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Description of a Program for Computing Eigenvalues and Eigenfunctions and Their First Derivatives with Respect to the Parameter of the Coupled Parametric Self-Adjoined Elliptic Differential Equations

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Brief description of 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 coupled parametric self-adjoined elliptic differential equations with the Dirichlet and/or Neumann type boundary conditions on the finite interval. The original problem is projected to the parametric homogeneous and nonhomogeneous 1D boundary-value problems for a set of ordinary second order differential equations which is solved by the finite element method. The program calculates also potential matrix elements – integrals of the eigenfunctions multiplied by their first derivatives with respect to the parameter. Parametric eigenvalues (so-called potential curves) and matrix elements computed by the POTHEA 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. As a test desk, the program is applied to the calculation of the potential curves and matrix elements of Schrödinger equation for a system of three charged particles with zero total angular momentum.

Key words and phrases: boundary value problem, finite element method, Kantorovich method.

1. Introduction

In this work we present a brief description of a POTHEA program for calculating with a given accuracy eigenvalues, eigenfunctions and their first derivatives with respect to the parameter of the coupled parametric self-adjoined elliptic differential equations with the Dirichlet and/or Neumann type boundary conditions on the finite interval [1]. The original problem is projected to the parametric homogeneous and nonhomogeneous 1D BVPs for a set of ordinary second order differential equations which is solved by the finite element method [2]. The program calculates also potential matrix elements – integrals of the eigenfunctions multiplied by their derivatives with respect to the parameter.

Potential curves and matrix elements computed by the POTHEA 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 [1, 3].

As a benchmark, we present calculation with a given accuracy of potential curves and matrix elements which is applied for calculation of ground state energy and first exited state energy of an helium atom in the framework of the Kantorovich method implemented like the close-coupled hyperspherical adiabatic approach [4]. 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.

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2. Statement of the Problem

Let us consider a boundary problem for a parametric two dimensional self-adjoined second order ordinary differential equation on the region $\Omega=[x_{\min},x_{\max}]\times[y_{\min},y_{\max}]$

$$\left(-\frac{1}{f_1(y)}\frac{\partial}{\partial y}f_2(y)\frac{\partial}{\partial y}-\frac{1}{f_3(y)}\frac{1}{f_4(x)}\frac{\partial}{\partial x}f_5(x)\frac{\partial}{\partial x}+U(x,y;z)-\varepsilon(z)\right)B(x,y;z)=0. \quad (1)$$

with the Dirichlet and/or Neumann type boundary conditions ($t=\min,\max$)

$$\lim_{y\to y_t} f_2(y)\partial_y B(x,y;z)=0 \text{ or } B(x,y_t;z)=0,\ x\in(x_{\min},x_{max}), \quad (2)$$

$$\lim_{x\to x_t} f_5(x)\partial_x B(x,y;z)=0 \text{ or } B(x_t,y;z)=0,\ y\in(y_{\min},y_{\max}).$$

Here $z\in[z_{\min},z_{\max}]$ is a parameter, functions $f_1(y)>0$, $f_2(y)>0$, $f_3(y)>0$, $f_4(x)>0$, $f_5(x)>0$, and $\partial_y f_2(y)$, $\partial_x f_5(x)$, $U(x,y;z)$, $\partial_z U(x,y;z)$ are continuous on the $(x,y)\in\Omega/\partial\Omega$. Also assume that the parametric boundary value problem (BVP) (1), (2) has only discrete spectrum.

The program executes the following steps.

In **Step 1** program calculates a set of $j_{\max}$ smallest eigenvalues $\varepsilon_1(z)<\varepsilon_2(z)<\ldots<\varepsilon_N(z)$, and $\varepsilon_1(z)\geqslant\alpha(z)$, and the corresponding eigenfunctions $\{B_j(x,y;z)\}_{j=1}^N \in F_z\sim\mathbf{L}_2(\Omega_{x,y})$, satisfying the orthogonality and normalization conditions

$$\int\limits_{y_{\min}}^{y_{\max}} \mathrm{d}y\, f_1(y) \int\limits_{x_{\min}}^{x_{\max}} \mathrm{d}x\, f_4(x)B_i(x,y;z)B_j(x,y;z)=\delta_{ij}, \quad (3)$$

where δ_{ij} is the Kronecker symbol, and $\alpha(z)>-\infty$ is the lower bound of the smallest eigenvalue of $\varepsilon_1(z)$.

In **Step 2** program computes a set of partial derivatives of eigenvalue $\partial\varepsilon_j(z)/\partial z$ and partial derivatives of eigenfunctions $\partial B_j(x,y;z)/\partial z$ with an accuracy of the same orders achieved for eigenvalues and eigenfunctions of the BVP (1)–(3), respectively.

