Symbolic-Numeric Algorithms for Solving BVPs for a System of ODEs of the Second Order: Multichannel Scattering and Eigenvalue Problems

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Abstract. Symbolic-numeric algorithms for solving multichannel scattering and eigenvalue problems of the waveguide or tunneling type for systems of ODEs of the second order with continuous and piecewise continuous coefficients on an axis are presented. The boundary-value problems are formulated and discretized using the FEM on a finite interval with interpolating Hermite polynomials that provide the required continuity of the derivatives of the approximated solutions. The accuracy of the approximate solutions of the boundary-value problems, reduced to a finite interval, is checked by comparing them with the solutions of the original boundary-value problems on the entire axis, which are calculated by matching the fundamental solutions of the ODE system. The efficiency of the algorithms implemented in the computer algebra system Maple is demonstrated by calculating the resonance states of a multichannel scattering problem on the axis for clusters of a few identical particles tunneling through Gaussian barriers.

Keywords: Eigenvalue problem · Multichannel scattering problem · System of ODEs · Finite element method

1 Introduction

At present, the physical processes of electromagnetic wave propagation in multilayered optical waveguide structures and metamaterials [8], near-surface quantum diffusion of molecules and clusters [5,7], and transport of charge carriers in quantum semiconductor structures [6] are a subject of growing interest and intense studies. The mathematical formulation of these physical problems leads to the boundary-value problems (BVPs) for partial differential equations, which are reduced by the Kantorovich method to a system of ordinary differential equations (ODEs) of the second order with continuous or piecewise continuous

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potentials in an infinite region (on axis or semiaxis). The asymptotic boundary conditions depend upon the kind of the considered physical problem, e.g., multichannel scattering, eigenvalue problem, or calculation of metastable states.

There is a number of unresolved problems in constructing calculation schemes and implementing them algorithmically. For example, the conventional calculation scheme for solving the scattering problem on axis was constructed only for the same number of open channels in the left-hand and right-hand asymptotic regions [1]. Generally, the lack of symmetry in the coefficient functions entering the ODE system with respect to the sign of the independent variable makes it necessary to construct more general calculation schemes. In the eigenvalue problem for bound or metastable states of the BVPs with piecewise constant potentials, the desired set of real or complex eigenvalues is conventionally calculated from the dispersion equation using the method of matching the general solutions with the unknown coefficients calculated from a system of algebraic equations. This method is quite a challenge, when the number of equations and/or the number of discontinuities of the potentials is large [8]. The aim of this paper is to present the construction of algorithms and programs implemented in the computer algebra systems Maple that allow progress in solving these problems and developing high-efficiency symbolic-numeric software.

In earlier papers [2,3], we developed symbolic-numeric algorithms of the finite element method (FEM) with Hermite interpolation polynomials (IHP) to calculate high-accuracy approximate solutions for a single ODE with piecewise continuous potentials and reduced boundary conditions on a finite interval. Here this algorithm is generalized to a set of ODEs and implemented as KANTBP 4M in the computer algebra system Maple [4]. For the multichannel scattering problem with piecewise constant potentials on the axis, the numerical estimates of the accuracy of the approximate solution of the BVP reduced to finite interval are presented using an auxiliary algorithm of matching the fundamental solutions at each boundary between the adjacent axis subintervals. The efficiency of the algorithms is demonstrated by the example of calculating the resonance and metastable states of the multichannel scattering problem on the axis for clusters formed by a few identical particles tunneling through Gaussian barriers.

The paper has the following structure. Section 2 formulates the eigenvalue problem and the multichannel scattering problem of the waveguide type for a system of ODEs with continuous and piecewise continuous coefficients on an axis. Sections 3 and 4 present the algorithms for solving the multichannel scattering problem and the eigenvalue problem. The comparative analysis of the solutions of the ODE system with piecewise constant potentials is given. In Sect. 5 the quantum transmittance induced by metastable states of clusters is analysed. Finally, the summary is given, and the possible use of algorithms and programs is outlined.

2 Formulation of the Boundary Value Problems

The symbolic-numeric algorithm realized in Maple is intended for solving the BVP and the eigenvalue problem for the system of second-order ODEs with respect to the unknown functions $\boldsymbol{\Phi}(z) = (\Phi_1(z), \ldots, \Phi_N(z))^T$ of the independent variable $z \in (z^{\min}, z^{\max})$ numerically using the Finite Element Method:

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

Here $f_B(z) > 0$ and $f_A(z) > 0$ are continuous or piecewise continuous positive functions, $\mathbf{I}$ is the identity 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 $\mathcal{H}_2^{s\geq1}(\Omega)$, providing the existence of nontrivial solutions subjected to homogeneous mixed 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 $N \times N$

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

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

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

One needs to note that the boundary conditions (2)–(4) can be applied to both ends of the domain independently, e.g. the boundary condition (2) to $z^{\min}$ and, at the same time, the boundary condition (4) to $z^{\max}$. The solution $\boldsymbol{\Phi}(z) \in \mathcal{H}_2^{s\geq1}(\bar{\Omega})$ of the BPVs (1)–(4) is determined using the Finite Element Method(FEM) by numerical calculation of stationary points for the symmetric quadratic functional

$$\boldsymbol{\Xi}(\boldsymbol{\Phi}, E, z^{\min}, z^{\max}) \equiv \int_{z^{\min}}^{z^{\max}} \boldsymbol{\Phi}^{\bullet}(z)\,(\mathbf{D} - E\,\mathbf{I})\,\boldsymbol{\Phi}(z)dz = \boldsymbol{\Pi}(\boldsymbol{\Phi}, E, z^{\min}, z^{\max}) + C,$$

$$C = -f^A(z^{\max})\boldsymbol{\Phi}^{\bullet}(z^{\max})\mathbf{G}(z^{\max})\boldsymbol{\Phi}(z^{\max}) + f^A(z^{\min})\boldsymbol{\Phi}^{\bullet}(z^{\min})\mathbf{G}(z^{\min})\boldsymbol{\Phi}(z^{\min}),$$

$$\boldsymbol{\Pi}(\boldsymbol{\Phi}, E, z^{\min}, z^{\max}) = \int_{z^{\min}}^{z^{\max}} \left[f^A(z)\frac{d\boldsymbol{\Phi}^{\bullet}(z)}{dz}\frac{d\boldsymbol{\Phi}(z)}{dz} + f^B(z)\boldsymbol{\Phi}^{\bullet}(z)\mathbf{V}(z)\boldsymbol{\Phi}(z) \right. \tag{5}$$

$$\left. + f^A(z)\boldsymbol{\Phi}^{\bullet}(z)\mathbf{Q}(z)\frac{d\boldsymbol{\Phi}(z)}{dz} - f^A(z)\frac{d\boldsymbol{\Phi}(z)^{\bullet}}{dz}\mathbf{Q}(z)\boldsymbol{\Phi}(z) - f^B(z)E\boldsymbol{\Phi}^{\bullet}(z)\boldsymbol{\Phi}(z)\right] dz,$$

where $\mathbf{G}(z) = \mathcal{R}(z) - \mathbf{Q}(z)$ is a symmetric matrix of the dimension $N \times N$, and the symbol $^{\bullet}$ denotes either the transposition ^{T}, or the Hermitian conjugation †.

