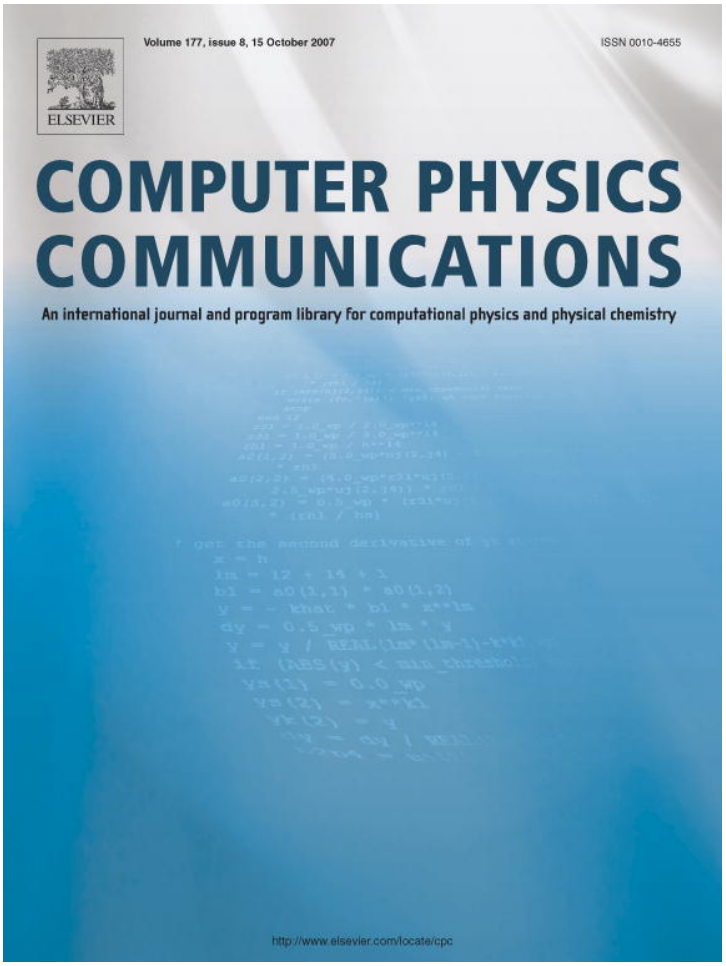

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KANTBP: A program for computing energy levels, reaction matrix and radial wave functions in the coupled-channel hyperspherical adiabatic approach ☆

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Abstract

A FORTRAN 77 program is presented which calculates energy values, reaction matrix and corresponding radial wave functions in a coupled-channel approximation of the hyperspherical adiabatic approach. In this approach, a multi-dimensional Schrödinger equation is reduced to a system of the coupled second-order ordinary differential equations on the finite interval with homogeneous boundary conditions of the third type. The resulting system of radial equations which contains the potential matrix elements and first-derivative coupling terms is solved using high-order accuracy approximations of the finite-element method. As a test desk, the program is applied to the calculation of the energy values and reaction matrix for an exactly solvable 2D-model of three identical particles on a line with pair zero-range potentials.

Program summary

Program title: KANTBP
Catalogue identifier: ADZH_v1_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADZH_v1_0.html
Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland
Licensing provisions: Standard CPC licence, http://cpc.cs.qub.ac.uk/licence/licence.html
No. of lines in distributed program, including test data, etc.: 4224
No. of bytes in distributed program, including test data, etc.: 31 232
Distribution format: tar.gz
Programming language: FORTRAN 77
Computer: Intel Xeon EM64T, Alpha 21264A, AMD Athlon MP, Pentium IV Xeon, Opteron 248, Intel Pentium IV
Operating system: OC Linux, Unix AIX 5.3, SunOS 5.8, Solaris, Windows XP
RAM: depends on (a) the number of differential equations; (b) the number and order of finite-elements; (c) the number of hyperradial points; and (d) the number of eigensolutions required. Test run requires 30 MB
Classification: 2.1, 2.4
External routines: GAULEG and GAUSSJ [W.H. Press, B.F. Flanery, S.A. Teukolsky, W.T. Vetterley, Numerical Recipes: The Art of Scientific Computing, Cambridge University Press, Cambridge, 1986]

☆ This paper and its associated computer program are available via the Computer Physics Communications homepage on ScienceDirect (http://www.sciencedirect.com/science/journal/00104655).

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Nature of problem: In the hyperspherical adiabatic approach [J. Macek, J. Phys. B 1 (1968) 831–843; U. Fano, Rep. Progr. Phys. 46 (1983) 97–165; C.D. Lin, Adv. Atom. Mol. Phys. 22 (1986) 77–142], a multi-dimensional Schrödinger equation for a two-electron system [A.G. Abrashkevich, D.G. Abrashkevich, M. Shapiro, Comput. Phys. Comm. 90 (1995) 311–339] or a hydrogen atom in magnetic field [M.G. Dimova, M.S. Kaschiev, S.I. Vinitsky, J. Phys. B 38 (2005) 2337–2352] is reduced by separating the radial coordinate ρ from the angular variables to a system of second-order ordinary differential equations which contain potential matrix elements and first-derivative coupling terms. The purpose of this paper is to present the finite-element method procedure based on the use of high-order accuracy approximations for calculating approximate eigensolutions for such systems of coupled differential equations.
Solution method: The boundary problems for coupled differential equations are solved by the finite-element method using high-order accuracy approximations [A.G. Abrashkevich, D.G. Abrashkevich, M.S. Kaschiev, I.V. Puzynin, Comput. Phys. Comm. 85 (1995) 40–64]. The generalized algebraic eigenvalue problem $\mathbf{AF} = E\mathbf{BF}$ with respect to pair unknowns $(E, \mathbf{F})$ arising after the replacement of the differential problem by the finite-element approximation is solved by the subspace iteration method using the SSPACE program [K.J. Bathe, Finite Element Procedures in Engineering Analysis, Englewood Cliffs, Prentice–Hall, New York, 1982]. The generalized algebraic eigenvalue problem $(\mathbf{A} - E\mathbf{B})\mathbf{F} = \lambda\mathbf{DF}$ with respect to pair unknowns $(\lambda, \mathbf{F})$ arising after the corresponding replacement of the scattering boundary problem in open channels at fixed energy value, E, is solved by the $\mathbf{LDL}^{\mathrm{T}}$ factorization of symmetric matrix and back-substitution methods using the DECOMP and REDBAK programs, respectively [K.J. Bathe, Finite Element Procedures in Engineering Analysis, Englewood Cliffs, Prentice–Hall, New York, 1982]. As a test desk, the program is applied to the calculation of the energy values and reaction matrix for an exactly solvable 2D-model of three identical particles on a line with pair zero-range potentials described in [Yu. A. Kuperin, P.B. Kurasov, Yu.B. Melnikov, S.P. Merkuriev, Ann. Phys. 205 (1991) 330–361; O. Chuluunbaatar, A.A. Gusev, S.Y. Larsen, S.I. Vinitsky, J. Phys. A 35 (2002) L513–L525; N.P. Mehta, J.R. Shepard, Phys. Rev. A 72 (2005) 032728-1-11; O. Chuluunbaatar, A.A. Gusev, M.S. Kaschiev, V.A. Kaschieva, A. Amaya-Tapia, S.Y. Larsen, S.I. Vinitsky, J. Phys. B 39 (2006) 243–269]. For this benchmark model the needed analytical expressions for the potential matrix elements and first-derivative coupling terms, their asymptotics and asymptotics of radial solutions of the boundary problems for coupled differential equations have been produced with help of a MAPLE computer algebra system.
Restrictions: The computer memory requirements depend on:

- (a) the number of differential equations;
- (b) the number and order of finite-elements;
- (c) the total number of hyperradial points; and
- (d) the number of eigensolutions required.

Restrictions due to dimension sizes may be easily alleviated by altering PARAMETER statements (see Long Write-Up and listing for details). The user must also supply subroutine POTCAL for evaluating potential matrix elements. The user should supply subroutines ASYMEV (when solving the eigenvalue problem) or ASYMSC (when solving the scattering problem) that evaluate the asymptotics of the radial wave functions at the right boundary point in case of a boundary condition of the third type, respectively.
Running time: The running time depends critically upon:

- (a) the number of differential equations;
- (b) the number and order of finite-elements;
- (c) the total number of hyperradial points on interval $[0, \rho_{\max}]$; and
- (d) the number of eigensolutions required.

The test run which accompanies this paper took 28.48 s without calculation of matrix potentials on the Intel Pentium IV 2.4 GHz.

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Keywords: Eigenvalue and multi-channel scattering problems; Kantorovich method; Finite element method; R-matrix calculations; Hyperspherical coordinates; Multi-channel adiabatic approximation; Ordinary differential equations; High-order accuracy approximations

1. Introduction

Development of stable numerical methods for solution of elliptic partial differential equation is one of the main problems of modern computational physics. Therefore elaboration of efficient, stable and high-accurate numerical schemes for solving the Schrödinger equation in a multi-dimensional space is an important task. Numerical solution of such equation has wide applications in various quantum-mechanical problems such as the modern calculations of the weakly bound states and elastic scattering in a system of three helium atoms considered as point particles with some short range pair potentials, i.e. a trimer of helium atoms [1], or in processes of ionization and recombination of antihydrogen in magnetic trap of modern laser physics experiments [2–4]. The above mentioned experiments require computer modeling of dynamics of exotic few-body Coulomb systems in external laser pulsed fields [5–7].

There are two conditions for elaborating numerical methods: to be stable and to have a high accuracy of calculations. The resulting system of ordinary second-order differential equations obtained after reduction of a multi-dimensional boundary problem

to a one-dimensional one is solved using high-order approximations of the Finite Element Method (FEM). In order to guarantee high-order accuracy of numerical solutions, the relevant potential matrix elements should be evaluated with the same level of accuracy as approximate solutions.

One of the most popular and widely used approaches for solving the quantum-mechanical three-body problem with pair Coulomb and point interactions is the adiabatic representation method [8–10]. In the framework of the hyperspherical coordinates formulation of this method [9–14], the hyperradius ρ is treated as a slowly varying adiabatic variable, analogous to the internuclear distance in the Born–Oppenheimer approximation for molecules [8]. From the mathematical point of view this approach is well known as the Kantorovich method (KM) for the reduction of a multi-dimension boundary problem to the one-dimensional one by using a set of solutions of an auxiliary parametric eigenvalue problem [15]. These solutions are obtained for a given set of values of the adiabatic variable, which plays here a role of an external parameter. The convergence of the adiabatic expansion in the hyperspherical coordinates is higher than the ones used in most conventional approaches based on the independent electron model. This is due to the fact that collective variables such as hyperradius $\rho = \sqrt{r_1^2 + r_2^2}$ and hyperangle $\alpha = \arctan(r_2/r_1)$ allow for more natural and accurate accounting of electron correlations in an atomic system (see, e.g., [9,12,16–18]) than the independent electron coordinates, r_1 and r_2.

An essential part in the implementation of the KM is the computation of variable coefficients (potential matrix elements) for the resulting system of the ordinary second-order differential equations. These coefficients are the integrals over eigenfunctions and their derivatives with respect to the adiabatic variable. In real applications, an efficient and stable computation of derivatives of the adiabatic eigenfunctions and the corresponding integrals with the accuracy comparable with the one achieved for adiabatic eigenfunctions presents a serious challenge for most of numerical approaches involved in various types of calculations within the adiabatic representation method [19].

This problem has been successfully solved in the paper [20]. A new method for computing variable coefficients (potential matrix elements of radial coupling) of a resulting system of ordinary second-order differential equations has been elaborated. It allows the calculation of the coefficients with the same precision as the adiabatic functions obtained as solutions of an auxiliary parametric eigenvalue problem. In the method proposed, a new boundary parametric problem with respect to unknown derivatives of eigenfunctions in the adiabatic variable (hyperradius) was formulated. An efficient, fast and stable algorithm for solving the boundary problem with the same accuracy for the adiabatic eigenfunctions and their derivatives was proposed. The method developed was tested on a parametric eigenvalue problem for a hydrogen atom on a three-dimensional sphere which has an analytical solution [21]. The accuracy, efficiency and robustness of the algorithm were studied in details. The method was also applied to the computation of the ground state energy of the helium atom and negative hydrogen ion [20], and low-excited states of a hydrogen atom in strong magnetic field [22]. The results obtained have shown an excellent agreement with the results of calculations by other methods.

The method of calculating the potential matrix elements of radial coupling suggested in paper [20] can be used in scattering calculations using some appropriate propagation scheme. In scattering calculations, in order to eliminate derivatives of the adiabatic surface eigenfunctions in hyperradius, the diabatic-by-sector approach is widely used [23]. The price for using this approximation is a slower convergence of the diabatic basis and therefore a larger number of hyperradial equations to be solved in order to get the required accuracy of the **S**-matrix elements [24,25]. Matrix elements computed by the method [20] can be directly incorporated in the popular hyperspherical close-coupling scheme. Applications of the method to scattering problems can be very useful and promising.

In this work we present program KANTBP for solving the eigenvalue and scattering problems for the multi-dimensional Schrödinger equation using the KM approach. In this method the multi-dimensional boundary problem is reduced to a system of ordinary differential equations of the second order with variable coefficients on a semi-axis with the help of expansion of the solution over a set of orthogonal solutions of an auxiliary parametric eigenvalue problem. Reduction of the boundary problem on a finite interval is implemented in the program with help of the Dirichlet, Neumann and third type boundary conditions in calculations of the eigenvalue problem for bound states and the third type boundary condition in a form appropriate for the **R**-matrix calculations of the multi-channel scattering problem [26–28]. Then a FEM is applied to construct numerical schemes for solving corresponding boundary problem for a system of ordinary differential equations with an accuracy of order $O(h^{p+1})$ in the grid step h. The order of approximation, p, depends on the smoothness of required solution. Note that variable coefficients of ordinary differential equations and the corresponding solutions can have a long-range asymptotic behavior [29]. That is why one has to be very careful in the formulation of the boundary problems under consideration. As a benchmark, we consider known exactly solvable 2D-model of three identical particles on a line with pair zero-range potentials [30–32] based on an adequate formulation of spectral problems and corresponding numerical schemes. For this benchmark model the needed analytical expressions for the potential matrix elements and first-derivative coupling terms, their asymptotics and asymptotics of radial solutions of the boundary problems for coupled differential equations have been produced with help of a MAPLE computer algebra system.