In **Step 3** program computes matrix elements defined by the integrals

$$H_{ij}(z)=H_{ji}(z)=\int\limits_{y_{\min}}^{y_{\max}} \mathrm{d}y\, f_1(y) \int\limits_{x_{\min}}^{x_{\max}} \mathrm{d}x\, f_4(x)\partial_z B_i(x,y;z)\partial_z B_j(x,y;z), \quad (4)$$

$$Q_{ij}(z)=-Q_{ji}(z)=-\int\limits_{y_{\min}}^{y_{\max}} \mathrm{d}y\, f_1(y) \int\limits_{x_{\min}}^{x_{\max}} \mathrm{d}x\, f_4(x)B_i(x,y;z)\partial_z B_j(x,y;z).$$

with an accuracy of the same order achieved for the corresponding eigenvalues of the BVP (1)–(3).

2.1. Reduction of the 2D BVP to the 1D BVP

Step 1.1. The partial wave function $B_i(x,y;z)$ is expanded over the orthonormal basis functions $\{\psi_j(x)\}_{j=1}^{j_{\max}}$:

$$B_i(x,y;z)=\sum_{j=1}^{j_{\max}}\psi_j(x)\xi_j^{(i)}(y;z). \quad (5)$$

In Eq. (5), the vector-functions $\boldsymbol{\xi}^{(i)}(y;z) = (\xi_1^{(i)}(y;z), \ldots, \xi_{j_{\max}}^{(i)}(y;z))^T$ are unknown. The functions $\psi_j(x)$ are determined as solutions of the following eigenvalue problem ($t = \min, \max$):

$$\left(-\frac{1}{f_4(x)}\frac{\mathrm{d}}{\mathrm{d}x}f_5(x)\frac{\mathrm{d}}{\mathrm{d}x} + U_0(x)\right)\psi_j(x) = \lambda_j\psi_j(x), \tag{6}$$

$$\lim_{x\to x_t} f_5(x)\frac{\mathrm{d}\psi_j(x)}{\mathrm{d}x} = 0 \quad \text{or} \quad \psi_j(x_t) = 0,$$

where $U_0(x)$ is a known function and

$$\int\limits_{x_{\min}}^{x_{\max}} \mathrm{d}x\, f_4(x)\psi_i(x)\psi_j(x) = \delta_{ij}. \tag{7}$$

Note, this problem can be numerically solved with a given accuracy by mens of the ODPEVP program [23].

Step 1.2. After minimizing the Rayleigh-Ritz variational functional, and using the expansion (5), Eq. (1) is reduced to a finite set of $j_{\max}$ ordinary second-order differential equations ($t = \min, \max$)

$$(\mathbf{D}(y;z) - \varepsilon_i(z)\,\mathbf{I})\,\boldsymbol{\xi}^{(i)}(y;z) = 0, \quad \mathbf{D}(y;z) = -\frac{1}{f_1(y)}\mathbf{I}\frac{\partial}{\partial y}f_2(y)\frac{\partial}{\partial y} + \mathbf{W}(y;z), \tag{8}$$

$$\lim_{y\to y_t} f_2(y)\partial_y\boldsymbol{\xi}^{(i)}(y;z) = 0 \quad \text{or} \quad \boldsymbol{\xi}^{(i)}(y_t;z) = 0. \tag{9}$$

Here $\mathbf{I}$, $\mathbf{W}(y;z)$ are symmetric matrices of dimension $j_{\max} \times j_{\max}$

$$I_{ij} = \delta_{ij} = \int\limits_{y_{\min}}^{y_{\max}} \mathrm{d}y\, f_1(y)\left(\boldsymbol{\xi}^{(i)}(y;z)\right)^T \boldsymbol{\xi}^{(j)}(y;z), \tag{10}$$

$$W_{ij}(y;z) = \frac{\lambda_i + \lambda_j}{2f_3(y)}\delta_{ij} + \int\limits_{x_{\min}}^{x_{\max}} \mathrm{d}x\, f_4(x)\,\psi_i(x)\left(U(x,y;z) - \frac{U_0(x)}{f_3(y)}\right)\psi_j(x).$$