Problem 1. For the multichannel scattering problem on the axis $z \in (-\infty, +\infty)$ at fixed energy $E \equiv \Re E$, the desired matrix solutions $\boldsymbol{\Phi}(z) \equiv \{\boldsymbol{\Phi}_v^{(i)}(z)\}_{i=1}^N$,

$\boldsymbol{\Phi}_v^{(i)}(z) = (\Phi_{1v}^{(i)}(z), \ldots, \Phi_{Nv}^{(i)}(z))^T$ (the subscript v takes the values $\rightarrow$ or $\leftarrow$ and indicates the initial direction of the incident wave) of the BVP 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 to obey the 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 the open channels $i = 1, ..., N_o$:

$$\boldsymbol{\Phi}_v(z \to \pm\infty) = \begin{cases} \begin{cases} \mathbf{X}^{(+)}(z)\mathbf{T}_v, & z \in [z^{\max}, +\infty), \\ \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z)\mathbf{R}_v, & z \in (-\infty, z^{\min}], \end{cases} & v = \rightarrow, \\ \begin{cases} \mathbf{X}^{(-)}(z) + \mathbf{X}^{(+)}(z)\mathbf{R}_v, & z \in [z^{\max}, +\infty), \\ \mathbf{X}^{(-)}(z)\mathbf{T}_v, & z \in (-\infty, z^{\min}], \end{cases} & v = \leftarrow, \end{cases} \tag{6}$$

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

$$\mathbf{S} = \begin{pmatrix} \mathbf{R}_{\rightarrow} & \mathbf{T}_{\leftarrow} \\ \mathbf{T}_{\rightarrow} & \mathbf{R}_{\leftarrow} \end{pmatrix}, \tag{7}$$

which is 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 $\boldsymbol{\Phi}(z)$ of the BVP 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 solution is to obey 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 $i = 1, ..., N_o$:

$$\begin{aligned} \boldsymbol{\Phi}_{\leftarrow}(z \to +\infty) &= \mathbf{X}^{(-)}(z) + \mathbf{X}^{(+)}(z)\mathbf{R}_{\leftarrow}, \quad z \in [z^{\max}, +\infty) \\ \text{or} \quad \boldsymbol{\Phi}_{\rightarrow}(z \to -\infty) &= \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z)\mathbf{R}_{\rightarrow}, \quad z \in (-\infty, z^{\min}], \end{aligned} \tag{8}$$

and obeying 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 (6), (8) have the form

$$LR: \boldsymbol{\Phi}_{\rightarrow}(z \to \pm\infty) = \begin{cases} \mathbf{X}_{\max}^{(\rightarrow)}(z)\mathbf{T}_{\rightarrow} + \mathbf{X}_{\max}^{(c)}(z)\mathbf{T}_{\rightarrow}^{c}, & z \to +\infty, \\ \mathbf{X}_{\min}^{(\rightarrow)}(z) + \mathbf{X}_{\min}^{(\leftarrow)}(z)\mathbf{R}_{\rightarrow} + \mathbf{X}_{\min}^{(c)}(z)\mathbf{R}_{\rightarrow}^{c}, & z \to -\infty \end{cases} \tag{9}$$

$$RL: \boldsymbol{\Phi}_{\leftarrow}(z \to \pm\infty) = \begin{cases} \mathbf{X}_{\max}^{(\leftarrow)}(z) + \mathbf{X}_{\max}^{(\rightarrow)}(z)\mathbf{R}_{\leftarrow} + \mathbf{X}_{\max}^{(c)}(z)\mathbf{R}_{\leftarrow}^{c}, & z \to +\infty, \\ \mathbf{X}_{\min}^{(\leftarrow)}(z)\mathbf{T}_{\leftarrow} + \mathbf{X}_{\min}^{(c)}(z)\mathbf{T}_{\leftarrow}^{c}, & z \to -\infty. \end{cases} \tag{10}$$

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 Eq. (9) and $\mathbf{X}_{\max}^{(\leftarrow)}(z) = \mathbf{X}^{(-)}(z), z \geq z^{\max}$ $\mathbf{X}_{\max}^{(\rightarrow)}(z) =$

$\mathbf{X}^{(+)}(z), z \geq z^{\max}$, $\mathbf{X}^{(\leftarrow)}_{\min}(z) = \mathbf{X}^{(-)}(z), z \leq z^{\min}$ in Eq. (10). It is assumed that the leading terms of the asymptotic solutions $\mathbf{X}^{(\pm)}(z)$ of the BVP at $z \leq z^{\min}$ and/or $z \geq z^{\max}$ have the following form:
in the open channels $V^t_{i_o i_o} < E$ are oscillating solutions $j=1,\ldots,N$, $i_o=1,\ldots,N_o$:

$$X^{(\pm)}_{i_o j}(z) \to \frac{\exp\left(\pm \imath p^t_{i_o} z\right)}{\sqrt{f_A(z) p^t_i}} \delta_{i_o j}, \quad p^t_{i_o} = \sqrt{\frac{f_B(z^t)}{f_A(z^t)}} \sqrt{E - V^t_{i_o i_o}} \tag{11}$$

in the closed channels $V^t_{i_c i_c} \geq E$ are exponentially decreasing solutions $j=1,\ldots,N$, $i_c=N_o+1,\ldots,N$

$$X^{(c)}_{i_c j}(z) \to \frac{1}{\sqrt{f_A(z)}} \exp\left(-p^t_{i_c}|z|\right) \delta_{i_c j}, \quad p^t_{i_c} = \sqrt{\frac{f_B(z^t)}{f_A(z^t)}} \sqrt{V^t_{i_c i_c} - E}. \tag{12}$$

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 $t = \min, \max$:

$$\frac{f_A(z)}{f_B(z)} = \frac{f_A(z^t)}{f_B(z^t)} + o(1), \quad V_{ij}(z) = V^t_{ii}\delta_{ij} + o(1), \quad Q^t_{ij}(z) = o(1). \tag{13}$$

In the procedure of solving the BVP (1)–(4), the corresponding symmetric quadratic functional (5) is used, where the symbol $^\bullet$ denotes the transposition and the complex conjugation † for real-valued potentials and the transposition ^{T} for complex-valued potentials required for discretisation of the problem using the FEM.

