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Algorithms for Solving the Parametric Self-Adjoint 2D Elliptic Boundary-Value Problem Using High-Accuracy Finite Element Method

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We consider the calculation schemes for solving elliptic boundary-value problems (BVPs) within the framework of the Kantorovich method that provides the reduction of an elliptic BVP to a system of coupled second-order ordinary differential equations (ODEs). The surface basis functions of the expansion depend on the independent variable of the ODEs parametrically. Here we use the basis functions calculated by means of the finite element method(FEM), as well as the probe parametric surface basis functions calculated in the analytical form.

We propose new calculation schemes and algorithms for solving the parametric self-adjoint elliptic boundary-value problem (BVP) in a 2D finite domain, using high-accuracy finite element method (FEM) with rectangular and triangular elements. The algorithm and the programs calculate with the given accuracy the eigenvalues, the surface eigenfunctions and their first derivatives with respect to the parameter of the BVP for parametric self-adjoint elliptic differential equation with the Dirichlet and/or Neumann type boundary conditions on the 2D finite domain, and the potential matrix elements, expressed as integrals of the products of surface eigenfunctions and/or their first derivatives with respect to the parameter. The parametric eigenvalues (potential curves) and the potential matrix elements computed by the program can be used for solving bound-state and multi-channel scattering problems for systems of coupled second-order ODEs by means of the Kantorovich method.

We demonstrate the efficiency of the proposed calculation schemes and algorithms in benchmark calculations of 2D elliptic BVPs describing quadrupole vibrations of a collective nuclear model.

Key words and phrases: parametric elliptic boundary-value problem, finite element method, Kantorovich method, systems of second-order ordinary differential equations

1. Introduction

The adiabatic representation is widely applied for solving multichannel scattering and bound-state problems for systems of several quantum particles in molecular, atomic and nuclear physics [1–4].

Such problems are described by elliptic boundary value problems (BVPs) in a multidimensional domain of the configuration space, solved using the Kantorovich method, i.e., the reduction to a system of self-adjoint ordinary differential equations(SODEs) using the basis of surface functions of an auxiliary BVP depending on the independent

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variable of the SODEs parametrically. The elements of matrices of variable coefficients of these SODEs including the matrix of the first derivatives are determined by the integrals of products of surface eigenfunctions and/or their first derivatives with respect to the parameter. Thus, the key problem of such method is to develop effective algorithms and programs for calculating with given accuracy the surface eigenfunctions and the corresponding eigenvalues of the auxiliary BVP, together with their derivatives with respect to the parameter, and the corresponding integrals that present the matrix elements of the effective potentials in the SODEs [5–7].

In this paper we propose new calculation schemes and algorithms for the solution of the parametric 2D elliptic boundary-value problem using high-accuracy finite element method (FEM) with rectangular and triangular elements. The algorithms were implemented in a package of programs that calculate with the given accuracy eigenvalues, eigenfunctions and their first derivatives with respect to the parameter of the parametric self-adjoint elliptic differential equations with the boundary conditions of the Dirichlet and/or Neumann type in the 2D finite domain and the integrals of products of the surface eigenfunctions and their first derivatives with respect to the parameter that express the matrix elements of the effective potentials in the SODEs.

We also propose a method of constructing the etalon potential in the auxiliary parametric BVP that allows the calculation of the parametric surface basis functions in the analytical form. These functions can be then used for the reduction of the original 2D BVP to the SODEs containing the additional potential matrix, representing the discrepancy between the original potential and the etalon one, averaged with the basis functions. The efficiency of the calculation schemes and algorithms is demonstrated by benchmark calculation of the 2D BVPs describing quadrupole vibrations in the collective nuclear model [4, 8, 9].

The structure of the paper is the following. In Section 2 the Kantorovich method for solving the 2D and 3D BVPs is considered. In Sections 3 and 4 the 2D FEM schemes and algorithms for solving the parametric 2D BVP and calculating derivatives with respect to the parameter together with the corresponding matrix elements are presented. In Section 5 the benchmark calculations of 2D FEM algorithms and programs are analyzed. In Conclusion we discuss the results and perspectives.

2. Kantorovich method with the etalon potential

Let us consider the BVP in the domain $\Omega(x_f, x_s) \subset \mathbf{R}^{n-1} \times \mathbf{R}^1$:

$$\left(-\frac{1}{f_{s1}(x_s)}\frac{\partial}{\partial x_s}f_{s2}(x_s)\frac{\partial}{\partial x_s}+\frac{D(x_f;x_s)}{f_{s3}(x_s)}+V(x_f,x_s)-E\right)\Psi(x_f,x_s)=0, \tag{1}$$

where $D(x_f; x_s)$ is a self-adjoint elliptic differential operator in the finite region $\Omega(x_f; x_s) \subset \mathbf{R}^{n-1}$, E is the spectral parameter, corresponding to the energy of the quantum system, $f_{si}(x_s) > 0$, $\partial_{x_s} f_{si}(x_s)$ and $V(x_f, x_s)$ $\partial_{x_s} V(x_f, x_s)$ are real-valued continuous bounded functions in $\Omega(x_f, x_s)$, and $\Psi(x_f, x_s)$ satisfies the Dirichlet and/or Neumann boundary condition (BC) at the boundary $\partial\Omega \equiv \partial\Omega(x_f, x_s)$ of the domain $\Omega(x_f, x_s)$ and the orthonormalization conditions

$$\langle\Psi_i|\Psi_j\rangle = \int_{\Omega(x_f,x_s)} f_{s1}(x_s)\Psi_i(x_f,x_s)\Psi_j(x_f,x_s)\mathrm{d}x_f^{n-1}\,\mathrm{d}x_s=\delta_{ij}. \tag{2}$$

The solution $\Psi(x_f, x_s)\in W_2^2(\Omega)$ of the BVP (1) is sought in the form of the Kantorovich expansion [3]

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

using the set of parametric eigenfunctions $\Phi_j(x_f;x_s) \in \mathcal{F}(x_s) \sim W_2^2(\Omega(x_f;x_s))$ of the parametric BVP in the domain $\Omega(x_f;x_s) \subset \mathbf{R}^{n-1}$

$$(D(x_f;x_s)-\varepsilon_j(x_s))\,\Phi(x_f;x_s)=0. \tag{4}$$

For example, $D(x_f;x_s)$ at $n-1=2$ is determined in a conventional form in Section 3. To avoid cumbersome notations, below we will use the simplest definition of $D(x_f;x_s)$ at $n-1=1$

$$D(x_f;x_s) = -\frac{\partial^2}{\partial x_f^2}+V_o(x_f;x_s,g(x_s)), \tag{5}$$

where $V_o(x_f;x_s,g(x_s))$ is the etalon potential 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 $x_s \in \Omega_{x_s}$ as a parameter. We assume that these functions obey the BCs

$$\Phi_j(x_f^{\min}(x_s);x_s)=0, \quad \Phi_j(x_f^{\max}(x_s);x_s)=0 \tag{6}$$

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

$$\langle\Phi_i|\Phi_j\rangle = \int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} \Phi_i(x_f;x_s)\Phi_j(x_f;x_s)\,\mathrm{d}x_f=\delta_{ij}. \tag{7}$$

Here $\varepsilon(x_s) : \varepsilon_1(x_s) < \ldots < \varepsilon_{j_{\max}}(x_s) < \ldots$ is the desired set of real eigenvalues.

During the simulation the etalon potential $V_0(x_f;x_s,g(x_s))$ in Eq. (5) will be chosen as $V_0(x_f;x_s,g(x_s)) = V(x_f,x_s)$ or calculated separately for different values of $x_s \in \Omega_{x_s}$ from the conditions

$$\min_{g(x_s)} \int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)} (V(x_f,x_s)-V_o(x_f;x_s,g(x_s))^2\,\mathrm{d}x_f. \tag{8}$$

If this parametric eigenvalue problem has no analytical solution, then it is solved numerically by the FEM: at $n-1=1$ using the program ODPEVP [6] and at $n-1=2$ using the program, implementing the algorithm presented in Section 3.

