED =       8807
```

```
               T O T A L   S Y S T E M   D A T A
               -------------------------------

     TOTAL NUMBER OF ALGEBRAIC EQUATIONS. . . . (NN ) =     1601
     TOTAL NUMBER OF MATRIX ELEMENTS. . . . . . (NWK) =     5601
     MAXIMUM HALF BANDWIDTH . . . . . . . . . . (MK ) =        5
     MEAN    HALF BANDWIDTH . . . . . . . . . . (MMK) =        3


     LAST ADDRESS OF ARRAY TOT USED =      12999


     LAST ADDRESS OF ARRAY TOT USED =      45256

 THERE ARE    0 ROOTS LOWER THEN SHIFT
 CONVERGENCE REACHED FOR RTOL 0.1000E-12
 I T E R A T I O N   N U M B E R   26
 RELATIVE TOLERANCE REACHED ON EIGENVALUES
  0.0000E+00 0.3826E-14 0.3197E-13 0.2584E-14 0.2651E-14 0.1134E-12

*******************************************************************************

    R O O T   N U M B E R     E I G E N V A L U E         D E R I V A T I V E
   ----------------------   ---------------------       --------------------
             1                -63.99999999998519       -15.99999999999546
             2                -12.99999999997674       -4.000000000007500
             3                0.8888888889180890       -1.777777777775382
             4                 11.00000000002065      -0.9999999999255478
             5                 21.44000000001866      -0.6400000012114990
             6                 33.22222222224192      -0.4444445049532144

*******************************************************************************



        R              E I G E N F U N C T I O N
        -        ---------------------------------------

     0.0000  0.45607017D+02 -.17888544D+02 0.13109228D+02 -.12649133D+02 0.13281250D+02 -.14196050D+02
     0.7854  0.85168492D-01 0.16398529D+01 0.59790078D-01 -.61977823D+00 0.95678611D+00 -.10614438D+01
     1.5708  0.15904728D-03 0.13362332D+00 0.87617699D+00 0.72882478D+00 -.68083352D+00 -.32293554D+00
     2.3562  0.29701169D-06 0.51038856D-02 0.13147060D+00 0.61601006D+00 0.12401978D+01 0.13223847D+01
     3.1416  0.55465260D-09 0.62383477D-04 0.30146728D-02 0.23621531D-01 0.87143859D-01 0.21527760D+00

*******************************************************************************



        R              I T S   D E R I V A T I V E
        -        ---------------------------------------

     0.0000  0.84636099D+01 -.29068884D+01 0.15425938D+01 -.11067645D+01 0.98392782D+00 -.96904963D+00
     0.7854  -.51085871D-01 -.10418382D+00 0.40991318D+00 -.31989712D+00 0.16210582D+00 0.28957439D-01
     1.5708  -.22031538D-03 -.66530808D-01 -.12005277D+00 0.23307684D+00 0.17446766D+00 -.27458383D+00
     2.3562  -.64469879D-06 -.46731036D-02 -.65118968D-01 -.16500181D+00 -.11862643D+00 0.11616782D+00
     3.1416  -.16395611D-08 -.87854421D-04 -.28022143D-02 -.16485488D-01 -.48298137D-01 -.98023856D-01

*******************************************************************************



          P O T E N T I A L   M A T R I C E S   H(I,J) A N D   Q(I,J):

     H-MATRIX AT THE PARAMETER =     8.00000
  0.1136D-01  -.1016D-01  -.9803D-03  0.3020D-02  -.3697D-02  0.3875D-02
  -.1016D-01  0.2972D-01  -.1652D-01  -.1065D-01  0.9211D-02  -.7225D-02
  -.9803D-03  -.1652D-01  0.5213D-01  -.2163D-01  -.1704D-01  0.8337D-02
  0.3020D-02  -.1065D-01  -.2163D-01  0.6997D-01  -.2275D-01  -.2062D-01
  -.3697D-02  0.9211D-02  -.1704D-01  -.2275D-01  0.7850D-01  -.2038D-01
  0.3875D-02  -.7225D-02  0.8337D-02  -.2062D-01  -.2038D-01  0.8015D-01