Problem 2. For the eigenvalue problem the code calculates a set of M energy eigenvalues E: $\Re E_1 \leq \Re E_2 \leq \ldots \leq \Re E_M$ and the corresponding set of eigenfunctions $\boldsymbol{\Phi}(z) \equiv \{\boldsymbol{\Phi}^{(m)}(z)\}_{m=1}^M$, $\boldsymbol{\Phi}^{(m)}(z) = (\Phi^{(m)}_1(z), \ldots, \Phi^{(m)}_N(z))^T$ from the space $\mathcal{H}^2_2$ for the system of N ordinary differential equations of the second order (1) subjected to the homogeneous boundary conditions of the first and/or second, and/or third kind (see (2)–(4)) at 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 normalisation and orthogonality conditions

$$\langle \boldsymbol{\Phi}^{(m)} | \boldsymbol{\Phi}^{(m')} \rangle = \int_{z^{\min}}^{z^{\max}} f_B(z) (\boldsymbol{\Phi}^{(m)}(z))^\bullet \boldsymbol{\Phi}^{(m')}(z) dz = \delta_{mm'}, \tag{14}$$

and the corresponding symmetric quadratic functional (5) is used, in which $^\bullet$ denotes the Hermitian conjugation † needed for discretisation of the problem by the FEM. In the case of complex valued potentials, the solutions are to obey the normalisation and orthogonality conditions (14), and the corresponding symmetric quadratic functional (5) is used, in which $^\bullet$ denotes the transposition ^{T}.

To solve the bound-state problem on the axis or on the semiaxis, the original problem is approximated by the BVP (1)–(4) on a finite interval $z \in (z^{\min}, z^{\max})$ under the boundary conditions of the third kind (4) with the given matrices $\mathcal{R}(z^t)$, which are independent of the unknown eigenvalue E, and the set of approximate eigenvalues and eigenfunctions is calculated. If the matrices $\mathcal{R}(z^t)$ depend on the unknown eigenvalue E, then $\mathcal{R}(z^t, E)$ is determined by the known asymptotic expansion of the desired solution. In this case, the Newtonian iteration scheme is implemented to calculate the approximate eigenfunctions and eigenvalues. The appropriate initial approximations are chosen from the solutions calculated previously with the boundary conditions independent of E.

Problem 3. For the calculation of metastable states with unknown complex eigenvalues E, the program solves the BVP for the set of equations (1) on a finite interval with the homogeneous conditions of the third kind (4), depending on the unknown eigenvalue E, using the appropriate symmetric quadratic functional (5). In this case, the symbol $^\bullet$ denotes the transposition ^{T}, which is necessary for the discretisation of the problem in the FEM. In contrast to the scattering problem, the asymptotic solutions for metastable states contain only outgoing waves, considered in the sufficiently large, but finite interval of the spatial variable. For the metastable states on the axis $z \in (-\infty, +\infty)$, the eigenfunctions obey the boundary conditions of the third kind (4), where the matrix $\mathcal{R}(z^t) = \text{diag}(\mathcal{R}(z^t))$ depends on the desired complex energy eigenvalue $E \equiv E_m = \Re E_m + \imath \Im E_m$, $\Im E_m < 0$ and is given by [9]

$$\mathcal{R}_{i_o i_o}(z^t, E_m) = \pm\sqrt{f_B(z^t)/f_A(z^t)}\sqrt{V^t_{i_o i_o} - E_m}, \quad t = \min, \max, \quad (15)$$

where $+$ or $-$ corresponds to $t = \max$ or $t = \min$, respectively, because the asymptotic solution of this problem contains only outgoing waves in the open channels $V^t_{i_o i_o} < \Re E$, $i_o = 1, \ldots, N_o$, while in the closed channels, there are only decay waves $V^t_{i_c i_c} > \Re E$, $i_c = N_o + 1, \ldots, N$

$$\mathcal{R}_{i_c i_c}(z^t, E_m) = \mp\sqrt{f_B(z^t)/f_A(z^t)}\sqrt{E_m - V^t_{i_c i_c}}, \quad t = \min, \max, \quad (16)$$

where $+$ or $-$ corresponds to $t = \min$ or $t = \max$, respectively.

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

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

$$(\boldsymbol{\Phi}^{(m')}|\boldsymbol{\Phi}^{(m)}) = (E_m - E_{m'})\left[\int_{z^{\min}}^{z^{\max}} (\boldsymbol{\Phi}^{(m')}(z))^T \boldsymbol{\Phi}^{(m)}(z) f_B(z) dz - \delta_{m'm}\right] + C_{m'm} = 0, \quad (17)$$

$$C_{m'm} = \sum_{t=\min,\max} \mp f_A(z^t)(\boldsymbol{\Phi}^{(m')}(z^t))^T[\mathcal{R}_{i_o i_o}(z^t, E_m) - \mathcal{R}_{i_o i_o}(z^t, E_{m'}) - 2\mathbf{Q}(z^t)]\boldsymbol{\Phi}^{(m)}(z^t),$$

where $+$ or $-$ corresponds to $t = \min$ or $t = \max$, respectively. Note that the orthogonality condition is derived by calculating the difference of two functionals (5) with the substitution of eigenvalues E_m, $E_{m'}$, eigenfunctions $\boldsymbol{\Phi}^{(m)}(z)$,

$\boldsymbol{\Phi}^{(m')}(z)$, and elements of matrices $\mathcal{R}(z^{\max}, E_m)$, $\mathcal{R}(z^{\min}, E_{m'})$ from Eq. (16). The calculation of the complex eigenvalues and eigenfunctions of metastable states is performed using the Newton iteration method. The appropriate initial approximations are chosen from the solutions calculated previously with the boundary conditions at fixed E.

3 The Algorithm for Solving the Scattering Problem

We consider a discrete representation of the solutions $\boldsymbol{\Phi}(z)$ of the problem (1)–(4) reduced by means of the FEM to the variational functional (5), on the finite-element grid, $\Omega^p_{h_j(z)}[z^{\min}, z^{\max}] = [z_0 = z^{\min}, z_l, l = 1, \ldots, np-1, z_{np} = z^{\max}]$, with the mesh points $z_l = z_{jp} = z^{\max}_j \equiv z^{\min}_{j+1}$ of the grid $\Omega^{h_j(z)}[z^{\min}, z^{\max}]$ and the nodal points $z_l = z_{(j-1)p+r}$, $r = 0, \ldots, p$ of the sub-grids $\Omega^{h_j(z)}_j[z^{\min}_j, z^{\max}_j]$, $j = 1, \ldots, n$.

