

KANTBP 4M - PROGRAM FOR SOLVING BOUNDARY PROBLEMS OF THE SYSTEM OF ORDINARY SECOND-ORDER DIFFERENTIAL EQUATIONS

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Environment: MAPLE (tested in versions 14, 16, 17 and 18) / Windows. (Intel Core I7 3.20 Ghz 8 GB RAM 64bit Windows 8.1; 2 x Xeon 3.2 GHz, 4 GB RAM 64bit Windows 7; PC Inter Pentium CPU 1.50 GHz 4GB 64bit Windows 8)

file kantbp4me.pdf contains detailed description,

file kantbp4m.mwt contains the program source code

files examplxx.txt (xx=01-16) contain examples of using of the code. For execution of the code for a selected examplxx.txt user should copy it to Maple worksheet via "copy/paste", or use Maple command << read "examplxx.txt" >>, or open file examplxx.txt by Maple choosing <<Maple Input >>.

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I. BOUNDARY VALUE AND EIGENVALUE PROBLEMS AND SYMMETRIC QUADRATIC FUNCTIONAL

The program KANTBP 4M is intended for solving the boundary value problem and eigenvalue problem for the system of ordinary differential equations of the second order with respect to the unknown functions $\Phi(z) = (\Phi_1(z), \dots, \Phi_N(z))^T$ of the independent variable $z \in \Omega(z^{\min}, z^{\max})$ numerically using the Finite Element Method:

$$(\mathbf{D} - E\mathbf{I}) \Phi^{(i)}(z) \equiv \left(-\frac{1}{f_B(z)} \mathbf{I} \frac{d}{dz} f_A(z) \frac{d}{dz} + \mathbf{V}(z) + \frac{f_A(z)}{f_B(z)} \mathbf{Q}(z) \frac{d}{dz} + \frac{1}{f_B(z)} \frac{d f_A(z) \mathbf{Q}(z)}{dz} - E\mathbf{I} \right) \Phi(z) = 0. \quad (1)$$

Here $f_B(z) > 0$ and $f_A(z) > 0$ are continuous or piecewise continuous positive functions, \mathbf{I} is the unit matrix, $\mathbf{V}(z)$ is a symmetric matrix, $V_{ij}(z) = V_{ji}(z)$, and $\mathbf{Q}(z)$ is an antisymmetric matrix, $Q_{ij}(z) = -Q_{ji}(z)$, of the effective potentials having the dimension $N \times N$. The elements of these matrices are continuous or piecewise continuous real or complex-valued coefficients from the Sobolev space $\mathcal{H}_2^{s \geq 1}(\Omega)$, providing the existence of nontrivial solutions subjected to homogeneous boundary conditions: Dirichlet and/or Neumann, and/or third-kind at the boundary points of the interval $z \in \{z^{\min}, z^{\max}\}$ at given values of the elements of the real or complex-valued matrix $\mathcal{R}(z^t)$ of the dimension $N \times N$

$$(I): \quad \Phi(z^t) = 0, \quad t = \min \text{ and/or } \max, \quad (2)$$

$$(II): \quad \lim_{z \rightarrow z^t} f_A(z) \left(\mathbf{I} \frac{d}{dz} - \mathbf{Q}(z) \right) = 0, \quad t = \min \text{ and/or } \max, \quad (3)$$

$$(III): \quad \left(\mathbf{I} \frac{d}{dz} - \mathbf{Q}(z) \right) \Big|_{z=z^t} = \mathcal{R}(z^t) \Phi(z^t), \quad t = \min \text{ and/or } \max. \quad (4)$$

The solution $\Phi(z) \in \mathcal{H}_2^{s \geq 1}(\bar{\Omega})$ of the BPVs (1)–(4) is reduced to the calculation of stationary points of a symmetric quadratic functional numerically using the Finite Element Method(FEM)

$$\Xi(\Phi, E, z^{\min}, z^{\max}) \equiv \int_{z^{\min}}^{z^{\max}} \Phi^\bullet(z) (\mathbf{D} - E\mathbf{I}) \Phi(z) dz = \Pi(\Phi, E, z^{\min}, z^{\max}) - f^A(z^{\max}) \Phi^\bullet(z^{\max}) \mathbf{G}(z^{\max}) \Phi(z^{\max}) + f^A(z^{\min}) \Phi^\bullet(z^{\min}) \mathbf{G}(z^{\min}) \Phi(z^{\min}), \quad (5)$$

$$\Pi(\Phi, E, z^{\min}, z^{\max}) = \int_{z^{\min}}^{z^{\max}} \left[f^A(z) \frac{d\Phi^\bullet(z)}{dz} \frac{d\Phi(z)}{dz} + f^B(z) \Phi^\bullet(z) \mathbf{V}(z) \Phi(z) + f^A(z) \Phi^\bullet(z) \mathbf{Q}(z) \frac{d\Phi(z)}{dz} - f^A(z) \frac{d\Phi(z)}{dz} \mathbf{Q}(z) \Phi(z) - f^B(z) E \Phi^\bullet(z) \Phi(z) \right] dz, \quad (6)$$

where $\mathbf{G}(z) = \mathcal{R}(z) - \mathbf{Q}(z)$ is a symmetric matrix of the dimension $N \times N$, \bullet denotes either the transposition T , or the Hermitian conjugation \dagger , i.e., the transposition with complex conjugation, depending on the type of the problem to be solved.

II. BRIEF DESCRIPTION OF THE CLASS OF PROBLEMS

Three classes of the boundary value problems are considered

1. For the multichannel scattering problem (examples: 07, 08, 11, 13, 14) on the axis $z \in (-\infty, +\infty)$ at fixed energy $E \equiv \Re E$ the desired matrix solutions $\Phi(z) \equiv \{\Phi_v^{(i)}(z)\}_{i=1}^N$, $\Phi_v^{(i)}(z) = (\Phi_{1v}^{(i)}(z), \dots, \Phi_{Nv}^{(i)}(z))^T$ (the subscript v takes the values \rightarrow or \leftarrow and means the initial direction of the incident wave from left to right or from right to left) the boundary value problem for the system of N ordinary differential equations of the second order (1) in the interval $z \in (z^{\min}, z^{\max})$ are calculated by the code. These matrix solutions are subjected to homogeneous third-kind boundary conditions (4) at the boundary points of the interval $z \in \{z^{\min}, z^{\max}\}$ with the asymptotes of the “incident wave + outgoing waves” type in open channels $i = 1, \dots, N_o$:

$$\Phi_v(z \rightarrow \pm\infty) = \begin{cases} \begin{cases} \mathbf{X}^{(+)}(z) \mathbf{T}_v, & z \in [z^{\max}, +\infty), \\ \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z) \mathbf{R}_v, & z \in (-\infty, z^{\min}], \end{cases} & v = \rightarrow, \\ \begin{cases} \mathbf{X}^{(-)}(z) + \mathbf{X}^{(+)}(z) \mathbf{R}_v, & z \in [z^{\max}, +\infty), \\ \mathbf{X}^{(-)}(z) \mathbf{T}_v, & z \in (-\infty, z^{\min}], \end{cases} & v = \leftarrow, \end{cases} \quad (7)$$

where \mathbf{T}_v and \mathbf{R}_v are unknown rectangular and square matrices of transmission and reflection amplitudes, respectively, to construct the scattering matrix \mathbf{S} of the dimension $N_o \times N_o$:

$$\mathbf{S} = \begin{pmatrix} \mathbf{R}_{\rightarrow} & \mathbf{T}_{\leftarrow} \\ \mathbf{T}_{\rightarrow} & \mathbf{R}_{\leftarrow} \end{pmatrix}, \quad (8)$$

which is the symmetric and unitary in the case of real-valued potentials.

For the multichannel scattering problem on a semiaxis $z \in (z^{\min}, +\infty)$ or $z \in (-\infty, z^{\max})$, the desired matrix solution $\Phi(z)$ of the boundary value problem for the system of N ordinary differential equations of the second order (1) is calculated in the interval $z \in (z^{\min}, z^{\max})$. This matrix solutions is subjected to the homogeneous third-kind boundary conditions (4) at the boundary point z^{\max} or z^{\min} of the interval, with the asymptotes of the ‘‘incident wave + outgoing waves’’ type in the open channels $i = 1, \dots, N_o$:

$$\begin{aligned} \Phi_{\leftarrow}(z \rightarrow +\infty) &= \mathbf{X}^{(-)}(z) + \mathbf{X}^{(+)}(z)\mathbf{R}_{\leftarrow}, & z \in [z^{\max}, +\infty) \\ \text{or } \Phi_{\rightarrow}(z \rightarrow -\infty) &= \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z)\mathbf{R}_{\rightarrow}, & z \in (-\infty, z^{\min}] \end{aligned} \quad (9)$$

and subjected to the homogeneous boundary conditions (Dirichlet and/or Neumann, and/or third-kind (see (2)–(4))) at the boundary point z^{\min} or z^{\max} to construct the scattering matrix $\mathbf{S} = \mathbf{R}_{\leftarrow}$ or $\mathbf{S} = \mathbf{R}_{\rightarrow}$, which is symmetric and unitary in the case of real-valued potentials.

In the solution of a multichannel scattering problem the closed channels are taken into account. In this case the asymptotic conditions (7), (9) have the form

$$\Phi_{\rightarrow}^{as} = \begin{cases} \mathbf{X}_{\max}^{(\rightarrow)}(z)\mathbf{T}_{\rightarrow} + \mathbf{X}_{\max}^{(c)}(z)\mathbf{T}_{\rightarrow}^c, & z \geq z^{\max}, \\ \mathbf{X}_{\min}^{(\rightarrow)}(z) + \mathbf{X}_{\min}^{(\leftarrow)}(z)\mathbf{R}_{\rightarrow} + \mathbf{X}_{\min}^{(c)}(z)\mathbf{R}_{\rightarrow}^c, & z \leq z^{\min}; \end{cases} \quad (10)$$

$$\Phi_{\leftarrow}^{as} = \begin{cases} \mathbf{X}_{\max}^{(\leftarrow)}(z) + \mathbf{X}_{\max}^{(\rightarrow)}(z)\mathbf{R}_{\leftarrow} + \mathbf{X}_{\max}^{(c)}(z)\mathbf{R}_{\leftarrow}^c, & z \geq z^{\max}, \\ \mathbf{X}_{\min}^{(\leftarrow)}(z)\mathbf{T}_{\leftarrow} + \mathbf{X}_{\min}^{(c)}(z)\mathbf{T}_{\leftarrow}^c, & z \leq z^{\min}; \end{cases} \quad (11)$$

where $\mathbf{X}_{\max}^{(\rightarrow)}(z) = \mathbf{X}^{(+)}(z)$, $z \geq z^{\max}$, $\mathbf{X}_{\min}^{(\rightarrow)}(z) = \mathbf{X}^{(+)}(z)$, $z \leq z^{\min}$, $\mathbf{X}_{\min}^{(\leftarrow)}(z) = \mathbf{X}^{(-)}(z)$, $z \leq z^{\min}$ in eqs.(10) and $\mathbf{X}_{\max}^{(\leftarrow)}(z) = \mathbf{X}^{(-)}(z)$, $z \geq z^{\max}$, $\mathbf{X}_{\min}^{(\leftarrow)}(z) = \mathbf{X}^{(+)}(z)$, $z \geq z^{\max}$, $\mathbf{X}_{\min}^{(\leftarrow)}(z) = \mathbf{X}^{(-)}(z)$, $z \leq z^{\min}$ in eqs.(11).

It is assumed that the leading terms of the asymptotic solutions $\mathbf{X}^{(\pm)}(z)$ of the boundary value problem at $z \leq z^{\min}$ and/or $z \geq z^{\max}$ have the following form: in the open channels $V_{i_o i_o}^t < E$ are oscillating solutions:

$$X_{i_o j}^{(\pm)}(z) \rightarrow \frac{\exp(\pm i p_{i_o}^t z)}{\sqrt{f_A(z) p_i^t}} \delta_{i_o j}, \quad p_{i_o}^t = \sqrt{\frac{f_B(z^t)}{f_A(z^t)}} \sqrt{E - V_{i_o i_o}^t} \quad j = 1, \dots, N, \quad i_o = 1, \dots, N_o, \quad (12)$$

in the closed channels $V_{i_c i_c}^t \geq E$ are exponentially decreasing solutions

$$X_{i_c j}^{(c)}(z) \rightarrow \frac{1}{\sqrt{f_A(z)}} \exp(-p_{i_c}^t |z|) \delta_{i_c j}, \quad p_{i_c}^t = \sqrt{\frac{f_B(z^t)}{f_A(z^t)}} \sqrt{V_{i_c i_c}^t - E} \quad j = 1, \dots, N, \quad i_c = N_o + 1, \dots, N. \quad (13)$$

These relations are valid if the coefficients of the equations with $z \leq z^{\min}$ and/or $z \geq z^{\max}$ satisfy the following conditions:

$$\frac{f_A(z)}{f_B(z)} = \frac{f_A(z^t)}{f_B(z^t)} + o(1), \quad t = \min, \max, \quad V_{ii}(z) = V_{ii}^t + o(1), \quad V_{ij}^t(z) = o(1), \quad Q_{ij}^t(z) = o(1), \quad i \neq j. \quad (14)$$

In this version of the program the more general case is not considered, but if the user knows the asymptotic behavior of the solutions, it is possible to apply them. For example, long-range effective potentials, decreasing $\sim z^{-k}$, $k \geq 1$, applied asymptotic expansions of solutions with leading members of (12). Examples of calculation of such expansions by means of recurrence relations are given in [3]. In solving the boundary value problem (1)–(4) the corresponding symmetric quadratic functional (5) is used, where \bullet denotes transpose and complex conjugate \dagger for real-valued potentials and transposition T for complex-valued potentials, required for discretization of the problem by the FEM. Detailed information on the solution of multi-channel scattering problem is given below. See Examples 11 and 13.

2. For the eigenvalue problem (examples: 02, 03, 04, 05, 06, 09, 10, 12, 15, 16) the code calculates a set of M energy eigenvalues E : $\Re E_1 \leq \Re E_2 \leq \dots \leq \Re E_M$ and the corresponding set of eigenfunctions $\Phi(z) \equiv \{\Phi^{(m)}(z)\}_{m=1}^M$, $\Phi^{(m)}(z) = (\Phi_1^{(m)}(z), \dots, \Phi_N^{(m)}(z))^T$ from the space \mathcal{H}_2^2 for the system of N ordinary differential equations of the second order (1) subjected to homogeneous boundary conditions: first and/or second, and/or third kind (see (2)–(4)) in the boundary points of the interval $z \in (z^{\min}, z^{\max})$. In the case of real-valued potentials the solutions are subjected to the normalization and orthogonality conditions

$$\langle \Phi^{(m)} | \Phi^{(m')} \rangle = \int_{z^{\min}}^{z^{\max}} f_B(z) (\Phi^{(m)}(z))^\dagger \Phi^{(m')}(z) dz = \delta_{mm'}, \quad (15)$$

and the corresponding symmetric quadratic functional (5) is used, in which \bullet denotes Hermitian conjugation \dagger , needed for discretization of the problem by the FEM.

In the case of complex valued potentials (examples 06 и 15) the solutions are subjected the normalization and orthogonality conditions

$$(\Phi^{(m)} | \Phi^{(m')}) = \int_{z^{\min}}^{z^{\max}} f_B(z) (\Phi^{(m)}(z))^T \Phi^{(m')}(z) dz = \delta_{mm'}, \quad (16)$$

and corresponding symmetric quadratic functional (5) is used, in which \bullet denotes the transposition T , needed for discretization of the problem by the FEM.

To solve the problem for bound states on the axis or on the semiaxis the initial problem is approximated by boundary value problem (1)–(4) on a finite interval $z \in (z^{\min}, z^{\max})$ with the boundary conditions of the third kind (4) with given matrices $\mathcal{R}(z^t)$, independing on an unknown eigenvalue E , and a set of approximate eigenvalues and eigenfunctions is calculated (examples 02–06, 09, 10, 12, 15–16). If the matrices $\mathcal{R}(z^t)$ are depended on an unknown eigenvalue E , then $\mathcal{R}(z^t, E)$ are determined by the known asymptotic expansion of the desirable solution. In this case, to calculate the approximate eigenfunctions and eigenvalues in the program, Newtonian iteration scheme is implemented. Appropriate initial approximations are chosen from solutions calculated previously with boundary conditions independing on E (Examples 04, 14, 15, 16).

3. For the calculation of metastable states (examples 14 and 15) with unknown complex eigenvalues E the program solves the boundary value problem for a system of equations (1) on a finite interval with homogeneous conditions of the third kind (4), depending on an unknown eigenvalue E , using the appropriate symmetrical quadratic functional (5), where \bullet denotes transposition T , which is necessary for the discretisation of the problem by the FEM. In contrast to the scattering problem, the asymptotic solutions for metastable states contain only outgoing waves, that are considered in a sufficiently large, but finite interval of the spatial variable [5]. For metastable states on the axis $z \in (-\infty, +\infty)$, the eigenfunctions obey the boundary conditions of the third kind (4), where the matrix $\mathcal{R}(\xi_0^t) = \text{diag}(\mathcal{R}(\xi_0^t))$ depends on the desired complex energy eigenvalue $E \equiv E_m = \Re E_m + i\Im E_m$, $\Im E_m < 0$ and is given by

$$\mathcal{R}_{i_o i_o}(z^{\max}, E_m) = \sqrt{\frac{f_B(z^{\max})}{f_A(z^{\max})}} \sqrt{V_{i_o i_o}^{\max} - E_m}, \quad \mathcal{R}_{i_o i_o}(z^{\min}, E_m) = -\sqrt{\frac{f_B(z^{\min})}{f_A(z^{\min})}} \sqrt{V_{i_o i_o}^{\min} - E_m}, \quad (17)$$

because the asymptotic solution of this problem contains only outgoing waves in the open channels $V_{i_o i_o}^t < \Re E$, $i_o = 1, \dots, N_o$, while only decay waves in closed channels $V_{i_c i_c}^t > \Re E$, $i_c = N_o + 1, \dots, N$

$$\mathcal{R}_{i_c i_c}(z^{\max}, E_m) = -\sqrt{\frac{f_B(z^{\max})}{f_A(z^{\max})}} \sqrt{E_m - V_{i_c i_c}^{\max}}, \quad \mathcal{R}_{i_c i_c}(z^{\min}, E_m) = \sqrt{\frac{f_B(z^{\min})}{f_A(z^{\min})}} \sqrt{E_m - V_{i_c i_c}^{\min}}. \quad (18)$$

For metastable states on the semiaxis $z \in (z^{\min}, +\infty)$ or $z \in (-\infty, z^{\max})$, the solution is subject to the boundary condition (4), (17) at the boundary point z^{\max} or z^{\min} and the boundary conditions of the first, second, or third kind (see (2), (3) or (4)) at the boundary point z^{\min} or z^{\max} .

In this case, the eigenfunctions obey the orthogonality and normalization conditions

$$\begin{aligned} (\Phi^{(m')} | \Phi^{(m)}) &= (E_m - E_{m'}) \left[\int_{z^{\min}}^{z^{\max}} (\Phi^{(m')})^T(z) \Phi^{(m)}(z) f_B(z) dz - \delta_{m'm} \right] + C_{m'm} = 0, \\ C_{m'm} &= -f_A(z^{\max}) (\Phi^{(m')})^T(z^{\max}) [\mathcal{R}_{i_o i_o}(z^{\max}, E_m) - \mathcal{R}_{i_o i_o}(z^{\max}, E_{m'}) - 2\mathbf{Q}(z^{\max})] \Phi^{(m)}(z^{\max}) \\ &+ f_A(z^{\min}) (\Phi^{(m')})^T(z^{\min}) [\mathcal{R}_{i_o i_o}(z^{\min}, E_m) - \mathcal{R}_{i_o i_o}(z^{\min}, E_{m'}) - 2\mathbf{Q}(z^{\min})] \Phi^{(m)}(z^{\min}). \end{aligned} \quad (19)$$

Note the orthogonality condition is derived by calculation of difference of two functionals (5) with substitution of eigenvalues $E_m, E_{m'}$, eigenfunctions $\Phi^{(m)}(z), \Phi^{(m')}(z)$ and elements of matrices $\mathcal{R}(z^{\max}, E_m), \mathcal{R}(z^{\min}, E_{m'})$ from formulas (17), (18). The calculation of the complex eigenvalues and eigenfunctions of the metastable states is performed using the Newton iteration method. Appropriate initial approximations are chosen from solutions calculated previously with boundary conditions at fixed E . In example 14 as the initial approximation an appropriate resonance transmission solution of the scattering problem at the resonance value of energy $E \equiv \Re E$ is taken. In example 15 as the initial approximation an appropriate solution of the bound state problem is taken.

III. FEM GENERATION OF ALGEBRAIC PROBLEMS

High-accuracy computational schemes for solving the BVP (1)–(4) can be derived from the variational functional (5), (6) basing on the FEM. The general idea of the FEM in one-dimensional space is to divide the interval $[z^{\min}, z^{\max}]$ into many small domains referred to as elements. The size of the elements can be defined free enough to account for physical properties or qualitative behavior of the desired solutions, such as smoothness.

The interval $\Delta = [z^{\min}, z^{\max}]$ is covered by a set of n elements $\Delta_j = [z_j^{\min}, z_j^{\max} \equiv z_{j+1}^{\min}]$ in such a way that $\Delta = \bigcup_{j=1}^n \Delta_j$. Thus, we obtain the grid

$$\Omega^{h_j(z)}[z^{\min}, z^{\max}] = \{z^{\min} = z_1^{\min}, z_j^{\max} = z_j^{\min} + h_j, j = 1, \dots, n-1, \\ z_n^{\max} = z_n^{\min} + h_n = z^{\max}\}, \quad (20)$$

where $z_j^{\min} \equiv z_{j-1}^{\max}$, $j = 2, \dots, n$ are the mesh points, and the steps $h_j = z_j^{\max} - z_j^{\min}$ are the lengths of the elements Δ_j .

The program features the ability to specify a quasi-uniform grid, for which $h_1 = h_2 = \dots = h_{n_1}$, $h_{n_1+1} = h_{n_1+2} = \dots = h_{n_1+n_2}$, $h_{n_1+n_2+1} = h_{n_1+n_2+2} = \dots = h_{n_1+n_2+n_3}$, i.e. interval $\Delta = [z^{\min}, z^{\max}]$ is first broken down into **nmesh** sub-intervals (in the general case of unequal length) each of which is divided into **ngrid**(r_0)= n_{r_0} subintervals of equal length.

