Математическое моделирование

UDC 519.632.4

Solution of the Boundary-Value Problem for a Systems of ODEs of Large Dimension: Benchmark Calculations in the Framework of Kantorovich Method

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We present benchmark calculations of the boundary-value problem (BVP) for a systems of second order ODEs of large dimension with help of KANTBP program using a finite element method. In practice, for solving the BVPs with the long-range potentials and a large number of open channels there is a necessity of solving boundary value problems of the large-scale systems of differential equations that require further investigation of convergence and stability of the algorithms and programs. With this aim we solve here the eigenvalue problem for an elliptic differential equation in a two-dimensional domain with Dirichlet boundary conditions. The solution is sought in the form of Kantorovich expansion over the parametric basis functions of one of the independent variables with the second variable treated as a parameter. The basis functions are calculated in an analytical form as solutions of the auxiliary parametric Sturm-Lioville problem for a second-order ODE. As a result, the two-dimensional problem is reduced to a boundary-value problem for a set of self-adjoint second-order ODEs for functions of the second independent variable. The discrete formulation of the problem is implemented using the finite element method. The efficiency, stability and convergence of the calculation scheme is shown by benchmark calculations for a triangle membrane with a degenerate spectrum.

Key words and phrases: benchmark calculations, boundary-value problem, large-scale systems of ODEs, Kantorovich method, finite element method

1. Introduction

The solving quantum tunneling problem or calculations of spectral and optical properties of electronic states in axially symmetric quantum dots and Helium-like atom (system of two-electron in the Coulomb field) is reduced to the solution of boundary-value problems (BVP) for elliptic differential equations with nonseparable variables in a finite domain [1–3]. One of the ways to solve these problems is implemented as a set of programs ODPEVP-POTHEA-KANTBP [4–6] basing on the Kantorovich method (KM) that provides the reduction of the initial problem to a set of self-adjoint second-order ODEs [7] with further discretization by the finite element method (FEM) [8]. In practice, for solving problems with the long-range potential and a large number of open channels there is a necessity of solving boundary value problems of the large-scale systems of the ODEs that require further investigation of convergence and stability of the algorithms and programs.

Testing such approach, algorithms and programs for the solution of two-dimensional BVPs and large-scale systems of the ODEs is the aim of the present work. We present a computational scheme for solving the eigenvalue problem for an elliptic differential equation in a two-dimensional finite domain with Dirichlet boundary conditions. The solution is sought in the form of Kantorovich expansion over the basis functions of one of the independent variables with the second variable treated as a parameter. The basis functions are calculated as a solution of the parametric eigenvalue problem for an ordinary

Received 12$^{\text{th}}$ July, 2016. The work was partially supported by the Russian Foundation for Basic Research (RFBR) (grant 14-01-00420). The reported study was partially funded within the Agreement No. 02.a03.21.0008 dated 24.11.2016 between the Ministry of Education and Science of the Russian Federation and RUDN University.

second-order differential equation. Finally, the initial problem is reduced to a BVP for a set of self-adjoint second-order differential equations for functions of the second independent variable. The discretization of the problems is carried out using the FEM with Lagrange interpolating polynomials. The result is used to formulate a generalized algebraic eigenvalue problem for higher-order matrices. We demonstrate the efficiency of the KANTBP program for solving the boundary-value problem for a systems of the ODEs of large dimension in benchmark calculations for the exactly solvable eigenvalue problem of a triangle membrane with the degenerate spectrum.

2. Kantorovich Method

Let us consider the 2D BVP in the two-dimensional domain $\Omega(x_f, x_s) \subset \mathbf{R}^2$:

$$\left(-\frac{\partial^2}{\partial x_s} - \frac{\partial^2}{\partial x_f} + V(x_f, x_s) - E\right)\Psi(x_f, x_s) = 0, \tag{1}$$

where $V(x_f, x_s)$ is a real-valued function and $\Psi(x_f, x_s)$ satisfies the Dirichlet condition at the boundary $\partial\Omega(x_f, x_s)$ of the domain $\Omega(x_f, x_s)$