The solution $\boldsymbol{\Phi}^h(z) \approx \boldsymbol{\Phi}(z)$ is sought in the form of a finite sum over the basis of local functions $N^g_\mu(z)$ at each nodal point $z = z_l$ of the grid $\Omega^p_{h_j(z)}[z^{\min}, z^{\max}]$ of the interval $z \in \Delta = [z^{\min}, z^{\max}]$ (see [2]):

$$\boldsymbol{\Phi}^h(z) = \sum_{\mu=0}^{L-1} \boldsymbol{\Phi}^h_\mu N^g_\mu(z),\ \boldsymbol{\Phi}^h(z_l) = \boldsymbol{\Phi}^h_{l\kappa^{\max}},\ \left.\frac{d^\kappa \boldsymbol{\Phi}^h(z)}{dz^\kappa}\right|_{z=z_l} = \boldsymbol{\Phi}^h_{l\kappa^{\max}+\kappa}, \tag{18}$$

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

The substitution of the expansion (18) into the variational functional (5) reduces the solution of the problem (1)–(4) to the solution of the algebraic problem with respect to the matrix functions, $\boldsymbol{\Phi}^h \equiv ((\boldsymbol{\chi}^{(1)})^h, \ldots, (\boldsymbol{\chi}^{(N_o)})^h)$ at $E = E^h$,

$$\mathbf{G}^p \boldsymbol{\Phi}^h \equiv (\mathbf{A}^p - E^h\, \mathbf{B}^p)\boldsymbol{\Phi}^h = \mathbf{M}\,\boldsymbol{\Phi}^h, \quad \mathbf{M} = \mathbf{M}^{\max} - \mathbf{M}^{\min}, \tag{19}$$

with the matrices $\mathbf{A}^p$ and $\mathbf{B}^p$ of the dimension $NL\times NL$ obtained by integration in the variational functional (5) (see, e.g., [2]). The matrices $\mathbf{M}^{\max}$ and $\mathbf{M}^{\min}$ arise due to the approximation of the boundary conditions of the third kind at the left-hand and right-hand boundaries of the interval $z \in (z^{\min}, z^{\max})$

$$\frac{d\boldsymbol{\Phi}^h(z)}{dz} = (\mathbf{G}(z) + \mathbf{Q}(z))\boldsymbol{\Phi}^h(z), \quad z = z^{\min}, \quad z = z^{\max}. \tag{20}$$

The elements of the matrix $\mathbf{M} = \{M_{l'_1,l'_2}\}^{NL}_{l'_1,l'_2=1}$ 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 $1, \ldots, N$ or to the interval $(L-\kappa_{\max})N + 1, \ldots, (L-\kappa_{\max})N + N$, where N is the number of equations (1) and L is the number of basis functions $N^g_\mu(z)$ in the expansion of the desired solutions (18) in the interval $z \in \Delta = [z^{\min}, z^{\max}]$.

Input. We present the matrix $\boldsymbol{\Phi}^h$ of the dimension $NL\times 1$ in the form of three submatrices: matrix $\boldsymbol{\Phi}_a$ of the dimension $N\times 1$, such that $(\boldsymbol{\Phi}_a)_{i1} = (\boldsymbol{\Phi}^h)_{i1}$, matrix $\boldsymbol{\Phi}_c$ of the dimension $N\times 1$, such that $(\boldsymbol{\Phi}_c)_{i1} = (\boldsymbol{\Phi}^h)_{(L-\kappa_{\max})N+i,1}$, and the matrix $\boldsymbol{\Phi}_b$ of the dimension $(L-2)N\times 1$ is derived by omitting the submatrices $\boldsymbol{\Phi}_a$ and $\boldsymbol{\Phi}_c$ from the solution matrix. Then the matrices in l.h.s. and r.h.s. of Eq. (19) take the form

$$(\mathbf{A}^p - E\,\mathbf{B}^p) = \begin{pmatrix} \mathbf{G}^p_{aa} & \mathbf{G}^p_{ab} & \mathbf{0} \\ \mathbf{G}^p_{ba} & \mathbf{G}^p_{bb} & \mathbf{G}^p_{bc} \\ \mathbf{0} & \mathbf{G}^p_{cb} & \mathbf{G}^p_{cc} \end{pmatrix}, \quad \mathbf{M} = \begin{pmatrix} -\mathbf{G}^p_{\min} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{G}^p_{\max} \end{pmatrix}. \tag{21}$$

The matrices $\mathbf{G}^p_{bb}$ of the dimension $(L-2)N\times(L-2)N$, $\mathbf{G}^p_{ba}$ and $\mathbf{G}^p_{bc}$ of the dimension $(L-2)N\times N$, $\mathbf{G}^p_{ab}$ and $\mathbf{G}^p_{cb}$ of the dimension $N\times(L-2)N$, $\mathbf{G}^p_{aa}$, $\mathbf{G}^p_{cc}$, of the dimension $N\times N$ are determined from the finite element approximation and considered as known. The existence of zero submatrices is related to the band structure of the matrix $\mathbf{G}^p$ from Eq. (19). The matrices $\mathbf{G}_{\min}$ and $\mathbf{G}_{\max}$ of the dimension $N\times N$ correspond to nonzero blocks of the matrix $\mathbf{M}$, and the matrices $\boldsymbol{\Phi}_a$ and $\boldsymbol{\Phi}_c$ of the dimension $N\times 1$, are given by the asymptotic values (9), (10) and will be considered below, the matrix $\boldsymbol{\Phi}_b$ of the dimension $(L-2)N\times 1$ is derived by omitting the submatrices $\boldsymbol{\Phi}_a$ and $\boldsymbol{\Phi}_c$ from the solution matrix. We rewrite problem (19) in the following form

$$\begin{aligned} \mathbf{G}^p_{aa}\boldsymbol{\Phi}_a + \mathbf{G}^p_{ab}\boldsymbol{\Phi}_b \qquad\qquad &= -\mathbf{G}^p_{\min}\boldsymbol{\Phi}_a, \\ \mathbf{G}^p_{ba}\boldsymbol{\Phi}_a + \mathbf{G}^p_{bb}\boldsymbol{\Phi}_b + \mathbf{G}^p_{bc}\boldsymbol{\Phi}_c &= \mathbf{0}, \\ \mathbf{G}^p_{cb}\boldsymbol{\Phi}_b + \mathbf{G}^p_{cc}\boldsymbol{\Phi}_c &= \mathbf{G}^p_{\max}\boldsymbol{\Phi}_c. \end{aligned} \tag{22}$$

Step 1. Let us eliminate $\boldsymbol{\Phi}_b$ from the problem. From the second equation, the explicit expression follows

$$\boldsymbol{\Phi}_b = -(\mathbf{G}^p_{bb})^{-1}\mathbf{G}^p_{ba}\boldsymbol{\Phi}_a - (\mathbf{G}^p_{bb})^{-1}\mathbf{G}^p_{bc}\boldsymbol{\Phi}_c, \tag{23}$$

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

$$\mathbf{G}^p_{bb}\boldsymbol{F}_{ba} = \mathbf{G}^p_{ba}, \qquad \mathbf{G}^p_{bb}\boldsymbol{F}_{bc} = \mathbf{G}^p_{bc}. \tag{24}$$

Since $\mathbf{G}^p_{bb}$ is a non-degenerate matrix, each of the matrix equations (24) has a unique solution

$$\boldsymbol{F}_{ba} = (\mathbf{G}^p_{bb})^{-1}\mathbf{G}^p_{ba}, \qquad \boldsymbol{F}_{bc} = (\mathbf{G}^p_{bb})^{-1}\mathbf{G}^p_{bc}. \tag{25}$$