The paper is organized as follows. In Section 2 we give a brief overreview of the problem. The construction of the finite-element high-order schemes is discussed in Section 3. A description of the KANTBP program is given in Section 4. Subroutine units are briefly described in Section 5. Test desk is discussed in Section 6.

2. Statement of the problem

In many cases the solution of a multi-dimensional quantum-mechanical problem is reduced to a solution of the time-independent Schrödinger equation for wave function $\Psi(\rho, \Omega)$

$$\big(\mathbf{H} + \mathbf{U}(\rho, \Omega)\big)\Psi(\rho, \Omega) = E\Psi(\rho, \Omega), \tag{1}$$

where $\mathbf{H}$ is the $d > 1$ dimensional Hamiltonian, $\mathbf{U}(\rho, \Omega)$ is the given potential, E is the energy of a system, ρ is the hyperradius, and Ω is the set of angular coordinates which describe the internal motion of system on sphere $S^{d-1}(\Omega)$. In the close coupling approximation, known in mathematics as the KM [15] the partial wave function $\Psi_i(\rho, \Omega)$ is expanded over the one-parametric basis functions $\{B_j(\Omega; \rho)\}_{j=1}^{N}$:

$$\Psi_i(\rho, \Omega) = \sum_{j=1}^{N} B_j(\Omega; \rho)\chi_j^{(i)}(\rho). \tag{2}$$

In Eq. (2), the vector-functions $\boldsymbol{\chi}^{(i)}(\rho) = (\chi_1^{(i)}(\rho), \ldots, \chi_N^{(i)}(\rho))^{\mathrm{T}}$ are unknown, and the surface functions $\mathbf{B}(\Omega; \rho) = (B_1(\Omega; \rho), \ldots, B_N(\Omega; \rho))^{\mathrm{T}}$ is an orthonormal basis with respect to the set of angular coordinates Ω for each value of hyperradius ρ which is treated here as a given parameter. In the Kantorovich approach [15], the functions $B_j(\Omega; \rho)$ are determined as solutions of the following parametric eigenvalue problem:

$$\left(-\frac{1}{\rho^2}\hat{\boldsymbol{\Lambda}}_{\Omega}^2 + 2\mathbf{U}(\rho, \Omega)\right)B_j(\Omega; \rho) = \varepsilon_j(\rho)B_j(\Omega; \rho), \tag{3}$$

where $\hat{\boldsymbol{\Lambda}}_{\Omega}^2$ is the generalized self-adjoint angular momentum operator. The eigenfunctions of this problem satisfy the same boundary conditions in angular variable Ω for $\Psi_i(\rho, \Omega)$ and are normalized as follows

$$\big\langle B_i(\Omega; \rho) \,\big|\, B_j(\Omega; \rho)\big\rangle_{\Omega} = \int B_i^*(\Omega; \rho)B_j(\Omega; \rho)\,\mathrm{d}\Omega = \delta_{ij}, \tag{4}$$

where "$*$" denotes the complex conjugate and δ_{ij} is the Kroneker symbol.

After minimizing the Rayleigh–Ritz variational functional (see [20]), and using the expansion (2) equation (1) is reduced to a finite set of N ordinary second-order differential equations for the $\boldsymbol{\chi}(\rho) \equiv \boldsymbol{\chi}^{(i)}(\rho)$

$$(\mathbf{L} - 2E\mathbf{I})\boldsymbol{\chi}(\rho) \equiv \left(-\frac{1}{\rho^{d-1}}\mathbf{I}\frac{\mathrm{d}}{\mathrm{d}\rho}\rho^{d-1}\frac{\mathrm{d}}{\mathrm{d}\rho} + \mathbf{V}(\rho) + \mathbf{Q}(\rho)\frac{\mathrm{d}}{\mathrm{d}\rho} + \frac{1}{\rho^{d-1}}\frac{\mathrm{d}\rho^{d-1}\mathbf{Q}(\rho)}{\mathrm{d}\rho} - 2E\mathbf{I}\right)\boldsymbol{\chi}(\rho) = 0. \tag{5}$$

Here $\mathbf{I}$, $\mathbf{V}(\rho)$ and $\mathbf{Q}(\rho)$ are matrices of dimension $N \times N$ whose elements are given by the relation

$$\begin{aligned}
V_{ij}(\rho) &= H_{ij}(\rho) + \frac{\varepsilon_i(\rho) + \varepsilon_j(\rho)}{2}\delta_{ij}, \qquad I_{ij} = \delta_{ij}, \\
H_{ij}(\rho) &= H_{ji}(\rho) = \left\langle \frac{\partial B_i(\Omega; \rho)}{\partial\rho} \,\middle|\, \frac{\partial B_j(\Omega; \rho)}{\partial\rho} \right\rangle_{\Omega}, \\
Q_{ij}(\rho) &= -Q_{ji}(\rho) = -\left\langle B_i(\Omega; \rho) \,\middle|\, \frac{\partial B_j(\Omega; \rho)}{\partial\rho} \right\rangle_{\Omega}.
\end{aligned} \tag{6}$$

Let us consider the general radial homogeneous boundary conditions for the partial function $\boldsymbol{\Psi}_i(\rho, \Omega)$ at the endpoints of the finite interval $0 < \rho < \rho_{\max} < \infty$:

$$\mu_1\frac{\partial\Psi_i(\rho, \Omega)}{\partial\rho} - \lambda_1\Psi_i(\rho, \Omega) = 0, \quad \rho = 0,\ \Omega \in S^{d-1}(\Omega), \tag{7}$$

$$\mu_2\frac{\partial\Psi_i(\rho, \Omega)}{\partial\rho} - \lambda_2\Psi_i(\rho, \Omega) = 0, \quad \rho = \rho_{\max},\ \Omega \in S^{d-1}(\Omega), \tag{8}$$

where μ_1, λ_1 are some constants and $\mu_2 = \mu_2(\rho_{\max})$, $\lambda_2 = \lambda_2(\rho_{\max})$ are some numbers depending on the $\rho = \rho_{\max}$. Since the adiabatic functions form a complete set, one can alternatively require that projections of (7) and (8) onto all adiabatic functions fulfill

$$\left\langle B_j(\Omega; \rho) \,\middle|\, \mu_l\frac{\partial\Psi_i(\rho, \Omega)}{\partial\rho} - \lambda_l\Psi_i(\rho, \Omega)\right\rangle_{\Omega} = 0, \quad l = 1, 2, \tag{9}$$

using which we obtain the following matrix homogeneous boundary conditions

$$\mu_l\left(\mathbf{I}\frac{\mathrm{d}}{\mathrm{d}\rho} - \mathbf{Q}(\rho)\right)\boldsymbol{\chi}(\rho) - \lambda_l\boldsymbol{\chi}(\rho) = 0, \quad l = 1, 2. \tag{10}$$

From here for $l = 1$, the left boundary condition imposed on function $\boldsymbol{\chi}(\rho)$ at $\rho = 0$ has one of the following form:

1. if $\lim_{\rho\to 0}\rho^{d-1}|V_{ii}(\rho)| = \infty$, we have the Dirichlet boundary condition

$$\boldsymbol{\chi}(0) = 0, \tag{11}$$

2. if $\lim_{\rho\to 0}\rho^{d-1}|V_{ii}(\rho)| < \infty$, we have the Neumann type boundary condition

$$\lim_{\rho\to 0}\rho^{d-1}\left(\mathbf{I}\frac{\mathrm{d}}{\mathrm{d}\rho} - \mathbf{Q}(\rho)\right)\boldsymbol{\chi}(\rho) = 0. \tag{12}$$

2.1. The bound state case

For the bound state problem the energy E and radial wave function $\boldsymbol{\chi}(\rho)$ are calculated. For large ρ the radial wave function $\boldsymbol{\chi}(\rho)$ satisfies the exponentially or power decreased asymptotic behavior. From Eq. (10) for $l = 2$, the right boundary condition imposed on function $\boldsymbol{\chi}(\rho)$ at $\rho = \rho_{\max}$ has one of the following form:

- if $\mu_2 = 0$, we have the Dirichlet boundary condition

$$\boldsymbol{\chi}(\rho_{\max}) = 0, \tag{13}$$

- if $\lambda_2 = 0$, we have the Neumann type boundary condition

$$\left(\mathbf{I}\frac{\mathrm{d}}{\mathrm{d}\rho} - \mathbf{Q}(\rho)\right)\boldsymbol{\chi}(\rho) = 0, \tag{14}$$

- if $\mu_2 \neq 0$ and $\lambda_2 \neq 0$, we have the homogeneous third type boundary condition

$$\left(\mathbf{I}\frac{\mathrm{d}}{\mathrm{d}\rho} - \mathbf{Q}(\rho)\right)\boldsymbol{\chi}(\rho) = \lambda\boldsymbol{\chi}(\rho), \tag{15}$$

i.e., $\lambda \equiv \lambda(\rho) = \lambda_2(\rho)/\mu_2(\rho)$ and $\boldsymbol{\chi}(\rho)$ should be the eigenvalue and corresponding eigenvector of the above eigenvalue problem. After substituting (15) in Eq. (5) we obtain the following eigenvalue problem at $\rho = \rho_{\max}$

$$\big(\mathbf{V}(\rho) + \mathbf{Q}^2(\rho)\big)\hat{\boldsymbol{\chi}}(\rho) = \mu(\rho)\hat{\boldsymbol{\chi}}(\rho), \qquad \hat{\boldsymbol{\chi}}(\rho) = \boldsymbol{\chi}(\rho), \tag{16}$$

where eigenvalues $\mu(\rho)$ and $\lambda(\rho)$ satisfy the following relation

$$\mu(\rho) = \frac{1}{\rho^{d-1}}\frac{\mathrm{d}\rho^{d-1}\lambda(\rho)}{\mathrm{d}\rho} + \lambda^2(\rho) + 2E. \tag{17}$$

Note that, the eigenvalue $\mu(\rho)$ should be a fixed value for the any E and $\lambda(\rho)$ at $\rho = \rho_{\max}$ and this condition plays a very important role in the future calculations.

2.2. The scattering case

Most physical matrix potentials $\mathbf{V}(\rho)$ and $\mathbf{Q}(\rho)$ satisfy the following asymptotic behavior at large ρ

$$V_{ij}(\rho) = \sum_{l=2}\frac{v_{ij}^{(l)}}{\rho^l}, \qquad Q_{ij}(\rho) = \sum_{l=1}\frac{q_{ij}^{(l)}}{\rho^l}, \quad \text{for } i \neq j, \tag{18}$$

$$V_{jj}(\rho) = \epsilon_j - \frac{2Z_j}{\rho} + \frac{l_j(l_j+d-2)}{\rho^2} + \sum_{l=3}\frac{v_{jj}^{(l)}}{\rho^l}, \tag{19}$$

where $\epsilon_1 \leqslant \cdots \leqslant \epsilon_N$ are the threshold energy values. For the scattering problem we need to obtain the reaction matrix $\mathbf{K}$ and radial wave functions at given momentum $2E > \epsilon_1$. For large ρ the radial wave functions $\{\boldsymbol{\chi}^{(i)}(\rho)\}_{i=1}^{N_o}$ satisfy the following asymptotic conditions

$$\chi_j^{(i)}(\rho) \to \frac{\sin(w_j(\rho))\delta_{ji} + \cos(w_j(\rho))K_{ji}}{\sqrt{k_j\rho^{d-1}}} + \mathrm{O}(\rho^{-(d+1)/2}), \quad j = \overline{1, N_o}, \tag{20}$$

$$\chi_j^{(i)}(\rho) \to \frac{\exp(-v_j(\rho))}{\sqrt{q_j\rho^{d-1}}} + \mathrm{O}\big(\rho^{-(d+1)/2}\exp\big(-v_j(\rho)\big)\big), \quad j = \overline{N_o+1, N}, \tag{21}$$

where

$$w_j(\rho) = k_j\rho + \frac{Z_j}{k_j}\ln(2k_j\rho) - \frac{2l_j+d-3}{4}\pi + \delta_j^c,$$
$$\delta_j^c = \arg\Gamma\left(\frac{2l_j+d-1}{2} - \iota\frac{Z_j}{k_j}\right),$$
$$v_j(\rho) = q_j\rho - \frac{Z_j}{q_j}\ln(2q_j\rho). \tag{22}$$

Here N_o is the number of open channels, δ_j^c is the known Coulomb phase shift, $\mathbf{K} = \{K_{ji}\}_{ji=1}^{N_o}$ is the required reaction matrix, $k_j = \sqrt{2E-\epsilon_j}$ for $j = \overline{1, N_o}$ and $q_j = \sqrt{\epsilon_j - 2E}$ for $j = \overline{N_o+1, N}$.