A. Interpolation Hermite Polynomials

In each element Δ_j we define the equidistant sub-grid $\Omega_j^{h_j(z)}[z_j^{\min}, z_j^{\max}] = \{z_{(j-1)p+r} = z_j^{\min}, z_{(j-1)p+r}, r = 1, \dots, p-1, z_{jp} = z_j^{\max}\}$ with the nodal points $z_r \equiv z_{(j-1)p+r}$ determined by the formula

$$z_{(j-1)p+r} = ((p-r)z_j^{\min} + rz_j^{\max})/p, \quad r = 0, \dots, p. \quad (21)$$

As a set of local functions $\{N_l(z, z_j^{\min}, z_j^{\max})\}_{l=0}^{l^{\max}}$, $l^{\max} = \sum_{r=0}^p \kappa_r^{\max}$ we will use the Interpolation Hermite Polynomials (IHPs) $\{\{\varphi_r^\kappa(z)\}_{r=0}^p\}_{\kappa=0}^{\kappa_r^{\max}-1}$ in the nodes z_r , $r = 0, \dots, p$ of the grid (21). The values of the functions $\varphi_r^\kappa(z)$ with their derivatives up to the order $(\kappa_r^{\max} - 1)$, i.e. $\kappa = 0, \dots, \kappa_r^{\max} - 1$, where κ_r^{\max} is referred to as the multiplicity of the node z_r , are determined by the expressions [6]

$$\varphi_r^\kappa(z_{r'}) = \delta_{rr'} \delta_{\kappa 0}, \quad \left. \frac{d^{\kappa'} \varphi_r^\kappa(z)}{dz^{\kappa'}} \right|_{z=z_{r'}} = \delta_{rr'} \delta_{\kappa \kappa'}. \quad (22)$$

To calculate the IHPs we introduce the auxiliary weight function

$$w_r(z) = \prod_{r'=0, r' \neq r}^p \left(\frac{z - z_{r'}}{z_r - z_{r'}} \right)^{\kappa_{r'}^{\max}}, \quad w_r(z_r) = 1. \quad (23)$$

The weight function derivatives can be presented as a product

$$\frac{d^\kappa w_r(z)}{dz^\kappa} = w_r(z) g_r^\kappa(z),$$

where the factor $g_r^\kappa(z)$ is calculated by means of the recurrence relations

$$g_r^\kappa(z) = \frac{dg_r^{\kappa-1}(z)}{dz} + g_r^1(z) g_r^{\kappa-1}(z), \quad (24)$$

with the initial conditions

$$g_r^0(z) = 1, \quad g_r^1(z) \equiv \frac{1}{w_r(z)} \frac{dw_r(z)}{dz} = \sum_{r'=0, r' \neq r}^p \frac{\kappa_{r'}^{\max}}{z - z_{r'}}.$$

We will seek for the IHPs $\varphi_r^\kappa(z)$ in the following form:

$$\varphi_r^\kappa(z) = w_r(z) \sum_{\kappa'=0}^{\kappa_r^{\max}-1} a_r^{\kappa, \kappa'} (z - z_r)^{\kappa'}. \quad (25)$$

Differentiating the function (25) by z at the point of z_r and using Eq. (23), we obtain

$$\left. \frac{d^{\kappa'} \varphi_r^\kappa(z)}{dz^{\kappa'}} \right|_{z=z_r} = \sum_{\kappa''=0}^{\kappa'} \frac{\kappa'!}{\kappa''! (\kappa' - \kappa'')!} g_r^{\kappa' - \kappa''}(z_r) a_r^{\kappa, \kappa''} \kappa''!. \quad (26)$$

Hence we arrive at the expression for the coefficients $a_r^{\kappa, \kappa'}$

$$a_r^{\kappa, \kappa'} = \left(\left. \frac{d^{\kappa'} \varphi_r^\kappa(z)}{dz^{\kappa'}} \right|_{z=z_r} - \sum_{\kappa''=0}^{\kappa'-1} \frac{\kappa'!}{\kappa''! (\kappa' - \kappa'')!} g_r^{\kappa' - \kappa''}(z_r) a_r^{\kappa, \kappa''} \kappa''! \right) / \kappa'!. \quad (27)$$

Taking Eq. (22) into account, we finally get:

$$a_r^{\kappa, \kappa'} = \begin{cases} 0, & \kappa' < \kappa, \\ 1/\kappa'!, & \kappa' = \kappa, \\ - \sum_{\kappa''=\kappa}^{\kappa'-1} \frac{1}{(\kappa' - \kappa'')!} g_r^{\kappa' - \kappa''}(z_r) a_r^{\kappa, \kappa''}, & \kappa' > \kappa. \end{cases}$$

Note that all degrees of interpolation Hermite polynomials $\varphi_r^\kappa(z)$ do not depend on κ and equal $p' = \sum_{r'=0}^p \kappa_{r'}^{\max} - 1$. Below we consider only the IHPs with the nodes of identical multiplicity $\kappa_r^{\max} = \kappa^{\max}$, $r = 0, \dots, p$. In this case, the degree of the polynomials is equal to $p' = \kappa^{\max}(p+1) - 1$. We introduce the following notation for such polynomials:

$$N_{\kappa^{\max}r+\kappa}(z, z_j^{\min}, z_j^{\max}) = \varphi_r^\kappa(z), \quad r = 0, \dots, p, \quad \kappa = 0, \dots, \kappa^{\max} - 1. \quad (28)$$

These IHPs form a basis in the space of polynomials having the degree $p' = \kappa^{\max}(p+1) - 1$ in the element $z \in [z_j^{\min}, z_j^{\max}]$ that have continuous derivatives up to the order $\kappa^{\max} - 1$ at the boundary points z_j^{\min} and z_j^{\max} of the element $z \in [z_j^{\min}, z_j^{\max}]$.

The interpolation Lagrange polynomials and interpolation Hermite polynomials with the multiplicity of nodes $\kappa^{\max} = 2, 3$ (and their first and second derivatives with respect to z) are shown in Fig. 1 – 3.

It is seen that the values of IHP $N_{\kappa^{\max}p+\kappa}(z, z_j^{\min}, z_j^{\max})$ and $N_\kappa(z, z_{j+1}^{\min}, z_{j+1}^{\max})$ (at $r = p$ and $r = 0$) and their derivatives up to the order $\kappa^{\max} - 1$ coincide at the mutual point $z_j^{\max} = z_{j+1}^{\min}$ of the adjacent elements. Moreover, the boundary points are nodes (zeros) of the multiplicity κ^{\max} of other IHPs, irrespective of the length of elements of $[z_j^{\min}, z_j^{\max}]$ and $[z_{j+1}^{\min}, z_{j+1}^{\max}]$. This allows the construction of a basis of piecewise and polynomial functions having continuous derivatives to the order of $\kappa^{\max} - 1$ in any set $\Delta = \bigcup_{j=1}^n \Delta_j = [z_j^{\min}, z_j^{\max}]$ of elements $\Delta_j = [z_j^{\min}, z_j^{\max} \equiv z_{j+1}^{\min}]$.

B. Generation of Algebraic Eigenvalue Problems

We consider a discrete representation of the solutions $\Phi(z)$ of the problem (1)–(4) reduced by means of the FEM to the variational functional (5), (6) on the finite-element grid,

$$\Omega_{h_j(z)}^p [z^{\min}, z^{\max}] = [z_0 = z^{\min}, z_l, l = 1, \dots, np - 1, z_{np} = z^{\max}], \quad (29)$$

with the mesh points $z_l = z_{jp} = z_j^{\max} \equiv z_{j+1}^{\min}$ of the grid $\Omega^{h_j(z)} [z^{\min}, z^{\max}]$ determined by Eq. (20) and the nodal points $z_l = z_{(j-1)p+r}$, $r = 0, \dots, p$ of the sub-grids $\Omega_j^{h_j(z)} [z_j^{\min}, z_j^{\max}]$, $j = 1, \dots, n$, determined by Eq. (21). The

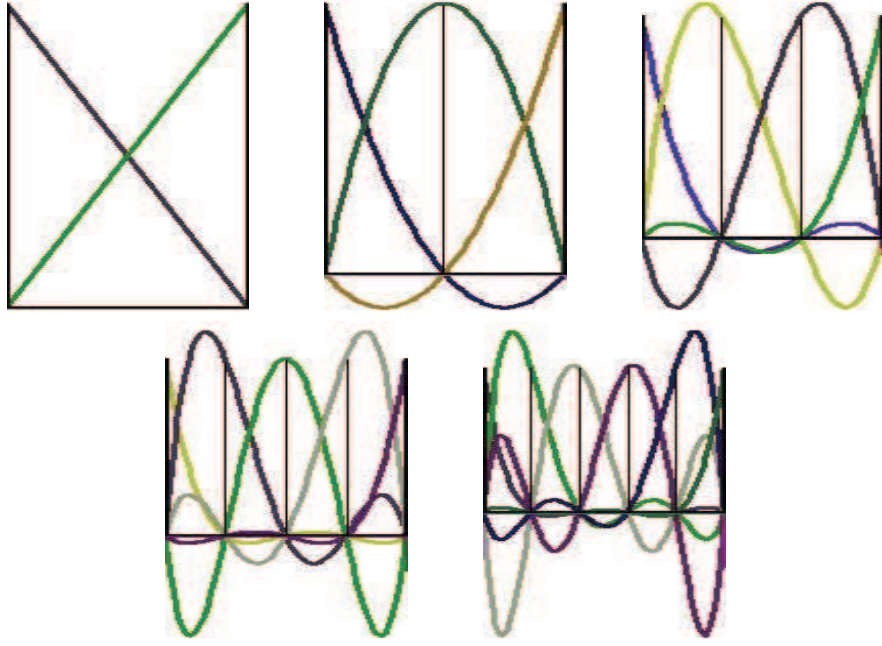


FIG. 1: The interpolation Lagrange polynomials up to the fifth order $p' = p = 1, 2, 3, 4, 5$, $\kappa^{\max} = 1$, The nodes z_r of interpolation Lagrange polynomials are shown by vertical lines.

solution $\Phi^h(z) \approx \Phi(z)$ is sought for in the form of a finite sum over the basis of local functions $N_\mu^g(z)$ at each nodal point $z = z_l$ of the grid $\Omega_{h_j}^p[z^{\min}, z^{\max}]$ of the interval $z \in \Delta = [z^{\min}, z^{\max}]$:

$$\Phi^h(z) = \sum_{\mu=0}^{L-1} \Phi_\mu^h N_\mu^g(z), \quad \Phi^h(z_l) = \Phi_{l\kappa^{\max}}^h, \quad \left. \frac{d^\kappa \Phi^h(z)}{dz^\kappa} \right|_{z=z_l} = \Phi_{l\kappa^{\max}+\kappa}^h \quad (30)$$

where $L = (pn + 1)\kappa^{\max}$ is the number of basis functions Φ_μ^h (matrices of dimensional $N \times 1$) at $\mu = l\kappa^{\max} + \kappa$ are the nodal values of the κ th derivatives of the function $\Phi^h(z)$ (including the function $\Phi^h(z)$ itself for $\kappa = 0$) at the points z_l .

The basis functions $N_\mu^g(z) \equiv N_{l\kappa^{\max}+\kappa}^g(z)$ are piecewise polynomials of the given order p' , their derivative of the order κ at the node z_l equals one, and the derivative of the order $\kappa' \neq \kappa$ at this node equals zero, while the values of the function $N_\mu^g(z)$ with all its derivatives up to the order $(\kappa^{\max} - 1)$ equal zero at all other nodes $z_{l'} \neq z_l$ of the grid $\Omega_{h_j}^p$, i.e., $\left. \frac{d^{\kappa'} N_{l\kappa^{\max}+\kappa}^g(z)}{dz^{\kappa'}} \right|_{z=z_{l'}} = \delta_{ll'} \delta_{\kappa\kappa'}$, $l = 0, \dots, np$, $\kappa = 0, \dots, \kappa^{\max} - 1$.

For the nodes z_l of the grid (29) that do not coincide with the mesh points z_j^{\max} of the grid (20), i.e., at $l \neq jp$, $j = 1 \dots n - 1$, the polynomial $N_\mu^g(z)$ at $\mu = ((j - 1)p + r)\kappa^{\max} + \kappa$ has the form

$$N_{(p(j-1)+r)\kappa^{\max}+\kappa}^g(z) = \begin{cases} N_{\kappa^{\max}r+\kappa}(z, z_j^{\min}, z_j^{\max}), & z \in \Delta_j; \\ 0, & z \notin \Delta_j, \end{cases} \quad (31)$$

i.e., it is defined as the IHP $N_{\kappa^{\max}r+\kappa}(z, z_j^{\min}, z_j^{\max})$ in the interval $z \in \Delta_j$ and zero otherwise. Since the points z_j^{\min} and z_j^{\max} are nodes of multiplicity κ^{\max} , such piecewise polynomial functions and their derivatives up to the order $\kappa^{\max} - 1$ are continuous in the entire interval Δ .

For the nodal points of the grid z_l of the grid (29) that coincide with one of the mesh points z_j^{\max} of the grid (20), belonging to two elements Δ_j and Δ_{j+1} , $j = 1 \dots n - 1$, i.e., for $l = jp$, the polynomial, whose derivative of the order κ equals one at the node z_l , has the form

$$N_{p\kappa^{\max}j+\kappa}^g(z) = \begin{cases} N_{\kappa^{\max}p+\kappa}(z, z_j^{\min}, z_j^{\max}), & z \in \Delta_j; \\ N_\kappa(z, z_{j+1}^{\min}, z_{j+1}^{\max}), & z \in \Delta_{j+1}; \\ 0, & z \notin \Delta_j \cup \Delta_{j+1}. \end{cases} \quad (32)$$

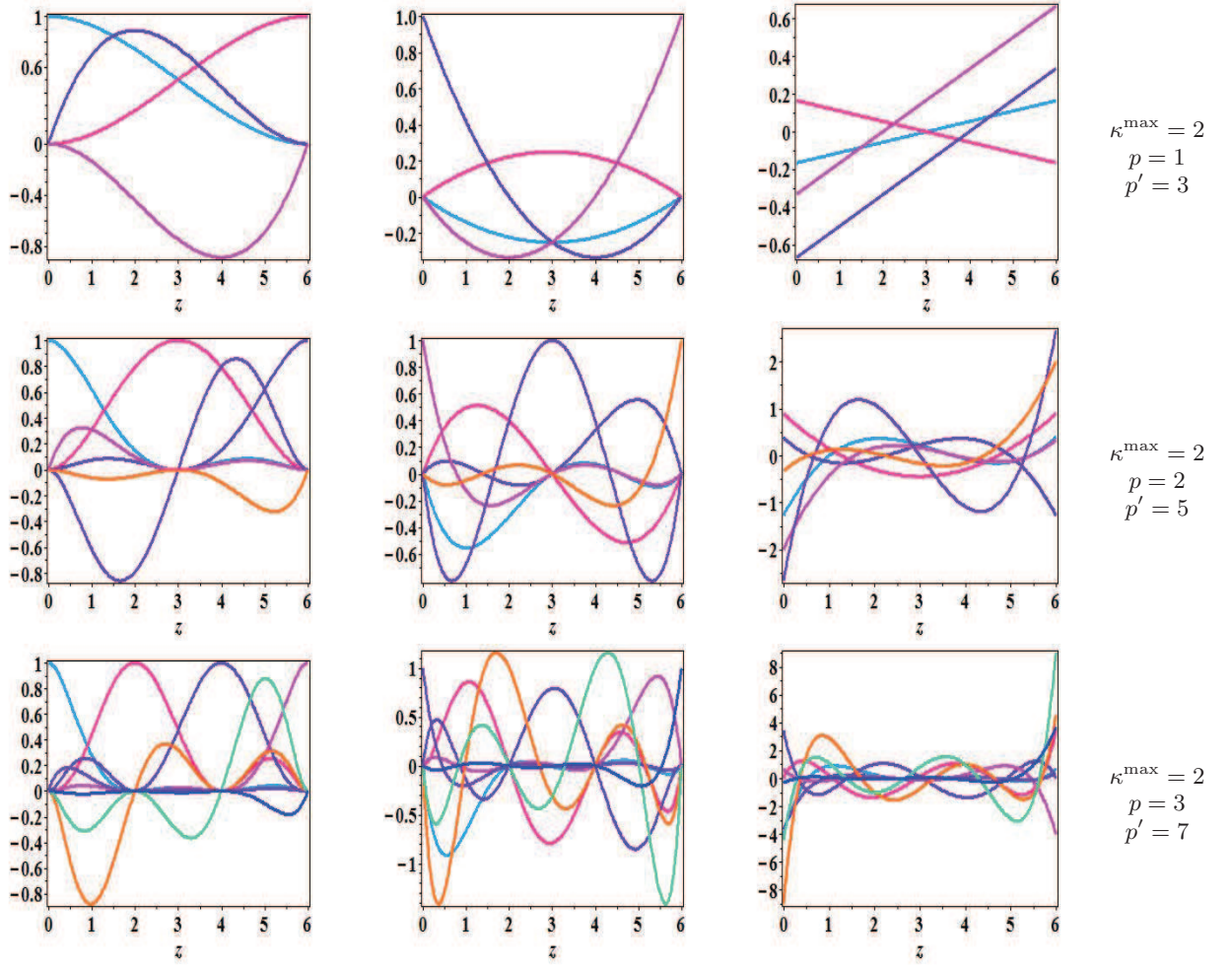


FIG. 2: The interpolation Hermite polynomials with the multiplicity of nodes $\kappa^{\max} = 2$ (left), their first (centre) and second (right) derivatives at $z_j^{\min} = 0$ $z_j^{\max} = 6$.

In other words, it is constructed by joining the polynomial $N_{p\kappa^{\max}+\kappa}(z, z_j^{\min}, z_j^{\max})$ defined in the element Δ_j with the polynomial $N_\kappa(z, z_{j+1}^{\min}, z_{j+1}^{\max})$ defined in the element Δ_{j+1} . These basis piecewise polynomial functions $N_\mu^g(z) \equiv N_{l\kappa^{\max}+\kappa}^g(z)$ are also continuous with all its derivatives of the order $\kappa^{\max} - 1$ in the interval $z \in \Delta$.

As an example, Figs. 4, 5 и 6 present the basis functions $N_\mu^g(z)$ a piecewise continuous polynomials of the order p' with IHPs with different κ^{\max} and p on the grid (29) of the three finite elements $n = 3$.

Fig. 4 shows the basis functions of Lagrangian elements of the first $p' = 1$, the second $p' = 2$ and the fourth $p' = 4$ order: $(\kappa^{\max}, p) = (1, 1)$, $(\kappa^{\max}, p) = (1, 2)$, $(\kappa^{\max}, p) = (1, 4)$. It is evident that at the boundary points of the finite elements, marked by vertical lines, the basis functions are continuous, and the fractures indicate the fact that their first derivatives are discontinuous.

Fig. 5 shows the basis functions of the third order $p' = 3$ with Lagrangian elements $(\kappa^{\max}, p) = (1, 3)$, and the Hermitian elements $(\kappa^{\max}, p) = (2, 1)$. Fig. 6 shows the basis function of the fifth order $p' = 5$ with Lagrangian elements $(\kappa^{\max}, p) = (1, 5)$, and the Hermitian elements $(\kappa^{\max}, p) = (2, 2)$ and $(\kappa^{\max}, p) = (3, 1)$. It is evident that the Hermitian elements, in contrast to the Lagrangian ones, in the boundary points of the finite elements have no fractures, i.e., both the basic functions and their first derivatives are continuous.

The modulo of the division number of basis functions μ on κ^{\max} shows the function (if μ is a multiple of κ^{\max}) or a derivative of order κ (if the modulo is equal to κ) in one of the nodes is taken as equal to unity: for basis functions with Hermitian elements with $\kappa^{\max} = 2$, the first derivatives in one of the nodes take the value equal to one, marked by odd numbers, but for the basis functions of a Hermitian elements of a $\kappa^{\max} = 3$, the first and second derivatives in one of the nodes take the value equal to one, marked with numbers 1,4,7,10 and 2,5,8,11, respectively.

The substitution of the expansion (30) into the variational functional (5), (6) reduces the solution of the problem (1)–(4) to the solution of the generalized algebraic eigenvalue problem with respect to the desired set of eigenvalues

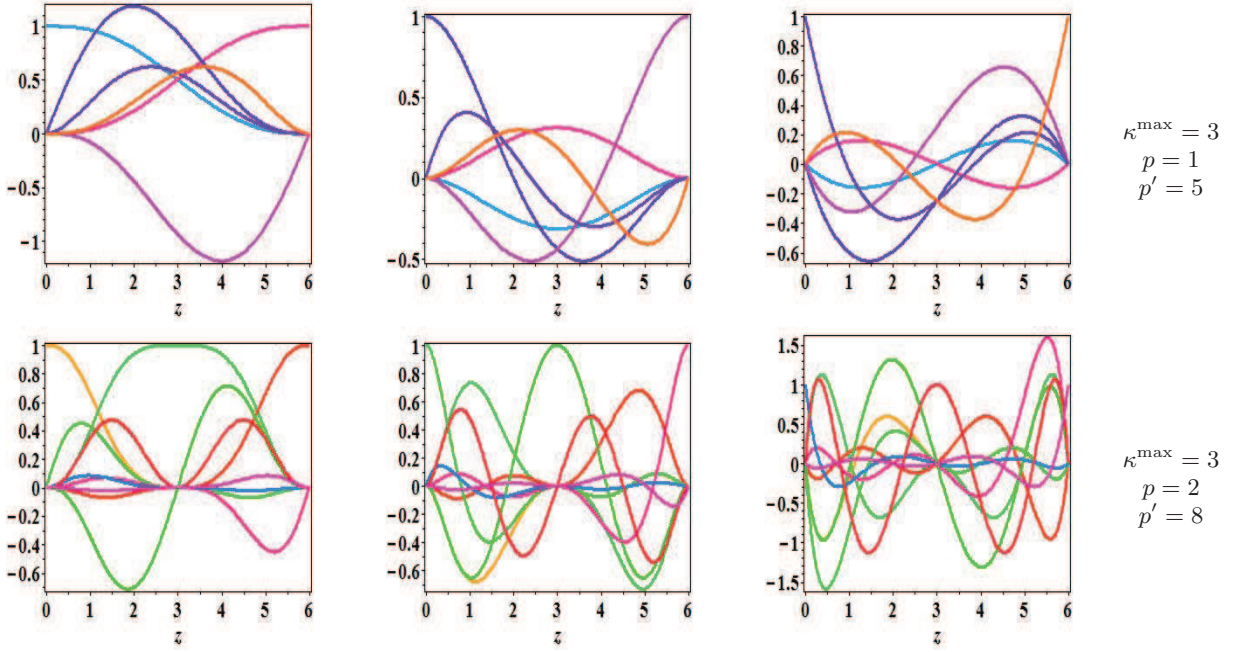


FIG. 3: The interpolation Hermite polynomials with the multiplicity of nodes $\kappa^{\max} = 3$ (left), their first (centre) and second (right) derivatives at $z_j^{\min} = 0$ $z_j^{\max} = 6$.