Step 2. Taking a derivative of the boundary problem (8)–(9) with respect to parameter z, we get that $\partial_z\boldsymbol{\xi}^{(i)}(y;z)$ can be obtained as a solution of the following boundary problem ($t = \min, \max$)

$$(\mathbf{D}(y;z) - \varepsilon_i(z)\,\mathbf{I})\,\frac{\partial\boldsymbol{\xi}^{(i)}(y;z)}{\partial z} = -\left[\frac{\partial}{\partial z}\left(\mathbf{W}(y;z) - \varepsilon_i(z)\,\mathbf{I}\right)\right]\boldsymbol{\xi}^{(i)}(y;z), \tag{11}$$

$$\lim_{y\to y_t} f_2(y)\partial_y(\partial_z\boldsymbol{\xi}^{(i)}(y;z)) = 0 \quad \text{or} \quad \partial_z\boldsymbol{\xi}^{(i)}(y_t;z) = 0. \tag{12}$$

The BVP (11)–(12) has a unique solution, if and only if:

$$\frac{\partial\varepsilon_i(z)}{\partial z} = \int\limits_{y_{\min}}^{y_{\max}} \mathrm{d}y\, f_1(y)\left(\boldsymbol{\xi}^{(i)}(y;z)\right)^T \frac{\partial_z\mathbf{W}(y;z)}{\partial z}\boldsymbol{\xi}^{(i)}(y;z), \tag{13}$$

$$\int\limits_{y_{\min}}^{y_{\max}} \mathrm{d}y f_1(y) \left(\boldsymbol{\xi}^{(i)}(y;r)\right)^T \frac{\partial \boldsymbol{\xi}^{(i)}(y;z)}{\partial z} = 0. \tag{14}$$

Step 3. The required matrix elements (4) are represented by

$$H_{ij}(z) = H_{ji}(z) = \int\limits_{y_{\min}}^{y_{\max}} \mathrm{d}y\, f_1(y) \left(\frac{\partial \boldsymbol{\xi}^{(i)}(y;z)}{\partial z}\right)^T \frac{\partial \boldsymbol{\xi}^{(j)}(y;z)}{\partial z}, \tag{15}$$

$$Q_{ij}(z) = -Q_{ji}(z) = -\int\limits_{y_{\min}}^{y_{\max}} \mathrm{d}y\, f_1(y) \left(\boldsymbol{\xi}^{(i)}(y;z)\right)^T \frac{\partial \boldsymbol{\xi}^{(j)}(y;z)}{\partial z}.$$

3. Test Desk

For a Helium atom with zero angular momentum in hyperspherical coordinates $x = \alpha$, $y = \vartheta$, $z = R$, by using weight functions $f_1(x) = f_2(x) = f_3(x) = \sin^2\alpha$, $f_4(y) = f_5(y) = \sin\vartheta$ and potential function

$$U(\alpha, \vartheta; R) = \frac{R}{2}\left(-\frac{2}{\sin(\alpha/2)} - \frac{2}{\cos(\alpha/2)} + \frac{1}{\sqrt{1-\sin(\alpha)\cos\vartheta}}\right),$$

we reduce boundary value problem (1)–(3) using expansion (5) with analytical solution of problem (6)–(7) in the form of Legendre polynomials $P_j(\cos\theta)$ to boundary problems (8)–(14). The later have been solved by the POTHEA program on finite element grids $\Omega_\alpha = \{0.(150)\pi/2\}$ with fourth-order Lagrange elements with accuracy $eps = 10^{-12}$ and the corresponding matrix elements $\mathbf{H}(z)$, $\mathbf{Q}(z)$ have been calculated with accuracy $eps = 10^{-6}$, at run time is 4 seconds.

The following values of numerical parameters and characters described in [1] have been used in the test run via the supplied input file POTHEA.INP:

```
&PARAMS TITLE='  PARAMETRIC 2D DIFFERENTIAL EQUATION  ',
        ICOUN=0,PARAM=10D0,NROOT=6,MDIM=12,NPOL=4,RTOL=1.D-12,
        NITEM=2000,SHIFT=-1.1D0,ICHK=1,IPRINT=0,IPRSTP=15,
        NMESH=3,RMESH=0.0D0,150.D0,1.570796326794896D0,
        NDIR=1, NDIL=12, NMDIL=0,IBOUND=4,
        FNOUT='3DNGSS.LPR',IOUT=7,POTEN='3DNGSS.PTN',IOUP=10,
        FMATR='3DNGSS.MAT',IOUM=11,EVWFN='3DNGSS.WFN',IOUF=1
&END
```

All calculation details of this problem were written into file POTHEA.LPR.