Let us consider the quadratic functional

$$\boldsymbol{\Xi}(\boldsymbol{\Phi}, E, \rho_{\max}) \equiv \int_0^{\rho_{\max}} \boldsymbol{\Phi}^{\mathrm{T}}(\rho)(\mathbf{L} - 2E\mathbf{I})\boldsymbol{\Phi}(\rho)\rho^{d-1}\,\mathrm{d}\rho$$
$$= \boldsymbol{\Pi}(\boldsymbol{\Phi}, E, \rho_{\max}) - \rho_{\max}^{d-1}\boldsymbol{\Phi}^{\mathrm{T}}(\rho_{\max})\boldsymbol{\Phi}(\rho_{\max})\boldsymbol{\Lambda}, \tag{23}$$

where $\boldsymbol{\Pi}(\boldsymbol{\Phi}, E, \rho_{\max})$ is the symmetric functional

$$\boldsymbol{\Pi}(\boldsymbol{\Phi}, E, \rho_{\max}) = \int_0^{\rho_{\max}} \left(\frac{\mathrm{d}\boldsymbol{\Phi}^{\mathrm{T}}(\rho)}{\mathrm{d}\rho}\frac{\mathrm{d}\boldsymbol{\Phi}(\rho)}{\mathrm{d}\rho} + \boldsymbol{\Phi}^{\mathrm{T}}(\rho)\mathbf{V}(\rho)\boldsymbol{\Phi}(\rho)\right.$$
$$\left. + \boldsymbol{\Phi}^{\mathrm{T}}(\rho)\mathbf{Q}(\rho)\frac{\mathrm{d}\boldsymbol{\Phi}(\rho)}{\mathrm{d}\rho} - \frac{\mathrm{d}\boldsymbol{\Phi}(\rho)^{\mathrm{T}}}{\mathrm{d}\rho}\mathbf{Q}(\rho)\boldsymbol{\Phi}(\rho) - 2E\boldsymbol{\Phi}^{\mathrm{T}}(\rho)\boldsymbol{\Phi}(\rho)\right)\rho^{d-1}\,\mathrm{d}\rho, \tag{24}$$

and $\boldsymbol{\Phi}(\rho) = \{\boldsymbol{\chi}^{(i)}(\rho)\}_{i=1}^{N_o}$ is the matrix-solution of dimension $N \times N_o$ which satisfies the following eigenvalue problem at $\rho = \rho_{\max}$

$$\frac{\mathrm{d}\boldsymbol{\Phi}(\rho)}{\mathrm{d}\rho} - \mathbf{Q}(\rho)\boldsymbol{\Phi}(\rho) = \boldsymbol{\Phi}(\rho)\boldsymbol{\Lambda}, \quad \boldsymbol{\Lambda} = \left\{\delta_{ij}\lambda^{(i)}\right\}_{ij=1}^{N_o}. \tag{25}$$

After using FEM, Eq. (23) can be approximated by the following problem at $\rho = \rho_{\max}$ (see details in Section 3)

$$\mathbf{G}(\rho)\boldsymbol{\Phi}(\rho) = \frac{\mathrm{d}\boldsymbol{\Phi}(\rho)}{\mathrm{d}\rho} - \mathbf{Q}(\rho)\boldsymbol{\Phi}(\rho), \tag{26}$$

where $\mathbf{G}(\rho)$ is the symmetric matrix of dimension $N \times N$. From here, we obtain the relation between $\boldsymbol{\Phi}(\rho)$ and its derivative at $\rho = \rho_{\max}$

$$\frac{\mathrm{d}\boldsymbol{\Phi}(\rho)}{\mathrm{d}\rho} = \mathbf{R}(\rho)\boldsymbol{\Phi}(\rho), \quad \mathbf{R}(\rho) = \mathbf{G}(\rho) + \mathbf{Q}(\rho). \tag{27}$$

After that, $\boldsymbol{\Phi}(\rho)$ and its derivative can be rewritten via the two independent fundamental regular and irregular asymptotic matrix-solutions $\boldsymbol{\Phi}_{\mathrm{reg}}(\rho) = \{\boldsymbol{\chi}_{\mathrm{reg}}^{(i)}(\rho)\}_{i=1}^{N_o}$, $\boldsymbol{\Phi}_{\mathrm{irr}}(\rho) = \{\boldsymbol{\chi}_{\mathrm{irr}}^{(i)}(\rho)\}_{i=1}^{N_o}$ of Eq. (5) and their derivatives at $\rho = \rho_{\max}$

$$\boldsymbol{\Phi}(\rho) = \boldsymbol{\Phi}_{\mathrm{reg}}(\rho) + \boldsymbol{\Phi}_{\mathrm{irr}}(\rho)\mathbf{K}, \qquad \frac{\mathrm{d}\boldsymbol{\Phi}(\rho)}{\mathrm{d}\rho} = \frac{\mathrm{d}\boldsymbol{\Phi}_{\mathrm{reg}}(\rho)}{\mathrm{d}\rho} + \frac{\mathrm{d}\boldsymbol{\Phi}_{\mathrm{irr}}(\rho)}{\mathrm{d}\rho}\mathbf{K}. \tag{28}$$

Using formula (27), we obtain the following matrix equation for the reaction matrix $\mathbf{K}$

$$\left(\frac{\mathrm{d}\boldsymbol{\Phi}_{\mathrm{irr}}(\rho)}{\mathrm{d}\rho} - \mathbf{R}(\rho)\boldsymbol{\Phi}_{\mathrm{irr}}(\rho)\right)\mathbf{K} = -\left(\frac{\mathrm{d}\boldsymbol{\Phi}_{\mathrm{reg}}(\rho)}{\mathrm{d}\rho} - \mathbf{R}(\rho)\boldsymbol{\Phi}_{\mathrm{reg}}(\rho)\right). \tag{29}$$

In addition, it should be noted that the regular and irregular functions satisfy the generalized Wronskian relation for large ρ

$$\mathbf{Wr}\big(\mathbf{Q}(\rho); \boldsymbol{\Phi}_{\mathrm{irr}}(\rho), \boldsymbol{\Phi}_{\mathrm{reg}}(\rho)\big) = \mathbf{I}_{oo}, \tag{30}$$

where $\mathbf{Wr}(\bullet; \mathbf{a}(\rho), \mathbf{b}(\rho))$ is a generalized Wronskian with a long derivative defined as

$$\mathbf{Wr}\big(\bullet; \mathbf{a}(\rho), \mathbf{b}(\rho)\big) = \rho^{d-1}\left[\mathbf{a}^{\mathrm{T}}(\rho)\left(\frac{\mathrm{d}\mathbf{b}(\rho)}{\mathrm{d}\rho} - \bullet\mathbf{b}(\rho)\right) - \left(\frac{\mathrm{d}\mathbf{a}(\rho)}{\mathrm{d}\rho} - \bullet\mathbf{a}(\rho)\right)^{\mathrm{T}}\mathbf{b}(\rho)\right]. \tag{31}$$

This Wronskian will be used to estimate a desirable accuracy of the above expansion. Here $\mathbf{I}_{oo}$ is the unit matrix of dimension $N_o \times N_o$ and Eq. (30) at $\rho = \rho_{\max}$ is equivalent to

$$\mathbf{Wr}\big(\mathbf{R}(\rho); \boldsymbol{\Phi}_{\mathrm{irr}}(\rho), \boldsymbol{\Phi}_{\mathrm{reg}}(\rho)\big) = \mathbf{Wr}\big(\mathbf{Q}(\rho); \boldsymbol{\Phi}_{\mathrm{irr}}(\rho), \boldsymbol{\Phi}_{\mathrm{reg}}(\rho)\big). \tag{32}$$

Note that, when some channels are closed, the left and right matrices of Eq. (29) are rectangle matrices. Therefore, we obtain the following formula for the reaction matrix $\mathbf{K}$

$$\mathbf{K} = -\mathbf{X}^{-1}(\rho_{\max})\mathbf{Y}(\rho_{\max}), \tag{33}$$

where

$$\begin{aligned}
\mathbf{X}(\rho) &= \left(\frac{\mathrm{d}\boldsymbol{\Phi}_{\mathrm{irr}}(\rho)}{\mathrm{d}\rho} - \mathbf{R}(\rho)\boldsymbol{\Phi}_{\mathrm{irr}}(\rho)\right)_{oo}, \\
\mathbf{Y}(\rho) &= \left(\frac{\mathrm{d}\boldsymbol{\Phi}_{\mathrm{reg}}(\rho)}{\mathrm{d}\rho} - \mathbf{R}(\rho)\boldsymbol{\Phi}_{\mathrm{reg}}(\rho)\right)_{oo},
\end{aligned} \tag{34}$$

are the square matrices of dimension $N_o \times N_o$ depended on the open–open matrix (channels).

2.3. Construction of the regular and irregular matrix-solutions

We can construct the regular and irregular matrix-solutions by various methods (see [33–37]). For example, we can find regular and irregular matrix-solutions $\boldsymbol{\Phi}_{\mathrm{reg}}(\rho)$, $\boldsymbol{\Phi}_{\mathrm{irr}}(\rho)$ of Eq. (5) with components $\boldsymbol{\chi}^{(i)}_{\mathrm{reg}}(\rho) = (\chi^{\mathrm{reg}}_{1i}(\rho), \ldots, \chi^{\mathrm{reg}}_{Ni}(\rho))^{\mathrm{T}}$ and $\boldsymbol{\chi}^{(i)}_{\mathrm{irr}}(\rho) = (\chi^{\mathrm{irr}}_{1i}(\rho), \ldots, \chi^{\mathrm{irr}}_{Ni}(\rho))^{\mathrm{T}}$ using the following asymptotic form for large ρ

$$\begin{aligned}
\chi^{\mathrm{reg}}_{ji}(\rho) &= \frac{\sin(w_i(\rho))}{\sqrt{k_i\rho^{d-1}}}\sum_{l=0}\frac{s^{(l,1)}_{ji}}{\rho^l} + \frac{\cos(w_i(\rho))}{\sqrt{k_i\rho^{d-1}}}\sum_{l=0}\frac{c^{(l,1)}_{ji}}{\rho^l}, \\
\chi^{\mathrm{irr}}_{ji}(\rho) &= \frac{\cos(w_i(\rho))}{\sqrt{k_i\rho^{d-1}}}\sum_{l=0}\frac{c^{(l,2)}_{ji}}{\rho^l} + \frac{\sin(w_i(\rho))}{\sqrt{k_i\rho^{d-1}}}\sum_{l=0}\frac{s^{(l,2)}_{ji}}{\rho^l},
\end{aligned} \tag{35}$$

with initial data

$$s^{(0,1)}_{ji} = \delta_{ji}, \quad c^{(0,1)}_{ji} = 0, \quad c^{(0,2)}_{ji} = \delta_{ji}, \quad s^{(0,2)}_{ji} = 0. \tag{36}$$

Substituting expansions (18), (19) and (35) into Eq. (5) and equating expressions of $\sin(w_i(\rho))$, $\cos(w_i(\rho))$, and again equating coefficients of expansion for the same powers of ρ, we arrive to a set of recurrence relations with respect to unknown coefficients $s^{(l,1)}_{ji}$, $s^{(l,2)}_{ji}$ and $c^{(l,1)}_{ji}$, $c^{(l,2)}_{ji}$. By means of initial data (36) we have a step-by-step procedure for determining of series coefficients $s^{(l,1)}_{ji}$, $s^{(l,2)}_{ji}$ and $c^{(l,1)}_{ji}$, $c^{(l,2)}_{ji}$ [38,39].

3. High-order approximations of the finite-element method

In order to solve numerically the Sturm–Liouville problem for Eq. (5) subject to the corresponding boundary conditions from Eqs. (11), (12) and (13), (14), (15), (25) the high-order approximations of the FEM [40,41] elaborated in our previous paper [42] have been used. Such high-order approximations of the FEM have been proved [42] to be very accurate, stable, and efficient for a wide set of quantum-mechanical problems. Computational schemes of the High-order of accuracy are derived from the Rayleigh–Ritz variationals functional for the bound state problem

$$\mathcal{R}_b(\boldsymbol{\chi}, E, \lambda) = \left\{\int_0^{\rho_{\max}}\sum_{i,j=1}^{N}[\chi H\chi]_{ij}\rho^{d-1}\,\mathrm{d}\rho - \lambda\rho_{\max}^{d-1}\sum_{j=1}^{N}\chi_j^2(\rho_{\max})\right\}\left\{\int_0^{\rho_{\max}}\sum_{j=1}^{N}\chi_j^2(\rho)\rho^{d-1}\,\mathrm{d}\rho\right\}^{-1}, \tag{37}$$

and for the scattering problem with $\boldsymbol{\chi}(\rho) \equiv \boldsymbol{\chi}^{(i)}(\rho)$ and $\lambda \equiv \lambda^{(i)}$

$$\mathcal{R}_s(\boldsymbol{\chi}, \lambda) = \left\{\int_0^{\rho_{\max}}\sum_{i,j=1}^{N}\big[\chi(H-2E)\chi\big]_{ij}\rho^{d-1}\,\mathrm{d}\rho\right\}\left\{\rho_{\max}^{d-1}\sum_{j=1}^{N}\chi_j^2(\rho_{\max})\right\}^{-1}, \tag{38}$$

on the basis of the FEM. Here

$$\begin{aligned}
[\chi H\chi]_{ij} &= \chi_i'(\rho)\chi_j'(\rho)\delta_{ij} + \chi_i(\rho)V_{ij}(\rho)\chi_j(\rho) + Q_{ij}(\rho)\big[\chi_i(\rho)\chi_j'(\rho) - \chi_i'(\rho)\chi_j(\rho)\big], \\
\big[\chi(H-2E)\chi\big]_{ij} &= [\chi H\chi]_{ij} - 2E\chi_i(\rho)\chi_j(\rho)\delta_{ij},
\end{aligned} \tag{39}$$

and symbol "′" denotes a derivative in ρ.

The general idea of the FEM in one-dimensional space is to divide interval $[0, \rho_{\max}]$ into many small domains called elements. The size of elements can be defined very freely so that physical properties can be taken into account.