E and eigenvectors $\{\{\Phi_{\nu\mu}^h\}_{\nu=0}^N\}_{\mu=0}^{L-1}$:

$$(\tilde{\mathbf{A}} - 2E\mathbf{B})\Phi^h = 0. \quad (33)$$

Here $\tilde{\mathbf{A}} = \mathbf{A}^{(2)} + \mathbf{A}^{(1)} + \mathbf{V} + \mathbf{M}^{\min} - \mathbf{M}^{\max}$ and positive defined \mathbf{B} are symmetric $LN \times LN$ stiffness and mass matrices of dimension $NL \times NL$

$$\begin{aligned}
A_{\nu_1, \nu_2; \mu_1+1, \mu_2+1}^{(2)} &= \sum_{(j, l_1, l_2) \in D} A_{\nu_1, \nu_2; l_1, l_2}^{(2)j}, & A_{\nu_1, \nu_2; l_1, l_2}^{(2)j} &= \int_{z_j^{\min}}^{z_j^{\max}} \delta_{\nu_1 \nu_2} f_A(z) \frac{dN_{l_1}(z, z_j^{\min}, z_j^{\max})}{dz} \frac{dN_{l_2}(z, z_j^{\min}, z_j^{\max})}{dz} dz, \\
A_{\nu_1, \nu_2; \mu_1+1, \mu_2+1}^{(1)} &= \sum_{(j, l_1, l_2) \in D} A_{\nu_1, \nu_2; l_1, l_2}^{(1)j}, & A_{\nu_1, \nu_2; l_1, l_2}^{(1)j} &= \int_{z_j^{\min}}^{z_j^{\max}} f_A(z) N_{l_1}(z, z_j^{\min}, z_j^{\max}) Q_{\nu_1 \nu_2}(z) \frac{dN_{l_2}(z, z_j^{\min}, z_j^{\max})}{dz} dz \\
&&& - \int_{z_j^{\min}}^{z_j^{\max}} f_A(z) \frac{dN_{l_1}(z, z_j^{\min}, z_j^{\max})}{dz} Q_{\nu_1 \nu_2}(z) N_{l_2}(z, z_j^{\min}, z_j^{\max}) dz, \\
V_{\nu_1, \nu_2; \mu_1+1, \mu_2+1} &= \sum_{(j, l_1, l_2) \in D} V_{\nu_1, \nu_2; l_1, l_2}^j, & V_{\nu_1, \nu_2; l_1, l_2}^j &= \int_{z_j^{\min}}^{z_j^{\max}} f_B(z) dz N_{l_1}(z, z_j^{\min}, z_j^{\max}) V_{\nu_1 \nu_2}(z) N_{l_2}(z, z_j^{\min}, z_j^{\max}), \\
B_{\nu_1, \nu_2; \mu_1+1, \mu_2+1} &= \sum_{(j, l_1, l_2) \in D} B_{\nu_1, \nu_2; l_1, l_2}^j, & B_{\nu_1, \nu_2; l_1, l_2}^j &= \int_{z_j^{\min}}^{z_j^{\max}} \delta_{\nu_1 \nu_2} f_B(z) N_{l_1}(z, z_j^{\min}, z_j^{\max}) N_{l_2}(z, z_j^{\min}, z_j^{\max}) dz, \quad (34)
\end{aligned}$$

where $D = \{j \in \{1, \dots, n\}, l_1 \in \{0, \dots, p'\}, l_2 \in \{0, \dots, p'\} | \mu_1 = p\kappa^{\max}(j-1) + l_1, \mu_2 = p\kappa^{\max}(j-1) + l_2\}$.

The matrices \mathbf{M}^{\max} and \mathbf{M}^{\min} with the dimension $NL \times NL$ have only one nonzero $N \times N$ sub-matrices each: $M_{\nu_1, \nu_2; 11}^{\min} = f_A(z^{\min}) R_{\nu_1, \nu_2}(z^{\min})$ and $M_{\nu_1, \nu_2; L+1-\kappa^{\max}, L+1-\kappa^{\max}}^{\max} = f_A(z^{\max}) R_{\nu_1, \nu_2}(z^{\max})$, respectively.

1. If the coefficients of the equation (33) are given in the tabular form, then we use the following matrix elements

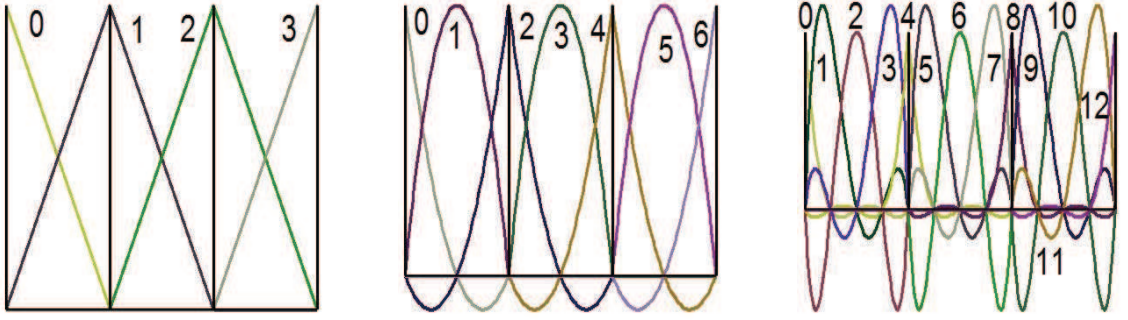


FIG. 4: The basis functions $N_{\mu}^g(z)$ of a Lagrangian elements of the first $p' = 1$, the second $p' = 2$ and the fourth $p' = 4$ order: $(\kappa^{\max}, p) = (1, 1)$, $(\kappa^{\max}, p) = (1, 2)$, $(\kappa^{\max}, p) = (1, 4)$ at $n = 3$ finite elements, marked by vertical lines.

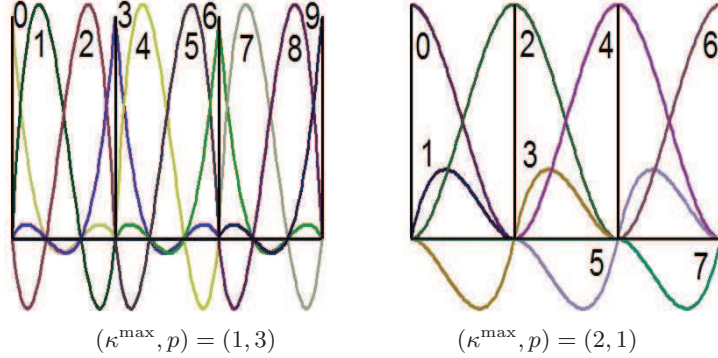


FIG. 5: The basis function $N_{\mu}^g(z)$ of fifth order $p' = 3$ with Lagrangian elements $(\kappa^{\max}, p) = (1, 4)$, and Hermitian elements $(\kappa^{\max}, p) = (2, 1)$ at $n = 3$ finite elements, marked by vertical lines.

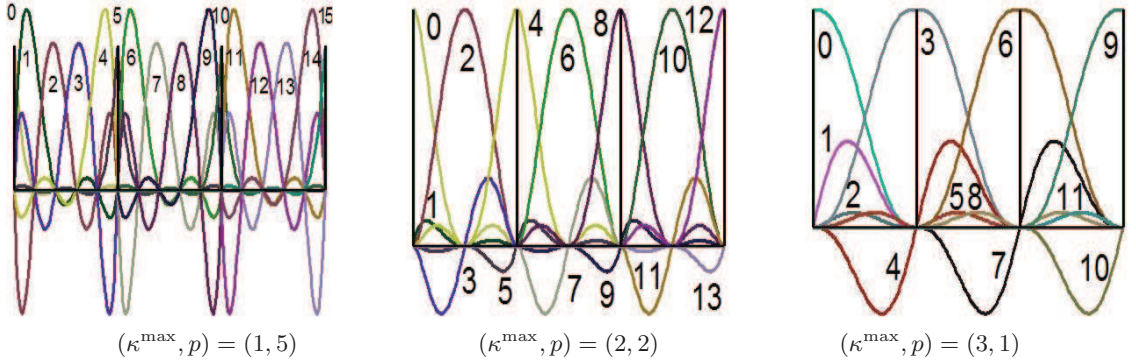


FIG. 6: The basis function $N_{\mu}^g(z)$ of fifth order $p' = 5$ with Lagrangian elements $(\kappa^{\max}, p) = (1, 5)$, and Hermitian elements $(\kappa^{\max}, p) = (2, 2)$ and $(\kappa^{\max}, p) = (3, 1)$ at $n = 3$ finite elements, marked by vertical lines.

$V_{l_1; l_2}(z^{\min}, z^{\max})$ from (34):

$$\int_{z_j^{\min}}^{z_j^{\max}} f_B(z) dz N_{L_1}(z, z_j^{\min}, z_j^{\max}) V(z) N_{L_2}(z, z_j^{\min}, z_j^{\max}) = \sum_{r=0}^p \sum_{\kappa=0}^{\kappa^{\max}-1} W_{l_1; l_2; \kappa^{\max} r + \kappa}^j(z_j^{\min}, z_j^{\max}) V^{(\kappa)}(z_{(j-1)p+r}),$$

where $W_{l_1; l_2; l_3}^j(z_j^{\min}, z_j^{\max})$ are determined by the integrals with IHPs

$$W_{l_1; l_2; l_3}^j(z_j^{\min}, z_j^{\max}) = \int_{z_j^{\min}}^{z_j^{\max}} f_B(z) N_{l_1}(z, z_j^{\min}, z_j^{\max}) N_{l_2}(z, z_j^{\min}, z_j^{\max}) N_{l_3}(z, z_j^{\min}, z_j^{\max}) dz.$$

The obtained expression will be exact for polynomial potentials of the order smaller than p' . Generally this decomposition leads to numerical eigenfunctions and eigenvalues with the accuracy of the order about $p' + 1$. If the integrals cannot be calculated in the analytical form, then the Gauss integration rule [7] with $p' + 1$ nodes is applied and held

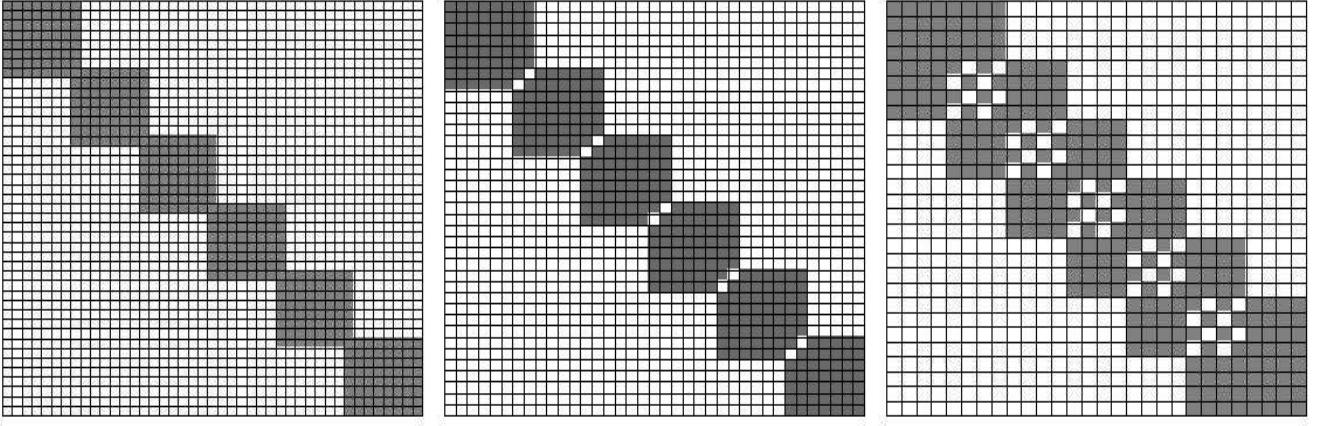


FIG. 7: The structure of the matrices $B_{L_1 L_2}$ and $A_{L_1 L_2}$ for the potential $V(z) = 0$ and $Q(z) = 0$ for the number of elements $n = 6$ in the entire interval (z^{\min}, z^{\max}) and different values of the multiplicity of nodes κ^{\max} and the number of subintervals p . From left to right: $(\kappa^{\max}, p) = (1, 7)$, $(\kappa^{\max}, p) = (2, 3)$, $(\kappa^{\max}, p) = (4, 1)$, the dimension of the matrices are $L \times L$, $L = \kappa^{\max}(np+1)$, equal to 43×43 , 38×38 , 28×28 , the total number of elements within blocks $(n(p^2+2p)+1)(\kappa^{\max})^2 = 379, 364, 304$ and bandwidth $2(p'+1) - \kappa^{\max} = 15, 14, 12$, respectively. At $N > 1$ each block is a matrix of dimension $N \times N$, i.e. \mathbf{B} and \mathbf{A} are matrices of the dimension of the matrix $NL \times NL$ to the total number of elements within blocks $N^2(n(p^2+2p)+1)(\kappa^{\max})^2$ and bandwidth $N(2(p'+1) - \kappa^{\max})$.

the theoretical estimations (35)

$$\begin{aligned}
A_{\nu_1, \nu_2; l_1, l_2}^{(2)j} &= \sum_{g=0}^{p'} \delta_{\nu_1, \nu_2} w_g f_A(z_g) \left. \frac{dN_{l_1}(z, z_j^{\min}, z_j^{\max})}{dz} \right|_{z=z_g} \left. \frac{dN_{l_2}(z, z_j^{\min}, z_j^{\max})}{dz} \right|_{z=z_g} \\
A_{\nu_1, \nu_2; l_1, l_2}^{(1)j} &= \sum_{g=0}^{p'} w_g f_A(z_g) N_{l_1}(z_g, z_j^{\min}, z_j^{\max}) Q_{\nu_1 \nu_2}(z_g) \left. \frac{dN_{l_2}(z, z_j^{\min}, z_j^{\max})}{dz} \right|_{z=z_g} \\
&\quad - \sum_{g=0}^{p'} w_g f_A(z_g) \left. \frac{dN_{l_1}(z, z_j^{\min}, z_j^{\max})}{dz} \right|_{z=z_g} Q_{\nu_1 \nu_2}(z_g) N_{l_2}(z_g, z_j^{\min}, z_j^{\max}) \\
V_{\nu_1, \nu_2; l_1, l_2}^j &= \sum_{g=0}^{p'} w_g f_B(z_g) N_{L_1}(z_g, z_j^{\min}, z_j^{\max}) V(z_g) N_{L_2}(z_g, z_j^{\min}, z_j^{\max}), \\
B_{\nu_1, \nu_2; l_1, l_2}^j &= \sum_{g=0}^{p'} \delta_{\nu_1, \nu_2} w_g f_B(z_g) N_{l_1}(z_g, z_j^{\min}, z_j^{\max}) N_{l_2}(z_g, z_j^{\min}, z_j^{\max})
\end{aligned}$$

where $z_g = (p' - g)z^{\min} + gz^{\max}$ and w_g , $g = \overline{0, p'}$ are gaussian nodes and weights of an orthogonal polynomial of degree $p' + 1$, on the element $z \in (z_j^{\min}, z_j^{\max})$.

Note, using the local coordinate $\eta \in [-1, 1]$ related to the absolute coordinate z as $z = z_j^{\min} + h_j(1+\eta)/2$, $\frac{dz}{d\eta} = h_j/2$, one should ordinary exploit the following expansions of the function and its first derivative

$$\begin{aligned}
\hat{\Phi}(z) &= \sum_{r=0}^p \sum_{\kappa=0}^{\kappa^{\max}-1} \hat{\Phi}_{\kappa^{\max}r+\kappa} N_{\kappa^{\max}r+\kappa}(\eta, -1, 1) \left(\frac{dz}{d\eta} \right)^{\kappa}, \\
\frac{d\hat{\Phi}(z)}{dz} &= \sum_{r=0}^p \sum_{\kappa=0}^{\kappa^{\max}-1} \hat{\Phi}_{\kappa^{\max}r+\kappa} \frac{dN_{\kappa^{\max}r+\kappa}(\eta, -1, 1)}{d\eta} \left(\frac{dz}{d\eta} \right)^{\kappa-1}.
\end{aligned}$$

3. The matrices $\tilde{A}_{\nu_1, \nu_2; l_1, l_2}$, $B_{\nu_1, \nu_2; l_1, l_2}$ и $V_{\nu_1, \nu_2; l_1, l_2}$ are symmetric, their dimension is $NL \times NL$, where $L = \kappa^{\max}(np+1)$. They consist of n sub-matrices with the dimension $\kappa^{\max}(p+1) \times \kappa^{\max}(p+1)$. The intersections of these sub-matrices are blocks having the dimension $\kappa^{\max} \times \kappa^{\max}$. These blocks include elements that equal zero in both matrices

$B_{\nu_1, \nu_2; l_1, l_2}$ and $\tilde{A}_{\nu_1, \nu_2; l_1, l_2}$ for $V(z) = 0$ and become nonzero in the matrix $\tilde{A}_{\nu_1, \nu_2; l_1, l_2}$, when $V(z) \neq 0$. The existence of such elements is a manifestation of the IHPs symmetry. The total number of elements in all these blocks is $(n(p^2 + 2p) + 1)(\kappa^{\max})^2$. Examples of banded matrix structures are shown in Fig. 7.

4. In the case of BC (II) the matrix elements of (34) are unchanged. To impose the BC (I) in z^{\min} one should omit the first row and the first column, while to apply the BC (I) in z^{\max} one should omit the row and the column with the number $L + 1 - \kappa^{\max}$. To impose the BC (III) in z^{\min} one should apply $\tilde{A}_{\nu_1, \nu_2; 1, 1} \rightarrow \tilde{A}_{\nu_1, \nu_2; 1, 1} + f_A(z^{\min})R(z^{\min})$, while to impose the BC (III) in z^{\max} one should apply $\tilde{A}_{\nu_1, \nu_2; L+1-\kappa^{\max}, L+1-\kappa^{\max}} \rightarrow \tilde{A}_{\nu_1, \nu_2; L+1-\kappa^{\max}, L+1-\kappa^{\max}} - f_A(z^{\max})R(z^{\max})$.

5. For small matrix dimensions ~ 100 , the desired solution of the problem generated at Step 2.3 is performed using the built-in procedures of the Maple LinearAlgebra package. For large matrix dimensions $\sim 100 \div 1000000$, the subspace iteration method is used, implemented in the Fortran program SSPACE [7] which is efficient for large-scale eigenvalue problems with symmetric band matrices[9].

The theoretical estimate for the \mathbf{H}^0 norm of the difference between the exact solution $\Phi_m(z) \in \mathcal{H}_2^2$ and the numerical one $\Phi_m^h(z) \in \mathbf{H}^{\kappa^{\max}}$ has the order of

$$|E_m^h - E_m| \leq c_1 h^{2p'}, \quad \|\Phi_m^h(z) - \Phi_m(z)\|_0 \leq c_2 h^{p'+1}, \quad (35)$$

where $h = \max_{1 < j < n} h_j$ is the maximal step of the grid [2].

C. The calculation scheme of multichannel scattering problem

We consider the solution of the algebraic problem with respect to the matrix solution $\Phi^h \equiv ((\chi^{(1)})^h, \dots, (\chi^{(N_o)})^h)$

$$\mathbf{G}^p \Phi^h \equiv (\mathbf{A}^p - E \mathbf{B}^p) \Phi^h = \mathbf{M} \Phi^h, \quad (36)$$

obtained by discretization with the help of Finite Element Method of high order of accuracy of variational functional (5), (6) corresponding to BVP (1), (4) that approximate of multichannel problem at fixed E . The matrices $\mathbf{A}^p = \mathbf{A}^{(2)} + \mathbf{A}^{(1)} + \mathbf{V}$ and $\mathbf{M} = \mathbf{M}^{\max} - \mathbf{M}^{\min}$ of dimension $NL \times NL$ are given in (34). Matrices \mathbf{M}^{\max} and \mathbf{M}^{\min} arise due to the approximation of boundary conditions of the third kind at the left and right boundaries of the interval $z \in (z^{\min}, z^{\max})$

$$\frac{d\Phi^h(z)}{dz} = (\mathbf{G}(z) + \mathbf{Q}(z))\Phi^h(z), \quad z = z^{\min}, \quad z = z^{\max}. \quad (37)$$

The elements of the matrix $\mathbf{M} = \{M_{l'_1, l'_2}\}_{l'_1, l'_2=1}^{NL}$ equal zero except those, for which both indexes $l'_1 = (l_1 - 1)N + \nu_1$, $l'_2 = (l_2 - 1)N + \nu_2$ belong to the interval $1, \dots, N$ or to the interval $(L - \kappa^{\max}N) + 1, \dots, (L - \kappa^{\max}N) + N$, where N is the number of equations (1) and L is a number of basis functions $N_\mu^g(z)$ in expansion of desired solutions (30) on interval $z \in \Delta = [z^{\min}, z^{\max}]$.

We rewrite the problem (36) in the following form

$$\begin{pmatrix} \mathbf{G}_{aa}^p & \mathbf{G}_{ab}^p & \mathbf{0} \\ \mathbf{G}_{ba}^p & \mathbf{G}_{bb}^p & \mathbf{G}_{bc}^p \\ \mathbf{0} & \mathbf{G}_{cb}^p & \mathbf{G}_{cc}^p \end{pmatrix} \begin{pmatrix} \Phi_a \\ \Phi_b \\ \Phi_c \end{pmatrix} = \begin{pmatrix} -\mathbf{G}_{\min}^p & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{G}_{\max}^p \end{pmatrix} \begin{pmatrix} \Phi_a \\ \Phi_b \\ \Phi_c \end{pmatrix}. \quad (38)$$

The matrices \mathbf{G}_{bb}^p of the dimension $(L - 2N) \times (L - 2N)$, \mathbf{G}_{ba}^p and \mathbf{G}_{bc}^p of the dimension $(L - 2N) \times N$, \mathbf{G}_{ab}^p and \mathbf{G}_{cb}^p of the dimension $N \times (L - 2N)$, \mathbf{G}_{aa}^p , \mathbf{G}_{cc}^p , of the dimension $N \times N$ are determined from finite element approximation and considered as known. Existence of zero submatrices are connected with band structure of matrix \mathbf{G}^p from (38). Matrices \mathbf{G}_{\min} and \mathbf{G}_{\max} of the dimension $N \times N$, and Φ_a and Φ_c of the dimension $N \times 1$, should be connected by with asymptotic expansion and will be considered below, matrix Φ_b of the dimension $(L - 2N) \times 1$ are derived by dropping submatrices Φ_a and Φ_c from matrix-solution.