Substituting the expansion (3) into Eq. (1) with Eqs. (6) and (7) taken into account, we arrive at the set of self-adjoint ODEs for the unknown vector functions $\boldsymbol{\chi}^{(i)}(x_s,E) \equiv \boldsymbol{\chi}^{(i)}(x_s)=(\chi_1^{(i)}(x_s),\ldots,\chi_{j_{\max}}^{(i)}(x_s))^T \in W_2^2(\Omega_{x_s})$:

$$\left(-\mathbf{I}\frac{1}{f_{s1}(x_s)}\frac{\mathrm{d}}{\mathrm{d}x_s}f_{s2}(x_s)\frac{\mathrm{d}}{\mathrm{d}x_s}+\mathbf{W}(x_s)-2E\,\mathbf{I}+ \right.$$
$$\left. +\frac{f_{s2}(x_s)}{f_{s1}(x_s)}\frac{\mathrm{d}\mathbf{Q}(x_s)}{\mathrm{d}x_s}+\frac{1}{f_{s1}(x_s)}\frac{\mathrm{d}f_{s2}(x_s)\mathbf{Q}(x_s)}{\mathrm{d}x_s}\right)\boldsymbol{\chi}^{(i)}(x_s)=0. \tag{9}$$

Here $\mathbf{I}$, $\mathbf{W}(x_s)$ and $\mathbf{Q}(x_s)$ are the $j_{\max}\times j_{\max}$ matrices

$$W_{ij}(x_s)=\frac{\varepsilon_i(x_s)}{f_{s3}(x_s)}\delta_{ij}+\frac{f_{s2}(x_s)}{f_{s1}(x_s)}H_{ij}(x_s)+V_{ij}(x_s), \quad I_{ij}=\delta_{ij}, \tag{10}$$

$$H_{ij}(x_s)=H_{ji}(x_s)=\int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)}\frac{\partial\Phi_i(x_f;x_s)}{\partial x_s}\frac{\partial\Phi_j(x_f;x_s)}{\partial x_s}\,\mathrm{d}x_f, \tag{11}$$

$$Q_{ij}(x_s)=-Q_{ji}(x_s)=-\int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)}\Phi_i(x_f;x_s)\frac{\partial\Phi_j(x_f;x_s)}{\partial x_s}\,\mathrm{d}x_f. \tag{12}$$

The effective potentials $V_{ij}(x_s)=V_{ji}(x_s)$ are calculated by integrating the difference $\delta V(x_f,x_s)=V(x_f,x_s)-V_o(x_f;x_s,g(x_s))$ with the basis functions:

$$V_{ij}(x_s)=\int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)}\Phi_i(x_f;x_s)\delta V(x_f,x_s)\Phi_j(x_f;x_s)\,\mathrm{d}x_f. \tag{13}$$

If the etalon potential is equal to the original one, $V_o(x_f;x_s,g(x_s))=V(x_f,x_s)$ then $V_{ij}(x_s)=0$. If the original potential $V(x_f,x_s)$ is presented in the tabular form, e.g., as in Ref. [4], then the etalon potential $V_o(x_f;x_s,g(x_s))$ can be considered as a certain approximation or interpolation of the original one, and the approximation error $\delta V(x_f,x_s)\neq 0$. In this case the etalon potential $V_o(x_f;x_s,g(x_s))$ can be determined minimizing $\delta V(x_f,x_s)$ in accordance with the condition (8) of the least squares method. Then the integrals $V_{ij}(x_s)$ of the approximation error $\delta V(x_f,x_s)$ averaged with the parametric basis functions are included into the final system of ODEs. It means that we take the approximation error of the original potential into account and require the solutions of the 2D BVP (1) to have the given accuracy, see, e.g., Section 5.4.

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

$$\boldsymbol{\chi}^{(p)}(x_s^t)=0,\ x_s^t=x_s^{\min},x_s^{\max},\ \int\limits_{x_s^{\min}}^{x_s^{\max}}f_{s1}(x_s)(\boldsymbol{\chi}^{(i)}(x_s))^T\boldsymbol{\chi}^{(j)}(x_s)\,\mathrm{d}x_s=\delta_{ij}. \tag{14}$$

3. FEM algorithm for solving the parametric 2D BVP

Let us consider a boundary value problem for the parametric self-adjoint 2D PDE in the domain $\Omega_{x,y}=(x_{\min},x_{\max})\times(y_{\min},y_{\max})$

$$\begin{gathered}(D(x,y;z)-\varepsilon_i(z))\,\Phi_i(x,y;z)=0,\\ D\equiv D(x,y;z)=-\frac{1}{f_1(x)}\frac{\partial}{\partial x}f_2(x,y)\frac{\partial}{\partial x}-\frac{1}{f_3(x)f_4(y)}\frac{\partial}{\partial y}f_5(x,y)\frac{\partial}{\partial y}+U(x,y;z),\end{gathered} \tag{15}$$

with the Dirichlet and/or Neumann boundary conditions

$$\begin{aligned}&\lim_{x\to x_t}f_2(x,y)\frac{\partial\Phi_i(x,y;z)}{\partial x}=0\ \text{or}\ \Phi_i(x_t,y;z)=0,\quad y\in[y_{\min},y_{\max}],\\ &\lim_{y\to y_t}f_5(x,y)\frac{\partial\Phi_i(x,y;z)}{\partial y}=0\ \text{or}\ \Phi_i(x,y_t;z)=0,\quad x\in[x_{\min},x_{\max}],\end{aligned} \tag{16}$$

where $t = \min, \max$. Here $z \in \Omega_z = [z_{\min}, z_{\max}]$ is a parameter, the functions $f_1(x) > 0$, $f_2(x,y) > 0$, $f_3(x) > 0$, $f_4(y) > 0$, $f_5(x,y) > 0$, and $\partial_x f_2(x,y)$, $\partial_y f_5(x,y)$, $U(x,y;z)$, $\frac{\partial U(x,y;z)}{\partial z}$ and $\frac{\partial \Phi_i(x,y;z)}{\partial z}$ are continuous and bounded for $(x,y) \in \Omega_{x,y}$. Also assume that the BVP (15), (16) has only the discrete spectrum, so that $\varepsilon(x_s) : \varepsilon_1(x_s) < \ldots < \varepsilon_{j_{\max}}(x_s) < \ldots$ is the desired set of real eigenvalues. The eigenfunctions satisfy the orthonormality conditions

$$\langle \Phi_i | \Phi_j \rangle = \int\limits_{x^{\min}}^{x^{\max}} \int\limits_{y^{\min}}^{y^{\max}} f_1(x) f_4(y) \Phi_i(x,y;z) \Phi_j(x,y;z)\, \mathrm{d}x\, \mathrm{d}y = \delta_{ij}. \tag{17}$$

The FEM calculation scheme is derived from the variational functional

$$\begin{aligned}\langle \Phi_i | D - \varepsilon(z) | \Phi_j \rangle = \int\limits_{x_{\min}}^{x_{\max}} \mathrm{d}x \int\limits_{y_{\min}}^{y_{\max}} \mathrm{d}y \Bigg(& f_4(y) f_2(x,y) \frac{\partial \Phi_i(x,y;z)}{\partial x} \frac{\partial \Phi_j(x,y;z)}{\partial x} + \\ & + \frac{f_1(x)}{f_3(x)} f_5(x,y) \frac{\partial \Phi_i(x,y;z)}{\partial y} \frac{\partial \Phi_j(x,y;z)}{\partial y} + \\ & + \Phi_i(x,y;z) f_1(x) f_4(y) (U(x,y;z) - \varepsilon(z)) \Phi_j(x,y;z) \Bigg). \end{aligned} \tag{18}$$

1. The domain $\Delta = [x_{\min}, x_{\max}] \times [y_{\min}, y_{\max}]$ is covered by the system of $n \times m$ subdomains $\Delta_{ij} = [x_{i-1}, x_i] \times [y_{j-1}, y_j]$ in such a way that $\Delta = \bigcup_{i=1}^{n} \bigcup_{j=1}^{m} \Delta_{ij}$. In each subdomain Δ_{ij} the nodes $\left\{x_{i,r}^p\right\}_{r=0}^p$ and $\left\{y_{j,r}^p\right\}_{r=0}^p$

$$x_{i,r}^p = x_{i-1} + \frac{h_i^x}{p} r, \quad h_i^x = x_i - x_{i-1}, \quad y_{j,r}^p = y_{j-1} + \frac{h_j^y}{p} r, \quad h_j^y = y_j - y_{j-1},$$

and the Lagrange elements $\left\{\phi_{i,r}^p(x)\right\}_{r=0}^p$ and $\left\{\psi_{j,r}^p(y)\right\}_{r=0}^p$

$$\phi_{i,r}^p(x) = \prod_{s=0, s\neq r}^{p} \frac{x - x_{i,s}^p}{x_{i,r}^p - x_{i,s}^p}, \quad \psi_{j,r}^p(y) = \prod_{s=0, s\neq r}^{p} \frac{y - y_{j,s}^p}{y_{j,r}^p - y_{j,s}^p}$$

are determined. By means of the Lagrange elements $\phi_{i,r}^p(x)$ and $\psi_{j,r}^p(y)$, we define the set of piecewise polynomial functions $N_l^p(x)$ and $M_l^p(y)$ as follows:

$$N_l^p(x) = \begin{cases} \begin{cases} \phi_{1,0}^p(x), & x \in \Delta_{1j}, \\ 0 & x \notin \Delta_{1j}, \end{cases} & l{=}0, \\ \begin{cases} \phi_{i,r}^p(x), & x \in \Delta_{ij}, \\ 0, & x \notin \Delta_{ij}, \end{cases} & l{=}r{+}p(i{-}1),\ r{=}\overline{1, p{-}1}, \\ \begin{cases} \phi_{i,p}^p(x), & x \in \Delta_{ij}, \\ \phi_{i+1,0}^p(x), & x \in \Delta_{i+1j}, \\ 0, & x \notin \Delta_{ij} \bigcup \Delta_{i+1j}, \end{cases} & l{=}ip,\ i{=}\overline{1, n{-}1}, \\ \begin{cases} \phi_{n,p}^p(x), & x \in \Delta_{nj}, \\ 0, & x \notin \Delta_{nj}, \end{cases} & l{=}np, \end{cases}$$