Now we cover the interval $\Delta = [0, \rho_{\max}]$ by a system of n subintervals $\Delta_j = [\rho_{j-1}, \rho_j]$ in such a way that $\Delta = \bigcup_{j=1}^{n} \Delta_j$. In each subinterval Δ_j the nodes

$$\rho_{j,r}^p = \rho_{j-1} + \frac{h_j}{p} r, \qquad h_j = \rho_j - \rho_{j-1}, \quad r = \overline{0, p}, \tag{40}$$

and the Lagrange elements $\{\phi_{j,r}^p(\rho)\}_{r=0}^p$

$$\phi_{j,r}^p(\rho) = \prod_{i=0, i\neq r}^{p} \frac{(\rho - \rho_{j,i}^p)}{(\rho_{j,r}^p - \rho_{j,i}^p)} \tag{41}$$

are determined. By means of the Lagrange elements $\phi_{j,r}^p(\rho)$, we define a set of local functions $N_l(\rho)$ as follows:

$$N_l^p(\rho) = \begin{cases} \begin{cases} \phi_{1,0}^p(\rho), & \rho \in \Delta_1, \\ 0, & \rho \notin \Delta_1, \end{cases} & l = 0, \\ \begin{cases} \phi_{j,r}^p(\rho), & \rho \in \Delta_j, \\ 0, & \rho \notin \Delta_j, \end{cases} & l = r + p(j-1),\ r = \overline{1, p-1}, \\ \begin{cases} \phi_{j,p}^p(\rho), & \rho \in \Delta_j, \\ \phi_{j+1,0}^p(\rho), & \rho \in \Delta_{j+1}, \\ 0, & \rho \notin \Delta_j \bigcup \Delta_{j+1}, \end{cases} & l = jp,\ j = \overline{1, n-1}, \\ \begin{cases} \phi_{n,p}^p(\rho), & \rho \in \Delta_n, \\ 0, & \rho \notin \Delta_n, \end{cases} & l = np. \end{cases} \tag{42}$$

The functions $\{N_l^p(\rho)\}_{l=0}^L$, $L = np$, form a basis in the space of polynomials of the pth order. Now, we approximate each function $\chi_\mu(\rho)$ by a finite sum of local functions $N_l^p(\rho)$

$$\chi_\mu(\rho) = \sum_{l=0}^{L} \chi_\mu^l N_l^p(\rho), \qquad \chi_\mu^l \equiv \chi_\mu^l(\rho_{j,r}^p). \tag{43}$$

For the bound state problem, after substituting expansion (43) into the variational functional (37) and minimizing it [40,41] we obtain that vector-solution $\boldsymbol{\chi}^h$ is the eigenvector of the generalized eigenvalue problem

$$(\mathbf{A}^p - \lambda^h \mathbf{M})\boldsymbol{\chi}^h = 2E^h \mathbf{B}^p \boldsymbol{\chi}^h. \tag{44}$$

Here $\mathbf{M}$ is a diagonal matrix with zero elements, except the last N elements that are equal $\rho_{\max}^{d-1}$, and in case of the Dirichlet and Neumann type boundary conditions $\lambda^h \equiv 0$. For the third type of boundary condition we use the following additional condition (17)

$$\mu = \frac{1}{\rho^{d-1}} \frac{\mathrm{d}\rho^{d-1}\lambda^h}{\mathrm{d}\rho} + (\lambda^h)^2 + 2E^h, \tag{45}$$

where μ is the first eigenvalue of the problem (16). In this case we use the following iterative scheme for solutions $\lambda \equiv \lambda^h$, $E \equiv E^h$ and $\boldsymbol{\chi} \equiv \boldsymbol{\chi}^h$

$$\begin{aligned} &(\mathbf{A}^p - \lambda^{(j-1)}\mathbf{M})\boldsymbol{\chi}^{(j-1)} = 2E^{(j-1)} \mathbf{B}^p \boldsymbol{\chi}^{(j-1)}, \\ &(\lambda^{(j)})^2 = \mu - \frac{\mathrm{d}\lambda^{(j-1)}}{\mathrm{d}\rho} - \frac{d-1}{\rho_{\max}} \lambda^{(j-1)} - 2E^{(j-1)}, \end{aligned} \tag{46}$$

with initial value $\lambda^{(0)}$.

To solve the scattering problem at a fixed value of energy E, after substituting expansion (43) into the variational functional (38) and minimizing it [40,41] we obtain that matrix-solution $\boldsymbol{\Phi}^h \equiv ((\boldsymbol{\chi}^{(1)})^h, \ldots, (\boldsymbol{\chi}^{(N_o)})^h)$ is a set of eigenvectors of a special eigenvalue problem

$$\mathbf{G}^p \boldsymbol{\Phi}^h \equiv (\mathbf{A}^p - 2E\mathbf{B}^p)\boldsymbol{\Phi}^h = \mathbf{M}\boldsymbol{\Phi}^h \boldsymbol{\Lambda}^h, \quad \boldsymbol{\Lambda}^h = \left\{\delta_{ij}(\lambda^{(i)})^h\right\}_{ij=1}^{N_o}, \tag{47}$$

where $\mathbf{M}^p$ is a diagonal matrix with zero elements except the last N elements equal to $\rho_{\max}^{d-1}$. Eq. (47) can be rewritten in the following form

$$\begin{pmatrix} \mathbf{G}_{aa}^p & \mathbf{G}_{ab}^p \\ \mathbf{G}_{ba}^p & \mathbf{G}_{bb}^p \end{pmatrix} \begin{pmatrix} \boldsymbol{\Phi}_a^h \\ \boldsymbol{\Phi}_b^h \end{pmatrix} = \rho_{\max}^{d-1} \begin{pmatrix} 0 & 0 \\ 0 & \mathbf{I} \end{pmatrix} \begin{pmatrix} \boldsymbol{\Phi}_a^h \\ \boldsymbol{\Phi}_b^h \end{pmatrix} \boldsymbol{\Lambda}^h, \quad \boldsymbol{\Phi}^h = \begin{pmatrix} \boldsymbol{\Phi}_a^h \\ \boldsymbol{\Phi}_b^h \end{pmatrix}, \tag{48}$$

where $\boldsymbol{\Phi}_a^h$ and $\boldsymbol{\Phi}_b^h \equiv \boldsymbol{\Phi}(\rho_{\max})$ are the matrix-solutions of dimension $(LN - N) \times N_o$ and $N \times N_o$, respectively. From here, we obtain the following eigenvalue problem with respect to $\boldsymbol{\Phi}_b^h$ and $\boldsymbol{\Lambda}^h$, of nonhomogeneous problem with respect to $\boldsymbol{\Phi}_b^h$ with right-hand side

from Eq. (25)

$$\left(\mathbf{G}^p_{bb} - \mathbf{G}^p_{ba}\left(\mathbf{G}^p_{aa}\right)^{-1}\mathbf{G}^p_{ab}\right)\boldsymbol{\Phi}^h_b = \rho_{\max}^{d-1}\boldsymbol{\Phi}^h_b\boldsymbol{\Lambda}^h \equiv \rho_{\max}^{d-1}\left(\frac{\mathrm{d}\boldsymbol{\Phi}^h_b}{\mathrm{d}\rho} - \mathbf{Q}(\rho_{\max})\boldsymbol{\Phi}^h_b\right), \tag{49}$$

and explicit expression for component, $\boldsymbol{\Phi}^h_a$,

$$\boldsymbol{\Phi}^h_a = -\left(\mathbf{G}^p_{aa}\right)^{-1}\mathbf{G}^p_{ab}\boldsymbol{\Phi}^h_b. \tag{50}$$

From Eqs. (27) and (49) we can obtain the relation between $\boldsymbol{\Phi}^h_b$ and its derivative

$$\begin{aligned}
&\frac{\mathrm{d}\boldsymbol{\Phi}^h_b}{\mathrm{d}\rho} = \mathbf{R}(\rho_{\max})\boldsymbol{\Phi}^h_b,\\
&\mathbf{R}(\rho_{\max}) = \rho_{\max}^{1-d}\left(\mathbf{G}^p_{bb} - \mathbf{G}^p_{ba}\left(\mathbf{G}^p_{aa}\right)^{-1}\mathbf{G}^p_{ab}\right) + \mathbf{Q}(\rho_{\max}),
\end{aligned} \tag{51}$$

i.e. we have found the required $\mathbf{R}(\rho_{\max})$ matrix without calculation of eigenvalue $\boldsymbol{\Lambda}^h$ and corresponding eigenvector $\boldsymbol{\Phi}^h$ of the eigenvalue problem (47). For calculating Eq. (51) consider the following auxiliary system of algebraic equation, as the determinant of the matrix $\mathbf{G}^p$ nonzero,

$$\begin{pmatrix} \mathbf{G}^p_{aa} & \mathbf{G}^p_{ab} \\ \mathbf{G}^p_{ba} & \mathbf{G}^p_{bb} \end{pmatrix}\begin{pmatrix} \mathbf{F}^p_a \\ \mathbf{F}^p_b \end{pmatrix} = \rho_{\max}^{d-1}\begin{pmatrix} 0 \\ \mathbf{I} \end{pmatrix}. \tag{52}$$

The above equation has solutions

$$\mathbf{F}^p_a = -\left(\mathbf{G}^p_{aa}\right)^{-1}\mathbf{G}^p_{ab}\mathbf{F}^p_b, \quad \mathbf{F}^p_b = \rho_{\max}^{d-1}\left(\mathbf{G}^p_{bb} - \mathbf{G}^p_{ba}\left(\mathbf{G}^p_{aa}\right)^{-1}\mathbf{G}^p_{ab}\right)^{-1}. \tag{53}$$

From here, our required $\mathbf{R}(\rho_{\max})$ matrix is equal to

$$\mathbf{R}(\rho_{\max}) = \left(\mathbf{F}^p_b\right)^{-1} + \mathbf{Q}(\rho_{\max}), \tag{54}$$

and required solution $\boldsymbol{\Phi}$ is calculated by formulae (50) and (53)

$$\boldsymbol{\Phi}^h_a = \mathbf{F}^p_a\left(\mathbf{F}^p_b\right)^{-1}\boldsymbol{\Phi}^h_b, \quad \boldsymbol{\Phi}^h_b = \boldsymbol{\Phi}_{\mathrm{reg}}(\rho_{\max}) + \boldsymbol{\Phi}_{\mathrm{irr}}(\rho_{\max})\mathbf{K}, \tag{55}$$

where reaction matrix $\mathbf{K}$ is evaluated from (33) and asymptotics of solution $\boldsymbol{\Phi}_{\mathrm{reg}}(\rho) = \{\boldsymbol{\chi}^{(i)}_{\mathrm{reg}}(\rho)\}_{i=1}^{N_o}$, $\boldsymbol{\Phi}_{\mathrm{irr}}(\rho) = \{\boldsymbol{\chi}^{(i)}_{\mathrm{irr}}(\rho)\}_{i=1}^{N_o}$ are determined in (28).

Let E_m and $\boldsymbol{\chi}_m(\rho)$ be the exact solutions of Eq. (44) and E^h_m and $\boldsymbol{\chi}^h_m(\rho)$ be the corresponding numerical solutions. Then the following estimations are valid [40]

$$\left|E^h_m - E_m\right| \leqslant c_1|E_m|h^{2p}, \qquad \left\|\boldsymbol{\chi}^h_m(\rho) - \boldsymbol{\chi}_m(\rho)\right\|_0 \leqslant c_2|E_m|h^{p+1}, \tag{56}$$

where h is the maximal step of the finite-element grid, m is the number of the corresponded solution, and the positive constants c_1 and c_2 do not depend on step h. Similar estimations are valid for approximate values of the eigenvalue $(\lambda^{(i)})^h$ and corresponding solution $(\boldsymbol{\chi}^{(i)}(\rho))^h$. The stiffness matrix $\mathbf{A}^p$ and the mass matrix $\mathbf{B}^p$ are symmetric and have a banded structure, and $\mathbf{B}^p$ matrix is positively defined. They have the following form

$$\mathbf{A}^p = \sum_{j=1}^{n}\mathbf{a}^p_j, \qquad \mathbf{B}^p = \sum_{j=1}^{n}\mathbf{b}^p_j, \tag{57}$$

where the local matrices $\mathbf{a}^p_j$ and $\mathbf{b}^p_j$ are calculated as

$$\begin{aligned}
\left(\mathbf{a}^p_j\right)^{qr}_{\mu\nu} = \int_{-1}^{+1}\Bigg\{&\delta_{\mu\nu}\frac{4}{h_j^2}\left(\phi^p_{j,q}\right)'(\rho)\left(\phi^p_{j,r}\right)'(\rho) + V_{\mu\nu}(\rho)\phi^p_{j,q}(\rho)\phi^p_{j,r}(\rho)\\
&+ Q_{\mu\nu}(\rho)\left[\phi^p_{j,q}(\rho)\left(\phi^p_{j,r}\right)'(\rho) - \left(\phi^p_{j,q}\right)'(\rho)\phi^p_{j,r}(\rho)\right]\frac{2}{h_j}\Bigg\}\rho^{d-1}\frac{h_j}{2}\,\mathrm{d}\eta,
\end{aligned}$$

$$\left(\mathbf{b}_j^p\right)_{\mu\nu}^{qr} = \delta_{\mu\nu} \int_{-1}^{+1} \phi_{j,q}^p(\rho)\phi_{j,r}^p(\rho)\rho^{d-1}\frac{h_j}{2}\,\mathrm{d}\eta, \tag{58}$$

$$\rho = \rho_{j-1} + 0.5h_j(1+\eta), \quad q,r = \overline{0,p},\ \mu,\nu = \overline{1,N}.$$

Integrals (58) are evaluated using the Gaussian quadrature formulae

$$\begin{aligned}\left(\mathbf{a}_j^p\right)_{\mu\nu}^{qr} &= \sum_{g=0}^{p}\left\{\delta_{\mu\nu}\frac{4}{h_j^2}\left(\phi_{j,q}^p\right)'(\rho_g)\left(\phi_{j,r}^p\right)'(\rho_g) + V_{\mu\nu}(\rho_g)\phi_{j,q}^p(\rho_g)\phi_{j,r}^p(\rho_g)\right.\\ &\quad\left. + Q_{\mu\nu}(\rho_g)\left[\phi_{j,q}^p(\rho_g)\left(\phi_{j,r}^p\right)'(\rho_g) - \left(\phi_{j,q}^p\right)'(\rho_g)\phi_{j,r}^p(\rho_g)\right]\frac{2}{h_j}\right\}\rho_g^{d-1}\frac{h_j}{2}w_g,\\ \left(\mathbf{b}_j^p\right)_{\mu\nu}^{qr} &= \sum_{g=0}^{p}\delta_{\mu\nu}\phi_{j,q}^p(\rho_g)\phi_{j,r}^p(\rho_g)\rho_g^{d-1}\frac{h_j}{2}w_g,\end{aligned} \tag{59}$$

where $\rho_g = \rho_{j-1} + 0.5h_j(1+\eta_g)$, η_g and w_g, $g = \overline{0,p}$ are the Gaussian nodes and weights.