We rewrite the problem (38) in the explicit form

$$\begin{aligned} \mathbf{G}_{aa}^p \Phi_a + \mathbf{G}_{ab}^p \Phi_b &= -\mathbf{G}_{\min}^p \Phi_a, \\ \mathbf{G}_{ba}^p \Phi_a + \mathbf{G}_{bb}^p \Phi_b + \mathbf{G}_{bc}^p \Phi_c &= \mathbf{0}, \\ \mathbf{G}_{cb}^p \Phi_b + \mathbf{G}_{cc}^p \Phi_c &= \mathbf{G}_{\max}^p \Phi_c. \end{aligned} \quad (39)$$

Let us eliminate Φ_b from the problem. From the second equation the explicit expression follows

$$\Phi_b = -(\mathbf{G}_{bb}^p)^{-1} \mathbf{G}_{ba}^p \Phi_a - (\mathbf{G}_{bb}^p)^{-1} \mathbf{G}_{bc}^p \Phi_c, \quad (40)$$

however, it requires the inversion of a large-dimension matrix. To avoid it, we consider the auxiliary problems

$$\mathbf{G}_{bb}^p \mathbf{F}_{ba} = \mathbf{G}_{ba}^p, \quad \mathbf{G}_{bb}^p \mathbf{F}_{bc} = \mathbf{G}_{bc}^p. \quad (41)$$

Since \mathbf{G}_{bb}^p is a nondegenerate matrix, each of the matrix equations (41) has a unique solution

$$\mathbf{F}_{ba} = (\mathbf{G}_{bb}^p)^{-1} \mathbf{G}_{ba}^p, \quad \mathbf{F}_{bc} = (\mathbf{G}_{bb}^p)^{-1} \mathbf{G}_{bc}^p. \quad (42)$$

Then, for the function Φ_b we have the expression

$$\Phi_b = -\mathbf{F}_{ba} \Phi_a - \mathbf{F}_{bc} \Phi_c, \quad (43)$$

and the problem (39) takes the form

$$\begin{aligned} \mathbf{G}_{aa}^p \Phi_a - \mathbf{G}_{ab}^p \mathbf{F}_{ba} \Phi_a - \mathbf{G}_{ab}^p \mathbf{F}_{bc} \Phi_c &= -\mathbf{G}_{\min}^p \Phi_a, \\ -\mathbf{G}_{cb}^p \mathbf{F}_{ba} \Phi_a - \mathbf{G}_{cb}^p \mathbf{F}_{bc} \Phi_c + \mathbf{G}_{cc}^p \Phi_c &= \mathbf{G}_{\max}^p \Phi_c. \end{aligned}$$

Thus, the algebraic problem (38) with the matrix of the dimension $L \times L$ is reduced to two algebraic problems with the matrices of the dimension $N \times N$

$$\begin{aligned} \mathbf{Y}_{aa}^p \Phi_a + \mathbf{Y}_{ac}^p \Phi_c &= -\mathbf{G}_{\min}^p \Phi_a, \\ \mathbf{Y}_{ca}^p \Phi_a + \mathbf{Y}_{cc}^p \Phi_c &= \mathbf{G}_{\max}^p \Phi_c. \end{aligned} \quad (44)$$

where \mathbf{Y}_{**}^p is determined via the solutions \mathbf{F}_{ba} and \mathbf{F}_{bc} of problems (41)

$$\begin{aligned} \mathbf{Y}_{aa}^p &= \mathbf{G}_{aa}^p - \mathbf{G}_{ab}^p \mathbf{F}_{ba}, & \mathbf{Y}_{ac}^p &= -\mathbf{G}_{ab}^p \mathbf{F}_{bc}, \\ \mathbf{Y}_{ca}^p &= -\mathbf{G}_{cb}^p \mathbf{F}_{ba}, & \mathbf{Y}_{cc}^p &= \mathbf{G}_{cc}^p - \mathbf{G}_{cb}^p \mathbf{F}_{bc}. \end{aligned} \quad (45)$$

Let us consider the solution (10) for the incident wave travelling from left to right

$$\Phi_{\rightarrow}(z \rightarrow \pm\infty) = \begin{cases} \mathbf{X}_{\max}^{(\rightarrow)}(z) \mathbf{T}_{\rightarrow} + \mathbf{X}_{\max}^{(c)}(z) \mathbf{T}_{\rightarrow}^c, & z > 0, \\ \mathbf{X}_{\min}^{(\rightarrow)}(z) + \mathbf{X}_{\min}^{(\leftarrow)}(z) \mathbf{R}_{\rightarrow} + \mathbf{X}_{\min}^{(c)}(z) \mathbf{R}_{\rightarrow}^c, & z < 0 \end{cases} \quad (46)$$

and solution (11) for incident wave from right to left

$$\Phi_{\leftarrow}(z \rightarrow \pm\infty) = \begin{cases} \mathbf{X}_{\max}^{(\leftarrow)}(z) + \mathbf{X}_{\max}^{(\rightarrow)}(z) \mathbf{R}_{\leftarrow} + \mathbf{X}_{\max}^{(c)}(z) \mathbf{R}_{\leftarrow}^c, & z > 0, \\ \mathbf{X}_{\min}^{(\leftarrow)}(z) \mathbf{T}_{\leftarrow} + \mathbf{X}_{\min}^{(c)}(z) \mathbf{T}_{\leftarrow}^c, & z < 0. \end{cases} \quad (47)$$

Here $\Phi_{\rightarrow}(z \rightarrow \pm\infty)$ and $\Phi_{\leftarrow}(z \rightarrow \pm\infty)$ are the matrix solutions of the dimension $1 \times N_o^L$ and $1 \times N_o^R$. In other words, there are N_o^L linearly independent solutions, describing the incident wave traveling from left to right and N_o^R linearly independent solution, describing the incident wave traveling from right to left, respectively. The matrices $\mathbf{X}_{\min}^{(\rightarrow)}(z)$, $\mathbf{X}_{\min}^{(\leftarrow)}(z)$ of the dimension $1 \times N_o^L$ and the matrices $\mathbf{X}_{\max}^{(\rightarrow)}(z)$, $\mathbf{X}_{\max}^{(\leftarrow)}(z)$ of the dimension $1 \times N_o^R$ represent the fundamental asymptotic solution at the left and right boundaries of the interval, describing the motion of the wave in the arrow direction. The matrices $\mathbf{X}_{\min}^{(c)}(z)$ of the dimension $1 \times (N - N_o^L)$ and $\mathbf{X}_{\max}^{(c)}(z)$ of the dimension $1 \times (N - N_o^R)$ are fundamental asymptotically decreasing solutions at the left and right boundaries of the interval. The elements of these matrices are column matrices of the dimension $N \times 1$.

It follows that the matrices of reflection amplitudes \mathbf{R}_{\rightarrow} and \mathbf{R}_{\leftarrow} are square matrices of the dimension $N_o^L \times N_o^L$ and $N_o^R \times N_o^R$, while the matrices of transmission amplitudes \mathbf{T}_{\rightarrow} , \mathbf{T}_{\leftarrow} are rectangular matrices of the dimension $N_o^R \times N_o^L$ and $N_o^L \times N_o^R$. The auxiliary matrices $\mathbf{R}_{\rightarrow}^c$, $\mathbf{T}_{\rightarrow}^c$, $\mathbf{R}_{\leftarrow}^c$ and $\mathbf{T}_{\leftarrow}^c$ are rectangular matrices of the dimension $(N - N_o^L) \times N_o^L$, $(N - N_o^R) \times N_o^L$, $(N - N_o^R) \times N_o^R$ и $(N - N_o^L) \times N_o^R$.

Then the components of the wave function take the form

$$\begin{aligned} (\Phi_a)_{i_o i_o^L} &= X_{i_o i_o^L}^{(\rightarrow)}(z^{\min}) + \sum_{i'_o=1}^{N_o^L} X_{i_o i'_o}^{(\leftarrow)}(z^{\min}) R_{i'_o i_o^L}^{(\rightarrow)} + \sum_{i'_c=1}^{N - N_o^L} X_{i_o i'_c}^{(c)}(z^{\min}) R_{i'_c i_o^L}^{(c \rightarrow)}, \\ (\Phi_c)_{i_o i_o^L} &= \sum_{i'_o=1}^{N_o^R} X_{i_o i'_o}^{(\leftarrow)}(z^{\max}) T_{i'_o i_o^L}^{(\rightarrow)} + \sum_{i'_c=1}^{N - N_o^R} X_{i_o i'_c}^{(c)}(z^{\max}) T_{i'_c i_o^L}^{(c \rightarrow)}, \\ (\Phi_a)_{i_o i_o^R} &= \sum_{i'_o=1}^{N_o^L} X_{i_o i'_o}^{(\rightarrow)}(z^{\min}) T_{i'_o i_o^R}^{(\leftarrow)} + \sum_{i'_c=1}^{N - N_o^L} X_{i_o i'_c}^{(c)}(z^{\min}) T_{i'_c i_o^R}^{(c \leftarrow)}, \\ (\Phi_c)_{i_o i_o^R} &= X_{i_o i_o^R}^{(\leftarrow)}(z^{\max}) + \sum_{i'_o=1}^{N_o^R} X_{i_o i'_o}^{(\rightarrow)}(z^{\max}) R_{i'_o i_o^R}^{(\leftarrow)} + \sum_{i'_c=1}^{N - N_o^R} X_{i_o i'_c}^{(c)}(z^{\max}) R_{i'_c i_o^R}^{(c \leftarrow)}, \end{aligned} \quad (48)$$

where the asymptotic solutions $\mathbf{X}^{(\rightarrow)}(z) \equiv \mathbf{X}^{(+)}(z)$, $\mathbf{X}^{(\leftarrow)}(z) \equiv \mathbf{X}^{(-)}(z)$ of the boundary value problem at $z \leq z^{\min}$ and/or $z \geq z^{\max}$ are given by Eqs. (12)–(13).

For the right-hand side of Eqs. (44) we have

$$\begin{aligned}
(\mathbf{G}_{\min}^p \Phi_a)_{i_o i_o^L} &= X'_{i_o i_o^L}{}^{(\rightarrow)}(z^{\min}) + \sum_{i'_o=1}^{N_o^L} X'_{i_o i'_o}{}^{(\leftarrow)}(z^{\min}) R_{i'_o i_o^L}{}^{(\rightarrow)} + \sum_{i'_c=1}^{N-N_o^L} X'_{i_o i'_c}{}^{(c)}(z^{\min}) R_{i'_c i_o^L}{}^{(c \rightarrow)}, \\
(\mathbf{G}_{\max}^p \Phi_c)_{i_o i_o^L} &= \sum_{i'_o=1}^{N_o^R} X'_{i_o i'_o}{}^{(\leftarrow)}(z^{\max}) T_{i'_o i_o^L}{}^{(\rightarrow)} + \sum_{i'_c=1}^{N-N_o^R} X'_{i_o i'_c}{}^{(c)}(z^{\max}) T_{i'_c i_o^L}{}^{(c \rightarrow)}, \\
(\mathbf{G}_{\min}^p \Phi_a)_{i_o i_o^R} &= \sum_{i'_o=1}^{N_o^L} X'_{i_o i'_o}{}^{(\rightarrow)}(z^{\min}) T_{i'_o i_o^R}{}^{(\leftarrow)} + \sum_{i'_c=1}^{N-N_o^L} X'_{i_o i'_c}{}^{(c)}(z^{\min}) T_{i'_c i_o^R}{}^{(c \leftarrow)}, \\
(\mathbf{G}_{\max}^p \Phi_c)_{i_o i_o^R} &= X'_{i_o i_o^R}{}^{(\leftarrow)}(z^{\max}) + \sum_{i'_o=1}^{N_o^R} X'_{i_o i'_o}{}^{(\rightarrow)}(z^{\max}) R_{i'_o i_o^R}{}^{(\leftarrow)} + \sum_{i'_c=1}^{N-N_o^R} X'_{i_o i'_c}{}^{(c)}(z^{\max}) R_{i'_c i_o^R}{}^{(c \leftarrow)}.
\end{aligned} \tag{49}$$

Substituting the equalities (48) and (49) into Eq. (44) we arrive at the system of nonhomogeneous equations $R_{i_o i_o^L}{}^{(\rightarrow)}$, $T_{i'_o i_o^L}{}^{(\rightarrow)}$, $R_{i'_o i_o^R}{}^{(\leftarrow)}$, $T_{i'_c i_o^L}{}^{(c \rightarrow)}$, $R_{i'_c i_o^R}{}^{(c \leftarrow)}$, $T_{i'_c i_o^R}{}^{(c \leftarrow)}$, which has a unique solution.

When solving the problem in the semiaxis with the Neumann or the third-kind boundary conditions on the boundary z^{\min} or z^{\max} of the semiaxis, the role of independent variables is played by the elements of the matrices Φ_a or Φ_c , instead of \mathbf{R} and \mathbf{T} , while for the Dirichlet boundary conditions we have $\Phi_a = 0$ or $\Phi_c = 0$, so that in this case the corresponding equation is not taken into account.

D. Algorithm for calculating the complex eigenvalues and eigenfunctions of metastable states

To calculate the complex eigenvalues and the corresponding eigenfunctions of metastable states we solve the algebraic problem (33) for the equation with respect to the pair of unknowns $u = \{\lambda^h, \Phi^h\}$:

$$\begin{cases} (\tilde{\mathbf{A}} - \lambda^h \mathbf{B}) \Phi^h = 0, & \lambda = 2E^h, \\ (\Phi^h, \mathbf{B} \Phi^h) - 1 = 0. \end{cases} \tag{50}$$

The equation of the Continuous Analog of Newton Method in the vicinity of the solution $u = \{\lambda_*^h, \Phi_*^h\}$ with respect to the unknowns $u(t) = \{\Phi(t), \lambda(t)\}$, $0 \leq t < \infty$ has the form

$$\begin{cases} (\tilde{\mathbf{A}} - \lambda \mathbf{B}) \frac{d\Phi}{dt} - \frac{d\lambda}{dt} \mathbf{B} \Phi = -(\tilde{\mathbf{A}} - \lambda \mathbf{B}) \Phi, \\ 2 \left(\frac{d\Phi}{dt}, \mathbf{B} \Phi \right) = 1 - (\Phi, \mathbf{B} \Phi), \end{cases} \tag{51}$$

where $\lambda(0)$ and $\Phi(0)$ denote the known initial approximation for the eigenvalue and the eigenfunction. Using the discrete representation of derivatives

$$\left. \frac{d\Phi}{dt} \right|_{t_k} \approx \frac{\Phi_{k+1} - \Phi_k}{\tau_k} = \mathbf{v}_k, \quad \left. \frac{d\lambda}{dt} \right|_{t_k} \approx \frac{\lambda_{k+1} - \lambda_k}{\tau_k} = \mu_k, \tag{52}$$

the discrete analog of Eq.(51) obtained using the grid $t_{k+1} = t_k + \tau_k$ with the step τ_k with respect to the pair of unknowns μ_k \mathbf{v}_k takes the form

$$\begin{cases} (\tilde{\mathbf{A}} - \lambda_k \mathbf{B}) \mathbf{v}_k - \mu_k \mathbf{B} \Phi_k = -\mathbf{r}_k, \\ 2 (\mathbf{v}_k, \mathbf{B} \Phi_k) = 1 - (\Phi_k, \mathbf{B} \Phi_k), \end{cases} \tag{53}$$

where $\lambda_0 = \lambda(0)$ and $\Phi_0 = \Phi(0)$ are initial approximation to the eigenvalue and the eigenvector. The iteration corrections \mathbf{r}_k and \mathbf{v}_k are given by formulas

$$\mathbf{r}_k = (\tilde{\mathbf{A}} - \lambda_k \mathbf{B}) \Phi_k, \quad \mathbf{v}_k = -\Phi_k + \mu_k \Theta_k. \tag{54}$$

The iteration corrections Θ_k and μ_k to the eigenvector Φ_k and to the eigenvalue λ_k are calculated from the algebraic problem

$$\begin{cases} (\tilde{\mathbf{A}} - \lambda_k \mathbf{B}) \Theta_k = \mathbf{B} \Phi_k, \\ 2\mu_k (\Theta_k, \mathbf{B} \Phi_k) = 1 + (\Phi_k, \mathbf{B} \Phi_k), \end{cases} \quad (55)$$

whereas the iteration corrections μ_k is calculated by means of the formula

$$\mu_k = \frac{1 + (\Phi_k, \mathbf{B} \Phi_k)}{2(\Theta_k, \mathbf{B} \Phi_k)}. \quad (56)$$

This option in the program is implemented, by default, when the value of the key **mukopt**=1.

The transition from Φ_k , λ_k at k -th step to Φ_{k+1} , λ_{k+1} at $k+1$ -th step is executed by using the formulas

$$\begin{cases} \Phi_{k+1} = \Phi_k + \tau_k \mathbf{v}_k = (1 - \tau_k) \Phi_k + \tau_k \mu_k \Theta_k, \\ \lambda_{k+1} = \lambda_k + \tau_k \mu_k. \end{cases} \quad (57)$$

Calculation of the optimal iteration step τ_k . To calculation the optimal iteration step τ_k , we use the following representation of the quantity \mathbf{r}_{k+1} at the $k+1$ -th step

$$\mathbf{r}_{k+1} = (\tilde{\mathbf{A}} - \lambda_{k+1} \mathbf{B}) \Phi_{k+1} = (\tilde{\mathbf{A}} - (\lambda_k + \tau_k \mu_k) \mathbf{B}) ((1 - \tau_k) \Phi_k + \tau_k \mu_k \Theta_k) = (1 - \tau_k) \mathbf{r}_k - \tau_k^2 \mu_k \mathbf{B} \mathbf{v}_k. \quad (58)$$

Then the expression for the discrepancy $\|\mathbf{r}_{k+1}\|^2$ takes the form

$$\|\mathbf{r}_{k+1}\|^2 = (1 - \tau_k)^2 \|\mathbf{r}_k\|^2 - 2(1 - \tau_k) \tau_k^2 \mu_k (\mathbf{r}_k, \mathbf{B} \mathbf{v}_k) + \tau_k^4 \mu_k^2 \|\mathbf{B} \mathbf{v}_k\|^2. \quad (59)$$

We denote $f(\tau_k) = \|\mathbf{r}_{k+1}\|^2$ and calculate its derivative

$$\begin{aligned} f'(\tau_k) &= 2(\tau_k - 1) \|\mathbf{r}_k\|^2 - 2(2\tau_k - 3\tau_k^2) \mu_k (\mathbf{r}_k, \mathbf{B} \mathbf{v}_k) + 4\tau_k^3 \mu_k^2 \|\mathbf{B} \mathbf{v}_k\|^2 \\ &= 4\mu_k^2 \|\mathbf{B} \mathbf{v}_k\|^2 \tau_k^3 + 6\mu_k (\mathbf{r}_k, \mathbf{B} \mathbf{v}_k) \tau_k^2 + 2[\|\mathbf{r}_k\|^2 - 2\mu_k (\mathbf{r}_k, \mathbf{B} \mathbf{v}_k)] \tau_k - 2\|\mathbf{r}_k\|^2. \end{aligned} \quad (60)$$

We see that $f'(0) = -2\|\mathbf{r}_k\|^2 < 0$ and $f'(2) = 2f(2) > 0$. Hence, the function $f(\tau_k)$ has at least one minimum in the interval $(0,2)$. Thus, it is possible to find an optimum value of the iteration parameter $\tau_k = \tau_k^*$, calculating the roots of the cubic equation $f'(\tau_k^*) = 0$. If it has three real roots, one should choose the one close to 1. In the program the option of choosing the optimal step τ_k is implemented with the key value of **mukopt**=1. By default, the program sets the value $\tau_k = 1$ when the value of the key is **mukopt**=0. The iterative process (55)–(57) is terminated, provided that $\|\mathbf{r}_{k+1}\|^2 \leq \epsilon$, where $0 < \epsilon \ll 1$ specifies the accuracy of the approximate solution.

Remark. Let $\tilde{\mathbf{A}}$, λ , Φ be complex numbers. Then μ_k , \mathbf{v}_k , \mathbf{r}_k are complex numbers and the discrepancy is determined by the relation

$$\begin{aligned} \|\mathbf{r}_{k+1}\|^2 &= ((1 - \tau_k) \mathbf{r}_k^* - \tau_k^2 \mu_k^* \mathbf{B} \mathbf{v}_k^*) ((1 - \tau_k) \mathbf{r}_k - \tau_k^2 \mu_k \mathbf{B} \mathbf{v}_k) \\ &= (1 - \tau_k)^2 \|\mathbf{r}_k\|^2 - 2(1 - \tau_k) \tau_k^2 \Re(\mathbf{r}_k^*, \mu_k \mathbf{B} \mathbf{v}_k)_1 + \tau_k^4 \|\mu_k \mathbf{B} \mathbf{v}_k\|^2, \end{aligned} \quad (61)$$

where $\|\mathbf{a}\|^2 = (\mathbf{a}^\dagger, \mathbf{a})_1$, and $(\mathbf{a}, \mathbf{b})_1 = \mathbf{a}^\dagger \mathbf{b}$.