for any j and

$$M_l^p(y) = \begin{cases} \begin{cases} \psi_{1,0}^p(y), & y \in \Delta_{i1}, \\ 0, & y \notin \Delta_{i1}, \end{cases} & l{=}0, \\ \begin{cases} \psi_{j,r}^p(y), & y \in \Delta_{ij}, \\ 0, & y \notin \Delta_{ij}, \end{cases} & l{=}r{+}p(j{-}1),\ r{=}\overline{1,p{-}1}, \\ \begin{cases} \psi_{j,p}^p(y), & y \in \Delta_{ij}, \\ \psi_{j+1,0}^p(y), & y \in \Delta_{ij+1}, \\ 0, & y \notin \Delta_{ij} \bigcup \Delta_{ij+1}, \end{cases} & l{=}jp,\ j{=}\overline{1,m{-}1}, \\ \begin{cases} \psi_{m,p}^p(y), & y \in \Delta_{im}, \\ 0, & y \notin \Delta_{im}, \end{cases} & l{=}mp, \end{cases}$$

for any i.

The functions $\{N_l^p(x)\}_{l=0}^{np}$ and $\{M_l^p(y)\}_{l=0}^{mp}$ form a basis in the space of polynomials of the p-th order. Now, the function $\Phi(x,y;z) \in \mathcal{F}_z^h \sim \mathcal{H}^1(\Omega_{h_x,h_y})$ is approximated by a finite sum of piecewise polynomial functions $N_l^p(x)$ and $M_l^p(y)$

$$\Phi^h(x,y;z) = \sum_{l_y=0}^{mp} \sum_{l_x=0}^{np} \xi^{l_x l_y}(z) N_{l_x}^p(x) M_{l_y}^p(y). \tag{19}$$

2. The domain $\Omega(x,y) = \bigcup_{q=1}^{Q} \Delta_q$, specified as a polygon in the plane ($x \equiv z_1, y \equiv z_2$) $\in \mathcal{R}^2$, is covered with finite elements, the triangles Δ_q with the vertices $(z_{11}, z_{21}), (z_{12}, z_{22}), (z_{13}, z_{23})$ (here $z_{ik} \equiv z_{ik;q}$, $i = \overline{1,2}$, $k = \overline{1,3}$, $q = \overline{1,Q}$). On each of the triangles Δ_q (the boundary is considered to belong to the triangle) the shape functions $\varphi_l^p(z_1,z_2)$ are introduced. For this purpose we divide the sides of the triangle into p equal parts and draw three families of parallel straight lines through the partition points. The straight lines of each family are numbered from 0 to p, so that the line passing through the side of the triangle has the number 0, and the line passing through the opposite vertex of the triangle has the number p.

Three straight lines from different families intersect in one point $A_l \in \Delta_q$, which will be numbered by the triplet (n_1, n_2, n_3), $n_i \geq 0$, $n_1 + n_2 + n_3 = p$, where n_1, n_2 and n_3 are the numbers of the straight lines passing parallel to the side of the triangle that does not contain the vertex (z_{11}, z_{21}), (z_{12}, z_{22}) and (z_{13}, z_{23}), respectively. The coordinates of this point $z_l = (z_{1l}, z_{2l})$ are determined by the expression $(z_{1l}, z_{2l}) = (z_{11}, z_{21})n_1/p + (z_{12}, z_{22})n_2/p + (z_{13}, z_{23})n_3/p$.

As shape functions we use the Lagrange triangular polynomials $\varphi_l^p(z_1,z_2)$ of the order p that satisfy the condition $\varphi_l^p(z_{1l'}, z_{2l'}) = \delta_{ll'}$, i.e., equal 1 in one of the points A_l and zero in the other points.

In this method the piecewise polynomial functions $N_l^p(z_1,z_2)$ in the domain Ω are constructed by joining the shape functions $\varphi_l^p(z_1,z_2)$ in the triangle Δ_q:

$$N_l^p(z_1,z_2) = \left\{ \varphi_l^p(z_1,z_2), A_l \in \Delta_q; 0, A_l \notin \Delta_q \right\}$$

and possess the following properties: functions $N_l^p(z_1,z_2)$ are continuous in the domain Ω; the functions $N_l^p(z_1,z_2)$ equal 1 in one of the points A_l and zero in the rest points; $N_l^p(z_{1l'}, z_{2l'}) = \delta_{ll'}$ in the entire domain Ω. Here l takes the values $l = \overline{1,N}$.

The functions $N_l^p(x,y)$ form a basis in the space of polynomials of the p-th order. Now, the function $\Phi(x,y;z) \in \mathcal{F}_z^h \sim \mathcal{H}^1(\Omega_{h_x,h_y})$ is approximated by a finite sum of piecewise basis functions $N_l^p(x,y)$

$$\Phi^h(x,y;z) = \sum_{l=1}^{N} \xi^l(z) N_l^p(x,y). \tag{20}$$

The vector function $\boldsymbol{\xi}_\nu^h = \{\xi_\nu^{l_x l_y}(z)\}_{l_y=0\,l_x=0}^{mp\;\;np}$ or $\boldsymbol{\xi}^h = \{\xi^l(z)\}_{l=1}^N$ has a generalized first-order partial derivative and belongs to the Sobolev space $\mathcal{H}^1(\Omega_{h_x,h_y})$ [10]. After substituting the expansion (19) or (20) into the variational functional (18) and minimizing it [10, 11], we obtain the generalized eigenvalue problem

$$\mathbf{A}^p \boldsymbol{\xi}^h = \varepsilon^h \mathbf{B}^p \boldsymbol{\xi}^h. \tag{21}$$

Here $\mathbf{A}^p$ is the stiffness matrix; $\mathbf{B}^p$ is the positive definite mass matrix; $\boldsymbol{\xi}^h$ is the vector approximating the solution on the finite-element grid; and ε^h is the corresponding eigenvalue. The matrices $\mathbf{A}^p$ and $\mathbf{B}^p$ have the following form:

$$\mathbf{A}^p = \sum_{j=1}^{m}\sum_{i=1}^{n} \mathbf{a}_{ji}^p,\ \mathbf{B}^p = \sum_{j=1}^{m}\sum_{i=1}^{n} \mathbf{b}_{ji}^p,\ \text{or } \mathbf{A}^p{=}\{a_{ll'}^p\}_{ll'=1}^N,\ \mathbf{B}^p{=}\{b_{ll'}^p\}_{ll'=1}^N,$$

where the local matrices $\mathbf{a}_{ji}^p$ and $\mathbf{b}_{ji}^p$ are calculated for rectangular elements as

$$\begin{aligned}
(\mathbf{a}_{ji}^p)_{\mu\nu}^{qr} = \int_{-1}^{+1}\int_{-1}^{+1} \Bigg\{ & f_2(x,y) f_4(y) \frac{4}{(h_i^x)^2} \frac{\mathrm{d}\phi_{i,q}^p(x)}{\mathrm{d}\eta_x} \frac{\mathrm{d}\phi_{i,r}^p(x)}{\mathrm{d}\eta_x} \psi_{j,\mu}^p(y)\psi_{j,\nu}^p(y) + \\
& + \frac{f_1(x)}{f_3(x)} f_5(x,y) \phi_{i,q}^p(x)\phi_{i,r}^p(x) \frac{4}{(h_j^y)^2} \frac{\mathrm{d}\psi_{j,\mu}^p(y)}{\mathrm{d}\eta_y} \frac{\mathrm{d}\psi_{j,\nu}^p(y)}{\mathrm{d}\eta_y} + \\
& + f_1(x) f_4(y) U(x,y;z) \phi_{i,q}^p(x)\phi_{i,r}^p(x)\psi_{j,\mu}^p(y)\psi_{j,\nu}^p(y) \Bigg\} \frac{h_i^x}{2}\frac{h_j^y}{2}\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y, \\
(\mathbf{b}_{ji}^p)_{\mu\nu}^{qr} = \int_{-1}^{+1}\int_{-1}^{+1} & f_1(x) f_4(y) \phi_{i,q}^p(x)\phi_{i,r}^p(x)\psi_{j,\mu}^p(y)\psi_{j,\nu}^p(y) \frac{h_i^x}{2}\frac{h_j^y}{2}\,\mathrm{d}\eta_x\,\mathrm{d}\eta_y,
\end{aligned} \tag{22}$$

$$x = x_{i-1} + 0.5h_i^x(1+\eta_x), \quad y = y_{j-1} + 0.5h_j^y(1+\eta_y), \quad \mu,\nu,q,r = \overline{0,p},$$

or the matrix elements $a_{ll'}^p$ and $b_{ll'}^p$ are calculated for triangular elements as