This way the following solution strategy can be used: since we know functions $\mathbf{V}(\rho)$ and $\mathbf{Q}(\rho)$ we choose first the FEM grid, then we calculate these matrix elements in the Gaussian points and finally we evaluate the integrals. This allow us to organize the calculation scheme for a system of N equations as follows. We evaluate the values of all matrix elements for these N equations in the Gaussian nodes and store them into the external file. Then we use it to investigate the convergence rate of the Kantorovich expansion as a function of number of equations.

In order to solve the generalized eigenvalue problem (44), the subspace iteration method [40,41] elaborated by Bathe [41] for the solution of large symmetric banded matrix eigenvalue problems has been chosen. This method uses a skyline storage mode, which stores components of the matrix column vectors within the banded region of the matrix, and is ideally suited for banded finite-element matrices. The procedure chooses a vector subspace of the full solution space and iterates upon the successive solutions in the subspace (for details, see [41]). The iterations continue until the desired set of solutions in the iteration subspace converges to within the specified tolerance on the Rayleigh quotients for the eigenpairs. Generally, 10–16 iterations are required for the subspace iterations to converge the subspace to within the prescribe tolerance. If matrix $\mathbf{A}^p - \lambda^h\mathbf{M}$ in Eq. (44) is not positively defined, problem (44) is replaced by the following problem:

$$\tilde{\mathbf{A}}^p\,\boldsymbol{\chi}^h = \tilde{E}^h\,\mathbf{B}^p\,\boldsymbol{\chi}^h, \quad \tilde{\mathbf{A}}^p = \mathbf{A}^p - \lambda^h\mathbf{M} - \alpha\mathbf{B}^p. \tag{60}$$

The number α (the shift of the energy spectrum) is chosen in such a way that matrix $\tilde{\mathbf{A}}^p$ is positive. The eigenvector of problem (44) is the same, and $E^h = \tilde{E}^h + \alpha$.

For the solution of Eq. (16) it is impossible to define some minimum shift, because a total set of eigenvalues, $\mu(\rho_{\max})$, should be defended on $\rho = \rho_{\max}$. But, we can use the following lower and upper bounds for the eigenvalues [43]

$$\left|\mu(\rho_{\max}) - f_{ii}\right| \leqslant \sum_{j=1, i\neq j}^{N} |f_{ij}|, \qquad f_{ij} = \left(\mathbf{V}(\rho_{\max}) + \mathbf{Q}^2(\rho_{\max})\right)_{ij}, \quad i = \overline{1,N}, \tag{61}$$

and from them we can determine the minimum shift of a full set of eigenvalues $\mu(\rho_{\max})$

$$\alpha = \min_{i=\overline{1,N}}\left(f_{ii} - \sum_{j=1, j\neq i}^{N}|f_{ij}|\right) - 1. \tag{62}$$

After that, we can rewrite (16) in the following form

$$\begin{aligned}&\left(\mathbf{V}(\rho_{\max}) + \mathbf{Q}^2(\rho_{\max}) - \alpha\mathbf{I}\right)\hat{\boldsymbol{\chi}}(\rho_{\max}) = \tilde{\mu}(\rho_{\max})\hat{\boldsymbol{\chi}}(\rho_{\max}),\\ &\mu(\rho_{\max}) = \tilde{\mu}(\rho_{\max}) + \alpha.\end{aligned} \tag{63}$$

In this case left matrix should be positively defined, and can be diagonalized by the generalized Jacobi method.

From the estimates above one can see that we have a high accuracy for calculating the bound states and corresponding wave functions of both (eigenvalues and continuous) cases. From this point of view, the main error in the solution depends only on the number of equations N and computer precision used in calculations.

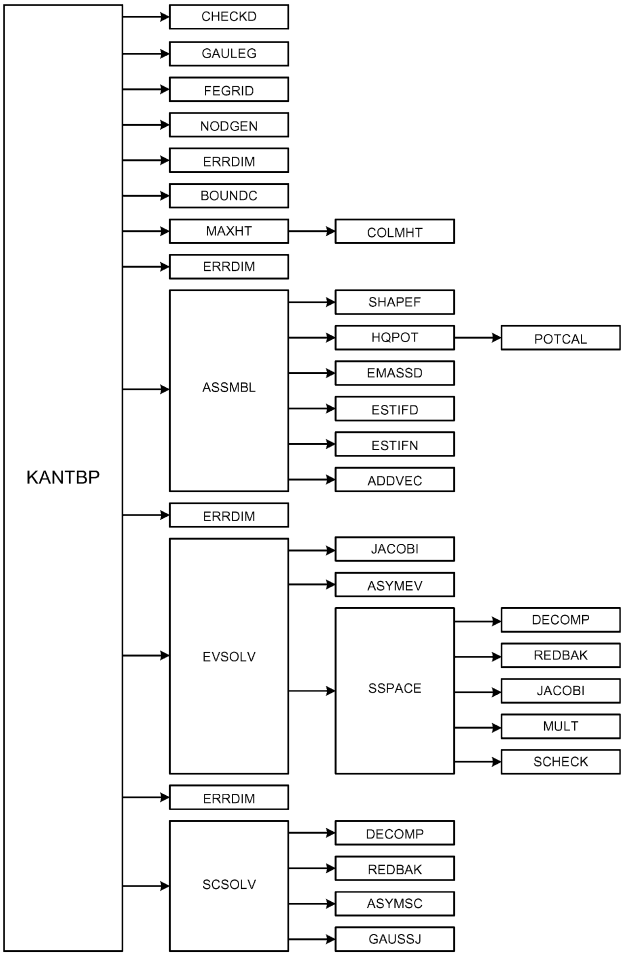

Fig. 1. Flow diagram of the KANTBP program.

4. Description of the program

Fig. 1 presents a flow diagram for the KANTBP program. The function of each subroutine is described in Section 5. The KANTBP program is called from the main routine (supplied by a user) which sets dimensions of the arrays and is responsible for the input data. In the present code each array declarator is written in terms of the symbolic names of constants. These constants are defined in the following PARAMETER statement in the main routine:
PARAMETER (MTOT = 9000000, MITOT = 900000, NMESH1 = 7, MDIM1 = 6) where

- MTOT is the dimension of the working DOUBLE PRECISION array TOT.
- MITOT is the dimension of the working INTEGER array ITOT.
- NMESH1 is the dimension of the DOUBLE PRECISION array RMESH containing the information about the subdivision of the hyperradial interval $[0, \rho_{\max}]$ on subintervals and number of elements on each one of them. NMESH1 is always odd and $\geqslant 3$.
- MDIM1 is the dimension of the DOUBLE PRECISION array THRSHL and INTEGER array NDIL containing information about a set of threshold values and numbers of coupled differential equations, respectively.

A more concrete assignment of these dimensions is discussed below. In order to change the dimensions of the code, all one has to do is to modify the single PARAMETER statement defined above in the main program unit.

The calling sequence for the subroutine KANTBP is:

```
 CALL KANTBP(TITLE,IPTYPE,NROOT,MDIM,IDIM,NPOL,RTOL,NITEM,
1            SHIFT,IPRINT,IPRSTP,NMESH,RMESH,NDIR,NDIL,NMDIL,
2            THRSHL,IBOUND,FNOUT,IOUT,POTEN,IOUP,FMATR,IOUM,
3            EVWFN,IOUF,TOT,ITOT,MTOT,MITOT)
```

where the arguments have the following type and meaning:

- POTCAL is the name of the user-supplied subroutine which calculates the potential matrices $\mathbf{V}(\rho)$ and $\mathbf{Q}(\rho)$ and should be written as follows:

```
      SUBROUTINE POTCAL(RHO,VV,QQ,MDIM,IOUT)
C.....................................................................
C.                                                                    .
C.    P R O G R A M                                                   .
C.                  TO CALCULATE THE POTENTIAL MATRIX ELEMENTS        .
C.                  VV AND QQ OF DIMENSION MDIM X MDIM IN POINT       .
C.                  RHO                                               .
C.                                                                    .
C.....................................................................
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION VV(MDIM,MDIM),QQ(MDIM,MDIM)
      RETURN
      END
```

- ASYMEV is the name of the user-supplied subroutine for the bound state problem which calculates the initial value $\lambda^{(0)}(\rho)$ for the homogeneous third boundary condition at $\rho = \rho_{\max}$ and should be written as follows:

```
      SUBROUTINE ASYMEV(RMAX,NDIM,MDIM,SHIFT,DLAMBDA,IOUT)
C.....................................................................
C.                                                                    .
C.    P R O G R A M                                                   .
C.                  TO CALCULATE THE INITIAL VALUE DLAMBDA FOR.       .
C.                  THE HOMOGENEOUS THIRD TYPE BOUNDARY CONDITION     .
C.                  AT RMAX                                           .
C.                                                                    .
C.....................................................................
      IMPLICIT REAL*8 (A-H,O-Z)
      RETURN
      END
```

- ASYMSC is the name of the user-supplied subroutine for the scattering problem which calculates the regular, irregular asymptotic matrix-solutions $\boldsymbol{\Phi}_{\mathrm{reg}}(\rho)$, $\boldsymbol{\Phi}_{\mathrm{irr}}(\rho)$ and their derivatives at $\rho = \rho_{\max}$ and should be written as follows:

```
      SUBROUTINE ASYMSC(RMAX,NDIM,NOPEN,QR,PREG,PIRR,DREG,DIRR,IOUT)
C.....................................................................
C.                                                                    .
C.    P R O G R A M                                                   .
C.                  TO CALCULATE THE REGULAR, IRREGULAR               .
C.                  ASYMPTOTIC MATRIX SOLUTIONS PREG, PIRR            .
C.                  AND THEIR DERIVATIVES DREG, DIRR AT RMAX          .
C.                                                                    .
C.....................................................................
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION  QR(NOPEN),PREG(NDIM,NOPEN),PIRR(NDIM,NOPEN),
     1           DREG(NDIM,NOPEN),DIRR(NDIM,NOPEN)
      RETURN
      END
```

Here in the ASYMEV, DLAMBDA is the initial value $\lambda^{(0)}$ and in the ASYMSC, array QR contains a set of momentum values, and NOPEN is the number of open channels. All parameters except VV, QQ, DLAMBDA, PREG, PIRR, DREG and DIRR in the subroutines POTCAL, ASYMEV and ASYMSC have the same meaning as described below and should not be changed by subroutines POTCAL, ASYMEV and ASYMSC.

4.1. Input data

TITLE	CHARACTER	title of the run to be printed on the output listing. The title should be no longer than 70 characters.
IPTYPE	INTEGER	IPTYPE contains information about type of the problem solved. If IPTYPE = 0 the program calculates the eigenvalue problem; otherwise, it calculates the scattering problem.
NROOT	INTEGER	number of eigenvalues (energy levels) and eigenvectors (radial wave functions) required. NROOT should be equals to 1 in case of IBOUND > 4 and not used for the scattering problem.
MDIM	INTEGER	maximum number of coupled differential equations.
IDIM	INTEGER	dimension of the envelope space.
NPOL	INTEGER	order of finite-element shape functions (interpolating Lagrange polynomials). Usually set to 6.
RTOL	REAL*8	convergence tolerance on eigenvalues (1.D–06 or smaller). This value is not used for the scattering problem.
NITEM	INTEGER	maximum number of iterations permitted (usually set to 16). This value is not used for the scattering problem.
SHIFT	REAL*8	For the eigenvalue problem, SHIFT contains the energy spectrum. If SHIFT = 0 the value of the energy shift is determined automatically by the program; otherwise, the NROOT eigenvalues and eigenvectors closest to the shift given are calculated (the nonzero value of SHIFT is recommended since it significantly speeds up the calculation). For the scattering problem, SHIFT contains the given double energy spectrum.
IPRINT	INTEGER	level of print: = 0—minimal level of print. The initial data, short information about the numerical scheme parameters, main flags and keys, and energy values calculated are printed out; = 1—radial functions calculated are printed out with step IPRSTP additionally; = 2—potential matrix is printed out with step IPRSTP; = 3—information about nodal point distribution is printed out; = 4—global matrices **A** and **B** are printed out additionally; = 5—the highest level of print. The local stiffness and mass matrices together with all current information about the course of the subspace iteration method solution of the generalized eigenvalue problem are printed out.
IPRSTP	INTEGER	step with which potential matrix and radial wave functions are printed out.
NMESH	INTEGER	dimension of array RMESH. NMESH always should be odd and $\geqslant 3$.
RMESH	REAL*8	array RMESH contains information about subdivision of interval $[0, \rho_{\max}]$ of hyperradius ρ on subintervals. The whole interval $[0, \rho_{\max}]$ is divided as follows: RMESH(1) = 0, RMESH(NMESH) = $\rho_{\max}$, and the values of RMESH(I) set the number of elements for each subinterval [RMESH(I − 1), RMESH(I + 1)], where I = 2, 4, . . . , NMESH − 1.
NDIR	INTEGER	dimension of array NDIL. If NDIR > MDIM the message about the error is printed and the execution of the program is stopped.
NDIL	INTEGER	array NDIL containing information about the set of numbers of coupled differential equations and always should be NDIL(NDIR) $\leqslant$ MDIM.
NMDIL	INTEGER	key parameter. If NMDIL = 0 the potential matrix elements of radial coupling are calculated and written to file POTEN; otherwise, they are read from file POTEN.
THRSHL	REAL*8	array THRSHL of dimension MDIM containing values of the thresholds. This array is not used for the eigenvalue problem.
IBOUND	INTEGER	parameter defining the type of boundary conditions set in the boundary points $\rho = 0$ and $\rho = \rho_{\max}$: = 1—the Dirichlet–Dirichlet boundary conditions: $\chi_i(0) = 0, \quad \chi_i(\rho_{\max}) = 0;$ = 2—the Dirichlet–Neumann boundary conditions: $\chi_i(0) = 0, \lim_{\rho \to \rho_{\max}} \chi_i'(\rho) = 0;$ = 3—the Neumann–Dirichlet boundary conditions: $\lim_{\rho \to 0} \rho^n \chi_i'(\rho) = 0, \chi_i(\rho_{\max}) = 0;$ = 4—the Neumann–Neumann boundary conditions: $\lim_{\rho \to 0} \rho^n \chi_i'(\rho) = 0, \lim_{\rho \to \rho_{\max}} \chi_i'(\rho) = 0.$ = 6—the Dirichlet—third type boundary conditions (only for NROOT = 1): at $\rho = 0$ the Dirichlet boundary condition