The iteration corrections Θ_k and μ_k to the eigenvector Φ_k and to the eigenvalue λ_k are calculated instead of (53) from the following algebraic problem:

$$\begin{cases} (\tilde{\mathbf{A}} - \lambda_k \mathbf{B}) \Theta_k = \mathbf{B} \Phi_k, \\ (\Phi_k, \mathbf{B} \Phi_k) \mu_k = (\Phi_k, (\tilde{\mathbf{A}} - \lambda_k \mathbf{B}) \Phi_k), \end{cases} \quad (62)$$

whereas the iteration corrections μ_k is calculated using the formula

$$(\Phi_k, \mathbf{B} \Phi_k) = 1, \quad \mu_k = \frac{(\Phi_k, (\tilde{\mathbf{A}} - \lambda_k \mathbf{B}) \Phi_k)}{(\Phi_k, \mathbf{B} \Phi_k)} = \frac{(\Phi_k, \mathbf{r}_k)}{(\Phi_k, \mathbf{B} \Phi_k)} = (\Phi_k, \mathbf{r}_k). \quad (63)$$

In the program this option is implemented, when the value of the key **mukc**=0. The transition from Φ_k , λ_k at the k -th step to Φ_{k+1} , λ_{k+1} at the $k+1$ -th step is executed by means of the formulas

$$\begin{cases} \tilde{\Phi}_{k+1} = \Phi_k + \tau_k \mathbf{v}_k = (1 - \tau_k) \Phi_k + \tau_k \mu_k \Theta_k, & \Phi_{k+1} = \frac{\tilde{\Phi}_{k+1}}{\sqrt{(\tilde{\Phi}_{k+1}, \mathbf{B} \tilde{\Phi}_{k+1})}}, \\ \lambda_{k+1} = \lambda_k + \tau_k \mu_k, \end{cases} \quad (64)$$

with the iteration step τ_k calculated using the formula [8]

$$\tau_k = \frac{\|\mathbf{r}_k\|^2}{\|\mathbf{r}_k\|^2 + \|\tilde{\mathbf{r}}_{k+1}\|^2} \leq 1, \quad (65)$$

where

$$\tilde{\mathbf{r}}_{k+1} = \left(\tilde{\mathbf{A}} - \lambda_{k+1} \mathbf{B} \right) \Phi_{k+1}, \quad (66)$$

and Φ_{k+1} , λ_{k+1} calculated by formula (64) at $\tau_k = 1$. In program the option of choosing the optimal step τ_k is implemented with the key value of **mukopt**=1. By default, the program made the value $\tau_k = 1$ when the value of the key **mukopt**=0.

The iterative process (62)–(65) in which μ_k is calculated using the formula (63) is terminated, using Eq. (66), under the condition that $\|\mathbf{r}_{k+1}\|^2 \leq \epsilon$, where $0 < \epsilon \ll 1$ is the specified accuracy of the approximate solution.

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IV. INPUT AND OUTPUT

This archive contains

File “kantbp4m.mwt” with procedure hermites() for solution of boundary problem for paragraph I,
Files with examples “examplexx.txt”.

In the process of work the program generates the work and output files, for example,

“hermites.dat” contains interpolation Hermite polynomials,

“inta.dat” contains integrals between polynomials Hermite and/or their derivatives, from which the stiffness and mass matrix are constructed,

“wfuncts**.dat” contains eigenvalues and eigenfunctions of the solved problem.

Accessing the program is as follows:

1. read “kantbp4m.mwt”; initialization of procedure;
2. ... (list of input data); input data;
3. hermites(); execution of procedure;
4. (output data); output data
the steps 2-4 are repeated.

A. List of input and output data

keypot (by default 1)

0 – approximation of a function by the interpolation Hermite polynomials,

1 – solution of the eigenvalue problem (calculations of first eigenvalues and eigenfunctions),

2 – solution of the scattering problem,

3 – solution of the eigenvalue problem by Newton method,

4 – matrices **A** and **B** from (33)–(34) are calculated and written in files “afem.dat” and “bfem.dat”.

z independent variable.

INPUT:

filenameh, **filenamew**, **filenameea**, **filenameei** (by default “hermites.dat”, “wfuncts*.dat”, “abfem.dat” and “inta.dat”, respectively) files for storing of intermediate and final results (see. below), where * means the value of counter nexec.

nexec counter (by default at the first start 1, further it is increased by 1) * in the name of file “wfuncts*.dat” takes values equal nexec.

zpoints (at keypot=0)

contains a list of nodes, in which the values of the approximated function and its derivatives is given in the form: $zpoints := [z_1, z_2, \dots, z_n]$.

fpoints (at keypot=0)

a list, containing the values of the approximated function and its derivatives in the points from the list zpoints is given in the form: $fvals := [[f(z_1), f'(z_1), \dots, f^{(\kappa_1)}(z_1)], [f(z_2), \dots, f^{(\kappa_2)}(z_2)], \dots, [f(z_n), \dots, f^{(\kappa_n)}(z_n)]]$.

psubint (by default 3)

the number of subintervals on p finite element (21), i.e. the number of nodes equals to psubint+1.

kappamax (by default 2)

multiplicity of nodes.

intprep (by default 1)

0 – integrals A , B and V , from which the stiffness and mass matrix are read from file filenameei. It used if previous execution was performed with same psubint and kappamax.

1 – integrals A , B and V are calculate and write to the file filenameei.

femmatcal (by default 0)

-1 – the stiffness matrix (AFEM) and the mass matrix (BFEM) without boundary conditions are read from file filenamea.

0 – the stiffness and the mass matrix are calculated, but are not written in file filenamea.

1 – the stiffness and the mass matrix are calculated, and are written in file filename, after that femmatcal takes value -1.

grid11(r0), r0=0,1,...,psubint, grid11(0):=-1, grid11(psubint):=1

distribution of the nodes in the interval [-1,1] (by default distribution of nodes is equidistant).

eqs (by default 0)

1,2,3,..., the number of equations N in (1)

0 one equation, at this indices of vpot, RBoundL, RBoundR are not written.

nmesh (by default 0)

1,2,3,..., the number of subintervals on domain $z \in [z^{\min}, z^{\max}]$ which divided on finite elements of equal length 0 on domain $z \in [z^{\min}, z^{\max}]$ the equidistant grid is used.

zmin, zmax (at nmesh=0)

boundary points z^{\min} and z^{\max} .

zmesh(r0), r0=0,1,...,nmesh, (at nmesh=1,2,3,...)

boundary points of nmesh subintervals

ngrid the number of finite elements on interval [zmin, zmax]. At nmesh=1,2,... is given in the form of array ngrid(1), ..., ngrid(nmesh) where ngrid(r0), r0=1,...,nmesh means the number of finite elements on subinterval [zmesh(r0-1), zmesh(r0)],

vpot are elements of matrix of effective potentials V_{ij} of the problem (1). Is given in the form:

vpot=... at nmesh=0 and eq=0

vpot(i0)=...; i0=1..nmesh; at nmesh=1,2,... and eq=0

vpot(i1,i2)=...; i1,i2=1...eq; at nmesh=0 and eq=1,2,...

vpot(i1,i2,i0)=...; i1,i2=1...eq; i0=1...nmesh; at nmesh=1,2,... at eq=1,2,...

Qap (at eqs=1,2,3,..., by default 0)

If matrix of effective potentials Q_{ij} is exist (1=yes, 0 - no).

qpot (at Qap=1)

are elements of matrix of effective potentials Q_{ij} of the problem (1). Is given in the form:

qpot(i1,i2)=...; i1,i2=1...eq; at nmesh=0 and eq=1,2,...

qpot(i1,i2,i0)=...; i1,i2=1...eq; i0=1...nmesh; at nmesh=1,2,... and eq=1,2,...

FFA (by default 1)

function $f_A(z)$. At nmesh=1,2,... and FFAD=-1 is given in the form of array FFA(1),...,FFA(nmesh).

FFB (by default 1)

function $f_B(z)$. At nmesh=1,2,... and FFBD=-1 is given in the form of array FFB(1),...,FFB(nmesh).

FFAD (by default 0, if $f_A(z)$ is monom of z , else 1)

0 – integrals A from (33)–(34) are calculated, using explicit expressions for FFA,

± 1 – integrals A are calculated, using expansions of FFA by interpolation Hermite polynomials, FFAD < 0 involves piecewise continuous $f_A(z)$.

FFBD (by default 0, if $f_B(z)$ is monom of z , else 1)

0 – integrals B , V and Q from (33)–(34) are calculated, using explicit expressions for FFB

± 1 – integrals B , V and Q are calculated, using expansions FFB and FFB*vpot by interpolation Hermite polynomials, FFBD < 0 involves piecewise continuous $f_B(z)$.

DirL, DirR (by default 2 at keypot=1 or 3 and 0 at keypot=2)

boundary condition in the left and right points of interval:

1 – Dirichlet condition,

2 – Neumann condition ,

3 – condition of third type,

0 – condition of third type that determined from the asymptotic solution (10), (11) of the multichannel scattering problem.

RBoundL, **RBoundR** (are given by user at DirL=3 and DirR=3, respectively, by default 0) relation $\mathcal{R}(z)$ of derivative of the solution to the solution see formula (4). At keypot=3 them may explicitly depend on formal parameter EEh, which correspond to the values of Eh. At eqs=1,2,..., are given in the form of matrix with dimension eqs \times eqs: RBoundL(11,l2), RBoundR(11,l2).

asymexp (at keypot=2, by default 0)

0 – asymptotic solutions of scattering problem are given by formulas (12) and (13),

1 – asymptotic solutions of scattering problem are given by user.

Lp2OC(l1) (at keypot=2, DirL=0, array of the dimension max(1,eqs), is given by user at asymexp=1)

the square of the wave number (p_{l1}^t) at $z \leq z^{\min}$ (see (12)), if > 0 , channel l1 is opened, if ≤ 0 , channel l1 is closed.

Rp2OC(l1) (at keypot=2, DirR=0, array of the dimension max(1,eqs), is given by user at asymexp=1)

the square of the wave number (p_{l1}^t) at $z \geq z^{\max}$ (see (12)), if > 0 , channel l1 is opened, если ≤ 0 , channel l1 is closed.

LBoundLR(l1,l2), **LBoundRL**(l1,l2), **LBoundC**(l1,l2) (at keypot=2, DirL=0, are matrices of the dimension max(1,eqs) \times max(1,eqs), in which the first index indicates the number of channel, and the second – the number of component of solution, are given by user at asymexp=1)

asymptotic solutions at $z \leq z^{\min}$, describing the waves incident from left to right, the waves incident from right to left and decreasing solutions for closed channels, respectively (see (12) and (13)).

DLBoundLR(l1,l2), **DLBoundRL**(l1,l2), **DLBoundC**(l1,l2) (at keypot=2, DirL=0, are matrices of the dimension max(1,eqs) \times max(1,eqs), are given by user at asymexp=1)

derivatives of asymptotic solutions LBoundLR(11,l2), LBoundRL(11,l2), LBoundC(11,l2) (see (12) and (13)).

RBoundLR(l1,l2), **RBoundRL**(l1,l2), **RBoundC**(l1,l2), **DRBoundLR**(l1,l2), **DRBoundRL**(l1,l2),

DRBoundC(l1,l2) (at keypot=2, DirR=0, are given at asymexp=1)

the same as LBoundLR(11,l2), LBoundRL(11,l2), LBoundC(11,l2), DLBoundLR(11,l2),

DLBoundRL(11,l2), DLBoundC(11,l2) but at $z \geq z^{\max}$ (see (12) and (13)).

numberf (at keypot=1 by default 5)

the number of eigenfunctions.

grprint (by default 1)

Are the graphics of eigenfunctions displayed (1-yes, 0 - no, -1 (at keypot=1 or 2) the program calculates only eigenvalues or S - matrix, 2 (at keypot=3) displayed intermediate results).

Eh (at keypot=2 or 3)

a fixed value of the energy E for the of scattering problem (at keypot=2) or an initial approximation for the eigenvalue (at keypot=3).

Phink (at keypot=3)

the initial approximation for eigenfunction, at eqs=1,2,... is given in the form of array Phink(1),...,Phink(eqs).

itermax (at keypot=3, by default 20)

the number of iterations, the calculations are also terminated at the achievement of accuracy $10^{3-\text{Digits}}$.

mukc (at keypot=3, by default 1)

method of calculation of iteration correction μ_k (1 – by formula (56), 0 – by formula (63)).

mukopt (по умолчанию 0)

Is the optimal value of iteration step τ_k calculated (1- yes, 0 - no).

gropts

a set of options for drawing, by default the real and imaginary parts of the solutions are displayed by the solid and dashed lines, and the color is changed from red for the first component to violet for the last component.

infopr (by default at the first execution is 1, after 0)

Is auxiliary information displayed (1-yes, 0 - no).

infoerr (at keypot=3, by default 1)

Are the intermediate eigenvalues, corrections and iteration step displayed (1 - yes, 0 - no).

normtp (at keypot 1 or 3, by default 1)

normalization condition (1 - by formula (15), 0 - by formula (16))

OUTPUT:

IHP (written to the file filenameh)

interpolation Hermite polynomials (25).

fun (at keypot=0, global)

the function, which interpolated from values fpoints on a grid zpoints.

eigvxx, xx=1, ..., numberf (at keypot=1, written to the file filenamew)

the eigenvalues.

eigfxx, xx=1, ..., numberf (at keypot=1, written to the file filenamew)

the eigenfunctions in the form of piecewise continuous polynomial. At eqs=1,2,... the number of components are added in parentheses: eigfxx(1), ..., eigfxx(eqs)

eigfLRr, **eigfLRi**, **eigfRLr**, **eigfRLi** (at keypot=2 и weigf>-1, written to the file filenamew)

the real and imaginary parts of the eigenfunctions Φ_{\leftarrow}^h and Φ_{\rightarrow}^h .

NOpenL, **NOpenR**, **NCloseL**, **NCloseR** (при keypot=2, global)

the numbers of open and closed channels.

RLRscat, **RRLscat**, **TLRscat**, **TRLscat**, **RLRscatc**, **RRLscatc**, **TLRscatc**, **TRLscatc** (at keypot=2, global, also written to the file filenamew)

the matrices of the reflection and transmission amplitudes, and the matrices of coefficients of asymptotic solutions in closed channels: $R_{\rightarrow}(E)$, $R_{\leftarrow}(E)$, $T_{\rightarrow}(E)$, $T_{\leftarrow}(E)$, $R_{\leftarrow}^c(E)$, $R_{\rightarrow}^c(E)$, $T_{\leftarrow}^c(E)$, $T_{\rightarrow}^c(E)$, respectively.

Smatr (at keypot=2, global)

S - matrix (8).

eigv (at keypot=3, written to the file filenamew)

the eigenvalue.

eigf (at keypot=3, written to the file filenamew)

the eigenfunctions in the form of piecewise continuous polynomial, the number of components are added in parentheses eigf(1), ..., eigf(max(1,eqs)).

Eh (at keypot=3, global)

eigenvalue of the discrete spectrum problem.

B. Notes

For such variables, when keypot are not specified, it is means that keypot>0.

For a short time, you can get results with an accuracy of the order of 8 significant digits. If you want to get results with a greater accuracy and the number of equations in the system is large, for example, such that the number of elements of the eigenvector in solving algebraic problem exceeds $NL > 10^3$, the calculation is best done in Fortran using a software package KANTBP [9].

Time of "silence" program when it is executed for the sample is not more than 1-3 minutes, long "silence" or hang can be caused by either too much order $p' = \kappa^{\max}(p + 1) - 1$ of the FEM scheme (p' is displayed as "Order of Finite Element Scheme"), or variable Digits or dimension of the algebraic problem $NL \times NL$ (NL is displayed as "Dimension of algebraic eigenvalue problem"), or the elements of the matrix algebraic problem is not calculated in the form of numbers, for example, presented as formal expressions. In the latter case it is recommended to start the program with keypot=4 and view the elements of the matrices in the files "afem.dat" and "bfem.dat".

V. EXAMPLES

Sample files are located in the same archive and called `examplexx.txt` (`xx=01-16`). For execution of the code for a selected `examplexx.txt` user should copy it to Maple worksheet via "copy/paste", or use Maple command `<< read "examplexx.txt" >>`, or open file `examplexx.txt` by Maple choosing `<<Maple Input >>`.

Examples of numerical solution of boundary value problems for systems of ODE on a finite interval with boundary conditions of the first, second and third type, that approximate the test quantum mechanical eigenvalue problems and the scattering problems on an infinite interval, and the problem of calculating the metastable states on a sufficiently large but finite interval. To control of an accuracy of the numerical solution computed error obtained when substituting the ODE, $\bar{\varepsilon}_m(z) = |(\mathbf{D}(z) - E_m^h)\Phi_m^h(z)|$, $z \in (z^{\min}, z^{\max})$. If the test problem has an analytical solution, it is calculated as the absolute value of the difference between the numerical and the known analytic solutions $\varepsilon_m(z) = |\Phi_m^h(z) - \Phi_m^{exact}(z)|$, $z \in (z^{\min}, z^{\max})$, $m = 1, 2, \dots, \text{numberf}$. Plots of calculated errors $\bar{\varepsilon}_m(z)$ and $\varepsilon_m(z)$ of eigenfunctions are displayed on the computer screen.

Since the eigenfunctions of the discrete spectrum of decay exponentially $\Phi_m^{as}(z) \sim \exp(-\sqrt{-E_m}|z|)$ in the $z \rightarrow \infty$, then the original problem is reduced to a boundary value problem for bound states in a finite interval with Dirichlet or Neumann conditions at the boundary points z^{\min} and z^{\max} interval and the normalization condition (15). Solutions of the reduced boundary problem differs from the solution of the original problem of the order of $\epsilon_m^{(1)} = \int_{-\infty}^{z^{\min}} \Phi_m^{as}(z)\Phi_m^{as}(z)dz + \int_{z^{\max}}^{+\infty} \Phi_m^{as}(z)\Phi_m^{as}(z)dz$ and actually determined by the sum of the exponents $\epsilon_m^{(1)} \approx (|\Phi_m^{as}(z^{\min})| + |\Phi_m^{as}(z^{\max})|)/(-2\sqrt{-E_m})$ in the boundary points of the interval. For a given value of error $\epsilon_m^{(1)}$, we have the estimate of required values of the boundary points z^{\min} and z^{\max} of a finite interval.

Example 01. The interpolation of function by the given values of the function and its derivatives on the grid

```

restart;read "kantbp4m.mwt";keypot:=0; 1
vv:=-99/8/cosh(z)^2; 2
zpoints:=[0, 5/4, 5/2, 3]; 3
fpoints:=[[subs(z=zpoints[1],vv)] 4
, [subs(z=zpoints[2],vv),seq(subs(z=zpoints[2],diff(vv,z$i)),i=1..4)] 5
, [subs(z=zpoints[3],vv),subs(z=zpoints[3],diff(vv,z))] 6
, [subs(z=zpoints[4],vv),subs(z=zpoints[4],diff(vv,z)),subs(z=zpoints[4],diff(vv,z,z))] 7
]; 8
hermites(); 9
fun1:=fun; 10
plot([fun1,vv],z=0..3);plot([fun1-vv],z=0..3); 11
12

```

Line 1: Initialization procedure.

Line 3: An approximated function.

Lines 4-9: It is assumed that there is a set of values of the function and its derivatives in the mesh points of a grid named 'zpoints': in first point value of function is given, in second point the values of function of the derivatives up to fourth order are given, in third point the values of function of the derivatives up to first order are given, and in fourth point the values of function of the derivatives up to second order are given.

Lines 10-12: interpolation of the function and verification : graphics of the calculated function and a difference between the calculated and approximated function

Example 02. Solution of the eigenvalue problem with Dirichlet, Neumann and third kind boundary conditions

Program calculates solutions of the eigenvalue problem (1) with the potential $V(z) = 0$ for different boundary conditions: Dirichlet, Neumann, and the third kind, for whose eigenvalues and functions are known in analytical form, for example, $E_n = 1, 4, 9, 16, \dots$ of Dirichlet boundary conditions and $E_n = 0, 1, 4, 9, \dots$ for Neumann boundary conditions.

```

restart;read "kantbp4m.mwt";          1
psubint:=3; kappamax:=2;            2
vpot:=0;                             3
ngrid:=4;zmin:=-Pi/2;zmax:=Pi/2;    4
numberf:=5;                           5
                                     6
DirL:=1;DirR:=1;                     7
hermites();                           8
                                     9
DirL:=2;DirR:=2;                    10
hermites();                           11
                                     12
DirL:=3;DirR:=3;RBoundL:=5;RBoundR:=5; 13
hermites();                           14
                                     15
                                     16
read "wfuncts1.dat":                 17
for ii from 1 to numberf do          18
plots[logplot]([abs(abs(eigf|ii)-abs(sin(ii*z+Pi*ii/2)/sqrt(Pi/2)))],z=zmin..zmax 19
, title=cat("test by comparison with ",convert(ii,string),"-th exact w.f.")); 20
plots[logplot]([abs(-diff(eigf|ii,z,z)-eigv|ii*eigf|ii)],z=zmin..zmax 21
, title=cat("test by substitution of ",convert(ii,string),"-th solution to ODE")); 22
od;                                   23
                                     24
read "wfuncts2.dat":                 25
for ii from 1 to numberf do          26
plots[logplot]([abs(abs(eigf|ii)-abs(cos((ii-1)*z+Pi*(ii-1)/2)/sqrt(Pi/'if'(ii=1,1,2))))] 27
,z=zmin..zmax 28
, title=cat("test by comparison with ",convert(ii,string),"-th exact w.f.")); 29
plots[logplot]([abs(-diff(eigf|ii,z,z)-eigv|ii*eigf|ii)],z=zmin..zmax 30
, title=cat("test by substitution of ",convert(ii,string),"-th solution to ODE")); 31
od;                                   32

```

Lines 1-2: Initialization of procedure, and the choice of parameters of finite element method.

Line 3: the effective potential of the problem.

Line 4: Select of the interval of integration and partition it into 4 equal sub-interval.

Line 5: Select the number of desired eigenfunctions.

Lines 7-8: The solution of the problem with Dirichlet boundary conditions. The eigenfunctions and eigenvalues are written to the file 'wfuncts1.dat' (see. filenameew).

Lines 10-11: The solution of the same problem, but with the Neumann boundary conditions. The eigenfunctions and eigenvalues are written to the file 'wfuncts2.dat'.

Lines 13-14: The solution of the same problem, but with boundary conditions of the third kind $\Phi'(z) = 5\Phi(z)$ in the $z = z^{\min}$ and $z = z^{\max}$. The eigenfunctions and eigenvalues are written to the file 'wfuncts3.dat'.

Lines 17-23: Display graphs of discrepancy of eigenfunctions for the problem with Dirichlet boundary conditions. The absolute value of the difference between the numerical and the known analytic solutions $\varepsilon_m(z) = |\Phi_m^{num}(z) - \Phi_m^{exact}(z)|$, $z \in (z^{\min}, z^{\max})$, $m = 1, 2, \dots, \text{numberf}$ and accuracy of numerical solutions obtained when substituting the TAC, $\bar{\varepsilon}_m(z) = |(\mathbf{D}(z) - E_m)\Phi_m^{num}(z)|$, $z \in (z^{\min}, z^{\max})$.

Lines 25-32: Display graphs of discrepancy of eigenfunctions $\varepsilon_m(z)$ and $\bar{\varepsilon}_m(z)$ for a problem with Neumann boundary conditions.