$$\Psi(x_f, x_s)\Big|_{(x_f,x_s)\in\partial\Omega(x_f,x_s)} = 0. \tag{2}$$

The solution $\Psi(x_f, x_s)\in W_2^2(\Omega)$ of the BVP (1)–(2) is sought in the form of Kantorovich expansion [7]

$$\Psi_i(x_f, x_s) = \sum_{j=1}^{j_{\max}} \Phi_j(x_f; x_s)\chi_j^i(x_s), \tag{3}$$

using the set of eigenfunctions of the parametric BVP

$$\left(-\frac{\partial^2}{\partial x_f} + V(x_f, x_s) - \epsilon_j(x_s)\right)\Phi_j(x_f; x_s) = 0, \tag{4}$$

defined in the interval $x_f \in (x_f^{\min}(x_s), x_f^{\max}(x_s)) = \Omega_{x_f}(x_s)$ and depending on the variable $x_s \in (x_s^{\min}, x_s^{\max}) = \Omega_{x_s}$ as a parameter. These functions obey the boundary conditions

$$\Phi_j(x_f^{\min}(x_s); x_s) = 0, \quad \Phi_j(x_f^{\max}(x_s); x_s) = 0 \tag{5}$$

at the boundary points $\{x_f^{\min}(x_s), x_f^{\max}(x_s)\} = \partial\Omega_{x_f}(x_s)$, of the interval $\Omega_{x_f}(x_s)$.

The eigenfunctions satisfy the orthonormality condition in the same interval $x_f \in \Omega_{x_f}(x_s)$:

$$\langle\Phi_i|\Phi_j\rangle = \int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f; x_s)\Phi_j(x_f; x_s)dx_f = \delta_{ij}. \tag{6}$$

In Eq. (4) $\epsilon_1(x_s) < \ldots < \epsilon_{j_{\max}}(x_s) < \ldots$ is the desired set of real-valued eigenvalues. If this parametric eigenvalue problem has no analytical solution, then it is solved numerically using the ODPEVP program [4] or in the case of two variables POTHEA program [5].

Substituting the expansion (3) into Eq. (1) with Eqs. (5) and (6) taken into account, we arrive at the set of self-adjoint ODEs for the unknown vector functions $\boldsymbol{\chi}^{(i)}(x_s, E) \equiv$

$\boldsymbol{\chi}^{(i)}(x_s) = (\chi_1^{(i)}(x_s), \ldots, \chi_{j_{\max}}^{(i)}(x_s))^T$:

$$\left(-\mathbf{I}\frac{d^2}{dx_s^2} + \mathbf{U}(x_s) - E\,\mathbf{I} + \frac{d\mathbf{Q}(x_s)}{dx_s} + \mathbf{Q}(x_s)\frac{d}{dx_s}\right)\boldsymbol{\chi}^{(i)}(x_s) = 0. \tag{7}$$

Here $\mathbf{U}(x_s)$ and $\mathbf{Q}(x_s)$ are matrices of the dimension $j_{\max} \times j_{\max}$

$$U_{ij}(x_s) = \epsilon_i(x_s)\delta_{ij} + H_{ij}(x_s), \tag{8}$$

$$H_{ij}(x_s) = H_{ji}(x_s) = \int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \frac{\partial \Phi_i(x_f; x_s)}{\partial x_s}\frac{\partial \Phi_j(x_f; x_s)}{\partial x_s} dx_f, \tag{9}$$

$$Q_{ij}(x_s) = -Q_{ji}(x_s) = -\int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f; x_s)\frac{\partial \Phi_j(x_f; x_s)}{\partial x_s} dx_f.$$

The solutions of the discrete spectrum $E : E_1 < E_2 < \ldots < E_v < \ldots$ that obey the boundary conditions at the points $x_s^t = \{x_s^{\min}, x_s^{\max}\} = \partial\Omega_{x_s}$, bounding the interval Ω_{x_s},

$$\boldsymbol{\chi}^{(p)}(x_s^t) = 0, \quad x_s^t = x_s^{\min}, x_s^{\max} \tag{10}$$

and the orthonormality conditions

$$\int\limits_{x_s^{\min}}^{x_s^{\max}} (\boldsymbol{\chi}^{(i)}(x_s))^T \boldsymbol{\chi}^{(j)}(x_s) dx_s = \delta_{ij}, \tag{11}$$

are calculated by means of the KANTBP program [6].