     Q-MATRIX AT THE PARAMETER =     8.00000
```

```
 0.1757D-15  -.7355D-01  0.3912D-01  -.3102D-01  0.2724D-01  -.2434D-01
 0.7355D-01  0.4427D-16  -.1332D+00  0.5842D-01  -.3716D-01  0.2635D-01
 -.3912D-01  0.1332D+00  0.1215D-15  -.1672D+00  0.5393D-01  -.3203D-01
 0.3102D-01  -.5842D-01  0.1672D+00  0.7797D-16  -.1844D+00  0.4495D-01
 -.2724D-01  0.3716D-01  -.5393D-01  0.1844D+00  -.4739D-16  -.1914D+00
 0.2434D-01  -.2635D-01  0.3203D-01  -.4495D-01  0.1914D+00  -.2222D-16
```

References

[1] O. Chuluunbaatar, A.A. Gusev, V.L. Derbov, M.S. Kaschiev, L.A. Melnikov, V.V. Serov, S.I. Vinitsky, J. Phys. A 40 (2007) 11485–11524.
[2] O. Chuluunbaatar, V.L. Derbov, A. Galtbayar, A.A. Gusev, M.S. Kaschiev, S.I. Vinitsky, T. Zhanlav, J. Phys. A 41 (2008) 295203-1–25.
[3] P.M. Krassovitskiy, N.Zh. Takibaev, Bull. Russian Acad. Sci. Phys. 70 (2006) 815–818.
[4] P.M. Krassovitskiy, S.I. Vinitsky, A.A. Gusev, O. Chuluunbaatar, Bull. Russian Acad. Sci. Phys. 73 (2009) 233–235.
[5] Yu.N. Demkov, J.D. Meyer, Eur. Phys. J. B 42 (2004) 361–365.
[6] M.G. Dimova, M.S. Kaschiev, S.I. Vinitsky, J. Phys. B 38 (2005) 2337–2352.
[7] E.M. Kazaryan, A.A. Kostanyan, H.A. Sarkisyan, Physica E 28 (2005) 423–430.
[8] O. Chuluunbaatar, A.A. Gusev, A.G. Abrashkevich, A. Amaya-Tapia, M.S. Kaschiev, S.Y. Larsen, S.I. Vinitsky, Comput. Phys. Comm. 177 (2007) 649–675.
[9] O. Chuluunbaatar, A.A. Gusev, S.I. Vinitsky, A.G. Abrashkevich, Comput. Phys. Comm. 179 (2008) 685–693.
[10] G. Strang, G.J. Fix, An Analysis of the Finite Element Method, Prentice-Hall, Englewood Cliffs, New York, 1973.
[11] K.J. Bathe, Finite Element Procedures in Engineering Analysis, Prentice-Hall, Englewood Cliffs, New York, 1982.
[12] O. Chuluunbaatar, A.A. Gusev, M.S. Kaschiev, V.A. Kaschieva, A. Amaya-Tapia, S.Y. Larsen, S.I. Vinitsky, J. Phys. B 39 (2006) 243–269.
[13] Yu.A. Kuperin, P.B. Kurasov, Yu.B. Melnikov, S.P. Merkuriev, Ann. Phys. 205 (1991) 330–361.
[14] O. Chuluunbaatar, A.A. Gusev, V.P. Gerdt, V.A. Rostovtsev, S.I. Vinitsky, A.G. Abrashkevich, M.S. Kaschiev, V.V. Serov, Comput. Phys. Comm. 178 (2008) 301–330.
[15] A.G. Abrashkevich, M.S. Kaschiev, S.I. Vinitsky, J. Comp. Phys. 163 (2000) 328–348.
[16] S.I. Vinitskii, L.G. Mardoyan, G.S. Pogosyan, A.N. Sissakian, T.A. Strizh, Phys. Atom. Nucl. 56 (1993) 321–327.
[17] W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes: The Art of Scientific Computing, Cambridge University Press, Cambridge, 1986.
[18] M. Abramowitz, I.A. Stegun, Handbook of Mathematical Functions, Dover, New York, 1965.