		(see the case 2) is used and at $\rho_{\max}$ the user-supplied subroutine ASYMEV for the calculation of initial value $\lambda^{(0)}(\rho_{\max})$ or user-supplied subroutine ASYMSC for the calculation of the regular, irregular asymptotic matrix-solutions $\boldsymbol{\Phi}_{\mathrm{reg}}(\rho)$, $\boldsymbol{\Phi}_{\mathrm{irr}}(\rho)$ and their derivatives at $\rho = \rho_{\max}$ are used; = 8—the Neumann—third type boundary conditions (only for NROOT = 1): at $\rho = 0$ the Neumann boundary condition (see the case 4) is used and at $\rho_{\max}$ the same boundary condition is used as in case 6. Here n = IDIM-1. IBOUND should always be equal to 6 or 8 for the scattering problem.
FNOUT	CHARACTER	name of the output file (up to 55 characters) for printing out the results of the calculation. It is system specific and may include a complete path to the file location.
IOUT	INTEGER	number of the output logical device for printing out the results of the calculation (usually set to 7).
POTEN	CHARACTER	name of the input/output file (up to 55 characters) containing potential matrix elements of radial coupling.
IOUP	INTEGER	number of the logical device for reading/storing data from/into file POTEN.
FMATR	CHARACTER	name of the scratch file (up to 55 characters) for storing stiffness matrix.
IOUM	INTEGER	number of the logical device for storing stiffness matrix.
EVWFN	CHARACTER	name of the output file (up to 55 characters) for storing the results of the calculation, namely, the energy values or reaction matrix, finite-element grid points, and radial wave functions. It is used only if IOUF > 0.
IOUF	INTEGER	number of the logical device for storing data into file EVWFN.
TOT	REAL*8	working vector of the DOUBLE PRECISION type.
ITOT	INTEGER	working vector of the INTEGER type.
MTOT	INTEGER	dimension of the DOUBLE PRECISION working array ITOT. The last address ILAST of array TOT is calculated and then compared with the given value of MTOT. If ILAST > MTOT the message about an error is printed and the execution of the program is aborted. In the last case, in order to carry out the required calculation it is necessary to increase the dimension MTOT of array TOT to the quantity ILAST taken from the message.
MITOT	INTEGER	dimension of the INTEGER working array ITOT. The last address ILAST of array ITOT is calculated and then compared with the given value of MITOT. If ILAST > MITOT the message about an error is printed and the execution of the program is aborted. In the last case, in order to carry out the required calculation it is necessary to increase the dimension MITOT of array ITOT to the quantity ILAST taken from the message.

4.2. Output data

The results of the calculation of energy values or reaction matrix and radial wave functions are written using unformatted segmented records into file EVWFN, according to the following operator:

```
      WRITE(IOUF)   NDIM,NN,NROOT,NGRID,(EIGV(I),I=1,NROOT)
     1              ,(XGRID(I),I=1,NGRID),((R(I,J),I=1,NN),J=1,NROOT)
```

or

```
      WRITE(IOUF)   NDIM,NN,NOPEN,NGRID,((RR(I,J),I=1,NOPEN),J=1,NOPEN)
     1              ,(XGRID(I),I=1,NGRID),((R(I,J),I=1,NN),J=1,NOPEN)
```

In the above, parameters presented in the WRITE statement have the following meaning:

- NDIM is the number of radial equations.
- NGRID is the number of finite-element grid points.
- NN = NGRID * NDIM.
- NROOT is the number of roots (energy levels).
- NOPEN is the number of open channels.
- Array EIGV contains the energy values calculated.
- Array RR contains the reaction matrix values calculated.
- Array XGRID contains the values of the finite-element grid points.
- Array R contains NROOT or NOPEN eigenfunctions each per NN elements in length stored in the following way: for each of the NGRID mesh points per NDIM elements of eigenfunction (see scheme below):

```
1-st root             2-nd root          ...   last root

              1                     1                       1
              2                     2                       2
1-st point    .       1-st point    .    ...   1-st point   .
              .                     .                       .
              .                     .                       .
           NDIM                  NDIM                    NDIM

              1                     1                       1
              2                     2                       2
2-nd point    .       2-nd point    .    ...    2-nd point   .
              .                     .                       .
              .                     .                       .
           NDIM                  NDIM                    NDIM
              .                     .                       .
              .                     .                       .
              .                     .                       .
              1                     1                       1
              2                     2                       2
last point    .       last point    .    ...    last point   .
              .                     .                       .
              .                     .                       .
           NDIM                  NDIM                    NDIM
```

5. Description of subprogram units

A flow diagram for the KANTBP program is presented in Fig. 1. The function of each subroutine is briefly described below. Additional details may be found in COMMENT cards within the program.

- Subroutine ADDVEC assembles the element stiffness and mass matrices into the corresponding global vector using a compact storage form.
- Subroutine ASSMBL controls the calculation of element stiffness and mass matrices and assembles them into the corresponding global matrices.
- User-supplied subroutine ASYMEV calculates the initial value $\lambda^{(0)}(\rho_{\max})$ of the bound state problem for the homogeneous third type boundary condition.
- User-supplied subroutine ASYMSC calculates the regular, irregular asymptotic matrix-solutions $\boldsymbol{\Phi}_{\mathrm{reg}}(\rho)$, $\boldsymbol{\Phi}_{\mathrm{irr}}(\rho)$ and their derivatives at $\rho = \rho_{\max}$ of the scattering problem.
- Subroutine BOUNDC sets the Dirichlet or Neumann boundary conditions.
- Subroutine COLMHT calculates column heights in banded matrix.
- Subroutine CHECKD prints error messages when input data are incorrect and stops the execution of program KANTBP.
- Subroutine DECOMP calculates $\mathbf{LDL}^{\mathrm{T}}$ factorization of stiffness matrix. This factorization is used in subroutine REDBAK to reduce and back-substitute the iteration vectors.
- Subroutine EMASSD calculates an element mass matrix.
- Subroutine ERRDIM prints error messages when high-speed storage requested by a user is exceeded and stops the execution of program KANTBP.
- Subroutine ESTIFD calculates a diagonal part of the local on element stiffness matrix.
- Subroutine ESTIFN calculates a nondiagonal part of the local on element stiffness matrix.
- Subroutine EVSOLV prepares all input data for the SSPACE program, prints out the calculated eigensolutions, and writes them into the file EVWFN, if necessary.
- Subroutine FEGRID calculates nodal points for the finite-element grid.
- Subroutine GAULEG [44] calculates nodes and weights of the Gauss–Legendre quadrature.
- Subroutine GAUSSJ [44] calculates linear equation solution by the Gauss–Jordan matrix inversion method.
- Subroutine HQPOT calculates potential matrix elements of radial coupling in the Gaussian nodes of the finite-element mesh.
- Subroutine JACOBI solves the generalized eigenproblem in subspace using the generalized Jacobi iteration.
- Subroutine MAXHT calculates addresses of diagonal elements in banded matrix.
- Subroutine MULT evaluates a product of the two vectors stored in compact form.
- Subroutine NODGEN generates a nodal point distribution for the finite-element grid.
- User-supplied subroutine POTCAL calculates the potential matrices $\mathbf{V}(\rho)$ and $\mathbf{Q}(\rho)$ of dimension MDIM $\times$ MDIM.

- Subroutine SCHECK evaluates shift for Sturm sequence check (called only if SHIFT = 0).
- Subroutine SCSOLV calculates the reaction matrix and radial function, and writes them into the file EVWFN, if necessary.
- Subroutine SHAPEF calculates shape functions of the given order and their derivatives with respect to the master element coordinate η at a specified value of ρ.
- Subroutine SSPACE [41] finds the smallest eigenvalues and the corresponding eigenvectors in the generalized eigenproblem using the subspace iteration method [41]. We have added to this program the possibility of finding the eigensolutions closest to the energy spectrum shift given and also the possibility of using the previously calculated eigenvectors as the starting vectors for inverse iterations. The list of arguments for this program is adequately commented in the routine; so, the interested reader is referred to the program listing for further details. Warning messages will be issued if the requested accuracy RTOL is not obtained after NITEM iterations or if the stiffness matrix **A** is not positively defined.

6. Test deck

The KANTBP program has been used and tested for a variety of physical problems [13,22,32,38,45–47]. Below we present exact solvable three-body benchmark for which the needed analytical expressions for the potential matrix elements and first-derivative coupling terms, their asymptotics and asymptotics of radial solutions of the boundary problems for coupled differential equations have been produced with help of a MAPLE computer algebra system.

We consider three identical particles in the center-of-mass reference frame (CMRF) described by the Jacobi coordinates,

$$\eta = \sqrt{\frac{1}{2}}(x_1 - x_2), \qquad \xi = \sqrt{\frac{2}{3}}\left(\frac{x_1 + x_2}{2} - x_3\right), \tag{64}$$

in the plane $\mathbf{R}^2$, where $\{\{x_1, x_2, x_3\} \in \mathbf{R}^3 \mid x_1 + x_2 + x_3 = 0\}$ are the Cartesian coordinates of the particles on a line. In polar coordinates

$$\eta = \rho\cos\theta, \qquad \xi = \rho\sin\theta, \quad -\frac{\pi}{6} < \theta \leqslant 2\pi - \frac{\pi}{6}, \quad 0 \leqslant \rho < \infty, \tag{65}$$

the Schrödinger equation for the wave function $\Psi(\rho,\theta)$ takes the form

$$-\frac{1}{2}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}\right)\Psi(\rho,\theta) + \mathbf{U}(\rho,\theta)\Psi(\rho,\theta) = E\Psi(\rho,\theta), \tag{66}$$

where E is the relative energy in the CMRF. To obtain an exact solution which can be used below for a comparison with the numerical results, we involve the sum of delta-functions for describing the pair interactions with identical finite strengths. Thus, $\mathbf{U}(\rho,\theta)$ assumes the form

$$\mathbf{U}(\rho,\theta) = g\sum_{l=-1}^{1}\delta\left(\sqrt{2}\rho\left|\cos\left(\theta - \frac{2\pi}{3}l\right)\right|\right), \tag{67}$$

where $g = \sqrt{2}c\bar{\kappa}$, and $\bar{\kappa} = \pi/6$ is the effective strength of the pair potential [31,48–50]. For the attractive case $c < 0$, we have the bound pair state $\phi_0(\eta) = \sqrt{\bar{\kappa}}\exp(-\bar{\kappa}|\eta|)$ with the energy $-\varepsilon_0^{(0)} = c^2\bar{\kappa}^2$, so that $2E = q^2 + \varepsilon_0^{(0)}$, where q is proportional to the relative momentum of the third particle with respect to the bound pair [31,32,49,50].

Using a six-fold symmetric representation compatible with (67), we formulate the following boundary problem corresponding to equation (66) for regular and bounded solution by the radial variable ρ [31]:

$$-\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}\right)\Psi(\rho,\theta) = 2E\Psi(\rho,\theta), \tag{68}$$

with boundary conditions by the angle variable $\theta_n \leqslant \theta < \theta_{n+1}$

$$\begin{aligned}&\frac{1}{\rho}\frac{\partial\Psi(\rho,\theta_i)}{\partial\theta} = (-1)^{i-n}c\bar{\kappa}\Psi(\rho,\theta_i),\\ &\Psi(\rho,\theta_{n+1}-0) = \Psi(\rho,\theta_{n+1}+0), \quad i = n, n+1,\end{aligned} \tag{69}$$

where $\theta_n = \bar{\kappa}(2n-1)$, $n = \overline{0,5}$.

Remark. Problem (66), (67) is exactly solvable model. For the discrete spectrum in attractive case we have exact energies for a ground state and a half-bound state

$$2E^b_{\text{exact}} = -4c^2\bar{\kappa}^2 = -c^2\frac{\pi^2}{9}, \qquad 2E^{hb}_{\text{exact}} = -c^2\bar{\kappa}^2 = -c^2\frac{\pi^2}{36}. \tag{70}$$

For the continuous spectrum in both the attractive and repulsive cases we have exact scattering matrix **S** [30,31] that connected with reaction matrix $\mathbf{K} = \mathbf{K}^{\mathrm{T}}$ by the conventional formulae $\mathbf{K} = \imath(\mathbf{I}+\mathbf{S})^{-1}(\mathbf{I}-\mathbf{S})$ or $\mathbf{S} = (\mathbf{I}+\imath\mathbf{K})(\mathbf{I}-\imath\mathbf{K})^{-1}$.

We consider here a formal expansion of the solution of Eqs. (66), (67) using a set of one-dimensional orthonormal basis functions $B_j(\theta;\rho) \in W_2^1(-\pi/6, 2\pi-\pi/6)$:

$$\Psi(\rho,\theta) = \sum_{j=1}^{N} B_j(\theta;\rho)\chi_j(\rho), \tag{71}$$

where the functions $B_j(\theta;\rho)$ are determined as solutions of the following one-dimensional parametric eigenvalue problem:

$$\begin{aligned}
&-\frac{1}{\rho^2}\frac{\partial^2 B_j(\theta;\rho)}{\partial\theta^2} = \varepsilon_j(\rho)B_j(\theta;\rho),\\
&\frac{1}{\rho}\frac{\partial B_j(\theta_i;\rho)}{\partial\theta} = (-1)^{i-n}c\bar{\kappa}B_j(\theta_i;\rho), \quad i = n, n+1,\\
&B_j(\theta_{n+1}-0;\rho) = B_j(\theta_{n+1}+0;\rho).
\end{aligned} \tag{72}$$

After substituting the expansion (71) into the Rayleigh–Ritz variational functional and minimizing the functional, the solution of Eq. (68) is reduced to a solution of the finite set of N ordinary second-order differential equations (5).