3. Benchmark Calculation: Triangular Membrane

As a benchmark example we consider the exactly solvable BVP for a triangular membrane in conventional variables $(x_f, x_s) \in \Omega(x_f, x_s)$

$$\left(-\frac{\partial^2}{\partial x_s^2} - \frac{\partial^2}{\partial x_f^2} - E\right)\Psi(x_f, x_s) = 0 \tag{12}$$

with the Dirichlet conditions at the boundary $\partial\Omega(x, y)$ of the region $\Omega(x_f, x_s)$

$$\Psi((x_f, x_s) \in \partial\Omega(x_f, x_s)) = 0. \tag{13}$$

In the considered case the parametric eigenvalue problem (4)–(6) has an exact solution, i.e., the parametric eigenfunctions $\Phi_i(x_f; x_s)$ and potential curves $\epsilon_i(x_s)$ are expressed in the analytical form

$$\epsilon_i(x_s) = \frac{\pi^2 i^2}{(x_f^{\max}(x_s) - x_f^{\min}(x_s))^2}, \quad \Phi_i(x_f; x_s) = \frac{\sqrt{2}\sin\left(\frac{\pi i (x_f - x_f^{\min}(x_s))}{x_f^{\max}(x_s) - x_f^{\min}(x_s)}\right)}{\sqrt{x_f^{\max}(x_s) - x_f^{\min}(x_s)}}. \tag{14}$$

With the basis functions (14) the integration in the effective potentials (9) can be carried out analytically, which yields the expressions

$$Q_{ij}(x_s) = -\frac{2ij}{i^2-j^2}\frac{\left((-1)^{i+j}\frac{dx_f^{\max}(x_s)}{dx_s} - \frac{dx_f^{\min}(x_s)}{dx_s}\right)}{x_f^{\max}(x_s) - x_f^{\min}(x_s)}, \quad j \neq i,$$

$$H_{ij}(x_s) = -\frac{4ij(i^2+j^2)}{(i^2-j^2)^2}\frac{\left((-1)^{i+j}\frac{dx_f^{\max}(x_s)}{dx_s} - \frac{dx_f^{\min}(x_s)}{dx_s}\right)\left(\frac{dx_f^{\max}(x_s)}{dx_s} - \frac{dx_f^{\min}(x_s)}{dx_s}\right)}{(x_f^{\max}(x_s) - x_f^{\min}(x_s))^2},$$

$$H_{ii}(x_s) = \frac{\pi^2 i^2}{3}\frac{\left(\frac{dx_f^{\max}(x_s)}{dx_s}\right)^2 + \left(\frac{dx_f^{\max}(x_s)}{dx_s}\right)\left(\frac{dx_f^{\min}(x_s)}{dx_s}\right) + \left(\frac{dx_f^{\min}(x_s)}{dx_s}\right)^2}{(x_f^{\max}(x_s) - x_f^{\min}(x_s))^2} + \\ + \frac{1}{4}\frac{\left(\frac{dx_f^{\max}(x_s)}{dx_s} - \frac{dx_f^{\min}(x_s)}{dx_s}\right)^2}{(x_f^{\max}(x_s) - x_f^{\min}(x_s))^2}.$$

In the symmetric case $x_f^{\max}(x_s) = -x_f^{\min}(x_s)$ the matrix elements H_{ij} and Q_{ij} between even and odd indexes equal zero and one can solve the BVP for even (e) and odd (o) solutions separately.

As a domain we chose the equilateral triangle with side equal to $4\pi/3$, in this case the eigenvalues $E_i = \mu^2 + \nu^2 + \mu\nu = 3, 7, 7, 12, 13, 13, 19, 19, 21, 21, 27, \ldots$, where $\mu, \nu = 1, 2, \ldots$, are integer [9].