Step 2. Then for the function $\boldsymbol{\Phi}_b$ we have the expression

$$\boldsymbol{\Phi}_b = -\boldsymbol{F}_{ba}\boldsymbol{\Phi}_a - \boldsymbol{F}_{bc}\boldsymbol{\Phi}_c, \tag{26}$$

and the problem (19) with the matrix of the dimension $NL\times NL$ is reduced to two algebraic problems with the matrices of the dimension $N\times N$

$$\begin{aligned} \mathbf{Y}^p_{aa}\boldsymbol{\Phi}_a + \mathbf{Y}^p_{ac}\boldsymbol{\Phi}_c &= -\mathbf{G}^p_{\min}\boldsymbol{\Phi}_a, \\ \mathbf{Y}^p_{ca}\boldsymbol{\Phi}_a + \mathbf{Y}^p_{cc}\boldsymbol{\Phi}_c &= \mathbf{G}^p_{\max}\boldsymbol{\Phi}_c, \end{aligned} \tag{27}$$

where $\mathbf{Y}^p_{**}$ is expressed in terms of the solutions $\boldsymbol{F}_{ba}$ and $\boldsymbol{F}_{bc}$ of the problems (24)

$$\mathbf{Y}^p_{aa} = \mathbf{G}^p_{aa} - \mathbf{G}^p_{ab}\boldsymbol{F}_{ba}, \quad \mathbf{Y}^p_{ac} = -\mathbf{G}^p_{ab}\boldsymbol{F}_{bc},$$
$$\mathbf{Y}^p_{ca} = -\mathbf{G}^p_{cb}\boldsymbol{F}_{ba}, \mathbf{Y}^p_{cc} = \mathbf{G}^p_{cc} - \mathbf{G}^p_{cb}\boldsymbol{F}_{bc}. \tag{28}$$

Note that the system of equations (28) is solved at **step 4** for each of $N_o^L + N_o^R$ incident waves.

Step 3. Consider the solution (9) for the incident wave travelling from left to right (LR) and the solution (10) for the incident wave travelling from right to left (RL). $\boldsymbol{\Phi}_{\rightarrow}(z{\rightarrow}\pm\infty)$ and $\boldsymbol{\Phi}_{\leftarrow}(z{\rightarrow}\pm\infty)$ are 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 $\mathbf{X}^{(\rightarrow)}_{\min}(z)$, $\mathbf{X}^{(\leftarrow)}_{\min}(z)$ of the dimension $1{\times}N_o^L$ and the matrices $\mathbf{X}^{(\rightarrow)}_{\max}(z)$, $\mathbf{X}^{(\leftarrow)}_{\max}(z)$ 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 $\mathbf{X}^{(c)}_{\min}(z)$ of the dimension $1{\times}(N - N_o^L)$ and $\mathbf{X}^{(c)}_{\max}(z)$ 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 $\mathbf{R}^c_{\rightarrow}$, $\mathbf{T}^c_{\rightarrow}$, $\mathbf{R}^c_{\leftarrow}$ and $\mathbf{T}^c_{\leftarrow}$ are rectangular matrices of the dimension $(N{-}N_o^L){\times}N_o^L$, $(N{-}N_o^R){\times}N_o^L$, $(N{-}N_o^R){\times}N_o^R$ and $(N{-}N_o^L){\times}N_o^R$. Then the components of the wave functions (9) and (10) take the form for LR and RL waves:

$$(\boldsymbol{\Phi}_a)_{i_o i_o^L} = X^{(\rightarrow)}_{i_o i_o^L}(z^{\min}) + \sum_{i'_o=1}^{N_o^L} X^{(\leftarrow)}_{i_o i'_o}(z^{\min}) R^{(\rightarrow)}_{i'_o i_o^L} + \sum_{i'_c=1}^{N-N_o^L} X^{(c)}_{i_o i'_c}(z^{\min}) R^{(c\rightarrow)}_{i'_c i_o^L},$$
$$(\boldsymbol{\Phi}_c)_{i_o i_o^L} = \sum_{i'_o=1}^{N_o^R} X^{(\leftarrow)}_{i_o i'_o}(z^{\max}) T^{(\rightarrow)}_{i'_o i_o^L} + \sum_{i'_c=1}^{N-N_o^R} X^{(c)}_{i_o i'_c}(z^{\max}) T^{(c\rightarrow)}_{i'_c i_o^L},$$
$$(\boldsymbol{\Phi}_a)_{i_o i_o^R} = \sum_{i'_o=1}^{N_o^L} X^{(\rightarrow)}_{i_o i'_o}(z^{\min}) T^{(\leftarrow)}_{i'_o i_o^R} + \sum_{i'_c=1}^{N-N_o^L} X^{(c)}_{i_o i'_c}(z^{\min}) T^{(c\leftarrow)}_{i'_c i_o^R}, \tag{29}$$
$$(\boldsymbol{\Phi}_c)_{i_o i_o^R} = X^{(\leftarrow)}_{i_o i_o^R}(z^{\max}) + \sum_{i'_o=1}^{N_o^R} X^{(\rightarrow)}_{i_o i'_o}(z^{\max}) R^{(\leftarrow)}_{i'_o i_o^R} + \sum_{i'_c=1}^{N-N_o^R} X^{(c)}_{i_o i'_c}(z^{\max}) R^{(c\leftarrow)}_{i'_c i_o^R},$$

where the asymptotic solutions $\mathbf{X}^{(\rightarrow)}(z){\equiv}\mathbf{X}^{(+)}(z)$, $\mathbf{X}^{(\leftarrow)}(z){\equiv}\mathbf{X}^{(-)}(z)$ of the BVP at $z{\le}z^{\min}$ and/or $z{\ge}z^{\max}$ are given by Eqs. (11)–(12). RL: The products in the r.h.s. of Eq. (27) in accordance with (4) and (20) are calculated via the first derivatives of the asymptotic solutions $X'^{(*)}_{**}(z^t) = \left.\frac{dX^{(*)}_{**}(z)}{dz}\right|_{z=z^t}$ for LR: $(\mathbf{G}^p_{\min}\boldsymbol{\Phi}_a)_{i_o i_o^L}$, $(\mathbf{G}^p_{\max}\boldsymbol{\Phi}_c)_{i_o i_o^L}$ and RL: $(\mathbf{G}^p_{\min}\boldsymbol{\Phi}_a)_{i_o i_o^R}$, $(\mathbf{G}^p_{\max}\boldsymbol{\Phi}_c)_{i_o i_o^R}$.