$$\begin{aligned}
a_{ll'}^p = \int_{\Delta_q} & f_1(x) f_4(y) \varphi_l^p(z_1,z_2)\varphi_{l'}^p(z_1,z_2) U(z_1,z_2;z)\,\mathrm{d}z_1\,\mathrm{d}z_2 + \\
& + \int_{\Delta_q} f_2(x,y) f_4(y) \frac{\partial\varphi_l^p(z_1,z_2)}{\partial z_1} \frac{\partial\varphi_{l'}^p(z_1,z_2)}{\partial z_1}\,\mathrm{d}z_1\,\mathrm{d}z_2 + \\
& + \int_{\Delta_q} \frac{f_1(x)}{f_3(x)} f_5(x,y) \frac{\partial\varphi_l^p(z_1,z_2)}{\partial z_2} \frac{\partial\varphi_{l'}^p(z_1,z_2)}{\partial z_2}\,\mathrm{d}z_1\,\mathrm{d}z_2 =
\end{aligned}$$

$$= |J| \int\limits_{\Delta} f_1(x) f_4(y) \varphi_l^p(z_1', z_2') \varphi_{l'}^p(z_1', z_2') U(z_1, z_2; z)\, \mathrm{d}z_1'\, \mathrm{d}z_2' +$$

$$+|J|^{-1} \int\limits_{\Delta} f_2(x,y) f_4(y) \left((z_{21}-z_{23}) \frac{\partial \varphi_l^p(z_1', z_2')}{\partial z_1'} + (z_{22}-z_{21}) \frac{\partial \varphi_l^p(z_1', z_2')}{\partial z_2'} \right) \times$$

$$\times \left((z_{21}-z_{23}) \frac{\partial \varphi_{l'}^p(z_1', z_2')}{\partial z_1'} + (z_{22}-z_{21}) \frac{\partial \varphi_{l'}^p(z_1', z_2')}{\partial z_2'} \right) \mathrm{d}z_1'\, \mathrm{d}z_2' +$$

$$+|J|^{-1} \int\limits_{\Delta} \frac{f_1(x)}{f_3(x)} f_5(x,y) \left((z_{11}-z_{13}) \frac{\partial \varphi_l^p(z_1', z_2')}{\partial z_1'} + (z_{12}-z_{11}) \frac{\partial \varphi_l^p(z_1', z_2')}{\partial z_2'} \right) \times$$

$$\times \left((z_{11}-z_{13}) \frac{\partial \varphi_{l'}^p(z_1', z_2')}{\partial z_1'} + (z_{12}-z_{11}) \frac{\partial \varphi_{l'}^p(z_1', z_2')}{\partial z_2'} \right) \mathrm{d}z_1'\, \mathrm{d}z_2', \quad (23)$$

$$b_{ll'}^p = \int\limits_{\Delta_q} f_1(x) f_4(y) \varphi_l^p(z_1, z_2) \varphi_{l'}^p(z_1, z_2)\, \mathrm{d}z_1\, \mathrm{d}z_2 =$$

$$= |J| \int\limits_{\Delta} f_1(x) f_4(y) \varphi_l^p(z_1', z_2') \varphi_{l'}^p(z_1', z_2')\, \mathrm{d}z_1'\, \mathrm{d}z_2', \quad (24)$$

where Δ_q is a triangular element with the vertices $(z_{11}, z_{21})(z_{12}, z_{22})(z_{13}, z_{23})$, Δ is the triangle with vertices $(0,0)(1,0)(0,1)$, and

$$J = \begin{vmatrix} \dfrac{\partial z_1}{\partial z_1'} & \dfrac{\partial z_1}{\partial z_2'} \\ \dfrac{\partial z_2}{\partial z_1'} & \dfrac{\partial z_2}{\partial z_2'} \end{vmatrix} = -z_{22}z_{13} + z_{22}z_{11} + z_{21}z_{13} + z_{23}z_{12} - z_{23}z_{11} - z_{21}z_{12}$$

is the Jacobian of the transformation from the global frame ($x \equiv z_1, y \equiv z_2$) to the local one (z_1', z_2'); $\mathrm{d}z_1 \mathrm{d}z_2 = J \mathrm{d}z_1' \mathrm{d}z_2'$ and (z_1, z_2) are expressed via (z_1', z_2') by the relations:

$$z_1 = z_{11} + (z_{12}-z_{11}) z_1' + (z_{13}-z_{11}) z_2',\ z_2 = z_{21} + (z_{22}-z_{21}) z_1' + (z_{23}-z_{21}) z_2'. \quad (25)$$

In this case we have explicit expression for shape functions $\varphi_l^p(z_1', z_2')$:

$$\varphi_l^p(z_1', z_2') = \prod_{n_1'=0}^{n_1-1} \frac{1 - z_1' - z_2' - n_1'/p}{n_1/p - n_1'/p} \prod_{n_2'=0}^{n_2-1} \frac{z_1' - n_2'/p}{n_2/p - n_2'/p} \prod_{n_3'=0}^{n_3-1} \frac{z_2' - n_3'/p}{n_3/p - n_3'/p}.$$

Remark. We start from the initial (global) coordinate frame ($x \equiv z_1, y \equiv z_2$) in which the coordinates of vertices of the triangle Δ_q are equal to $(z_{11}, z_{21}), (z_{12}, z_{22}), (z_{13}, z_{23})$, and the local coordinate frame ($x \equiv z_1', y \equiv z_2'$) in which the coordinates of the same vertices of the triangle Δ are equal to $(z_{11}', z_{21}') = (0,0), (z_{12}', z_{22}') = (1,0), (z_{13}', z_{23}') = (0,1)$.

We seek the relation between the global and the local coordinates of the triangle vertices in the form

$$z_1 = c_{10} + c_{11} z_1' + c_{12} z_2',\ z_2 = c_{20} + c_{21} z_1' + c_{22} z_2'. \quad (26)$$

Substituting the coordinates of three vertices in the global and the local frame into Eq.(26), we obtain the system of algebraic equations for calculating the coefficients c_{**}:

$$z_{11}{=}c_{10},\ z_{21}{=}c_{20},\quad z_{12}{=}c_{10}{+}c_{11},\ z_{22}{=}c_{20}{+}c_{21},\quad z_{13}{=}c_{10}{+}c_{12},\ z_{23}{=}c_{20}{+}c_{22}.$$

Substituting the calculated coefficients into Eq.(26), we arrive at the formula (25) for the transformation of coordinates $(z_1, z_2) \to (z_1', z_2')$, from which we express the inverse transformation of coordinates $(z_1', z_2') \to (z_1, z_2)$

$$z_1'{=}{-}J^{-1}(z_{23}z_{11}{-}z_{21}z_{13}){+}J^{-1}(z_{23}{-}z_{21})z_1{-}J^{-1}(z_{13}{-}z_{11})z_2,$$

$$z_2'{=}J^{-1}(z_{22}z_{11}{-}z_{21}z_{12}){+}J^{-1}({-}z_{22}{+}z_{21})z_1{+}J^{-1}(z_{12}{-}z_{11})z_2,$$

$$J{=}({-}z_{22}z_{13}{+}z_{22}z_{11}{+}z_{21}z_{13}{+}z_{23}z_{12}{-}z_{23}z_{11}{-}z_{21}z_{12}),$$

where J^{-1} is the Jacobian of the inverse transformation from the local frame (z_1', z_2') to the global one $(x \equiv z_1, y \equiv z_2)$: $\mathrm{d}z_1'\mathrm{d}z_2' = J^{-1}\mathrm{d}z_1\mathrm{d}z_2$.

The integrals (22) and (23)–(24) are evaluated using the Gaussian quadrature of the order $p+1$. Note that in the present approach the maximum half-band width of the matrices $\mathbf{A}^p$ and $\mathbf{B}^p$ is small compared to their dimension and is not greater than $(p+1)(p+1)$.

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 the skyline storage mode which stores the 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 the matrix $\mathbf{A}^p$ in Eq. (21) is not positively defined, the problem (21) is replaced with the following problem:

$$\tilde{\mathbf{A}}^p\,\boldsymbol{\xi}^h = \tilde{\varepsilon}^h\,\mathbf{B}^p\,\boldsymbol{\xi}^h,\quad \tilde{\mathbf{A}}^p = \mathbf{A}^p - \alpha\mathbf{B}^p. \tag{27}$$

The number α (the shift of the energy spectrum) is chosen such that the matrix $\tilde{\mathbf{A}}^p$ is positive defined. The eigenvector of the problem (27) is the same, and $\varepsilon^h = \tilde{\varepsilon}^h + \alpha$.