Case 1, x_f is paralleled to a triangle side and x_s belong to a triangle height:

$$x_f^{\max}(x_s) = 2\pi/3 - x_s/\sqrt{3}, \quad x_f^{\min}(x_s) = -2\pi/3 + x_s/\sqrt{3}, \quad x_s^{\min} = 0, \quad x_s^{\max} = 2\pi/\sqrt{3}.$$

Case 2, x_s is paralleled to a triangle side and x_f belong to a triangle height:

$$x_f^{\max}(x_s) = 2\pi/\sqrt{3} - \sqrt{3}|x_s|, \quad x_f^{\min}(x_s) = 0, \quad x_s^{\min} = -2\pi/3, \quad x_s^{\max} = 2\pi/3.$$

In both cases taking into account the symmetry properties of the equilateral triangle, we apply the FEM for discretization of the BVP (7)–(11) using finite element grid $\Omega_{x_s} = (0(2)3v/4(2)v)$, $v = x_s^{\max} - 0.002$, where the number of finite elements in each subinterval is presented in parentheses, and Lagrangian interpolation polynomials of $p' = 12$th order, which provides the accuracy $O(h^{p'+1})$ of the vector-eigenfunctions $\boldsymbol{\chi}^{(i)}(x_s, E) \equiv \boldsymbol{\chi}^{(i)}(x_s) = (\chi_1^{(i)}(x_s), \ldots, \chi_{j_{\max}}^{(i)}(x_s))^T$ and $O(h^{2p'})$ of the eigenvalues E_i, where $h = 3v/8$ is the maximal element length [8].

The numerical calculations of eigenvalue problem (7)–(11) were carried out till $j_{\max} = 280$ using the new version of the program KANTBP 2.0 implemented in Fortran. In Fig. 1 some typical examples of profiles of the eigenfunctions are presented, corresponding to the exact doubly degenerate eigenvalues E_2^e=E_1^o=7, E_4^e=E_2^o=13, and E_5^e=E_3^o=19.

Achieved the discrepancy $\delta E_i^\sigma = E_i^\sigma - E_i$ of the order of 10^{-8} for the eigenvalues that is shown in the Table 1. One can see from the table that the convergence rate of the Kantorovich expansion (3) is the order $j_{\max}^{-3}$, which corresponds to the theoretical estimations given by the perturbation theory. Similar rate of convergence takes place also in solving of the parametric 2D BVP for a Helium atom [5] and 2D BVP for quadratic membrane [10].

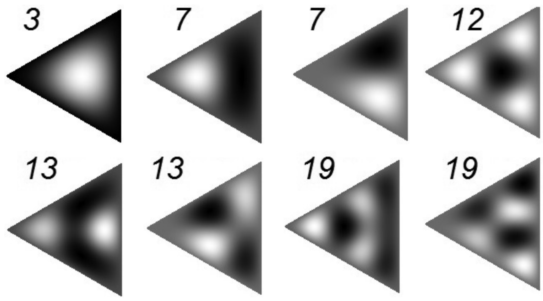

Figure 1. Eigenfunctions $\Psi(x, y)$ of bound states of the 2D boundary-value problem (12), (13) composed by the components $\chi_j^{(i)}(x_s)$ of the eigenfunctions of the BVP for system of ODEs (7)–(11) and parametric functions $\Phi_i\,(x_f; x_s)$ from (14)

Table 1

The discrepancy $\delta E_i^\sigma = E_i^{\sigma;\mathrm{calc}} - E_i^\sigma$, $\sigma = e, o$, vs a number $j_{\max}$ of even (e) and odd (o) basis functions (14) of Kantorovich expansion (3)