Step 4. Substituting the expressions (29) and their derivatives into Eq. (27), we form and solve the system of inhomogeneous equations for LR at $i_o^L = 1, ..., N_o^L$

$$
\begin{aligned}
&\sum_{i'_o=1}^{N_o^L}\left(X'^{(\leftarrow)}_{i_o i'_o}(z^{\min}) + \sum_{j_o=1}^{N}(\mathbf{Y}^p_{aa})_{i_o j_o}X^{(\leftarrow)}_{j_o i'_o}(z^{\min})\right)R^{(\rightarrow)}_{i'_o i_o^L}\\
&+\sum_{i'_c=1}^{N-N_o^L}\left(X'^{(c)}_{i_o i'_c}(z^{\min}) + \sum_{j_o=1}^{N}(\mathbf{Y}^p_{aa})_{i_o j_o}X^{(c)}_{j_o i'_c}(z^{\min})\right)R^{(c\rightarrow)}_{i'_c i_o^L}\\
&+\sum_{i'_o=1}^{N_o^R}\sum_{j_o=1}^{N}(\mathbf{Y}^p_{ac})_{i_o j_o}X^{(\leftarrow)}_{j_o i'_o}(z^{\max})T^{(\rightarrow)}_{i'_o i_o^L} + \sum_{i'_c=1}^{N-N_o^R}\sum_{j_o=1}^{N}(\mathbf{Y}^p_{ac})_{i_o j_o}X^{(c)}_{j_o i'_c}(z^{\max})T^{(c\rightarrow)}_{i'_c i_o^L}\\
&= -X'^{(\rightarrow)}_{i_o i_o^L}(z^{\min}) - \sum_{j_o=1}^{N}(\mathbf{Y}^p_{aa})_{i_o j_o}X^{(\rightarrow)}_{j_o i_o^L}(z^{\min}),\\
&+\sum_{i'_o=1}^{N_o^L}\sum_{j_o=1}^{N}(\mathbf{Y}^p_{ca})_{i_o j_o}X^{(\leftarrow)}_{j_o i'_o}(z^{\min})R^{(\rightarrow)}_{i'_o i_o^L} + \sum_{i'_c=1}^{N-N_o^L}\sum_{j_o=1}^{N}(\mathbf{Y}^p_{ca})_{i_o j_o}X^{(c)}_{j_o i'_c}(z^{\min})R^{(c\rightarrow)}_{i'_c i_o^L}\\
&+\sum_{i'_o=1}^{N_o^R}\left(-X'^{(\leftarrow)}_{i_o i'_o}(z^{\max}) + \sum_{j_o=1}^{N}(\mathbf{Y}^p_{cc})_{i_o j_o}X^{(\leftarrow)}_{j_o i'_o}(z^{\max})\right)T^{(\rightarrow)}_{i'_o i_o^L}\\
&+\sum_{i'_c=1}^{N-N_o^R}\left(-X'^{(c)}_{i_o i'_c}(z^{\max}) + \sum_{j_o=1}^{N}(\mathbf{Y}^p_{cc})_{i_o j_o}X^{(c)}_{j_o i'_c}(z^{\max})\right)T^{(c\rightarrow)}_{i'_c i_o^L})\\
&= -\sum_{j_o=1}^{N}(\mathbf{Y}^p_{ca})_{i_o j_o}X^{(\rightarrow)}_{j_o i_o^L}(z^{\min}),
\end{aligned}
$$

or a similar one for RL at $i_o^R = 1, ..., N_o^R$ that has a unique solution.

Remark. When solving the problem on a semiaxis with the Neumann or the third-kind boundary conditions at the boundary $z^{\min}$ or $z^{\max}$ of the semiaxis, the role of unknowns is played by the elements of the matrices $\boldsymbol{\Phi}_a$ or $\boldsymbol{\Phi}_c$, instead of $\mathbf{R}$ and $\mathbf{T}$, while for the Dirichlet boundary conditions, we have $\boldsymbol{\Phi}_a = 0$ or $\boldsymbol{\Phi}_c = 0$, so that in this case the corresponding equation is not taken into account.

4 The BVP with Piecewise Constant Potentials

The accuracy of the approximate solutions of the reduced BVPs on the finite interval calculated by FEM is checked by comparison with the solutions of the

BVPs for the system of Eq. (1) at $f_A(z) = f_A$, $f_B(z) = f_B$, $Q_{ij}(z) = 0$ on the entire axis with the matrix of piecewise constant potentials

$$V_{ij}(z) = V_{ji}(z) = \{V_{ij;1}, z \le z_1; \ldots ; V_{ij;k-1}, z \le z_{k-1}; V_{ij;k}, z > z_{k-1}\}. \quad (30)$$

Algorithm for solving the BVP by matching the fundamental solutions. In the algorithm, the following series of steps are implemented in two cycles $i_o = i_o^L = 1, ..., N_o^L$ and $i_o = i_o^R = 1, ..., N_o^R$:

Step 1. In the intervals $z \in (-\infty, z_1)$, $z \in (z_{k-1}, +\infty)$, one of the asymptotic states of the multichannel scattering problem is constructed, $\boldsymbol{\Phi}_0 \equiv \boldsymbol{\Phi}_a = \{(\boldsymbol{\Phi}_a)_i \equiv (\boldsymbol{\Phi}_a)_{ii_o^L} \text{ or } (\boldsymbol{\Phi}_a)_{ii_o^R}\}$ and $\boldsymbol{\Phi}_k \equiv \boldsymbol{\Phi}_c = \{(\boldsymbol{\Phi}_c)_i \equiv (\boldsymbol{\Phi}_c)_{ii_o^L} \text{ or } (\boldsymbol{\Phi}_c)_{ii_o^R}\}$, corresponding to Eq. (9) or (10), its explicit form given in Eq. (29).

Step 2. In the cycle by l for each of the internal subintervals $z \in [z_{l-1}, z_l]$, $l = 2, \ldots, k-1$, the general solution is calculated that depends on $2N$ parameters $C_{2N(l-2)+1}, \ldots, C_{2N(l-1)}$, $\boldsymbol{\Phi}_l = \mathbf{X}_{l;1}C_{2N(l-2)+1} + \ldots + \mathbf{X}_{l;2N}C_{2N(l-1)}$, of the ODE system (1) with constant coefficients $V_{ij;l}$ from (30), the spectral parameter E being fixed, and the first derivative of the obtained solution is calculated.

Step 3: In the cycle by l, the differences $\boldsymbol{\Phi}_l(z_l) - \boldsymbol{\Phi}_{l-1}(z_l)$ and $(d/dz)(\boldsymbol{\Phi}_l(z) - \boldsymbol{\Phi}_{l-1}(z))|_{z_l}$, $l = 1, \ldots, k$ are calculated and set equal to zero. As a result, the system of $2N(k-1)$ inhomogeneous equations with respect to $2N(k-1)$ unknown expansion coefficients $C_1, \ldots, C_{2N(k-2)}$, as well as the corresponding elements of the matrices $\mathbf{T}_*$, $\mathbf{R}_*$ listed in Eq. (29) are obtained and solved.

Remark. For solving the bound state problem or calculating metastable states, the algorithm is modified as follows.