4. The algorithm for calculating the parametric derivatives of eigenfunctions and the matrices of effective potentials

Taking a derivative of the boundary problem (15)–(17) with respect to the parameter z, we find that $\partial_z\Phi_i(x, y; z)$ is a solution of the following boundary problem

$$(D(x,y;z){-}\varepsilon_i(z))\,\frac{\partial\Phi_i(x,y;z)}{\partial z}{=}{-}\left[\frac{\partial}{\partial z}\,(U(x,y;z){-}\varepsilon_i(z))\right]\Phi_i(x,y;z), \tag{28}$$

$$\lim_{x\to x_t} f_2(x,y)\frac{\partial^2\Phi_i(x,y;z)}{\partial x\partial z} = 0 \ \text{ or } \ \frac{\partial\Phi_i(x_t,y;z)}{\partial z} = 0,\ y\in[y_{\min}, y_{\max}],$$

$$\lim_{y\to y_t} f_5(x,y)\frac{\partial^2\Phi_i(x,y;z)}{\partial y\partial z} = 0 \ \text{ or } \ \frac{\partial\Phi_i(x,y_t;z)}{\partial z} = 0,\ x\in[x_{\min}, x_{\max}],$$

where $t = \min, \max$. The parametric BVP (28), (29) has a unique solution, if and only if it satisfies the conditions

$$\frac{\partial\varepsilon_i(z)}{\partial z}=\int\limits_{x_{\min}}^{x_{\max}}\int\limits_{y_{\min}}^{y_{\max}}\mathrm{d}x\,\mathrm{d}y f_1(x)f_4(y)\left(\Phi_i(x,y;z)\right)\frac{\partial U(x,y;z)}{\partial z}\Phi_i(x,y;z), \tag{29}$$

$$\int\limits_{x_{\min}}^{x_{\max}}\int\limits_{y_{\min}}^{y_{\max}}\mathrm{d}x\,\mathrm{d}y f_1(x)f_4(y)\left(\Phi_i(x,y;z)\right)\frac{\partial\Phi_i(x,y;z)}{\partial z}=0. \tag{30}$$

Below we present an efficient numerical method that allows the calculation of $\partial_z\Phi_i(x,y;z)$ with the same accuracy as achieved for the eigenfunctions of the BVP (15)–(17) and the use of it for computing the matrices of the effective potentials defined as

$$\begin{aligned}H_{ij}(z)=H_{ji}(z)&=\int\limits_{x_{\min}}^{x_{\max}}\mathrm{d}x\,f_1(x)\int\limits_{y_{\min}}^{y_{\max}}\mathrm{d}y\,f_4(y)\frac{\partial\Phi_i(x,y;z)}{\partial z}\frac{\partial\Phi_j(x,y;z)}{\partial z},\\ Q_{ij}(z)=-Q_{ji}(z)&=-\int\limits_{x_{\min}}^{x_{\max}}\mathrm{d}x\,f_1(x)\int\limits_{y_{\min}}^{y_{\max}}\mathrm{d}y\,f_4(y)\Phi_i(x,y;z)\frac{\partial\Phi_j(x,y;z)}{\partial z}.\end{aligned} \tag{31}$$

The boundary problem (28)–(30) is reduced to the linear system of inhomogeneous algebraic equations with respect to the unknown $\partial\boldsymbol{\xi}^h/\partial z$:

$$\mathbf{L}\frac{\partial\boldsymbol{\xi}^h}{\partial z}\equiv(\mathbf{A}^p-\varepsilon^h\mathbf{B}^p)\frac{\partial\boldsymbol{\xi}^h}{\partial z}=b,\quad b=-\left(\frac{\partial\mathbf{A}^p}{\partial z}-\frac{\partial\varepsilon^h}{\partial z}\mathbf{B}^p\right)\boldsymbol{\xi}^h. \tag{32}$$

The normalization condition (17), the condition of orthogonality between the function and its parametric derivative (30), and the additional conditions (29) for the solution of (32) read as

$$\left(\boldsymbol{\xi}^h\right)^T\mathbf{B}^p\boldsymbol{\xi}^h=1,\quad\left(\frac{\partial\boldsymbol{\xi}^h}{\partial z}\right)^T\mathbf{B}^p\boldsymbol{\xi}^h=0,\quad\frac{\partial\varepsilon^h}{\partial z}=\left(\boldsymbol{\xi}^h\right)^T\frac{\partial\mathbf{A}^p}{\partial z}\boldsymbol{\xi}^h. \tag{33}$$

Then the potential matrix elements $H^h_{ij}(z)$ and $Q^h_{ij}(z)$ (31) corresponding to Eqs. (11)–(12) can be calculated using the formulas

$$H^h_{ij}(z)=\left(\frac{\partial\boldsymbol{\xi}^h_i}{\partial z}\right)^T\mathbf{B}^p\frac{\partial\boldsymbol{\xi}^h_j}{\partial z},\quad Q^h_{ij}(z)=-\left(\boldsymbol{\xi}^h_i\right)^T\mathbf{B}^p\frac{\partial\boldsymbol{\xi}^h_j}{\partial z}. \tag{34}$$

Since ε^h is an eigenvalue of (21), the matrix $\mathbf{L}$ in Eq. (32) is degenerate. In this case the algorithm for solving Eq. (32) can be written in three steps as follows:

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

$$\bar{\mathbf{L}}\mathbf{v}=\bar{\mathbf{b}},\quad\bar{\mathbf{L}}\mathbf{w}=\mathbf{d}, \tag{35}$$

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

$$\bar{L}_{ss'}=\begin{cases}L_{ss'}, & (s-S)(s'-S)\neq 0,\\ \delta_{ss'}, & (s-S)(s'-S)=0,\end{cases}$$

$$\bar{b}_s = \begin{cases} b_s, & s \neq S, \\ 0, & s = S, \end{cases} \qquad d_s = \begin{cases} L_{sS}, & s \neq S, \\ 0, & s = S, \end{cases}$$

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

Step k2. Evaluate the coefficient γ

$$\gamma = -\frac{\gamma_1}{(\mathbf{D}_S - \gamma_2)}, \quad \gamma_1 = \mathbf{v}^T\mathbf{B}^p\boldsymbol{\xi}^h, \quad \gamma_2 = \mathbf{w}^T\mathbf{B}^p\boldsymbol{\xi}^h, \quad \mathbf{D}_S = (\mathbf{B}^p\boldsymbol{\xi}^h)_S. \tag{36}$$

Step k3. Evaluate the vector $\partial_z\boldsymbol{\xi}^h$

$$\frac{\partial\xi_s^h}{\partial z} = \begin{cases} v_s - \gamma w_s, & s \neq S, \\ \gamma, & s = S. \end{cases} \tag{37}$$

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

Let $D(x, y; z)$ in Eq. (15) be a continuous and bounded positively defined operator on the space $\mathcal{H}^1$ with the energy norm, $\varepsilon_i(z)$, $\Phi_i(x, y; z) \in \mathcal{H}^2$ being the exact solutions of Eqs. (15)–(17), and $\varepsilon_i^h(z)$, $\Phi_i^h(x, y; z) \in \mathcal{H}^1$ being the corresponding numerical solutions. Then the following estimates are valid [10, 12]

$$\left|\varepsilon_i(z) - \varepsilon_i^h(z)\right| \leqslant c_1 h^{2p}, \quad \left\|\Phi_i(x, y; z) - \Phi_i^h(x, y; z)\right\|_0 \leqslant c_2 h^{p+1}, \tag{38}$$

where

$$\|\Phi_i(x, y; z)\|_0^2 = \int\limits_{x_{\min}}^{x_{\max}} \int\limits_{y_{\min}}^{y_{\max}} f_2(x, y)\,\mathrm{d}x f_5(x, y)\,\mathrm{d}y \Phi_i(x, y; z)\Phi_i(x, y; z),$$

h is the largest distance between any two points in Δ_q (see [12], p. 161), p is the order of the finite elements, i is the number of the corresponding solutions, and the constants c_1 and c_2 are independent of the step h.

The following theorem can be formulated.

Theorem 1. *Let $D(x, y; z)$ in Eq. (15) be a continuous and bounded positively defined operator on the space $\mathcal{H}^1$ with the energy norm. Also let $\partial_z U(x, y; z)$ be continuous and bounded for each value of the parameter z. Then for the exact values of the solutions $\partial_z\varepsilon_i(z)$, $\partial_z\Phi_i(x, y; z) \in \mathcal{H}^2$, $H_{ij}(z)$, $Q_{ij}(z)$ from (28)–(31) and the corresponding numerical values $\partial_z\varepsilon_i^h(z)$, $\partial_z\Phi_i^h(x, y; z) \in \mathcal{H}^1$, $H_{ij}^h(z)$, $Q_{ij}^h(z)$ from (32)–(34) the following estimates are valid:*

$$\left|\frac{\partial\varepsilon_i(z)}{\partial z} - \frac{\partial\varepsilon_i^h(z)}{\partial z}\right| \leqslant c_3 h^{2p}, \quad \left\|\frac{\partial\Phi_i(x, y; z)}{\partial z} - \frac{\partial\Phi_i^h(x, y; z)}{\partial z}\right\|_0 \leqslant c_4 h^{p+1},$$
$$\left|Q_{ij}(z) - Q_{ij}^h(z)\right| \leqslant c_5 h^{2p}, \quad \left|H_{ij}(z) - H_{ij}^h(z)\right| \leqslant c_6 h^{2p}, \tag{39}$$

where h is the largest distance between any two points of the finite element Δ_q, p is the order of finite elements, i, j are the numbers of the corresponding solutions, and the constants c_3, c_4, c_5 and c_6 are independent of the step h.