Test Run Output

```
 PROBLEM:   PARAMETRIC 2D DIFFERENTIAL EQUATION
 ********

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

     NUMBER OF DIFFERENTIAL EQUATIONS. . . . . (MDIM  ) =     12
     NUMBER OF ENERGY LEVELS REQUIRED. . . . . (NROOT ) =      6
     NUMBER OF FINITE ELEMENTS . . . . . . . . (NELEM ) =    150
```

```
     NUMBER OF GRID POINTS . . . . . . . . . . . (NGRID ) =    601
     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 EIGENVALUE . . . . . . . . . . . (SHIFT ) =   -1.10000
     CONVERGENCE TOLERANCE . . . . . . . . . . (RTOL  ) =   0.100000E-11
     VALUE OF PARAMETER. . . . . . . . . . . . (PARAM ) =    10.0000

    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       150        0.000   0.01047   0.00262      1.571

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

     TOTAL NUMBER OF ALGEBRAIC EQUATIONS. . . . (NN ) =     7212
     TOTAL NUMBER OF MATRIX ELEMENTS. . . . . . (NWK) =   262878
     MAXIMUM HALF BANDWIDTH . . . . . . . . . . (MK ) =       60
     MEAN    HALF BANDWIDTH . . . . . . . . . . (MMK) =       36


     NDIM, MDIM=       12       12

 THERE ARE    0 ROOTS LOWER THEN SHIFT
 CONVERGENCE REACHED FOR RTOL 0.1000E-11
 I T E R A T I O N   N U M B E R   68
 RELATIVE TOLERANCE REACHED ON EIGENVALUES
  0.0000E+00 0.4385E-15 0.5146E-14 0.1811E-13 0.7383E-15 0.1124E-11

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

    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                 -106.1449119429294      -20.49786509377458
            2                 -32.40954538140649      -5.355570130015161
            3                 -30.37792481031590      -5.456241767021648
            4                 -21.97501254692271      -3.414051588534342
            5                 -19.24789115244545      -3.025292223400815
            6                 -15.24989121658901      -2.766774467691610

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

          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 =    10.00000
  0.7530D-02  0.7277D-02  -.4429D-02  -.2551D-02  0.1761D-02  -.6160D-03
  0.7277D-02  0.2831D-01  -.4826D-02  0.8100D-02  -.7355D-03  0.9388D-03
  -.4429D-02  -.4826D-02  0.1766D-01  -.1222D-02  0.5248D-02  -.2412D-02
  -.2551D-02  0.8100D-02  -.1222D-02  0.2799D-01  -.4505D-02  0.1145D-02
  0.1761D-02  -.7355D-03  0.5248D-02  -.4505D-02  0.1618D-01  -.7024D-02
  -.6160D-03  0.9388D-03  -.2412D-02  0.1145D-02  -.7024D-02  0.1048D-01

     Q-MATRIX AT THE PARAMETER =    10.00000
  0.1003D-14  0.4752D-01  -.2558D-01  0.2470D-01  -.1301D-01  0.6895D-02
  -.4752D-01  0.2947D-15  0.1519D-01  0.1397D+00  -.2136D-01  0.5194D-02
  0.2558D-01  -.1519D-01  -.2203D-15  -.1770D-02  0.9586D-01  -.5406D-01
  -.2470D-01  -.1397D+00  0.1770D-02  0.5867D-16  -.2047D-01  0.3502D-02
  0.1301D-01  0.2136D-01  -.9586D-01  0.2047D-01  -.9482D-16  -.8956D-02
  -.6895D-02  -.5194D-02  0.5406D-01  -.3502D-02  0.8956D-02  0.3119D-16
```

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Описание программы вычисления собственных значений и собственных функций и их первых производных по параметру для параметрической самосопряжённой системы эллиптических дифференциальных уравнений

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Представлено краткое описание программ на языке Фортран 77 для расчёта с заданной точностью собственных значений, собственных функций и их первых производных по параметру для параметрической самосопряжённой системы эллиптических дифференциальных уравнений на конечном интервале с граничными условиями Дирихле и/или Неймана. Исходная задача проецируется на параметрические однородные и неоднородные одномерные краевые задачи для системы обыкновенных дифференциальных уравнений второго порядка, решаемые методом конечных элементов. Программа рассчитывает также потенциальные матричные элементы — интегралы от собственных функций, умноженные на их первые производные по параметру. Собственные значения, зависящие от параметра (так называемые потенциальные кривые) и матричных элементов, рассчитываемые программой POTHEA, могут быть использованы для решения с помощью программы KANTBP задач на связанные состояния и многоканальные задачи рассеяния для системы второго порядка обыкновенных дифференциальных уравнений. В качестве теста программа использована для расчёта потенциальных кривых и матричных элементов уравнения Шрёдингера для системы трёх заряженных частиц с нулевым полным угловым импульсом.

Ключевые слова: краевая задача, метод конечных элементов, метод Канторовича.