Example 03. The solution of the eigenvalue problem for the Schrödinger equation with the one-dimensional harmonic oscillator potential and the radial equation for the d-dimensional harmonic oscillator

The original problem for bound states is formulated for the Schrödinger equation of d-dimensional harmonic oscillator

$$(\mathbf{D} - E_m) \Phi_m(z) = \left(-\frac{1}{z^{d-1}} \frac{d}{dz} z^{d-1} \frac{d}{dz} + z^2 - E_m \right) \Phi_m(z) = 0,$$

has an analytical solution - the eigenvalues E_m^{exact} and the eigenfunctions of $\Phi_m^{exact}(z)$, normalized by the condition (15) on infinite interval $z \in (-\infty, +\infty)$ at $d = 1$ ($E_m^{exact} = 1, 3, 5, 7, \dots$), or semi-infinite interval $z \in (0, +\infty)$ at $d \geq 2$ ($E_m^{exact} = d, d + 4, d + 8, \dots$).

The original problem is reformulated as eigenvalues problem (1) with boundary conditions (2) and the normalization condition (15) (if $d \geq 2$, then at $z = z^{min}$ the boundary condition (3) is applied), at $f_B(z) = f_A(z) = z^{d-1}$, $N = 1$, $V(z) \equiv V_{11}(z) = z^2$.

```

restart;read "kantbp4m.mwt"; 1
psubint:=3;kappamax:=2; 2
vpot:=(z)^2; 3
ngrid:=14;zmin:=-7;zmax:=7; 4
numberf1:=10;numberf:=numberf1;filenamew:="1dosc.dat"; 5
hermites(); 6

intprep:=1;ddim:=5;filenamew:="5dosc.dat"; 8
vpot:=(z)^2; ngrid:=7; 9
FFA:=z^(ddim-1);FFB:=z^(ddim-1); 10
zmin:=0;zmax:=7;numberf2:=5;numberf:=numberf2; 11
hermites(); 12

read "1dosc.dat": 14
oscfun1(0):=0; 15
for ii from 1 to numberf1 do 16
oscfun1(ii):='if'(ii=1 17
,exp(-z^2/2)/sqrt(sqrt(Pi)) 18
,sqrt(2)*z/sqrt(ii-1)*oscfun1(ii-1)-sqrt(ii-2)/sqrt(ii-1)*oscfun1(ii-2)); 19
plots[logplot]([abs(abs(eigf||ii)-abs(oscfun1(ii))))],z=zmin..zmax 20
,title=cat("1d osc: test by comparison with ",convert(ii,string),"-th exact w.f.")); 21
print(%); 22
plots[logplot]([abs(-diff(eigf||ii,z,z)+z^2*eigf||ii-Re(eigv||ii)*eigf||ii)],z=zmin..zmax 23
,title=cat("1d osc: test by substitution of ",convert(ii,string),"-th solution to ODE")); 24
print(%); 25
od: 26

read "5dosc.dat": 29
for ii from 1 to numberf2 do 30
oscfun(ii):=sqrt(2*GAMMA(ii-1+(ddim)/2)/GAMMA((ii-1)+1)) 31
/GAMMA(ddim/2) 32
*exp(-z^2/2)*hypergeom([-ii+1],[ddim/2],z^2); 33
plots[logplot]([abs(abs(eigf||ii)-abs(oscfun(ii))))],z=zmin..zmax 34
,title=cat(convert(ddim,string),"d osc: test by comparison with " 35
,convert(ii,string),"-th exact w.f.")); 36
print(%); 37
plots[logplot]([abs(-1/FFB*diff(FFA*diff(eigf||ii,z,z)+z^2*eigf||ii-Re(eigv||ii)*eigf||ii)] 38
,z=zmin..zmax,title=cat(convert(ddim,string),"d osc: test by substitution of " 39
,convert(ii,string),"-th solution to ODE")); 40
print(%); 41
od: 42

```

Lines 1-2: Initialization of procedures, and the choice of parameters of finite element method.

Line 3: The effective potential of the problem.

Line 4: Select the interval of integration tasks and splitting it into 14 equal intervals.

Lines 5-6: Calculation of the first 10 of the eigenfunctions and eigenvalues of a one-dimensional harmonic oscillator.

Lines 8-12: Calculating the first 10 eigenfunctions and eigenvalues of the problem for the d-dimensional harmonic oscillator. The matrix elements are re-read again. This is important, if FFAD=0 or FBBD=0.

Lines 14-26: Display of plots of errors $\varepsilon_m(z)$ and $\bar{\varepsilon}_m(z)$ for the one-dimensional harmonic oscillator.

Lines 29-42: Display of plots of errors eigenfunctions $\varepsilon_m(z)$ and $\bar{\varepsilon}_m(z)$ for the d-dimensional harmonic oscillator.

Example 04. The solution of the eigenvalue problem for the radial equation with Coulomb potential

The original problem for bound states is formulated for the Schrödinger equation with Coulomb potential

$$(\mathbf{D} - E_n) \Phi_n(z) = \left(-\frac{1}{z^{d-1}} \frac{d}{dz} z^{d-1} \frac{d}{dz} - \frac{2}{z} - E_n \right) \Phi_n(z) = 0,$$

which has an analytical solution – eigenvalues E_n^{exact} and the eigenfunctions of $\Phi_n^{exact}(z)$, normalized by the condition (15) in the semi-infinite interval $z \in (0, +\infty)$ in the ($d \geq 2$) -dimensional space, In particular, for the $d = 3$, $E_n^{exact} = -1/n^2$, $n = 1, 2, \dots$

Firstly, the eigenvalue problem (1) with boundary conditions (3) and the normalization condition (15) at $f_B(z) = f_A(z) = z^2$, $N = 1$, $V(z) \equiv V_{11}(z) = -2/z$ is solved, then the boundary conditions (3) are replaced by boundary conditions (4), depending on the eigenvalue E_n , and the solutions are performed by Newton method.

```

restart; read "kantbp4m.mwt"; 1
psubint:=3; kappamax:=2; 2
3
FFA:=z^2;FFB:=FFA; 4
FFAD:=0; FFBD:=0; #choose 1 or 0; 5
6
nmesh:=12; for i from 1 to nmesh do vpot(i):=-2/(z);ngrid(i):=1;od; 7
8
zmesh(0):=1/32;for i from 1 to nmesh do zmesh(i):=zmesh(i-1)+2^i/64;od; 9
10
numberf:=5; hermites(); 11
12
read "wfuncts1.dat": 13
for i from 1 to nmesh do ngrid(i):=4;od; 14
15
DirL:=3;DirR:=3;keypote:=3; 16
17
18
RBoundL := (-1-(1/3*(EEh-2))*zmesh(0) 19
+ (1/6*(2*EEh-1))*zmesh(0)^2 20
+ (1/90*(-10*EEh+2+3*EEh^2))*zmesh(0)^3) 21
/ (1-zmesh(0) - (1/6*(EEh-2))*zmesh(0)^2 + (1/18*(2*EEh-1))*zmesh(0)^3 22
+ (1/360*(-10*EEh+2+3*EEh^2))*zmesh(0)^4); 23
24
RBoundR:=-sqrt(-EEh+subs(z=zmesh(nmesh),vpot(nmesh))); 25
Digits:=16; 26
for ii from 1 to numberf do 27
Phink:=eigf||ii: 28
Eh:=eigv||ii; 29
hermites(); 30
od: 31
32
for ii from 1 to numberf do 33
read cat("wfuncts",convert(ii+1,string),".dat"): 34
plots[logplot]([abs(abs(eigf(1))-abs(2/ii^(3/2)*exp(-z/ii)*hypergeom([-ii+1],[2],2*z/ii)))] 35
,z=zmesh(0)..zmesh(nmesh) 36
,title=cat("test by comparison with ",convert(ii,string),"-th exact w.f.")); 37
print(%); 38
plots[logplot]([abs(-1/z^2*diff(z^2*diff(eigf(1),z),z)-2/z*eigf(1)-eigv*eigf(1))] 39
,z=zmesh(0)..zmesh(nmesh) 40
,title=cat("test by comparison with ",convert(ii,string),"-th exact w.f.")); 41
print(%); 42
od: 43

```

Lines 1-2: Initialization of procedure, and the choice of parameters of finite element method.

Line 4: Determination of $f_A(z)$ and $f_B(z)$

Line 5: Choosing a method of calculating of the integrals to generate algebraic problem.

Lines 7 and 9: Firstly, the problem with Neumann boundary conditions is solved on a nonuniform grid $\Omega_z = \{1/32, 1/16, 1/8, \dots, 64, 128\}$, the effective potential should be set on on each of the sub-intervals.

Line 11: First five eigenfunctions and eigenvalues are calculated and written to the file 'wfuncts1.dat' (see. filenameew) .

Line 13: First five eigenfunctions and eigenvalues are read from the file 'wfuncts1.dat' .

Line 14: Sets a more dense irregular grid $\Omega'_z = \{1/32, 5/128, 3/64, 7/128, 1/16, 5/64, 3/32, 7/64, 1/8, \dots, 64, 80, 96, 112, 128\}$, where each subinterval Ω_z divided into 4 parts.

Line 16: Select the options for solving the problem by Newton's method with boundary conditions of the third kind.

Lines 19-25: Sets the asymptotic terms of the asymptotic expansions of the solution at $z \rightarrow 0$ and $z \rightarrow +\infty$.

Lines 26-31: Precision of the first five eigenfunctions and eigenvalues of Newton's method.

Lines 33-43: Displaying of graphs of errors $\varepsilon_n(z)$ and $\bar{\varepsilon}_n(z)$ of eigenfunctions for solving the problem by Newton's method.

Example 05. The solution of the eigenvalue problem with a one-dimensional Pöschl-Teller potential

The original problem for bound states is formulated on an infinite interval of $z \in (-\infty, +\infty)$ for the Schrödinger equation with the Pöschl-Teller potential

$$(\mathbf{D} - E_m) \Phi_m(z) = \left(-\frac{d^2}{dz^2} + \frac{-\lambda(\lambda-1)}{\cosh(z)^2} - E_m \right) \Phi_m(z) = 0, \quad (67)$$

with solutions are known in analytical form – eigenvalues E_m^{exact} and the eigenfunctions of $\Phi_m^{exact}(z)$ normalized by the condition (15) at $z^{\min} \rightarrow -\infty$ and $z^{\max} \rightarrow +\infty$. For the chosen $\lambda = 11/2$, there are five eigenvalues $E_m^{exact} = [-20.25, -12.25, -6.25, -2.25, -0.25]$.

The eigenvalues problem (1) with boundary conditions (3) and the normalization condition (15) at $f_B(z) = f_A(z) = 1$, $N = 1$ and $V(z) \equiv V_{11}(z) = \frac{-\lambda(\lambda-1)}{\cosh(z)^2}$ is solved. The program calculates five numerical eigenfunctions and eigenvalues.

A.A. Gusev, et al, Lecture Notes in Computer Science 8660, pp. 138–154 (2014)

```

restart;read "kantbp4m.mwt";
psubint:=3;kappamax:=2;

nmesh:=5;
for i from 1 to nmesh do ngrid(i):=4;vpot(i):=-99/4/cosh(z)^2;od;
zmesh(0):=-20;zmesh(1):=-5;zmesh(2):=-1;
zmesh(3):=1;zmesh(4):=5;zmesh(5):=20;

numberf:=5;hermites();

read "wfuncts1.dat":
ptfun(1) := (8/35)*sqrt(70)/(cosh(z)^(9/2)*sqrt(Pi));
ptfun(2) := (8/5)*sqrt(10)*sinh(z)/(cosh(z)^(9/2)*sqrt(Pi));
ptfun(3) := -(2/7)*sqrt(14)*(-8+7*cosh(z)^2)/(cosh(z)^(9/2)*sqrt(Pi));
ptfun(4) := -(2/5)*sqrt(10)*sinh(z)*(-8+5*cosh(z)^2)/(cosh(z)^(9/2)*sqrt(Pi));
ptfun(5) := (1/5)*sqrt(5)*(16-20*cosh(z)^2+5*cosh(z)^4)/(cosh(z)^(9/2)*sqrt(Pi));

for ii from 1 to 5 do
plots[logplot]([abs(abs(eigf||ii)-abs(ptfun(ii)))],z=zmesh(0)..zmesh(nmesh)
,title=cat("PT: test by comparison with ",convert(ii,string),"-th exact w.f."));
print(%);
plots[logplot]([abs(-diff(eigf||ii,z,z)+vpot(1)*eigf||ii-Re(eigv||ii)*eigf||ii)]
,z=zmesh(0)..zmesh(nmesh)
,title=cat("PT: test by substitution of ",convert(ii,string),"-th solution to ODE"));
print(%);
od:

```

Lines 1-2: Initialization of procedure, and the choice of parameters of finite element method.

Lines 4-7: The problem is solved in the quasi-uniform grid $\Omega_z = \{-20(4) - 5(4) - 1(4)1(4)5(4)20\}$, where the number in parentheses denotes the number of subinterval finite element, each of $n_{\text{mesh}} = 5$ subintervals effective potential must be specified.

Line 9: The solution of the problem with Neumann boundary conditions. Calculation of first five eigenfunctions and eigenvalues.

Lines 11-26: Display graphs errors $\varepsilon_m(z)$ and $\bar{\varepsilon}_m(z)$ of eigenfunctions.

Example 06. The solution of the eigenvalue problem with a one-dimensional potential Scarf (complex Pöschl-Teller potential)

The original problem for bound states is formulated on an infinite interval $z \in (-\infty, +\infty)$ for the Schrödinger equation with the Scarf potential

$$(\mathbf{D} - E_m) \Phi_m(z) = \left(-\frac{d^2}{dz^2} + \frac{V_1}{\cosh(z)^2} + i \frac{V_2 \sinh(z)}{\cosh(z)^2} - E_m \right) \Phi_m(z) = 0, \quad (68)$$

solutions are known in analytical form: - eigenvalues E_m^{exact} and the eigenfunctions of $\Phi_m^{exact}(z)$ normalized by the condition (16) at $z^{\min} \rightarrow -\infty$ and $z^{\max} \rightarrow +\infty$.

The eigenvalue problem (1) with boundary conditions (3) and the normalization condition (16) at $f_B(z) = f_A(z) = 1$, $N = 1$ and $V(z) \equiv V_{11}(z) = \frac{V_1}{\cosh(z)^2} + i \frac{V_2 \sinh(z)}{\cosh(z)^2}$ is solved.

A.A. Gusev, et al, Lecture Notes in Computer Science 9301, pp. 182–197 (2015);

```

restart;Digits:=12; read "kantbp4m.mwt";          1
keypot:=1;psubint:=3;kappamax:=2;                2
                                                    3
nmesh:=3;                                         4
ngrid(1):=4;ngrid(2):=ngrid(1);ngrid(3):=ngrid(1); 5
zmesh(0):=-12;zmesh(1):=-2;zmesh(2):=2;zmesh(3):=12; 6
V1:=2;V2:=3;                                     7
vpot(1):=-V1/cosh(z)^2-V2*I*sinh(z)/cosh(z)^2;    8
vpot(2):=vpot(1);vpot(3):=vpot(1);              9
                                                    10
numberf:=2;hermites();                           11
                                                    12
for n from 0 to numberf-1 do                       13
En:=evalf(-(n+1/2-1/2*(sqrt(1/4+V1+V2)+sqrt(1/4+V1-V2)))^2); 14
od;                                                15
                                                    16
read "wfunctsl.dat":                               17
for ii from 1 to numberf do                        18
  plots[logplot]([abs(-diff(eigf||ii+I*eigfi||ii,z,z) 19
    +(vpot(1)-eigv||ii)*(eigf||ii+I*eigfi||ii))],z=zmesh(0)..zmesh(nmesh) 20
  ,title=cat("Scarf: test by substitution of ",convert(ii,string),"-th solution to ODE")); 21
od;                                                22

```

Lines 1-2: Initialization of procedure, and the choice of parameters of finite element method.

Lines 4-9: The problem is solved in the quasi-uniform grid $\Omega_z = \{-12(4) - 2(4)2(4)12\}$, where the number in brackets denotes the number of subinterval finite element, each of $n_{\text{mesh}}:=3$ subintervals effective potential must be specified.

Line 11: Calculating and writing to the file 'wfunctsl.dat' (see. filenamew) two eigenfunctions and eigenvalues.

Lines 13-15: The analytical expressions for the eigenvalues E_m are given to verify the accuracy of approximate eigenvalues E_m^h .

Lines 17-22: Display graphs of error of numerical solution $\bar{\varepsilon}_m(z)$.

Example 07. The solution of the scattering problem for one-dimensional Pöschl-Teller potential

The original scattering problem is formulated on an infinite interval $z \in (-\infty, +\infty)$ for the Schrödinger equation with the Pöschl-Teller potential

$$(\mathbf{D} - E) \Phi(z) = \left(-\frac{d^2}{dz^2} + \frac{-\lambda(\lambda-1)}{\cosh(z)^2} - E \right) \Phi(z) = 0, \quad (69)$$

and has solutions known in analytical form: eigenfunctions $\Phi_m^{exact}(z)$, and the transmission T_v reflection and R_v .

Because the effective potential symmetric with respect to $z = 0$ solution of the problem can be constructed from even and odd solutions of the original scattering problems, but on a semiaxis $z \in (0, +\infty)$, with the Neumann or the Dirichlet boundary conditions at $z = 0$, respectively.

The boundary value problem (1) with boundary conditions (3) which are determined from the asymptotic solution (10), (11), of scattering problem $f_B(z) = f_A(z) = 1$, $N = 1$ and $V(z) \equiv V_{11}(z) = \frac{-\lambda(\lambda-1)}{\cosh(z)^2}$ is solved.

```

restart;Digits:=16; read "kantbp4m.mwt";
keypot:=2;psubint:=2;kappamax:=3;

lambda:=11/2;
#lambda:=1/2+7/sqrt(2)*I;
vpot:=-expand(lambda*(lambda-1))/cosh(z)^2;

Eh:=7.0;
zmin:=0;zmax:=8;ngrid:=12;DirL:=1;
hermites();Rr11:=RRLscat;

DirL:=2; hermites();Rr12:=RRLscat;

zmin:=-8;zmax:=8;DirL:=0;ngrid:=24; hermites();

"tests";
"|R<-|^2+|T<-|^2-1"=abs(TRLscat[1,1])^2+abs(RRLscat[1,1])^2-1;
"|R>|^2+|T>|^2-1"=abs(TLRscat[1,1])^2+abs(RLRscat[1,1])^2-1;
"|Reven|^2-1"=abs(Rr11[1,1])^2-1; "|Rodd|^2-1"=abs(Rr12[1,1])^2-1;
"( Reven+Rodd)/2-R<- "=(Rr11[1,1]+Rr12[1,1])/2-RRLscat[1,1];
"(-Reven+Rodd)/2-T<- "=(-Rr11[1,1]+Rr12[1,1])/2-TRLscat[1,1];
"(Reven+Rodd)/2-T> "=(Rr11[1,1]+Rr12[1,1])/2-RLRscat[1,1];
"(-Reven+Rodd)/2-T> "=(-Rr11[1,1]+Rr12[1,1])/2-TLRscat[1,1];

k:=sqrt(Eh):p:=evalf(sinh(Pi*k)/sin(Pi*lambda)):
"|Rexact|^2-|R<-|^2"=1/(1+p^2)-abs(RRLscat[1,1])^2;
"|Texact|^2-|T<-|^2"=p^2/(1+p^2)-abs(TRLscat[1,1])^2;

read "wfuncts1.dat":
plots[logplot]([abs(-diff(eigfRLr(1,1)+I*eigfRLi(1,1),z,z)
+(vpot-Eh)*(eigfRLr(1,1)+I*eigfRLi(1,1))),z=0..zmax
,title=cat("PT: test by substitution of odd solution to ODE"));

read "wfuncts2.dat":
plots[logplot]([abs(-diff(eigfRLr(1,1)+I*eigfRLi(1,1),z,z)
+(vpot-Eh)*(eigfRLr(1,1)+I*eigfRLi(1,1))),z=0..zmax
,title=cat("PT: test by substitution of even solution to ODE"));

read "wfuncts3.dat":
plots[logplot]([abs(-diff(eigfRLr(1,1)+I*eigfRLi(1,1),z,z)
+(vpot-Eh)*(eigfRLr(1,1)+I*eigfRLi(1,1))),z=zmin..zmax
,title=cat("PT: test by substitution of RL solution to ODE"));
plots[logplot]([abs(-diff(eigfLRLr(1,1)+I*eigfLRLi(1,1),z,z)

```

```

+(vpot-Eh)*(eigfLRr(1,1)+I*eigfLRi(1,1))] ,z=zmin..zmax 44
,title=cat("PT: test by substitution of LR solution to ODE"); 45

```

Lines 1-2: Initialization of procedure, and the choice of parameters of finite element method.

Lines 4-6: The effective potential of the problem.

Line 8: Sets the fixed value of the energy for the scattering problem

Lines 9-10: solving boundary value problems (1) on a uniform grid with Dirichlet boundary conditions (2) at $z = 0$ and the third kind (4) at $z = z^{max}$ with asymptotic solutions of the scattering problem on the semiaxis (9), (12).

Line 12: The decision of the boundary problem (1) on a uniform grid with Neumann boundary conditions (3) at $z = 0$ and the third kind (4) at $z = z^{max}$ with asymptotic solutions of the scattering problem on the semiaxis (9), (12).

Line 14: The decision of the boundary problem (1) on a uniform grid with the boundary of the Third Kind (4) at z^{min} and $z = z^{max}$ with asymptotic solutions scattering on the axis (7), (12).

Lines 16-27: Checking errors ($\simeq 0$) of implementation relations for the amplitudes of the reflection and transmission $|R_{\leftarrow}|^2 + |T_{\leftarrow}|^2 - 1 = 0$, $|R_{\rightarrow}|^2 + |T_{\rightarrow}|^2 - 1 = 0$, $|R_{\text{even}}|^2 - 1 = 0$, $|R_{\text{odd}}|^2 - 1 = 0$, Communication between the amplitudes of reflection on the half and amplitudes of the reflection and transmission axis $(R_{\text{even}} + R_{\text{odd}})/2 - R_{\leftarrow} = 0$, $(-R_{\text{even}} + R_{\text{odd}})/2 - T_{\leftarrow} = 0$, $(R_{\text{even}} + R_{\text{odd}})/2 - R_{\rightarrow} = 0$, $(-R_{\text{even}} + R_{\text{odd}})/2 - T_{\rightarrow} = 0$, and comparing the reflection and transmission coefficients with known analytical value $|R_{\rightarrow}^{\text{exact}}|^2 = |R_{\leftarrow}^{\text{exact}}|^2 = 1/(1 + p^2)$, $|T_{\rightarrow}^{\text{exact}}|^2 = |T_{\leftarrow}^{\text{exact}}|^2 = p^2/(1 + p^2)$, $p = \sinh(\pi\sqrt{E})/\sin(\pi\lambda)$.