The proof is straightforward following the proof schemes in accordance with [10, 13].

5. Benchmark calculations

5.1. The solution of 2D BVP in the triangular domain

As a benchmark example we consider the exactly solvable BVP for a membrane in the form of equilateral triangle with side equal to $4\pi/3$, in the conventional variables $(x, y) \in \Omega(x, y)$

$$\left(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \varepsilon_i\right) \Phi_i(x, y) = 0 \tag{40}$$

with the Dirichlet or Neumann conditions at the boundary $\partial\Omega(x, y)$ of the region $\Omega(x, y)$. In both cases the eigenvalues ε_i are integer [14–16].

The BVPs were solved on the uniform finite-element grid composed of n^2 equilateral triangles with the side equal to $4\pi/(3n)$. In Table 1 we present the estimations of the finite-element scheme order p depending on the size of elements.

Table 1

Discrepancies $\delta\varepsilon_i(n) = |\varepsilon_i^h(n) - \varepsilon_i|$ of the first $\varepsilon_1 = 3$ and the fourth $\varepsilon_4 = 3$ eigenvalues of the BVP(40) with Dirichlet and Neumann boundary conditions, respectively, and the Runge coefficients $\mathbf{Ru}_i = \log_2((\delta\varepsilon_i(n) - \delta\varepsilon_i(2n))/(\delta\varepsilon_i(2n) - \delta\varepsilon_i(4n)))$ for the schemes of the first $p = 1$ and the second $p = 2$ orders; n is the number of elements

p	n	$\delta\varepsilon_1(n)$	$\delta\varepsilon_1(2n)$	$\delta\varepsilon_1(4n)$	Ru_1
1	6	0.06914677126132	0.01717343333794	0.00428595766335	2.011
2	3	0.00470310603030	0.00030790240009	0.00001932528605	3.928
p	n	$\delta\varepsilon_4(n)$	$\delta\varepsilon_4(2n)$	$\delta\varepsilon_4(4n)$	Ru_4
1	6	0.06914677126135	0.01717343333808	0.00428595766371	2.011
2	3	0.00470310603029	0.00030790240005	0.00001932528593	3.928

They are seen to correspond rigorously to the theoretical estimations (38) of the order $O(h^{2p})$ of the eigenvalues approximation. The first eight eigenfunctions of the BVPs (40) with the Neumann and Dirichlet boundary conditions are shown in Figs. 1 and 2.

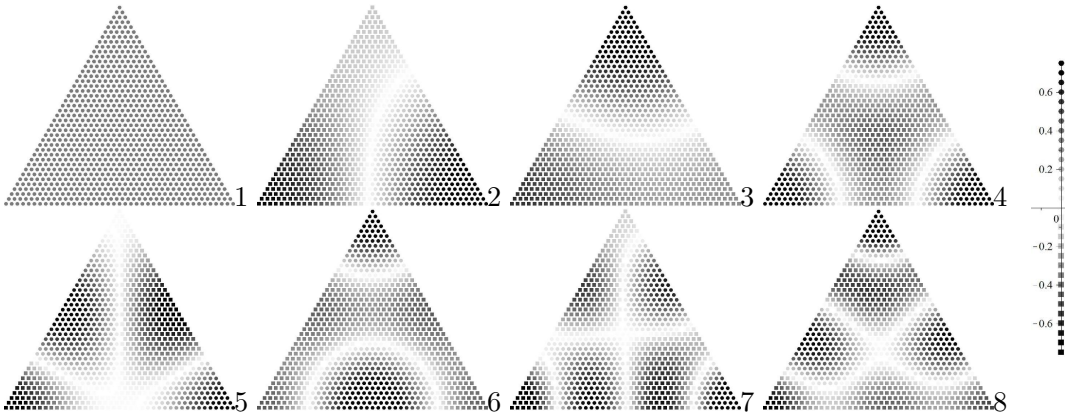

Figure 1. The first eight eigenfunctions of the BVPs (40) in the triangle region with the Neumann boundary conditions. The eigenvalues $\varepsilon_i = 0, 1, 1, 3, 4, 4, 7, 7$ at $i = 1, ..., 8$.

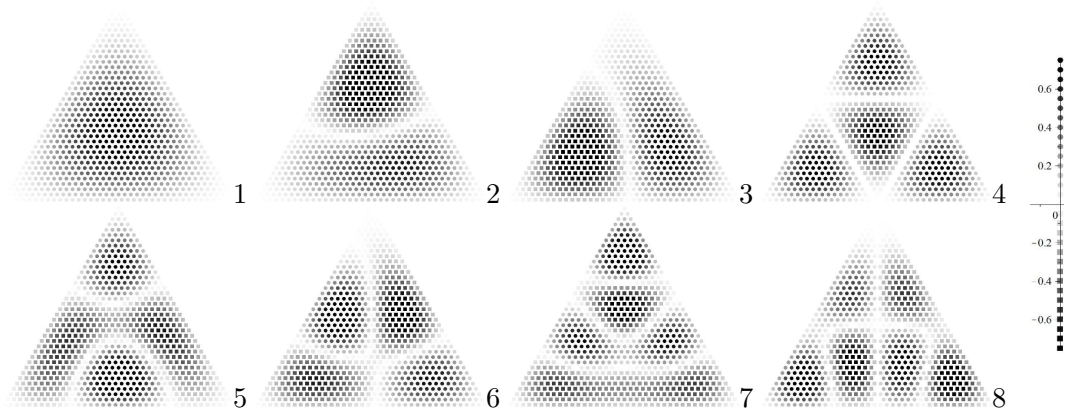

Figure 2. The first eight eigenfunctions of the BVP (40) in the triangle region with the Dirichlet boundary conditions. The eigenvalues $\varepsilon_i = 3, 7, 7, 12, 13, 13, 19, 19$ at $i = 1, ..., 8$.

5.2. Solution of the parametric 2D BVP for the oscillator potential

We consider the parametric 2D BVP (15)–(17) at $f_1(x) = f_2(x, y) = f_3(x) = f_4(y) = f_5(x, y) = 1$, with the potential function

$$U(x, y; z) \equiv U(z_1, z_2; z_3) = (z_1 - z_3)^2 + (3/2)^2 z_2, \tag{41}$$

which has the known spectrum $\varepsilon_{j=\{j_1,j_2\}} = (2(j_1 - 1) + 1) + 3/2(2(j_2 - 1) + 1)$ and the eigenfunctions $\Phi_{j_1,j_2}(z_1, z_2; z_3) = \Phi_{j_1-1}(z_1; z_3)\Phi_{j_2-1}(z_2; 0)$, where $\Phi_{j_1}(z_1; z_3)$ and $\Phi_{j_2-1}(z_2; 0)$ are determined in (45) at $\omega_1(x_s) = 1$, $z_{01}(x_s = z_3) = z_3$ and $\omega_2(x_s) = 3/2$, $z_{02}(x_s) = 0$, respectively. The matrix elements $Q_{i=\{i_1,i_2\},j=\{j_1,j_2\}}$ and $H_{i=\{i_1,i_2\},j=\{j_1,j_2\}}$ are calculated in the analytical form

$$\begin{aligned} Q_{ij}(x_s) &= \delta_{i_2 j_2} \mathrm{sign}(j_1 - i_1) \frac{\sqrt{2n}}{2} \delta_{|j_1 - i_1|,1}, \\ H_{ij}(x_s) &= \delta_{i_2 j_2} \left(\frac{(2n+1)}{2} \delta_{j_1 - i_1, 0} - \frac{\sqrt{n(n-1)}}{2} \delta_{|j_1 - i_1|,2} \right) \end{aligned} \tag{42}$$

where $n = \max(i_1, j_1) - 1$.

Solving the BVP, we use 294 finite elements, i.e. *equilateral triangles* with the side equal to 1 that form a regular hexagon with the vertices $\{(7\cos \pi n/3,\ 7 \sin \pi n/3)\}_{n=0}^{5}$. In each element the interpolation polynomials of the six order were applied. Stiffness and mass matrices with dimensions of 5167×5167 were used. The calculated eigenvalues ε_i^h are: $\varepsilon_i^h = (2.500000001,\ 4.500000002,\ 5.500000005,\ 6.500000014,\ 7.500000025)$, and the exact ones ε_i are: $\varepsilon_i = (2.5,\ 4.5,\ 5.5,\ 6.5,\ 7.5)$.