$j_{\max}$	δE_1^e	δE_2^e	δE_3^e	δE_4^e	δE_{10}^e	δE_1^o	δE_2^o	δE_7^o
								case 1
6	1.36(-4)	5.44(-4)	2.45(-3)	1.29(-3)	2.32(-2)	6.67(-4)	2.59(-3)	2.47(-2)
13	1.37(-5)	5.41(-5)	2.35(-4)	1.22(-4)	2.02(-3)	7.44(-5)	2.85(-4)	2.35(-3)
28	1.39(-6)	5.49(-6)	2.37(-5)	1.22(-5)	1.99(-4)	7.98(-6)	3.05(-5)	2.44(-4)
60	1.42(-7)	5.62(-7)	2.42(-6)	1.25(-6)	2.03(-5)	8.41(-7)	3.21(-6)	2.56(-5)
130	1.41(-8)	5.56(-8)	2.39(-7)	1.23(-7)	2.01(-6)	8.42(-8)	3.22(-7)	2.56(-6)
280	1.43(-9)	5.54(-9)	2.41(-8)	1.24(-8)	2.05(-7)	8.56(-9)	3.26(-8)	2.59(-7)
								case 2
6	8.69(-4)	8.21(-3)	1.83(-2)	2.43(-2)	0.95	1.13(-3)	8.79(-3)	4.84(-2)
13	1.01(-4)	8.93(-4)	1.79(-3)	2.33(-3)	3.57(-2)	1.34(-4)	9.97(-4)	3.10(-3)
28	1.13(-5)	9.82(-5)	1.93(-4)	2.52(-4)	3.48(-3)	1.50(-5)	1.10(-4)	3.27(-4)
60	1.21(-6)	1.05(-5)	2.07(-5)	2.70(-5)	3.65(-4)	1.62(-6)	1.18(-5)	3.48(-5)
130	1.24(-7)	1.07(-6)	2.10(-6)	2.73(-6)	3.68(-5)	1.64(-7)	1.20(-6)	3.52(-6)
280	1.29(-8)	1.09(-7)	2.13(-7)	2.78(-7)	3.74(-6)	1.68(-8)	1.22(-7)	3.58(-7)
exact	E_1^e=3	E_2^e=7	E_3^e=12	E_4^e=13	E_{10}^e=37	E_1^o=7	E_2^o=13	E_7^o=37

For the number $j_{\max}$ of the parametric basis functions increased to 280, that requires more RAM and computer time are needed. The dimension of the mass and stiffness matrices and their half-width are following: $(12 \cdot 4 + 1)j_{\max} \times (12 \cdot 4 + 1)j_{\max}$ and $(12 \cdot 2 + 1)j_{\max}$: 294×294 and 150 for $j_{\max} = 6$, 2940×2940 and 1500 for $j_{\max} = 60$, 13720×13720 and 7000 for $j_{\max} = 280$. The calculation time was about 1 seconds for $j_{\max} = 6$, 15 seconds for $j_{\max} = 60$ and 455 seconds for $j_{\max} = 280$ in the double precision of Fortran-77 using the PC Intel Core i5 3.33GHz, 4Gb, 64 bit Windows 7.

4. Conclusion

We show and estimate the rate of convergence of Kantorovich expansion (3) in benchmark calculations for the exactly solvable eigenvalue problem of a triangle membrane with the degenerate spectrum, together with the efficiency and stability of the KANTBP program for solving the boundary-value problem for systems of the ODEs of a large dimension.

The proposed benchmark model can be used for testing of algorithms and programs for solving the BVPs for systems of the ODEs or generalized algebraic eigenvalue problems of a large dimension.

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УДК 519.632.4

Решение краевых задач для систем ОДУ большой размерности: эталонные расчеты в рамках метода Канторовича

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Представлены эталонные расчеты краевой задачи для систем ОДУ второго порядка большой размерности с помощью программы KANTBP с использованием метода конечных элементов. На практике для решения краевых задач с дальнодействующими потенциалами и большого числа открытых каналов необходимо решать краевые задачи для систем дифференциальных уравнений большой размерности, которые также требуют изучения сходимости и устойчивости алгоритмов и программ. С этой целью в данной работе решена задача на собственные значения для эллиптического дифференциального уравнения в двумерной области с граничными условиями Дирихле. Решение ищется в виде разложения Канторовича по параметрическим базисным функциям одной из независимых переменных, при этом вторая независимая переменная рассматривается как параметр. Базисные функции вычисляются в аналитическом виде как решения вспомогательной параметрической задачи Штурма–Лиувилля для ОДУ второго порядка. В результате, двумерная задача сводится к краевой задаче для самосопряжённой системы ОДУ второго порядка относительно второй независимой переменной. Дискретизация задачи выполнена в рамках метода конечных элементов. Эффективность, устойчивость и сходимость вычислительной схемы продемонстрирована эталонными расчетами для треугольной мембраны с вырожденным спектром.

Ключевые слова: тестовые расчеты, краевая задача, системы ОДУ большой размерности, метод Канторовича, метод конечных элементов

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