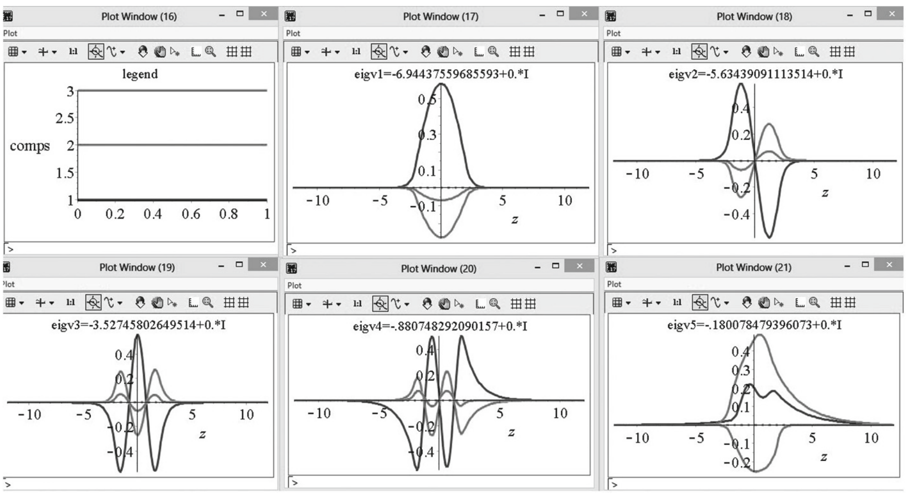

Fig. 1. A screenshot of the FEM algorithm run showing the components of five solutions $\boldsymbol{\Phi}_m^h(z)$, $m = 1, ..., 5$, of the bound state problem.

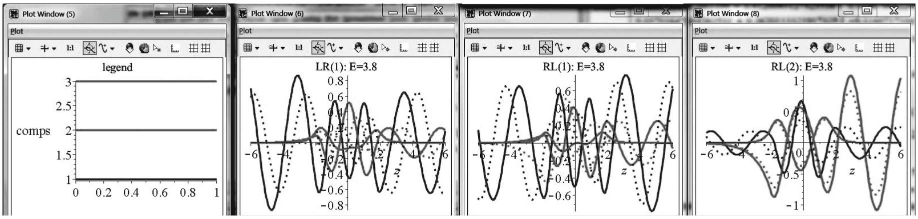

Fig. 2. The screenshot of the FEM algorithm run, showing the real (solid lines) and the imaginary (dotted lines) components of the solution of the scattering problem for the wave incident from the left, LR(1), and the waves incident from the right from the first, RL(1), and the second RL(2) open channels.

1. The sequence of **steps 1–3** is performed only once.
2. At **Step 1**, instead of the asymptotic expressions (9) and (10), one uses

$$\boldsymbol{\Phi}(z \to \pm\infty) = \left\{ \mathbf{X}^{(c)}_{\max}(z)\mathbf{C}_{+},\, z \to +\infty,\, \mathbf{X}^{(c)}_{\min}(z)\mathbf{C}_{-},\, z \to -\infty, \right\} \quad (31)$$

where $\mathbf{C}_{\pm}$ is a column matrix with the dimension $1{\times}N$, and $\mathbf{X}^{(c)}_{*}(z)$ is the specially selected fundamental solution that for bound states should decrease exponentially at $z \to \pm\infty$, while for metastable states must describe diverging waves in open channels and decrease exponentially in closed channels.
3. In **step 3**, a system of $2N(k-1)$ linear homogeneous algebraic equations for $2N(k-1)+1$ unknown coefficients $C_1, \ldots, C_{2N(k-2)}$ and the corresponding elements of the matrices $\mathbf{C}_{\pm}$, which is nonlinear and transcendent with respect to the spectral parameter E, is obtained and solved.

Benchmark Calculations. We solved the BVP for the system of equations (1) with the effective potentials (30) and the third-kind boundary conditions (4) on a finite interval, which is determined from the asymptotic solutions (9), (10), (11), (12) of the multichannel scattering problem on the axis

$$\mathbf{V}(z)=\left\{ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 10 \end{pmatrix}, z < -2;\ \begin{pmatrix} -5 & 4 & 4 \\ 4 & 0 & 4 \\ 4 & 4 & 10 \end{pmatrix}, -2 \le z \le 2;\ \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 10 \end{pmatrix}, z > 2 \right\}.$$

For solving the BVP the uniform finite-element grid $z^{\min}=-6$, $h_{j=1,\ldots,30}=0.4$, $z^{\max}=6$ with seventh-order Hermitian elements $(\kappa^{\max}, p)=(2,3)$, $p'=7$ preserving the continuity of the first derivative in the approximate solutions was chosen. The calculations were performed with 16 significant digits. Given $E=3.8$, for the wave incident from the left there is one open channel, $N_o^L=1$, and for the wave incident from the right, there are two open channels, $N_o^R=2$. The comparison of FEM results with those of solving the system of algebraic equations yields the error estimate $accuracy = S_{an} - S_{matr} \sim 10^{-13}$. for the computation of the square matrices of reflection amplitudes $\mathbf{R}_{\to}$ and $\mathbf{R}_{\leftarrow}$, having the dimension $1{\times}1$ and $2{\times}2$, and the rectangular matrices of transmission amplitudes $\mathbf{T}_{\to}$ and

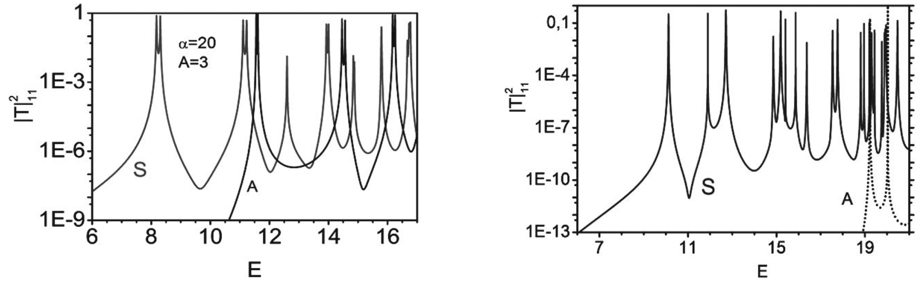

Fig. 3. The total probability $|\mathbf{T}|^2_{11}$ of transmission through the repulsive Gaussian barrier versus the energy E (in oscillator units) at σ=1/10, α=20 for the cluster of three (n=3, left panel) and four (n=4, right panel) identical particles initially being in the in the ground symmetric (solid lines) and antisymmetric (dashed lines) state.

$\mathbf{T}_{\leftarrow}$ having the dimension 2×1 and 1×2. With the error of the same order, the conditions of symmetry, $\mathbf{S} - \mathbf{S}^T$ and S-matrix unitarity $\mathbf{S}\mathbf{S}^{dag} - \mathbf{I}$ are satisfied. For five eigenvalues, the differences $\delta E_m = |E_m^h - E_m^{ex}|$ between the results of two above methods appeared to be of the order of 10^{-9} in the calculations performed with 12 significant figures. The components $\mathbf{\Phi}_m$ of the bound state solutions and the solutions $\mathbf{\Phi}_v$ of the scattering problem on a finite-element grid are shown in Figs. 1 and 2. The running time for this example using KANTBP 4M implemented in Maple 16 is 232 s for the PC Intel Pentium CPU 1.50 GHz 4 GB 64 bit Windows 8.