The calculated matrices Q_{ij}^h and H_{ij}^h, $i, j = 1, ..., 5$ from Eq. (34) of the parametric 2D BVP with the potential function (41) are

$$Q_{ij}^h = \begin{pmatrix} -0.00000000 & 0.70710678 & -0.00000000 & -0.00000000 & 0.00000000 \\ -0.70710678 & -0.00000000 & -0.00000000 & 1.00000000 & 0.00000000 \\ -0.00000000 & 0.00000000 & 0.00000000 & -0.00000000 & 0.70710678 \\ 0.00000000 & -1.00000000 & 0.00000000 & -0.00000000 & 0.00000000 \\ -0.00000000 & 0.00000000 & -0.70710678 & 0.00000000 & 0.00000000 \end{pmatrix},$$

$$H_{ij}^h = \begin{pmatrix} 0.50000000 & -0.00000000 & 0.00000000 & -0.70710678 & 0.00000000 \\ -0.00000000 & 1.49999999 & -0.00000000 & -0.00000000 & -0.00000000 \\ 0.00000000 & -0.00000000 & 0.49999999 & -0.00000000 & 0.00000000 \\ -0.70710678 & -0.00000000 & -0.00000000 & 2.50000001 & -0.00000000 \\ 0.00000000 & -0.00000000 & 0.00000000 & -0.00000000 & 1.49999999 \end{pmatrix}$$

From the comparison of the calculated and the exact values of ε_i and Q_{ij}, H_{ij} from (42), one can see that the achieved accuracy of results is of the order of 8–9 significant digits.

The parametric surface eigenfunctions and their derivatives with respect to the parameter under the dipole splitting are shown in Fig. 3.

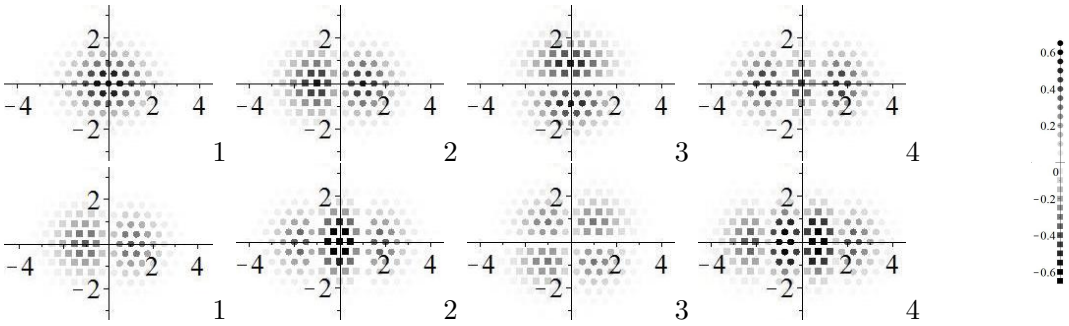

Figure 3. The first four eigenfunctions of the parametric 2D BVP with the potential function (41) and their derivatives with respect to the parameter at $z = 0$.

5.3. The solution of 2D BVP for the C_{3v} oscillator potential

Let us consider the 2D BVP (15)–(17) for $x{=}a_{22}$, $y{=}a_{20}$ with the potential function $U(x,y) = 2mV(x,y)$ and the spectral parameter $\varepsilon = 2mE$, and $f_1(x) = f_2(x,y) = f_3(x) = f_4(y) = f_5(x,y) = 1$. The quadrupole potential energy is approximated by the quartic potential:

$$V(a_{22},a_{20}){=}c_1(a_{22}^2{+}a_{20}^2){+}c_2(a_{22}^2a_{20}{-}a_{20}^3/3){+}c_3(a_{22}^2{+}y^2)^2{+}c_0 \tag{43}$$

We use the set of parameters $c_1{=}{-}120$, $c_2{=}240$, $c_3{=}1200$, $c_0{=}65/16$ that provide a crude approximation for the shape of $^{156}_{64}\mathrm{Gd}_{92}$, which has been fitted in the following points[1]: the minima at $(a_{22},a_{20}){=}(0,1/4)$, $V(0,1/4){=}0$; the maxima at $(a_{22},a_{20}){=}(0,0)$, $V(0,0){=}65/16$; and the saddle point at $(a_{22},a_{20}){=}(0,-1/5)$, $V(0,-1/5){=}729/400$ (see Fig. 4).

We choose the mass parameter to be $m{=}B_2{=}124$. Thus, there are ground and doubly degenerate excited states, localized in three wells.

The BVP was solved using three algorithms (and the forth in Section 5.4):

1. The solution of the BVP was calculated using the FEM scheme from Section 3 on the *rectangular* grid $[-0.4,-0.3,...,0.4]\times[-0.4,-0.3,...,0.4]$ with Lagrange interpolation polynomials of the order $p = 12$. The first 18 eigenvalues were calculated with 9 significant digits and are presented in Table 2.

[1]The fitting points in our parametrization are related to those of Ref. [4] as $a_{22} = \sqrt{2}\alpha_{22}, a_{20} = \alpha_{20}$.

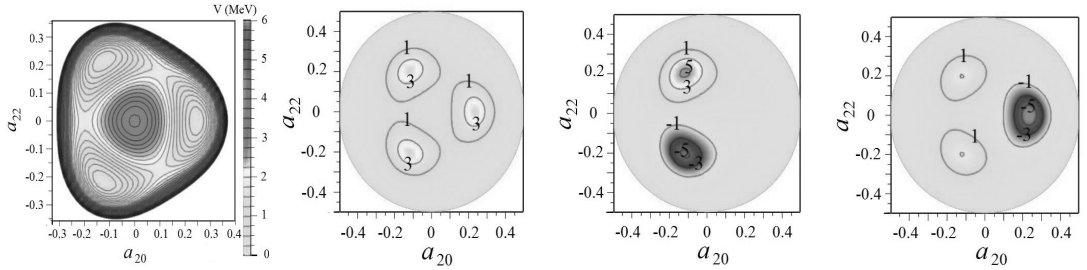

Figure 4. The potential energy of the C_{3v} oscillator having the quadrupole shape, the eigenfunction $\Psi_1(a_{22}, a_{20})$ of the ground state (irr. A1) and the degenerate eigenfunctions $\Psi_2(a_{22}, a_{20})$ (irr. E1) and $\Psi_3(a_{22}, a_{20})$ (irr. E2)

Table 2

The first energy levels of the 2D BVP using triangular $\varepsilon_i^{\triangle}$ and rectangular $\varepsilon_i^{\square}$ finite elements and the Kantorovich method ε_i^h using $j_{\max}$=28 parametric basis functions, classified by irrs (Class.) of the C_{3v} point group, E_i (MeV)

i	$\varepsilon_i^{\triangle}$	$\varepsilon_i^{\square}$	ε_i^h	$E_i^h{=}\varepsilon_i^h/2m$	Class.
1	381.754344	381.754355	381.754351	1.53933206	A1
2	387.240633	387.240644	387.240641	1.56145419	E1
3	387.240633	387.240646	387.240641	1.56145419	E2
4	617.024951	617.024967	617.024963	2.48800388	E1
5	617.024951	617.024989	617.024963	2.48800388	E2
6	667.104970	667.105020	667.104992	2.68993948	A2
7	695.166557	695.166590	695.166575	2.80309103	A1
8	785.680037	785.680100	785.680078	3.16806483	E1
9	785.680037	785.680136	785.680078	3.16806483	E2
10	898.045395	898.045497	898.045434	3.62115094	A1
11	915.823095	915.823200	915.823167	3.69283535	E1
12	915.823095	915.823309	915.823167	3.69283535	E2
13	993.158636	993.158784	993.158708	4.00467221	E2
14	993.158636	993.158872	993.158708	4.00467221	E1
15	1063.73690	1063.73709	1063.73692	4.28926178	A1
16	1119.21670	1119.21668	1119.21649	4.51296973	A2
17	1174.72840	1174.71177	1174.71166	4.73674057	E1
18	1174.75531	1174.71183	1174.71166	4.73674057	E2

2. In the solution of the BVP we used 54 finite elements in the form of *equilateral triangles* with the side equal to 1/6, forming a regular hexagon with the vertices $\{(0.5\cos\pi n/3,\ 0.5\sin\pi n/3)\}_{n=0}^{5}$. In each finite element the interpolation polynomials of the fifth order were applied. The stiffness and the mass 721×721 matrices were used. The calculated eigenvalues are presented in Table 2.

3. The problem (1)–(43) was also solved using the Kantorovich method implemented in the FEM program KANTBP 2 [5], with $j_{\max}$=28 parametric basis functions calculated using the FEM program ODPEVP [6]. The solution was calculated in the domain $\sqrt{a_{20}^2+a_{22}^2}<1/2$ with Dirichlet BCs at the boundary $\sqrt{a_{20}^2+a_{22}^2}=1/2$ using the scheme presented in Section 2. The calculations were performed in the case of $(x_f, x_s)= (a_{22}, a_{20})$ as well as $(x_f, x_s)=(a_{20}, a_{22})$ on the FE grid $\{-1/2, -1/3, -1/6, 0, 1/6, 1/3, 1/2\}$ with Lagrange interpolation polynomials of the order $p = 12$.