Lines 29-45: displaying graphs of error of numerical solution $\bar{\varepsilon}_m(z)$.

Example 08. The solution of the scattering problem for one-dimensional Scarf potential

The original scattering problem is formulated on an infinite interval $z \in (-\infty, +\infty)$ for the Schrödinger equation with the Scarf potential

$$(\mathbf{D} - E)\Phi(z) = \left(-\frac{d^2}{dz^2} + \frac{V_1}{\cosh(z)^2} + i\frac{V_2 \sinh(z)}{\cosh(z)^2} - E \right) \Phi(z) = 0, \quad (70)$$

and has solutions known in analytical form: eigenfunctions $\Phi_m^{exact}(z)$, and the transmission T_v reflection and R_v .

The boundary value problem (1) with boundary conditions (3) which are determined from the asymptotic solution (10), (11), of scattering problem at $f_B(z) = f_A(z) = 1$, $N = 1$, $V(z) \equiv V_{11}(z) = \frac{V_1}{\cosh(z)^2} + i\frac{V_2 \sinh(z)}{\cosh(z)^2}$ is solved.

```

restart;Digits:=12;read "kantbp4m.mwt";
keypot:=2; psubint:=2; kappamax:=3;

V1:=2;V2:=3;
vpot:=V1/cosh(z)^2+V2*I*sinh(z)/cosh(z)^2;

Eh:=2.0;
zmin:=-12;zmax:=12;ngrid:=60;
hermites();

"tests";
k:=sqrt(Eh);
gp:=sqrt(V1+V2-1/4);
gm:=sqrt(V1-V2-1/4);
TK:=evalf((sinh(2*Pi*k))^2
/((sinh(2*Pi*k))^2+2*cosh(2*Pi*k)*cosh(Pi*gp)*cosh(Pi*gm)+cosh(Pi*gp)^2+cosh(Pi*gm)^2));
RL:=evalf((2*cosh(Pi*gp)*cosh(Pi*gm)+cosh(Pi*gp)^2*exp(-2*Pi*k)+cosh(Pi*gm)^2*exp(2*Pi*k))
/((sinh(2*Pi*k))^2+2*cosh(2*Pi*k)*cosh(Pi*gp)*cosh(Pi*gm)+cosh(Pi*gp)^2+cosh(Pi*gm)^2));
RR:=evalf((2*cosh(Pi*gp)*cosh(Pi*gm)+cosh(Pi*gp)^2*exp(2*Pi*k)+cosh(Pi*gm)^2*exp(-2*Pi*k))
/((sinh(2*Pi*k))^2+2*cosh(2*Pi*k)*cosh(Pi*gp)*cosh(Pi*gm)+cosh(Pi*gp)^2+cosh(Pi*gm)^2));
"|Texact|^2-|T->|^2"=TK-abs(TLRscat[1,1])^2;
"|Texact|^2-|T<-|^2"=TK-abs(TRLscat[1,1])^2;
"|Rexact|^2-|R->|^2"=RL-abs(RLRscat[1,1])^2;
"|Rexact|^2-|R<-|^2"=RR-abs(RRLscat[1,1])^2;

read "wfunctsl.dat";
plots[logplot]([abs(-diff(eigfRLr(1,1)+I*eigfRLi(1,1),z)
+(vpot-Eh)*(eigfRLr(1,1)+I*eigfRLi(1,1))),z=zmin..zmax
,title=cat("Scarf: test by substitution of RL solution to ODE"));
plots[logplot]([abs(-diff(eigfLRr(1,1)+I*eigfLRi(1,1),z)
+(vpot-Eh)*(eigfLRr(1,1)+I*eigfLRi(1,1))),z=zmin..zmax
,title=cat("Scarf: test by substitution of LR solution to ODE"));

```

Lines 1-2: - Initialization procedures, and the choice of parameters of finite element method.

Lines 4-5: The effective potential of the problem.

Line 7: Setting a fixed value of the energy for the scattering problem

Lines 8-9: The decision of the boundary problem (1) on a uniform grid with the boundary of the third kind (4) at z^{\min} and $z = z^{\max}$ with asymptotic solutions of the scattering problem for axis (7), (12).

Lines 11-24: A comparison of the reflection coefficients and passing to known analytical values $|R_{\rightarrow}^{\text{exact}}|^2$, $|R_{\leftarrow}^{\text{exact}}|^2$, $|T_{\rightarrow}^{\text{exact}}|^2 = |T_{\leftarrow}^{\text{exact}}|^2$.

Lines 26-32: displaying graphs of error of numerical solution $\bar{\varepsilon}_m(z)$.

Example 09. The solution of the eigenvalue problem for square well potential

The original problem for bound states is formulated on an infinite interval $z \in (-\infty, +\infty)$ for the Schrödinger equation with the piecewise constant potential

$$(\mathbf{D} - E_m) \Phi_m(z) = \left(-\frac{d^2}{dz^2} + V(z) - E_m \right) \Phi_m(z) = 0, \quad V(z) = \{V_0, |z| \leq a; 0, \text{otherwise}\},$$

solutions are known in analytical form: – eigenvalues E_m^{exact} and the eigenfunctions of $\Phi_m^{exact}(z)$ normalized by the condition (16) at $z^{\min} \rightarrow -\infty$ and $z^{\max} \rightarrow +\infty$.

The eigenvalue problem (1) with boundary conditions (3) and the normalization condition (16) at $f_B(z) = f_A(z) = 1$, $N = 1$ with the above $V(z)$ is solved.

```

restart;read "kantbp4m.mwt";
psubint:=6; kappamax:=1;

V:=-50;a:=1;
nmesh:=3; vpot(1):=0;vpot(2):=V;vpot(3):=0;
ngrid(1):=10;ngrid(2):=20;ngrid(3):=10;
zmesh(0):=-5;zmesh(1):=-a;zmesh(2):=a;zmesh(3):=5;

numberf:=5;hermites();

"test";
eq3:=tan(sqrt(E-V)*a)=sqrt(-E)/sqrt(E-V);
eq3a:=tan(sqrt(E-V)*a)=-sqrt(E-V)/sqrt(-E);
ExactEigenvalues=sort({seq(fsolve(eq3,E=V+n^2/a^2),n=1..ceil(evalf(a*sqrt(-V))))
,seq(fsolve(eq3a,E=V+n^2/a^2),n=1..ceil(evalf(a*sqrt(-V))))});

```

Lines 1-2: Initialization procedures, and the choice of parameters of finite element method.

Lines 4-7: The problem is solved in the quasi-uniform grid $\Omega_z = \{-5(10) - a(20)a(10)5\}$, where the number in brackets indicates the number of finite elements each of $n_{mesh} = 3$ subintervals. It is important to point potential breaks coincide with nodes z_{mesh}^* .

Line 9: Calculation and write to the file 'wfunct1.dat' (see. `filenamew`) five eigenfunctions and eigenvalues.

Lines 11-15: the exact eigenvalues of the problem is the solution of algebraic equations 'eq3' and 'eq3a' for the depth of the potential well V and a width $2a$.

Example 10. The solution of the eigenvalue problem for the system of equations with square well potentials

The original problem for bound states is formulated on an infinite interval $z \in (-\infty, +\infty)$ for the system of equations

$$\begin{aligned} -\frac{d^2\Phi_1(z)}{dz^2} + V_{11}(z)\Phi_1(z) + V_{12}(z)\Phi_2(z) + \dots + V_{1N}(z)\Phi_N(z) - E\Phi_1(z) &= 0, \\ -\frac{d^2\Phi_2(z)}{dz^2} + V_{21}(z)\Phi_1(z) + V_{22}(z)\Phi_2(z) + \dots + V_{2N}(z)\Phi_N(z) - E\Phi_2(z) &= 0, \\ \vdots \\ -\frac{d^2\Phi_N(z)}{dz^2} + V_{N1}(z)\Phi_1(z) + V_{N2}(z)\Phi_2(z) + \dots + V_{NN}(z)\Phi_N(z) - E\Phi_N(z) &= 0, \end{aligned}$$

with the matrix of piecewise constant potentials

$$V_{ij}(z) = V_{ji}(z) = \{V_{ij;1}, z \leq z_1; V_{ij;2}, z \leq z_2; \dots; V_{ij;k-1}, z \leq z_{k-1}; V_{ij;k}, z > z_{k-1}\}.$$

The set of eigenvalues $E_1^{ex} < E_2^{ex} < \dots < E_m^{ex}$ and the eigenfunctions of $\Phi_1^{ex}(z), \Phi_2^{ex}(z), \dots, \Phi_m^{ex}(z)$ normalized by the condition (15) at $z^{\min} \rightarrow -\infty$ and $z^{\max} \rightarrow +\infty$, can be calculated at $f_B(z) = f_A(z) = 1$, $N = 3$ using a representation of their eigenfunctions as a linear combination of trigonometric and exponential functions depending on the spectral parameter E , with unknown coefficients. However, the need to find the roots of nonlinear equations, which is the required 'exact' eigenvalues of the original problem.

Since the eigenfunctions of the discrete spectrum decay exponentially as $z \rightarrow \infty$, then the original problem is reduced to a boundary value problem (1) with the above $V_{ij}(z) = 0$ and $Q_{ij}(z) = 0$ for bound states in a finite interval with Dirichlet conditions at the boundary points $z^{\min} < z_1$ and $z^{\max} > z_{k-1}$, the interval and the normalization condition (15) that is solved numerically by finite element method using KANTBP 4M .

```
restart;read "kantbp4m.mwt";Digits:=12; 1
eqs:=3;psubint:=8;kappamax:=1; 2
keypote:=1;DirL:=1;DirR:=1; 3
4
nmesh:=3; ngrid(1):=10;ngrid(2):=10;ngrid(3):=10; 5
zmesh(0):=-12;zmesh(1):=-2;zmesh(2):=2;zmesh(3):=12; 6
7
vpot(1,1,1):=0;vpot(2,2,1):=5;vpot(3,3,1):=10; 8
vpot(1,2,1):=0;vpot(1,3,1):=0;vpot(2,3,1):=0; 9
vpot(2,1,1):=0;vpot(3,1,1):=0;vpot(3,2,1):=0; 10
11
vpot(1,1,2):=-5;vpot(2,2,2):=0;vpot(3,3,2):=10; 12
vpot(1,2,2):=4;vpot(1,3,2):=4;vpot(2,3,2):=4; 13
vpot(2,1,2):=4;vpot(3,1,2):=4;vpot(3,2,2):=4; 14
15
vpot(1,1,3):=0;vpot(2,2,3):=0;vpot(3,3,3):=0; 16
vpot(1,2,3):=0;vpot(1,3,3):=0;vpot(2,3,3):=0; 17
vpot(2,1,3):=0;vpot(3,1,3):=0;vpot(3,2,3):=0; 18
19
numberf:=5; hermites(); 20
21
read "example10test.txt"; 22
```

Lines 1-3: The initialization of procedure, the choice of options for solving the problem on their eigenvalues for the three equations with Dirichlet boundary conditions and the choice of parameters of finite element method.

Lines 4-5: The problem is solved in the quasi-uniform grid $\Omega_z = \{-6(10) - 2(10)2(10)6\}$, where the number in brackets denotes the number of subinterval finite element, each of nmesh:=3 sub-intervals must be given effective potentials. It is important to point potential breaks coincide with nodes zmesh(*) .

Lines 8-18: Setting the effective potentials.

Line 20: Calculation, display and recording in a file 'wfunct1.dat' (see filenamew) five eigenfunctions $\Phi_1^h(z), \dots, \Phi_5^h(z)$ and its eigenvalues of $E_1^h < E_2^h < \dots < E_5^h$.

Line 22: File "example10test.txt" contains a helper program for example10test for systems of nonlinear equations with thirteen trigonometric and exponential functions, depending on the desired spectral parameter, and 12 linear with respect to the unknown parameters the expansion coefficients of the desired eigenvector - function of the original problem on their eigenvalues on the axis. This program is designed for the calculation of the spectrum only in a special case, eqs=3 and nmesh=3 and vpot(i,j,1)=vpot(i,j,3)=0 for $i \neq j$ and may be at be finalized by the user.

The first step to using the built-in procedures dsolve sought the general solution of the ODE with constant coefficients vpot(i,j,2) which is valid on the interval $z \in [zmesh(1), zmesh(2)]$, the derivative of the solution is calculated also.

The second step uses the asymptotic solutions proportional $A||i) \cdot \exp(\sqrt{-Eh+vpot(i,i,1)} \cdot x_{min})$ and $A||i+3) \cdot \exp(-\sqrt{-Eh+vpot(i,i,3)} \cdot x_{max})$, just under $z \leq zmesh(1)$ and $z \geq zmesh(2)$ and their derivatives of z .

In the third step calculates the difference between the solutions obtained in the first step and asymptotic solutions in the third step, and the difference between the derivatives thereof, whereupon the difference values with the substitution $z = zmesh(1)$ or $z = zmesh(2)$ equal to zero.

After the third step, we have a system of nonlinear equations with thirteen trigonometric and exponential functions, depending on the desired spectral parameter E , and 12 linear with respect to the unknown parameters ($A||1), \dots, A||6)$ of the asymptotic solutions and $_C||1), \dots, _C||6)$ from the general solution of the ODE). In order to calculate the non-trivial solutions, in the system of equations adding Equation $A||1)^2 + \dots + A||6)^2 - 1 = 0$. The result is a rather complicated system of nonlinear equations.

In the fourth step, the system of nonlinear equations for thirteen unknowns 13 (the spectral parameter E , 12 and the parameters ($A||1), \dots, A||6), _C||1), \dots, _C||6)$) solved numerically using the built-in procedure fsolve. As compared values desired spectral parameter E , displays only the value of the desired spectral parameter E . What would be an iterative process for solving nonlinear problems converge to different values of the spectral parameter E , the initial conditions for the unknown coefficients in a system of nonlinear equations are randomly generated by a built-in procedure rand, with the procedure for solving fsolve run $2 \cdot \text{numberf}$ times.

During testing, it became clear that to compute eigenvalues $E_1^{ex} < E_2^{ex} < \dots < E_m^{ex}$, which are displayed on the screen for comparison with the eigenvalues of $E_1^h < E_2^h < \dots < E_s^h$, calculated by finite element method, the number of repetitions $2 \cdot \text{numberf}$ not enough ie too often the solution converges to one of the eigenvalues. In this case, the command « read "example10test.txt"; » to be repeated again. As a reminder of this output displays the following warning:

"Eigenvalues given by solution of set of exact equations:"; "if not all, please repeat command « read "example10test.txt" "; »";

Attempts should be discontinued if the user sees all the eigenvalues calculated by the finite element method, or the user will bother to run this command.

Example 11. The solution of the multichannel scattering problem for the system of equations with square well potentials

The original multichannel scattering problem at fixed E is formulated on an infinite interval $z \in (-\infty, +\infty)$ for the system of equations

$$\begin{aligned} -\frac{d^2\Phi_1(z)}{dz^2} + V_{11}(z)\Phi_1(z) + V_{12}(z)\Phi_2(z) + \dots + V_{1N}(z)\Phi_N(z) - E\Phi_1(z) &= 0, \\ -\frac{d^2\Phi_2(z)}{dz^2} + V_{21}(z)\Phi_1(z) + V_{22}(z)\Phi_2(z) + \dots + V_{2N}(z)\Phi_N(z) - E\Phi_2(z) &= 0, \\ \vdots \\ -\frac{d^2\Phi_N(z)}{dz^2} + V_{N1}(z)\Phi_1(z) + V_{N2}(z)\Phi_2(z) + \dots + V_{NN}(z)\Phi_N(z) - E\Phi_N(z) &= 0, \end{aligned}$$

with the matrix of piecewise constant potentials

$$V_{ij}(z) = V_{ji}(z) = \{V_{ij;1}, z \leq z_1; V_{ij;2}, z \leq z_2; \dots; V_{ij;k-1}, z \leq z_{k-1}; V_{ij;k}, z > z_{k-1}\},$$

solutions of them are calculated using a representation of eigenfunctions as a linear combination of trigonometric and exponential functions with unknown coefficients.

The boundary value problem (1) with the above $V_{ij}(z) = 0$ and $Q_{ij}(z) = 0$ with boundary conditions (4) which are determined from the asymptotic solution (10), (11), of multichannel scattering problem at $f_B(z) = f_A(z) = 1$, $N = 3$.

```

restart;read "kantbp4m.mwt";Digits:=12;          1
eqs:=3;psubint:=8;kappamax:=1;                  2
keypote:=2;DirL:=0;DirR:=0;                     3
                                                    4
nmesh:=3;                                         5
ngrid(1):=10;ngrid(2):=10;ngrid(3):=10;          6
zmesh(0):=-6;zmesh(1):=-2;zmesh(2):=2;zmesh(3):=6; 7
                                                    8
vpot(1,1,1):=0;vpot(2,2,1):=5;vpot(3,3,1):=10;  9
vpot(1,2,1):=0;vpot(1,3,1):=0;vpot(2,3,1):=0; 10
vpot(2,1,1):=0;vpot(3,1,1):=0;vpot(3,2,1):=0; 11
                                                    12
vpot(1,1,2):=-5;vpot(2,2,2):=0;vpot(3,3,2):=10; 13
vpot(1,2,2):=4;vpot(1,3,2):=4;vpot(2,3,2):=4; 14
vpot(2,1,2):=4;vpot(3,1,2):=4;vpot(3,2,2):=4; 15
                                                    16
vpot(1,1,3):=0;vpot(2,2,3):=0;vpot(3,3,3):=0; 17
vpot(1,2,3):=0;vpot(1,3,3):=0;vpot(2,3,3):=0; 18
vpot(2,1,3):=0;vpot(3,1,3):=0;vpot(3,2,3):=0; 19
                                                    20
Eh:=3.8;                                          21
hermites();                                      22
                                                    23
"tests:";                                         24
"S-S^T"=Smatr-Transpose(Smatr);                 25
"S.S^\dag-I"=Smatr.HermitianTranspose(Smatr)-Matrix(NOpenR+NOpenL,shape=identity); 26
                                                    27
read "example11test.txt";                         28

```

Lines 1-3: The initialization of procedure, the choice of options for solving of the scattering problem for 3 equations on the axis, and the choice of parameters of finite element method.

Lines 4-5: The problem is solved in the quasi-uniform grid $\Omega_z = \{-6(10) - 2(10)2(10)6\}$, where the number in brackets denotes the number of subinterval finite element, each of nmesh:=3 subintervals effective potentials must be specified. It is important to point potential breaks coincide with nodes zmesh(*).

Lines 9-19: Setting the effective potentials.

Line 21: Sets the fixed value of the energy for the scattering problem.

Line 22: The solution of the boundary problem (1) in the quasi-uniform grid with the boundary of the third kind (4) at z^{\min} and $z = z^{\max}$ with asymptotic solutions of the scattering problem for axis (7), (12). Displays the S-matrix and its eigenfunctions.

Lines 24-26: Checking unitary and the symmetry of the S-matrix.

Line 28: The calculation of the S-matrix elements using a representation of eigenfunctions as a linear combination of trigonometric and exponential functions, and their comparison with the output to the screen with the previously counted using KANTBP 4M, calculated by FEM.

Example 12. The solution of the eigenvalue problem for the system of equations obtained by Kantorovich method for the Helmholtz equation in a rectangular region

We consider approximate solution of boundary value problem for the Helmholtz equation in a square with a side equal to π in new coordinates $z = (x + y)/\sqrt{2}$, $z' = (x - y)/\sqrt{2}$ which are diagonals of square, with Dirichlet conditions on boundary of the region. The solution $\Psi(z, z')$ is sought in the framework of Kantorovich expansions $\Psi^{(m)}(z, z') = \sum_{j=1}^N \Phi_j(z; z') \Psi_j^{(m)}(z)$ over basis functions $\Phi_i(z'; z)$, $z'^{\max}(z) = \pi/\sqrt{2} - |z|$, $z'^{\min}(z) = -\pi/\sqrt{2} + |z|$, corresponding to eigenvalues $\epsilon_i(z)$ at each value of parameter $z \in (z^{\min}, z^{\max})$:

$$\epsilon_i(z) = \frac{\pi^2 i^2}{(z'^{\max}(z) - z'^{\min}(z))^2}, \quad \Phi_i(z'; z) = \frac{\sqrt{2} \sin\left(\frac{\pi i(z' - z'^{\min}(z))}{z'^{\max}(z) - z'^{\min}(z)}\right)}{\sqrt{z'^{\max}(z) - z'^{\min}(z)}}, \quad (71)$$

Substitution of expansion to Helmholtz equation and averaging over basis $\Phi_i(z'; z)$ reduces to system of ODE w.r.t. $z \in (z^{\min}, z^{\max})$:

$$\begin{aligned} -\frac{d^2 \Phi_1^{(m)}(z)}{dz^2} + V_{11}(z) \Phi_1^{(m)}(z) + V_{12}(z) \Phi_2^{(m)}(z) + Q_{12}(z) \frac{d\Phi_2^{(m)}(z)}{dz} + \frac{dQ_{12}(z) \Phi_2^{(m)}(z)}{dz} + \dots - E_m \Phi_1^{(m)}(z) &= 0, \\ -\frac{d^2 \Phi_2^{(m)}(z)}{dz^2} + V_{21}(z) \Phi_1^{(m)}(z) + Q_{21}(z) \frac{d\Phi_1^{(m)}(z)}{dz} + \frac{dQ_{21}(z) \Phi_1^{(m)}(z)}{dz} + V_{22}(z) \Phi_2^{(m)}(z) + \dots - E_m \Phi_2^{(m)}(z) &= 0, \\ &\vdots \\ -\frac{d^2 \Phi_N^{(m)}(z)}{dz^2} + V_{N1}(z) \Phi_1^{(m)}(z) + Q_{N1}(z) \frac{d\Phi_1^{(m)}(z)}{dz} + \frac{dQ_{N1}(z) \Phi_1^{(m)}(z)}{dz} \\ &+ V_{N2}(z) \Phi_2^{(m)}(z) + Q_{N2}(z) \frac{d\Phi_2^{(m)}(z)}{dz} + \frac{dQ_{N2}(z) \Phi_2^{(m)}(z)}{dz} + \dots - E_m \Phi_N^{(m)}(z) &= 0, \end{aligned} \quad (72)$$

where effective potentials $Q_{ij}(z)$ and $V_{ij}(z)$ are given by analytic expressions

$$\begin{aligned} Q_{ij}(z) &= -\frac{4ij}{i^2 - j^2} \frac{1}{\pi\sqrt{2} - 2|z|} \frac{|z|}{z}, \quad V_{ij}(z) = -\frac{16ij(i^2 + j^2)}{(i^2 - j^2)^2} \frac{1}{(\pi\sqrt{2} - 2|z|)^2}, \\ V_{ii}(z) &= \frac{4\pi^2 i^2 + 3}{3} \frac{1}{(\pi\sqrt{2} - 2|z|)^2}, \quad j \neq i, \quad j - i \bmod 2 = 0. \end{aligned}$$

This system is divided into two subsystems of which are determined by the even (with odd indices j and i) and odd solutions (with even indices j and i). The program calculates approximate even and odd eigenvalues E_m that may be compared with known one $E_m^{exact} = 2, 5, 5, 8, 10, 10, \dots$ — the sum of squares of natural numbers, and one can see that $E_m - E_m^{exact} \sim N^{-3}$.