5 Quantum Transmittance Induced by Metastable States

In Ref. [5], the problem of tunneling of a cluster of n identical particles, coupled by pair harmonic oscillator potentials, through the Gaussian barriers $V(x_i) = \alpha/(2\pi\sigma^2)^{1/2} \exp(-x_i^2/\sigma^2)$, $i = 1, ..., n$, with averaging over the basis of the cluster eigenfunctions was formulated as a multichannel scattering problem for the system of ODEs (1) with the center-of-mass independent variable $z = (x_1 + ... + x_n)/\sqrt{n}$ and the boundary conditions (4) that follow from the asymptotic conditions (6) at $f_A(z) = 1$, $f_B(z) = 1$, $Q_{ij}(z) = 0$. The elements $V_{ij}(z)$ of the effective potentials matrix were calculated analytically and plotted in [5].

Let us apply the technique developed in the present paper and implemented as KANTBP 4M to the tunneling problem for the cluster comprising three and four identical particles in symmetric (S) and antisymmetric (A) states.

At first we solve the scattering problem with fixed energy $E = \Re E$. The solutions of the BVP were discretised on the finite-element grid $\Omega_h = (-11(11)11)$ for $n = 3$ and $\Omega_h = (-13(13)13)$ for $n = 4$, with the number of Lagrange elements of the twelfth order $p' = 12$ shown in brackets. The boundary points of the interval z^t were chosen in accordance with the required accuracy of the approximate solution $\max\{|V_{ij}(z^t)/\alpha|; i, j = 1, ..., j_{\max}\} < 10^{-8}$. The number N of the cluster basis functions in the expansion of solutions of the original problem

[5] and, correspondingly, the number of equations for S-states for $n = 3, 4$ was chosen equal to $N = 21, 39$ and for A-states $N = 16, 15$. The results of the calculations for three and four particles are presented in Fig. 3. The resonance values of energy $E = E_l^{S(A)}$ and the corresponding maximal values of the transmission coefficient $|\mathbf{T}|^2_{11}$ clearly visible in Fig. 3 are presented in Table 1.

Table 1. The first resonance energy values $E_l^{S(A)}$, at which the maximum of the transmission coefficient $|\mathbf{T}|^2_{11}$ is achieved, and the complex energy eigenvalues $E_m^M = \Re E_m^M + \imath \Im E_m^M$ of the metastable states for symmetric S (antisymmetric A) states of $n = 3$ and $n = 4$ particles at $\sigma = 1/10$, $\alpha = 20$.

l	E_l^S	$\|T\|^2_{11}$	m	E_m^M
1	8.175	0.775	1	8.175−ı5.1(−3)
	8.306	0.737	2	8.306−ı5.0(−3)
2	11.111	0.495	3	11.110−ı5.6(−3)
	11.229	0.476	4	11.229−ı5.5(−3)
3	12.598	0.013	5	12.598−ı6.4(−3)
			6	12.599−ı6.3(−3)
4	13.929	0.331	7	13.929−ı4.5(−3)
	14.003	0.328	8	14.004−ı4.6(−3)
5	14.841	0.014	9	14.841−ı3.5(−3)
	14.877	0.008	10	14.878−ı3.5(−3)

l	E_l^A	$\|T\|^2_{11}$	m	E_m^M
1	11.551	1.000	1	11.551−ı1.8(−3)
	11.610	1.000	2	11.610−ı2.0(−3)
2	14.459	0.553	3	14.459−ı2.9(−3)
	14.564	0.480	4	14.565−ı2.7(−3)

l	E_l^S	$\|T\|^2_{11}$	m	E_m^M
1	10.121	0.321	1	10.119−ı4.0(−3)
			2	10.123−ı4.0(−3)
2	11.896	0.349	3	11.896−ı6.3(−5)
3	12.713	0.538	4	12.710−ı4.5(−3)
	12.717	0.538	5	12.720−ı4.5(−3)
4	14.858	0.017	6	14.857−ı4.3(−3)
			7	14.859−ı4.3(−3)
5	15.188	0.476	8	15.185−ı3.9(−3)
			9	15.191−ı3.9(−3)
6	15.405	0.160	10	15.405−ı1.4(−5)
7	15.863	0.389	11	15.863−ı5.3(−5)

l	E_l^A	$\|T\|^2_{11}$	m	E_m^M
1	19.224	0.177	1	19.224−ı4.0(−4)
			2	19.224−ı4.0(−4)
2	20.029	0.970	3	20.029−ı3.3(−7)

For metastable states, the eigenfunctions obey the boundary conditions of the third kind (4), where the matrices $\mathcal{R}(z^t) = \text{diag}(\mathcal{R}(z^t))$ depend on the desired complex energy eigenvalue, $E \equiv E_m^M = \Re E_m^M + \imath \Im E_m^M$, $\Im E_m^M < 0$, are given by (15), (16), since the asymptotic solutions of this problem contain only outgoing waves in the open channels. In this case, the eigenfunctions obey the orthogonality and normalisation conditions (17). The discretisation of the solutions of the BVP was implemented on the above finite-element grid. The algebraic eigenvalue problem was solved using the Newton method with the optimal choice of the iteration step [3] using the additional condition $\Xi_h(\boldsymbol{\Phi}^{(m)}, E_m, z^{\min}, z^{\max}) = 0$ obtained as a result of the discretisation of the functional (5) and providing the upper estimates for the approximate eigenvalue. As the initial approximation we used the real eigenvalues and the eigenfunctions orthonormalised by the condition that the expression in square brackets in Eq. (17) is zero. They were found as a result of solving the bound-state problem with the functional (5) at $\mathcal{R}(z^t) = 0$ on the grid $\Omega_h = (-5(5)5)$ for $n = 3$ and $n = 4$. The results of the calculations performed with the variational functional (5), (17), defined in the interval $[z^{\min}, z^{\max}]$, for the complex values of energy of the metastable states

$E_m^M \equiv E_m = \Re E_m^M + \imath \Im E_m^M$ for $n = 3$ and $n = 4$ are presented in Table 1. The resonance values of energy corresponding to these metastable states are responsible for the peaks of the transmission coefficient, i.e., the quantum transparency of the barriers. The position of peaks presented in Fig. 3 is seen to be in quantitative agreement with the real part $\Re E_m^M$, and the half-width of the $|\mathbf{T}|_{11}^2(E_l)$ peaks agrees with the imaginary part $\Gamma = -2\Im E_m^M$ of the complex energy eigenvalues $E_m^M = \Re E_m^M + \imath \Im E_m^M$ of the metastable states by the order of magnitude.

6 Summary and Perspectives

The developed approach, algorithms, and programs can be adapted and applied to study the waveguide modes in a planar optical waveguide, the quantum diffusion of molecules and micro-clusters through surfaces, and the fragmentation mechanism in producing very neutron-rich light nuclei.

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