As was shown in paper [48] the boundary problem (72) has the analytical solutions for the attractive case

$$B_1(\theta;\rho) = \sqrt{\frac{y_1^2-x^2}{\pi(y_1^2-x^2)-x}}\cosh\left[6y_1\left(\theta-\frac{n\pi}{3}\right)\right], \qquad \varepsilon_1(\rho) = -\frac{36y_1^2(\rho)}{\rho^2}, \tag{73}$$

$$B_j(\theta;\rho) = \sqrt{\frac{y_j^2+x^2}{\pi(y_j^2+x^2)+x}}\cos\left[6y_j\left(\theta-\frac{n\pi}{3}\right)\right], \qquad \varepsilon_j(\rho) = \frac{36y_j^2(\rho)}{\rho^2}, \quad j\geqslant 2, \tag{74}$$

and for the repulsive case the index j stats from 1 in Eq. (74). The transcendental equations for the attractive case

$$\begin{aligned}
&y_1(\rho)\tanh\bigl(\pi y_1(\rho)\bigr) = -x, \quad 0\leqslant y_1(\rho) < \infty, \quad x = c\frac{\pi}{36}\rho,\\
&y_j(\rho)\tan\bigl(\pi y_j(\rho)\bigr) = x, \quad j-\frac{3}{2} < y_j(\rho) < j-1,
\end{aligned} \tag{75}$$

and for the repulsive case

$$y_j(\rho)\tan\bigl(\pi y_j(\rho)\bigr) = x, \quad x = c\frac{\pi}{36}\rho, \quad j-1 < y_j(\rho) < j-\frac{1}{2}, \tag{76}$$

follow from problems (72). Roots $y_j(\rho)$ of these equations are calculated numerically with a given accuracy for fixed values ρ from the considering interval $\Delta = [0, \rho_{\max}]$. The potential matrices $\mathbf{V}(\rho)$ and $\mathbf{Q}(\rho)$ are defined by formulas (6) and calculated by the analytical expressions using $y_j(\rho)$ and parameter x.

For the attractive case needed matrix elements $H_{ij}(\rho)$ and $Q_{ij}(\rho)$ for $i, j = \overline{1, N}$ read as follows:

$$\begin{aligned}
&H_{11}(\rho) = -\left(\frac{c\pi}{36}\right)^2\frac{1}{\tilde{y}_1^6}\left[\frac{4\pi^2y_1^4-\tilde{y}_1^4}{4\tilde{y}_1^2}+\frac{\pi^2y_1^2}{3}\left(\tilde{y}_1^2+4x\right)\right],\\
&H_{1j}(\rho) = H_{j1}(\rho) = \left(\frac{c\pi}{36}\right)^2\frac{(-1)^{1+j}y_1y_j}{\tilde{y}_1^3\tilde{y}_j^3}\left[2\pi(\pi x^2+x)\left(\frac{1}{\tilde{y}_1^2}-\frac{1}{\tilde{y}_j^2}\right)+\pi+2\pi^2x+\frac{4(y_1^2\tilde{y}_j^2+\tilde{y}_1^2y_j^2)}{(y_1^2+y_j^2)^2}\right],\\
&Q_{1j}(\rho) = -Q_{j1}(\rho) = -\frac{c\pi}{18}\frac{(-1)^{1+j}y_1y_j}{(y_1^2+y_j^2)\tilde{y}_1\tilde{y}_j},\\
&\tilde{y}_1 = \sqrt{\pi(y_1^2-x^2)-x},
\end{aligned} \tag{77}$$

and

$$\begin{aligned}
&H_{jj}(\rho) = -\left(\frac{c\pi}{36}\right)^2\frac{1}{\tilde{y}_j^6}\left[\frac{4\pi^2y_j^4-\tilde{y}_j^4}{4\tilde{y}_j^2}-\frac{\pi^2y_j^2}{3}\left(\tilde{y}_j^2-4x\right)\right],\\
&H_{ij}(\rho) = H_{ji}(\rho) = \left(\frac{c\pi}{36}\right)^2\frac{(-1)^{i+j}y_iy_j}{\tilde{y}_i^3\tilde{y}_j^3}\left[2\pi(\pi x^2+x)\left(\frac{1}{\tilde{y}_i^2}+\frac{1}{\tilde{y}_j^2}\right)-\pi-2\pi^2x+\frac{4(y_i^2\tilde{y}_j^2+\tilde{y}_i^2y_j^2)}{(y_i^2-y_j^2)^2}\right],\\
&Q_{ij}(\rho) = -Q_{ji}(\rho) = -\frac{c\pi}{18}\frac{(-1)^{i+j}y_iy_j}{(y_i^2-y_j^2)\tilde{y}_i\tilde{y}_j},
\end{aligned}$$

$$\tilde{y}_j = \sqrt{\pi(y_j^2 + x^2) + x}, \quad i, j = \overline{2, N}. \tag{78}$$

For the repulsive case one will be used only the formula (78) but with i, j starting from 1, i.e., $i, j = \overline{1, N}$.

Comments: The above matrix potentials are included in the subroutine POTCAL by default. Interaction constant c is accessed via general common block COMMON/IPROB/CCONST.

We consider a reduction of the boundary problem from semi-axis to finite interval using known asymptotic behavior of variable coefficients $H_{ij}(\rho)$, $Q_{ij}(\rho)$ and $\varepsilon_j(\rho)$ and solutions $\chi_j(\rho)$ for a large value of radial variable ρ [31,32]. For the attractive case the first threshold value ϵ_1 is equal to $-c^2\bar{\kappa}^2$, other threshold values are equal to zero and for the repulsive case all threshold values ϵ_j are equal to zero. In the left boundary point we have used Neumann boundary condition (12).

6.1. Bound state problem with the attractive interaction

In case of the attractive interaction, the above problem has the bound state energies and corresponded wave functions $\chi_j(\rho)$ that satisfy the following asymptotics for large ρ [32]

$$\chi_1(\rho) \to \frac{\exp(-\bar{q}\rho)}{\sqrt{\rho}}, \quad \chi_j(\rho) \to C_j \frac{\exp(-\bar{q}\rho)}{\rho^3}. \tag{79}$$

Here $\bar{q}^2 = -2E + \epsilon_1 \geqslant 0$, and C_j is the independent constant in ρ. For the calculation of the ground state energy, we have used the right boundary condition

$$\chi_j(\rho_{\max}) = 0. \tag{80}$$

The following values of numerical parameters and characters have been used in the test run via the supplied input file 3DDGSS.INP

```
&PARAM TITLE='  Ground state energy level of the 2D problem  ',
       IPTYPE=0,NROOT=1,MDIM=6,IDIM=2,NPOL=4,RTOL=1.D-15,
       NITEM=20,SHIFT=-1.1D0,IPRINT=0,IPRSTP=100,
       NMESH=5,RMESH=0.0D0,100.D0,10.D0,150.D0,50.D0,
       NDIR=2, NDIL=1,6, NMDIL=0,
       IBOUND=3,
       FNOUT='3DNGSS.LPR',IOUT=7,POTEN='3DNGSS.PTN',IOUP=10,
       FMATR='3DNGSS.MAT',IOUM=11,EVWFN='3DNGSS.WFN',IOUF=0
&END
```

6.2. Half-bound state problem with the attractive interaction

From formula (79) we obtain the homogeneous third type boundary condition at $\rho = \rho_{\max}$

$$\begin{aligned}
\lim_{\rho\to\rho_{\max}} \frac{d\chi_1(\rho)}{d\rho} &= -\left(\frac{1}{2\rho_{\max}} + \bar{q}\right)\chi_1(\rho_{\max}),\\
\lim_{\rho\to\rho_{\max}} \frac{d\chi_j(\rho)}{d\rho} &= -\left(\frac{3}{\rho_{\max}} + \bar{q}\right)\chi_j(\rho_{\max}).
\end{aligned} \tag{81}$$

In this case we choose initial value $\lambda^{(0)} = -(1/(2\rho_{\max}) + \bar{q})$, which is corrected during calculations. This function is included in the subroutine ASYMEV by default. The following values of numerical parameters and characters have been used in the test run via the supplied input file 3DDHSS.INP

```
&PARAM TITLE='  Half bound state energy level of the 2D problem  '
       IPTYPE=0,NROOT=1,MDIM=6,IDIM=2,NPOL=4,RTOL=1.D-13,
       NITEM=100,SHIFT=-0.2742D0,IPRINT=0,IPRSTP=100,
       NMESH=5,RMESH=0.0D0,100.D0,10.D0,1500.D0,500.D0,
       NDIR=2, NDIL=1,6, NMDIL=0,
       IBOUND=8,
       FNOUT='3DNHBS.LPR',IOUT=7,POTEN='3DNHBS.PTN',IOUP=10,
       FMATR='3DNHBS.MAT',IOUM=11,EVWFN='3DNHBS.WFN',IOUF=0
&END
```

6.3. Scattering problem with the attractive interaction

For scattering problem we have used the following two independent fundamental asymptotic solutions $\chi_{ji}^{(\mathrm{reg})}(\rho)$, $\chi_{ji}^{(\mathrm{irr})}(\rho)$ for large ρ: for $i = 1$

$$\begin{aligned}
\chi_{11}^{(\mathrm{reg})}(\rho) &= \frac{1}{\sqrt{q\rho}}\sin(q\rho),\\
\chi_{11}^{(\mathrm{irr})}(\rho) &= \frac{1}{\sqrt{q\rho}}\cos(q\rho),\\
\chi_{j1}^{(\mathrm{reg})}(\rho) &= +\frac{1}{\sqrt{q}}\cos(q\rho)\frac{c_{j1}^{(3)}}{\rho^3},\\
\chi_{j1}^{(\mathrm{irr})}(\rho) &= -\frac{1}{\sqrt{q}}\sin(q\rho)\frac{c_{j1}^{(3)}}{\rho^3},
\end{aligned} \tag{82}$$

for $i \neq 1$, $j = 1$

$$\begin{aligned}
\chi_{1i}^{(\mathrm{reg})}(\rho) &= +\frac{(-1)^{1+i}}{\sqrt{k}}\cos(k\rho+\delta^{(0)})\frac{c_{1i}^{(3)}}{\rho^3},\\
\chi_{1i}^{(\mathrm{irr})}(\rho) &= -\frac{(-1)^{1+i}}{\sqrt{k}}\sin(k\rho+\delta^{(0)})\frac{c_{1i}^{(3)}}{\rho^3},
\end{aligned} \tag{83}$$

and for $i \neq 1$, $j \neq 1$

$$\begin{aligned}
\chi_{ii}^{(\mathrm{reg})}(\rho) &= \frac{(-1)^{i+1}}{\sqrt{k\rho}}\left(\sin(k\rho+\delta^{(0)})\left(1+\frac{s_{ii}^{(2)}}{\rho^2}\right)+\cos(k\rho+\delta^{(0)})\left(\frac{c_{ii}^{(1)}}{\rho}+\frac{c_{ii}^{(2)}}{\rho^2}\right)\right),\\
\chi_{ii}^{(\mathrm{irr})}(\rho) &= \frac{(-1)^{i+1}}{\sqrt{k\rho}}\left(\cos(k\rho+\delta^{(0)})\left(1+\frac{s_{ii}^{(2)}}{\rho^2}\right)-\sin(k\rho+\delta^{(0)})\left(\frac{c_{ii}^{(1)}}{\rho}+\frac{c_{ii}^{(2)}}{\rho^2}\right)\right),\\
\chi_{ji}^{(\mathrm{reg})}(\rho) &= \frac{(-1)^{i+1}}{\sqrt{k\rho}}\left(\sin(k\rho+\delta^{(0)})\left(\frac{s_{ji}^{(1)}}{\rho}+\frac{s_{ji}^{(2)}}{\rho^2}\right)+\cos(k\rho+\delta^{(0)})\frac{c_{ji}^{(2)}}{\rho^2}\right),\\
\chi_{ji}^{(\mathrm{irr})}(\rho) &= \frac{(-1)^{i+1}}{\sqrt{k\rho}}\left(\cos(k\rho+\delta^{(0)})\left(\frac{s_{ji}^{(1)}}{\rho}+\frac{s_{ji}^{(2)}}{\rho^2}\right)-\sin(k\rho+\delta^{(0)})\frac{c_{ji}^{(2)}}{\rho^2}\right).
\end{aligned} \tag{84}$$

Here $k_1 \equiv q = \sqrt{2E-\epsilon_1}$, $k_j \equiv k = \sqrt{2E}$, $j = \overline{2,N}$ and

$$\begin{aligned}
c_{j1}^{(3)} &= -q\frac{72}{c^2\pi^2}Q_{j1}^{(5/2)}, \qquad c_{1i}^{(3)} = k\frac{72}{c^2\pi^2}Q_{1i}^{(5/2)},\\
s_{ii}^{(2)} &= -\frac{(4\epsilon_i^{(2)}-1)(4\epsilon_i^{(2)}-9)}{128k^2}+\frac{1}{2}\sum_{l=2,l\neq i}^{N}Q_{il}^{(2)}Q_{li}^{(2)}, \quad i\neq 1,\\
c_{ii}^{(1)} &= \frac{4\epsilon_i^{(2)}-1}{8k}, \qquad c_{ii}^{(2)} = \frac{\epsilon_i^{(3)}}{4k},\\
s_{ji}^{(1)} &= -Q_{ji}^{(2)}, \qquad s_{ji}^{(2)} = \frac{1}{2}\left(\sum_{l=2,l\neq j,l\neq i}^{N}Q_{jl}^{(2)}Q_{li}^{(2)}-Q_{ji}^{(3)}\right), \quad j\neq 1,\ i\neq 1,\\
c_{ji}^{(2)} &= -\frac{(2\epsilon_j^{(2)}+2\epsilon_i^{(2)}-1)Q_{ji}^{(2)}}{8k},\\
Q_{j1}^{(5/2)} &= -\frac{216(-1)^{j+1}(2j-3)}{|c|^{3/2}\pi^2}, \qquad Q_{1i}^{(5/2)} = \frac{216(-1)^{1+i}(2i-3)}{|c|^{3/2}\pi^2},\\
Q_{ij}^{(2)} &= \frac{18(-1)^{i+j}(2i-3)(2j-3)}{c\pi^2(i-j)(i+j-3)}, \qquad Q_{ij}^{(3)} = -\frac{36}{c\pi^2}Q_{ij}^{(2)},\\
\epsilon_i^{(2)} &= (6i-9)^2, \qquad \epsilon_i^{(3)} = -\frac{72}{c\pi^2}\epsilon_i^{(2)}.
\end{aligned} \tag{85}$$