The code solves the eigenvalues problem for the system of equations (72) with Dirichlet conditions (2) at $z^{\min} = -\pi/\sqrt{2}$ and $z^{\max} = \pi/\sqrt{2}$ and normalization conditions (15).

```

restart;read "kantbp4m.mwt"; 1
eqs:=6; 2
psubint:=7; kappamax:=1; 3
nmesh2:=2;nmesh:=2*nmesh2; 4
Qap:=1; 5
 6
DirL:=1;DirR:=1; 7
 8
for i0 from 1 to nmesh do ngrid(i0):=4;od; 9
zmesh(0):=-Pi/sqrt(2)+1/20; 10
zmesh(1):=zmesh(0)*7/8; 11
zmesh(2):=0; 12
zmesh(3):=-zmesh(1); 13
zmesh(4):=-zmesh(0); 14
 15

```

```

for par from 0 to 1 do
for nn1 from 1 to eqs do
for nn2 from 1 to eqs do
n1:=2*nn1-1+par;
n2:=2*nn2-1+par;
if (n1=n2)
then
for i0 from 1 to nmesh2 do
vpot(nn1,nn1,nmesh2+i0):=(1/3)*(4*n1^2*Pi^2+3)/(Pi*sqrt(2)-2*z)^2;
vpot(nn1,nn1,i0):=(1/3)*(4*n1^2*Pi^2+3)/(Pi*sqrt(2)+2*z)^2;
qpot(nn1,nn1,i0):=0;qpot(nn1,nn1,nmesh2+i0):=0;
od;
else
for i0 from 1 to nmesh2 do
vpot(nn1,nn2,nmesh2+i0):=(16*(n1^2+n2^2))*n1*n2/((n1-n2)^2*(n1+n2)^2*(Pi*sqrt(2)-2*z)^2);
vpot(nn1,nn2,i0):=(16*(n1^2+n2^2))*n1*n2/((n1-n2)^2*(n1+n2)^2*(Pi*sqrt(2)+2*z)^2);
qpot(nn1,nn2,nmesh2+i0):= 4*n1*n2/((n1+n2)*(n1-n2)*(Pi*sqrt(2)-2*z));
qpot(nn1,nn2,i0):=-4*n1*n2/((n1+n2)*(n1-n2)*(Pi*sqrt(2)+2*z)) ;
od;
fi;
od;od:
numberf:=5;
hermites();
od;

```

Lines 1-4: The initialization of procedure and the choice of the number of equations in the system and the parameters of the finite element method.

Line 5: Selecting the availability of effective potentials Q_{ij} in the ODEs.

Line 7: Setting the Dirichlet boundary conditions.

Lines 9-14: Setting the quasi-uniform grid with four finite elements on each of the sub-intervals. Since effective potentials are interrupted at $z = 0$, it is important that one of z_{mesh} (*) was zero.

Lines 16-39: The solution of the problem at first for the even, and then to the odd sub-systems, which are written to files 'wfunct1.dat' and 'wfunct2.dat' (see. filenamew). It includes job effective potentials (lines 17-36) and the calculation of the five eigenfunctions and eigenvalues (lines 37-38).

Example 13. The solution of the multichannel scattering problem of tunneling of two identical particles with the oscillator interaction through the potential barrier

Code solves the multichannel scattering problem on an axis for a system of equations (1) at $Q_{ij}(z) = 0$, $f_A(z) = f_B(z) = 1$ and $V_{ij}(z)$, given in analytical form, with asymptotic boundary conditions (10)–(13), obtained by Galerkin method for the problem of tunneling of two identical particles with coordinates x_1 и x_2 the harmonic oscillator interaction $V_{osc}(x_1 - x_2) = (x_1 - x_2)^2/2$ through the Gaussian potential barrier $V_g(x_s) = \alpha/(\sigma\sqrt{2\pi}) \exp(-x_s^2/\sigma^2)$, $s = 1, 2$, $\sigma = 0.1$, $\alpha = \text{alpha}$ (in this example $\alpha = 5$). Because the effective potentials $V_{ij}(z)$ are symmetric with respect to $z = 0$: $V_{ij}(z) = \int_{-\infty}^{+\infty} dx \Phi_i^{osc}(x)(V_g((z-x)/\sqrt{2}) + V_g((z+x)/\sqrt{2}))\Phi_j^{osc}(x)$, where $\Phi_j^{osc}(x)$ are even eigenfunctions of harmonic oscillator with potential $V_{osc}(x) = x^2$ and eigenvalues $E_i^{osc} = 1, 5, 9, 13, 17, \dots$ (which determine threshold energies E), then in the example under consideration the program calculates solutions Φ_{even} and Φ_{odd} of the multichannel scattering problems, respectively, on a semiaxis $z \in (0, +\infty)$, with the Neumann or the Dirichlet boundary conditions at $z = 0$. In the example under consideration the checking the unitarity and symmetry of the S-matrix and the relations between the matrices of reflection amplitudes on the semiaxis and the matrices of reflection and transmission amplitudes on the axis, $(\mathbf{R}_{\text{even}} + \mathbf{R}_{\text{odd}})/2 - \mathbf{R}_{\leftarrow} = 0$, $(-\mathbf{R}_{\text{even}} + \mathbf{R}_{\text{odd}})/2 - \mathbf{T}_{\leftarrow} = 0$ is performed.

The problem was formulated in: A.A. Gusev et al, Resonant tunneling of the few bound particles through repulsive barriers, Physics of Atomic Nuclei 77, pp. 389–413 (2014).

```

restart;read "kantbp4m.mwt";Digits:=8; 1
eqs:=5;psubint:=3;kappamax:=2;keypot:=2; 2
 3
alpha:=5; 4
vpot(1, 1) := (10/51)*2^(1/2)*51^(1/2)*exp(-(50/51)*z^2)/Pi^(1/2); 5
vpot(2, 1) := 6
... 7
vpot(5, 5) := ...; 8
 9
for i from 1 to eqs do 10
  for i1 from i+1 to eqs do 11
    vpot(i1,i):=alpha*vpot(i1,i);vpot(i,i1):=vpot(i1,i); 12
  od; 13
  vpot(i,i):=alpha*vpot(i,i)+[1,5,9,13,17][i]; 14
od; 15
 16
Eh:=5.45; 17
zmin:=-6;zmax:=6;ngrid:=40; 18
DirL:=0;DirR:=0; 19
hermites();NOpen:=NOpenL+NOpenR; 20
RLRscat0:=RLRscat;TLRscat0:=TLRscat;RRLscat0:=RRLscat;TRLscat0:=TRLscat;Smatr0:=Smatr; 21
 22
DirL:=1;zmin:=0;ngrid:=20; 23
hermites();RRLscat1:=RRLscat;Smatr1:=Smatr; 24
 25
DirL:=2; 26
hermites();RRLscat2:=RRLscat;Smatr2:=Smatr; 27
 28
"tests;"; 29
"S.S^\dag-I"=HermitianTranspose(Smatr0).Smatr0-Matrix(NOpen,shape=identity); 30
"even: S.S^\dag-I"=HermitianTranspose(Smatr1).Smatr1-Matrix(NOpenR,shape=identity); 31
"odd: S.S^\dag-I"=HermitianTranspose(Smatr2).Smatr2-Matrix(NOpenR,shape=identity); 32
"S-S^T"=Transpose(Smatr0)-Smatr0; 33
"even: S-S^T"=Transpose(Smatr1)-Smatr1; 34
"odd: S-S^T"=Transpose(Smatr2)-Smatr2; 35
"(Reven+Rodd)/2-R<-"=(RRLscat1+RRLscat2)/2-RRLscat0; 36
"(-Reven+Rodd)/2-T<-"=(-RRLscat1+RRLscat2)/2-TRLscat0; 37

```

Lines 1-2: - The initialization of procedure, the choice of options for solving the scattering problem for 5 equations and parameters of the finite element method.

Lines 4-15: Setting the effective potentials $V_{ij}(z)$ (see file 'example13.txt')

Line 17: Sets the fixed value of the energy for the scattering problem

Lines 18-21: The solution of the boundary problem (1) on a uniform grid with the boundary of the third kind (4) at z^{\min} and $z = z^{\max}$ with asymptotic solutions (7), (12) of the scattering problem on an axis. Assigning variables RLRscat0, TLRscat0, RRLscat0, TRLscat0, Smatr0, the matrices of reflection and transmission amplitudes and the S - matrix.

Lines 23-24: The decision of the boundary problem (1) on a uniform grid with Dirichlet boundary conditions (2) at $z = 0$ and the third kind (4) at $z = z^{\max}$ c asymptotic solutions (9), (12) of the scattering problem on a semiaxis. Assigning variables RRLscat1, Smatr1, the matrix of reflection amplitudes and S - matrix.

Lines 26-27: The decision of the boundary problem (1) on a uniform grid with Neumann boundary conditions (3) at $z = 0$ and the third kind (4) at $z = z^{\max}$ c asymptotic solutions (9), (12) of the scattering problem on a semiaxis. Assigning variables RRLscat2, Smatr2, the matrix of reflection amplitudes and S - matrix.

Lines 29-37: Checking unitarity and the symmetry of the S-matrix and the relations between the matrices of reflection amplitudes on the semiaxis and the matrices of reflection and transmission amplitudes on the axis: $(\mathbf{R}_{\text{even}} + \mathbf{R}_{\text{odd}})/2 - \mathbf{R}_{\leftarrow} = 0$, $(-\mathbf{R}_{\text{even}} + \mathbf{R}_{\text{odd}})/2 - \mathbf{T}_{\leftarrow} = 0$.

Example 14. Calculation of metastable states (as the initial approximation the resonance transmission solution of the scattering problem is taken)

The example of calculation of metastable states for two barriers (Pöschl-Teller or Scarf potentials), located at a distance $2d$

$$(\mathbf{D} - E_m) \Phi_m(z) = \left(-\frac{d^2}{dz^2} + \frac{V_1}{\cosh(z-d)^2} + i \frac{V_2 \sinh(z-d)}{\cosh(z-d)^2} + \frac{V_1}{\cosh(z+d)^2} + i \frac{V_2 \sinh(z+d)}{\cosh(z+d)^2} - E_m \right) \Phi_m(z) = 0. \quad (73)$$

As the initial approximation to Newtonian scheme the resonance transmission solution of the scattering problem localized between barriers is taken.

See for details:

A.A. Gusev, et al, Lecture Notes in Computer Science 9301, pp. 182–197 (2015)

```

restart;Digits:=12;read "kantbp4m.mwt";
keypot:=2;psubint:=6;kappamax:=1;
zmin:=-20;zmax:=20;ngrid:=80;DirL:=0;DirR:=0;

#choose one of four
#V1:=2;V2:=1;d12:=7/2;Eh:=0.360240;
V1:=2;V2:=1;d12:=7/2;Eh:=1.036324;
#V1:=2;V2:=0;d12:=7/2;Eh:=0.310918;
#V1:=2;V2:=0;d12:=7/2;Eh:=1.025359;
vpot:=V1/cosh(z-d12)^2+V2*I*sinh(z-d12)/cosh(z-d12)^2
      +V1/cosh(z+d12)^2+V2*I*sinh(z+d12)/cosh(z+d12)^2;

hermites();
abs(TLRscat[1,1])^2;

read "wfunctsl.dat":
keypot:=3;
Phink:=eigfRLr(1,1)+I*eigfRLi(1,1):
DirL:=3;DirR:=3;
RBoundL:=-sqrt(-EEh);RBoundR:=sqrt(-EEh);
normtp:=0;
itermax:=20;
hermites();

```

Lines 1–14 Calculation of initial approximation.

Lines 16–23 Calculation of metastable states.

Lines 1-3: Initialization of procedure selection of options for solving the problem of scattering on the axis with the boundary conditions of the third kind, and the choice of parameters of finite element method and a uniform grid.

Lines 5-11: Setting the effective potential and its eigenvalues (It is also the initial approximation for the eigenvalue in the Newtonian scheme). The eigenvalues of the corresponding resonant transmission selected in advance. A choice of 4 sets of parameters.

Lines 13-14: The solution of the scattering problem on the axis and check that there is a complete transmission (resonance transparency).

Line 16: Read file with the solution of the scattering problem.

Line 17: Select the options to clarify solution by Newton's method.

Frame 18: The initial approximation for eigenfunctions.

Lines 19-20: Setting the boundary conditions of the third kind.

Lines 21-23: Selecting the type of the normalization, the maximum number of iterations and the solution of the problem by Newton's method.

Example 15. Calculation of metastable states (as the initial approximation the solution of the eigenvalue problem is taken)

The example of calculation of metastable states for two barriers (Pöschl-Teller or Scarf potentials), located at a distance $2d$

$$(\mathbf{D} - E_m) \Phi_m(z) = \left(-\frac{d^2}{dz^2} + \frac{V_1}{\cosh(z-d)^2} + i \frac{V_2 \sinh(z-d)}{\cosh(z-d)^2} + \frac{V_1}{\cosh(z+d)^2} + i \frac{V_2 \sinh(z+d)}{\cosh(z+d)^2} - E_m \right) \Phi_m(z) = 0. \quad (74)$$

As the initial approximation for the Newtonian scheme the resonance solution of the eigenvalue problem localized between barriers is taken.

See for details:

A.A. Gusev, et al, Lecture Notes in Computer Science 9301, pp. 182–197 (2015)

```

restart;Digits:=12;
read "kantbp4m.mwt";
keypot:=1;psubint:=6;kappamax:=1;

zmin:=-20;zmax:=20;ngrid:=20;numberf:=13;
DirL:=3;DirR:=3;
RBoundL:=-0.04-0.4*I;RBoundR:=0.04+0.4*I;
#V1:=2;V2:=1;d12:=7/2;sts:=7,12;
V1:=2;V2:=0;d12:=7/2;sts:=7,12;
vpot:=V1/cosh(z-d12)^2+V2*I*sinh(z-d12)/cosh(z-d12)^2
      +V1/cosh(z+d12)^2+V2*I*sinh(z+d12)/cosh(z+d12)^2;

hermites();

read "wfuncts1.dat":
keypot:=3;
zmin:=-20;zmax:=20;ngrid:=80;
normtp:=0;
itermax:=20;
RBoundL:=-sqrt(-EEh);RBoundR:=sqrt(-EEh);
for ii in sts do
  Eh:=eigv(ii);
  Phink:=eigf(1,ii)+I*eigfi(1,ii);
  hermites();
od:

```

Lines 1–13 Calculation of initial approximation.

Lines 15–25 Calculation of complex eigenvalues and eigenfunctions of metastable states.

Lines 1-3: - Initialization procedure, the key task `keypot: = 1`; for solving the boundary value problem with the boundary conditions of the third kind: calculating a set of complex eigenvalues and the corresponding eigenfunctions, and the choice of parameters of finite element method.

Lines 5-7: Setting a uniform grid, the amount calculated the discrete spectrum and the boundary conditions of the third kind, which, unlike the boundary conditions of the third kind, defined in the line 20, does not depend on the desired eigenvalue. Note. In this example, the potential for exponentially decreasing initial approximation to the desired solution calculated for a given boundary condition of the third kind with coefficients $\mathcal{R}(z^{max}) = -\mathcal{R}(z^{min}) = \sqrt{-E_0}$, where the value of E_0 chosen from the vicinity of the desired eigenvalues E_1 and E_2 .

Lines 8-11: Assignment of the effective potential. A choice of 2 sets of parameter values. List of rooms eigenfunctions localized between the barriers (they are also the initial approximation for eigenfunctions) is the value chosen in advance local variable `sts`

Line 13: Solution of the discrete spectrum.

Line 15: Read file with the solution of the discrete spectrum.

Line 16: Choosing options to refine the solution by Newton's method.

Line 17: Specifying the new uniform grid.

Lines 18-19: The choice of the normalization condition and the maximum number of iterations.

Line 20: Set a new boundary conditions of the third kind, which in contrast to the boundary conditions of the third kind, given in line 7, depend on the desired eigenvalue.

Lines 21–25: Decision of the boundary problem by Newton's method, where the primary approximations used its eigenfunction, from the list of sts, localized at the origin and the corresponding eigenvalues.

Example 16. Application of program for solving the boundary value problem for the Schrödinger equation with cubic nonlinearity

The program can be used to prepare solutions of the boundary problem in the interval $z \in (0, 8)$ nonlinear Schrödinger equation

$$\left(-\frac{1}{2z} \frac{d}{dz} z \frac{d}{dz} + \frac{z^2}{2} - E_m\right) \Phi_m(z) + \lambda(\Phi_m(z))^3 = 0, \quad \lim_{z \rightarrow 0} z \frac{d\Phi_m(z)}{dz} = 0, \quad \Phi_m(8) = 0, \quad \int_0^8 z dz |\Phi_m(z)|^2 = 1. \quad (75)$$

For this, the equation (75) can be rewritten in the form

$$\left(-\frac{1}{2z} \frac{d}{dz} z \frac{d}{dz} + \frac{z^2}{2} + \lambda(\Phi_m(z))^2 - E\right) \Phi_m(z) = 0, \quad \lim_{z \rightarrow 0} z \frac{d\Phi_m(z)}{dz} = 0, \quad \Phi_m(8) = 0, \quad \int_0^8 z dz |\Phi_m(z)|^2 = 1 \quad (76)$$

and solve it by the method of simple iterations.

As a first approximation $\Phi_m^{(0)}(z)$ we use solutions (75) at $\lambda = 0$

$$\left(-\frac{1}{2z} \frac{d}{dz} z \frac{d}{dz} + \frac{z^2}{2} - E_m^{(0)}\right) \Phi_m^{(0)}(z) = 0, \quad \lim_{z \rightarrow 0} z \frac{d\Phi_m^{(0)}(z)}{dz} = 0, \quad \Phi_m^{(0)}(8) = 0, \quad \int_0^8 z dz |\Phi_m^{(0)}(z)|^2 = 1,$$

each next approximation $\Phi_m^{(k)}(z)$, $E_m^{(k)}$ is given from the previous one $\Phi_m^{(k-1)}(z)$, $E_m^{(k-1)}$ by solving the Newton's method the following boundary value problem:

$$\left(-\frac{1}{2z} \frac{d}{dz} z \frac{d}{dz} + \frac{z^2}{2} + \lambda(\Phi_m^{(k-1)}(z))^2 - E_m^{(k)}\right) \Phi_m^{(k)}(z) = 0, \quad \lim_{z \rightarrow 0} z \frac{d\Phi_m^{(k)}(z)}{dz} = 0, \quad \Phi_m^{(k)}(8) = 0, \quad \int_0^8 z dz |\Phi_m^{(k)}(z)|^2 = 1.$$

```

restart;Digits:=16;
read "kantbp4m.mwt";
psubint:=10;kappamax:=1;

zmin:=0;zmax:=8;ngrid:=4;
FFA:=z;FFB:=2*z;
DirL:=2;DirR:=1;
lambdaa:=2;eps:=10^(-6);
filenamew:="init.dat";
eqs:=1;
vpot(1,1):=z^2/2;
numberf:=4;
keypote:=1;
hermites();

keypote:=3;
grprint:=0;
for ii from 1 to numberf do
  filenamew:=cat("fun",convert(ii,string),".dat");
  itermax:=5; iters:=0;
  read "init.dat";
  vpot(1,1):=z^2/2+(eigf||ii(1))^2*lambdaa;
  Eh:=eigv||ii;
  Phink(1):=(eigf||ii(1));
  hermites();
  Ehs:=Eh;ii1:=0;itermax:=2;
  while ii1=0 do
    iters:=iters+1;
    print("iteration=", iters);
    read filenamew;
    vpot(1,1):=z^2/2+eigf(1)^2*lambdaa;
    Eh:=eigv;

```

```

    Phink(1):=eigf(1):                                     33
    hermites();                                          34
    if(abs(Ehs-Eh)<eps) then ii1:=1; fi;                 35
    Ehs:=Eh;                                           36
od:od:                                                 37
                                                    38
for ii from 1 to numberf do                             39
  read cat("fun",convert(ii,string),".dat");           40
  plot(eigf(1),z=zmin..zmax);                          41
  plots[logplot](abs(-1/2/z*diff(z*diff(eigf(1),z),z)  42
    +(z^2/2-eigv)*eigf(1)+eigf(1)^3*lambdadaa),z=zmin..zmax); 43
od;                                                    44

```

Lines 1-3: Initialization procedures, and the choice of parameters of finite element method.

Line 5: Setting a uniform grid.

Line 6: Identify $f_A(z)$ and $f_B(z)$

Line 7: Setting the boundary conditions Neumann-Dirichlet.

Line 8: Setting parameters of problem.

Line 9: Specify the file name to be written in the first approximations to the desired solutions.

Lines 10-11: Selecting eqs=1 for solutions of one equation, while, in contrast to eqs=0, vpot is an array of the dimension 1x1.

Lines 12-13: Selecting calculate a set of four of eigenfunctions and eigenvalues.

Line 14: The solution of the eigenvalue problem.

Lines 16-17: The choice of options refinement solutions by Newton's method without displaying the plots of calculation results on the screen.

Lines 18 and 37: The beginning and end of a cycle in which the computed solution of the boundary problem for the nonlinear Schrödinger equation.

Line 19: For each from numberf solutions the name of file for storing next approximations (the file will be overwritten each time).

Lines 20 and 26: Set the number of iterations to perform the Newton's method.

Lines 20 and 28-29: Count the number of iterations.

Lines 21 and 30: read a file from the first and $(k - 1)$ -th approximations.

Lines 22 and 31: Overriding effective potential for the calculation of the next approximation.

Lines 23 and 32: The initial approximation for the eigenvalue for further refinement solving the boundary problem by Newton's method.

Lines 24 and 33: The initial approximation for the eigenfunction for later refinement solving the boundary problem by Newton's method.

Lines 25 and 34: Clarification of boundary problem solution by Newton.

Lines 35 and 36: Check the condition of the completion of an iteration process.

Lines 39-44: Display graphs of four computed eigenfunctions and errors $\bar{\varepsilon}_m(z)$ of the numerical solution.