The point symmetry group C_{3v} of the problem (1), (43) has four irreducible representations (irrs.) A1, A2, E1 and E2 to classify the solutions, the E-type states being doubly degenerate [17,18]. The calculated eigenvalues are presented in Table 2. The first eigenfunctions for each of the irrs. A1, E1, E2 are shown in Fig. 4.

5.4. Parametric surface functions for KM in the analytical form

Let us consider the BVP for Eq. (5) with the etalon potential $V_o(x_f; x_s, g(x_s))$:

$$\begin{gathered}\left(-\frac{\partial^2}{\partial x_f^2}+V_o(x_f; x_s, g)-\varepsilon_i(x_s)\right)\Phi_i(x_f; x_s)=0,\\ V_o(x_f, x_s, g)=V_0(x_s)+\omega^2(x_s)(x_f-z_0(x_s))^2,\end{gathered} \tag{44}$$

where $g(x_s)$ is the set of parameters, $g(x_s) = \{V_0(x_s), \omega^2(x_s), z_0(x_s)\}$. In the considered case the parametric eigenvalue problem (5)–(7) has an exact solution, i.e., the parametric eigenfunctions $\Phi_i(x_f; x_s)$ and potential curves $\varepsilon_i(x_s)$ are expressed in the analytical form

$$\begin{gathered}\varepsilon_i(x_s) = V_0(x_s)+\omega(x_s)(2(i-1)+1),\\ \Phi_1(x_f; x_s) = \frac{\omega^{1/4}(x_s)}{\pi^{1/4}}\exp\left(-\omega(x_s)(x_f-z_0(x_s))^2/2\right),\\ \Phi_i(x_f; x_s) = \frac{\sqrt{2}\sqrt{\omega(x_s)}(x_f-z_0(x_s))}{\sqrt{i-1}}\Phi_{i-1}(x_f; x_s) - \frac{\sqrt{i-2}}{\sqrt{i-1}}\Phi_{i-2}(x_f; x_s).\end{gathered} \tag{45}$$

The integration in the effective potentials (11) with the basis functions (45) is carried out analytically, which yields the expressions

$$Q_{ij}(x_s)=\mathrm{sign}(j-i)\left(\frac{\sqrt{2n\omega(x_s)}}{2}\frac{\mathrm{d}z_0(x_s)}{\mathrm{d}x_s}\delta_{|j-i|,1}-\frac{\sqrt{n(n-1)}}{4}\frac{\mathrm{d}\omega(x_s)}{\mathrm{d}x_s}\delta_{|j-i|,2}\right),$$

$$\begin{aligned}H_{ij}(x_s)=&\left(\frac{n^2+n+1}{8\omega^2(x_s)}\delta_{j-i,0}-\frac{\sqrt{n(n-1)(n-2)(n-3)}}{16\omega^2(x_s)}\delta_{|j-i|,4}\right)\left(\frac{\mathrm{d}\omega(x_s)}{\mathrm{d}x_s}\right)^2+\\ &+\left(\frac{\omega(x_s)(2n+1)}{2}\delta_{j-i,0}-\frac{\omega(x_s)\sqrt{n(n-1)}}{2}\delta_{|j-i|,2}\right)\left(\frac{\mathrm{d}z_0(x_s)}{\mathrm{d}x_s}\right)^2-\\ &-\left(\frac{n\sqrt{2n}}{4\sqrt{\omega(x_s)}}\delta_{|j-i|,1}+\frac{\sqrt{2n(n-1)(n-2)}}{4\sqrt{\omega(x_s)}}\delta_{|j-i|,3}\right)\frac{\mathrm{d}z_0(x_s)}{\mathrm{d}x_s}\frac{\mathrm{d}\omega(x_s)}{\mathrm{d}x_s},\end{aligned}$$

where $n=\max(i,j)-1$. The effective potentials are calculated by integrating the difference $V(x_f,x_s)-V_o(x_f;x_s)$ with the basis functions:

$$V_{ij}(x_s)=\int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)}\Phi_i(x_f;x_s)(V(x_f,x_s)-V_o(x_f;x_s))\Phi_j(x_f;x_s)\,\mathrm{d}x_f.$$

During the simulation the adiabatic parameters $V_0(x_s)$, $\omega(x_s)$, $z_0(x_s)$ of the etalon potential (44) were found from the conditions

$$\min_{V_0(x_s),\omega^2(x_s),z_0(x_s)}\int\limits_{x_f^{\min}(x_s)}^{x_f^{\max}(x_s)}(V(x_fx_s)-V_o(x_f;x_s))^2\,\mathrm{d}x_f. \tag{46}$$

For the potential (43) from the condition (46) we have

$$\omega(x_s)=\sqrt{2m}\sqrt{\frac{960}{7}+240x_s+2400x_s^2},\ z_0(x_s)=0,\quad \text{at}\quad x_s=a_{20},\quad x_f=a_{22},$$
$$\omega(x_s)=\sqrt{2m}\sqrt{\frac{960}{7}+2400x_s^2},\ z_0(x_s)=-\frac{7(20x_s^2-1)}{80(35x_s^2+2)},\quad \text{at } x_s=a_{22},\quad x_f=a_{20}.$$

We performed the calculations for these parameters in the case when $(x_f,x_s)=(a_{22},a_{20})$, as well as $(x_f,x_s)=(a_{20},a_{22})$. The results coincide with those of the calculations of ε_i^h performed in the previous Section 5.3 and presented in Table 2 with 9 significant digits.

6. Conclusion

We elaborated new calculation schemes and algorithms for solving the parametric 2D elliptic BVP using the high-accuracy FEM with rectangular (22) and triangular (23)–(24) elements. The algorithm and the programs calculate with the given accuracy the eigenvalues, the eigenfunctions and their first derivatives with respect to the parameter of the parametric self-adjoint elliptic differential equations with boundary conditions of the Dirichlet and/or Neumann type in the finite 2D domain (15)–(17), (18) and the corresponding inhomogeneous boundary-value problem (28)–(33), obtained by taking a parametric derivative of the original 2D BVP. The program also calculates the potential matrix elements, the integrals of the eigenfunctions multiplied by their first derivatives with respect to the parameter (34). The parametric eigenvalues (potential curves) and the matrix elements computed by the program can be used for solving the bound-state and multi-channel scattering problems for a system of the coupled second-order ODES with using the Kantorovich method. We demonstrated the efficiency of the proposed calculation schemes, algorithms and codes by the example of solving the boundary-value problem of a quadruple vibration collective nuclear model.

We proposed the construction of parametric surface functions in the analytical form as eigenfunctions of the etalon equation (44), which provides the solution of the 2D BPV with given accuracy and reduces the expenditures of computer resources compared to the conventional basis, numerically calculated using FEM. One can construct parametric functions using different types of etalon potentials, e.g., that of the two-center problem with harmonic oscillator potentials [19]. This approach can be generalized for the BVP in a multidimensional domain using, e.g., the multistep Kantorovich method [3].

The proposed algorithms and codes can be adapted and applied to the analysis of quantum transparency effect, to the study of resonance three-body scattering problems, the quantum diffusion of molecules, the penetration of micro-clusters through surfaces, the fragmentation mechanism in producing very neutron-rich light nuclei, and heavy-ion collisions, as well as the microscopic study of tetrahedral-symmetric nuclei.

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Алгоритмы для решения параметрической самосопряжённой эллиптической краевой задачи в двумерной области методом конечных элементов высокого порядка точности

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Рассмотрены вычислительные схемы решения краевых эллиптических задач в рамках метода Канторовича — редукции эллиптической краевой задачи к системе обыкновенных дифференциальных уравнений второго порядка с использованием поверхностных функций, зависящих от независимой переменной системы обыкновенных дифференциальных уравнений как параметра, вычисленные как методом конечных элементов, так и пробных параметрических поверхностных базисных функций, вычисленных в аналитической виде.

Предложены новые вычислительные схемы и алгоритмы для решения параметрической самосопряжённой эллиптической краевой задачи в двумерной области, используя метод конечных элементов высокого порядка точности с прямоугольными и треугольными элементами.

Комплексы программ, реализующие алгоритмы, вычисляют с заданной точностью собственные значения, собственные функции и их первые производные по параметру, связанные с параметрической самосопряжённой краевой задачей для эллиптических дифференциальных уравнений с условиями Дирихле или Неймана на границе в конечной двумерной области, а также потенциальные матричные элементы – интегралы от произведения собственных функций и их первых производных по параметру. Параметрические собственные значения (так называемые потенциальные кривые) и матричные элементы, вычисленные с помощью комплекса программ, можно применять для решения задачи на связанные состояния и многоканальной задачи рассеяния для системы обыкновенных дифференциальных уравнений второго порядка с помощью метода Канторовича.

Эффективность предложенных схем расчёта и алгоритмов демонстрируется решением двумерных эллиптических краевых задач, описывающих квадрупольные колебания в коллективной модели атомного ядра.

Ключевые слова: параметрические эллиптические краевые задачи, метод конечных элементов, метод Канторовича, системы ОДУ второго порядка

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