In order to compare with results [31], $\delta^{(0)} = \pi/4$, and $2E = 0.085844322191962$ ($q = 0.6$) have been chosen. The above matrix-solutions are included in the subroutine ASYMSC by default for $c < 0$. The following values of numerical parameters and characters have been used in the test run via the supplied input file 3DDSCM.INP

```
&PARAS TITLE='  Reaction matrix of the 2D problem - I  ',
       IPTYPE=1,MDIM=6,IDIM=2,NPOL=4,
       SHIFT=0.858443221919622D-1,IPRINT=0,IPRSTP=150,
       NMESH=5,RMESH=0.0D0,2000.D0,100.D0,4000.D0,2000.D0,
       NDIR=2, NDIL=1,6, NMDIL=0,
       THRSHL=-0.274155677808037D0,0.D0,0.D0,0.D0,0.D0,0.D0,
       IBOUND=8,
       FNOUT='3DNSCM.LPR',IOUT=7,POTEN='3DNSCM.PTN',IOUP=10,
       FMATR='3DNSCM.MAT',IOUM=11,EVWFN='3DNSCM.WFN',IOUF=0
&END
```

6.4. Scattering problem with the repulsive interaction

In case of the repulsive interaction, we have used asymptotic solutions (84) with

$$
\begin{aligned}
&s_{ii}^{(2)} = -\frac{(4\epsilon_i^{(2)} - 1)(4\epsilon_i^{(2)} - 9)}{128k^2} + \frac{1}{2}\sum_{l\neq i, l=1}^{N} Q_{il}^{(2)} Q_{li}^{(2)},\\
&c_{ii}^{(1)} = \frac{4\epsilon_i^{(2)} - 1}{8k}, \qquad c_{ii}^{(2)} = \frac{\epsilon_i^{(3)}}{4k},\\
&s_{ji}^{(1)} = -Q_{ji}^{(2)}, \qquad s_{ji}^{(2)} = \frac{1}{2}\left(\sum_{l=1, l\neq j, l\neq i}^{N} Q_{jl}^{(2)} Q_{li}^{(2)} - Q_{ji}^{(3)}\right),\\
&c_{ji}^{(2)} = -\frac{(2\epsilon_j^{(2)} + 2\epsilon_i^{(2)} - 1) Q_{ji}^{(2)}}{8k},\\
&Q_{ij}^{(2)} = \frac{18(-1)^{i+j}(2i-1)(2j-1)}{c\pi^2(i-j)(i+j-1)}, \qquad Q_{ij}^{(3)} = -\frac{36}{c\pi^2} Q_{ij}^{(2)},\\
&\epsilon_i^{(2)} = (6i-3)^2, \qquad \epsilon_i^{(3)} = -\frac{72}{c\pi^2}\epsilon_i^{(2)},
\end{aligned}
\tag{86}
$$

and indexes i, j start from 1. In order to compare with results [31], $\delta^{(0)} = \pi/4$, and $2E = 0.01$ ($k = 0.1$) have been chosen. The matrix-solutions (84), (86) are included in the subroutine ASYMSC by default for $c > 0$. The following values of numerical parameters and characters have been used in the test run via the supplied input file 3DDSCP.INP

```
&PARAS TITLE='  Reaction matrix of the 2D problem - II  ',
       IPTYPE=1,MDIM=6,IDIM=2,NPOL=4,
       SHIFT= 0.01D0,IPRINT=0,IPRSTP=150,
       NMESH=7,RMESH=0.0D0,2000.D0,100.D0,4000.D0,2000.D0,
       2000.D0,11000.D0,
       NDIR=2, NDIL=1,6, NMDIL=0,
       THRSHL= 0.D0,0.D0,0.D0,0.D0,0.D0,0.D0,
       IBOUND=8,
       FNOUT='3DNSCP.LPR',IOUT=7,POTEN='3DNSCP.PTN',IOUP=10,
       FMATR='3DNSCP.MAT',IOUM=11,EVWFN='3DNSCP.WFN',IOUF=0
&END
```

These four tests run approximately for 1.01 s, 11.01 s, 7.06 s and 9.39 s without calculation of matrix potentials on the Intel Pentium IV 2.4 GHz, respectively. Total run time is 28.48 s.

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Appendix A. Test run output

```
 PROBLEM:   Ground state energy level of the 2D problem
 ********

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

     NUMBER OF DIFFERENTIAL EQUATIONS...... (MDIM  ) =      6
     NUMBER OF ENERGY LEVELS REQUIRED...... (NROOT ) =      1
     NUMBER OF FINITE ELEMENTS............. (NELEM ) =    250
     NUMBER OF GRID POINTS................. (NGRID ) =   1001
     ORDER  OF SHAPE FUNCTIONS............. (NPOL  ) =      4
     ORDER  OF GAUSS-LEGENDRE QUADRATURE... (NGQ   ) =      5
     NUMBER OF SUBSPACE ITERATION VECTORS.. (NC    ) =      2
     DIMENSION OF ENVELOPE SPACE........... (IDIM  ) =      2
     BOUNDARY CONDITION CODE............... (IBOUND) =      3
     SHIFT OF DOUBLE ENERGY SPECTRUM....... (SHIFT ) =   -1.10000
     CONVERGENCE TOLERANCE................. (RTOL  ) =   0.100000E-14


    SUBDIVISION OF RHO-REGION ON THE FINITE-ELEMENT GROUPS:
    ******************************************************

   NO OF  NUMBER OF  BEGIN OF  LENGTH OF    GRID     END OF
   GROUP  ELEMENTS   INTERVAL   ELEMENT     STEP    INTERVAL
   -----  ---------  --------  ---------  --------  --------
     1       100        0.000   0.10000   0.02500     10.000
     2       150       10.000   0.26667   0.06667     50.000


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

     TOTAL NUMBER OF ALGEBRAIC EQUATIONS.... (NN ) =     1000
     TOTAL NUMBER OF MATRIX ELEMENTS........ (NWK) =     3496
     MAXIMUM HALF BANDWIDTH................. (MK ) =        5
     MEAN    HALF BANDWIDTH................. (MMK) =        3


     NDIM, MDIM=         1         6

 THERE ARE    0 ROOTS LOWER THEN SHIFT
 CONVERGENCE REACHED FOR RTOL 0.1000E-14
 I T E R A T I O N   N U M B E R    6
 RELATIVE TOLERANCE REACHED ON EIGENVALUES
  0.3955E-18

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

    R O O T   N U M B E R     E I G E N V A L U E
   ----------------------   --------------------
             1               -0.5482213063633842

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


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

     TOTAL NUMBER OF ALGEBRAIC EQUATIONS.... (NN ) =     6000
     TOTAL NUMBER OF MATRIX ELEMENTS........ (NWK) =   110856
```

```
     MAXIMUM HALF BANDWIDTH..................... (MK ) =       30
     MEAN    HALF BANDWIDTH..................... (MMK) =       18


     NDIM, MDIM=         6         6

 THERE ARE    0 ROOTS LOWER THEN SHIFT
 CONVERGENCE REACHED FOR RTOL 0.1000E-14
 I T E R A T I O N   N U M B E R    6
 RELATIVE TOLERANCE REACHED ON EIGENVALUES
  0.2729E-16

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

    R O O T   N U M B E R     E I G E N V A L U E
   ----------------------   --------------------
             1                -0.5483113526413836

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



 PROBLEM:   Half bound state energy level of the 2D problem
 ********


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

     NUMBER OF DIFFERENTIAL EQUATIONS...... (MDIM  ) =      6
     NUMBER OF ENERGY LEVELS REQUIRED...... (NROOT ) =      1
     NUMBER OF FINITE ELEMENTS............. (NELEM ) =   1600
     NUMBER OF GRID POINTS................. (NGRID ) =   6401
     ORDER  OF SHAPE FUNCTIONS............. (NPOL  ) =      4
     ORDER  OF GAUSS-LEGENDRE QUADRATURE... (NGQ   ) =      5
     NUMBER OF SUBSPACE ITERATION VECTORS.. (NC    ) =      2
     DIMENSION OF ENVELOPE SPACE........... (IDIM  ) =      2
     BOUNDARY CONDITION CODE............... (IBOUND) =      8
     SHIFT OF DOUBLE ENERGY SPECTRUM....... (SHIFT ) =  -0.274200
     CONVERGENCE TOLERANCE................. (RTOL  ) =   0.100000E-12


    SUBDIVISION OF RHO-REGION ON THE FINITE-ELEMENT GROUPS:
    ******************************************************

   NO OF  NUMBER OF  BEGIN OF  LENGTH OF    GRID     END OF
   GROUP  ELEMENTS   INTERVAL   ELEMENT     STEP    INTERVAL
   -----  ---------  --------  ---------  --------  --------
     1       100        0.000   0.10000   0.02500     10.000
     2      1500       10.000   0.32667   0.08167    500.000


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

     TOTAL NUMBER OF ALGEBRAIC EQUATIONS.... (NN ) =     6401
     TOTAL NUMBER OF MATRIX ELEMENTS........ (NWK) =    22401
     MAXIMUM HALF BANDWIDTH................. (MK ) =        5
     MEAN    HALF BANDWIDTH................. (MMK) =        3


     NDIM, MDIM=         1         6
```

```
 THERE ARE    1 ROOTS LOWER THEN SHIFT
 CONVERGENCE REACHED FOR RTOL 0.1000E-12
 I T E R A T I O N   N U M B E R    9
 RELATIVE TOLERANCE REACHED ON EIGENVALUES
  0.6835E-14
 I T E R A T I O N   N U M B E R   22
 RELATIVE TOLERANCE REACHED ON LAMBDA
  0.4462E-13

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

    R O O T   N U M B E R     E I G E N V A L U E          L A M B D A
   ----------------------   ---------------------      ----------------
             1               -0.1370771705679387      -0.6232569850201794E-03

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


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

     TOTAL NUMBER OF ALGEBRAIC EQUATIONS.... (NN ) =    38406
     TOTAL NUMBER OF MATRIX ELEMENTS........ (NWK) =   710421
     MAXIMUM HALF BANDWIDTH................. (MK ) =       30
     MEAN    HALF BANDWIDTH................. (MMK) =       18


     NDIM, MDIM=         6         6

 THERE ARE    1 ROOTS LOWER THEN SHIFT
 CONVERGENCE REACHED FOR RTOL 0.1000E-12
 I T E R A T I O N   N U M B E R    9
 RELATIVE TOLERANCE REACHED ON EIGENVALUES
  0.1629E-13
 I T E R A T I O N   N U M B E R   15
 RELATIVE TOLERANCE REACHED ON LAMBDA
  0.7793E-13

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

    R O O T   N U M B E R     E I G E N V A L U E          L A M B D A
   ----------------------   ---------------------      ----------------
             1               -0.1370777081621216      -0.1131640030879691E-02

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


 PROBLEM:   Reaction matrix of the 2D problem - I
 ********


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

     NUMBER OF DIFFERENTIAL EQUATIONS..... (MDIM  ) =      6
     NUMBER OF FINITE ELEMENTS............ (NELEM ) =   6000
     NUMBER OF GRID POINTS................ (NGRID ) =  24001
     ORDER OF SHAPE FUNCTIONS............. (NPOL  ) =      4
     ORDER OF GAUSS-LEGENDRE QUADRATURE... (NGQ   ) =      5
     DIMENSION OF ENVELOPE SPACE.......... (IDIM  ) =      2
```

```
     BOUNDARY CONDITION CODE.............. (IBOUND) =      8
     DOUBLE ENERGY SPECTRUM............... (SHIFT ) =   0.858443E-01


    SUBDIVISION OF RHO-REGION ON THE FINITE-ELEMENT GROUPS:
    ******************************************************

   NO OF  NUMBER OF  BEGIN OF  LENGTH OF    GRID     END OF
   GROUP  ELEMENTS   INTERVAL   ELEMENT     STEP    INTERVAL
   -----  ---------  --------  ---------  --------  --------
     1      2000        0.000   0.05000   0.01250    100.000
     2      4000      100.000   0.47500   0.11875   2000.000


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

     TOTAL NUMBER OF ALGEBRAIC EQUATIONS.... (NN ) =    24001
     TOTAL NUMBER OF MATRIX ELEMENTS........ (NWK) =    84001
     MAXIMUM HALF BANDWIDTH................. (MK ) =        5
     MEAN    HALF BANDWIDTH................. (MMK) =        3


     NDIM, MDIM=         1         6

     NUMBER OF OPEN CHANNELS......... (NOPEN) =      1
     VALUE OF I-TH MOMENTUM.......... (I,QR ) =      1  0.6000E+00

           C H E C K  W R O N S K I A N
          ------------------------------
   1.00000

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

           R E A C T I O N   M A T R I X
          -------------------------------
  -.224884

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


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

     TOTAL NUMBER OF ALGEBRAIC EQUATIONS.... (NN ) =   144006
     TOTAL NUMBER OF MATRIX ELEMENTS........ (NWK) =  2664021
     MAXIMUM HALF BANDWIDTH................. (MK ) =       30
     MEAN    HALF BANDWIDTH................. (MMK) =       18


     NDIM, MDIM=         6         6

     NUMBER OF OPEN CHANNELS......... (NOPEN) =      6
     VALUE OF I-TH MOMENTUM.......... (I,QR ) =      1  0.6000E+00
     VALUE OF I-TH MOMENTUM.......... (I,QR ) =      2  0.2930E+00
     VALUE OF I-TH MOMENTUM.......... (I,QR ) =      3  0.2930E+00
     VALUE OF I-TH MOMENTUM.......... (I,QR ) =      4  0.2930E+00
     VALUE OF I-TH MOMENTUM.......... (I,QR ) =      5  0.2930E+00
     VALUE OF I-TH MOMENTUM.......... (I,QR ) =      6  0.2930E+00

           C H E C K  W R O N S K I A N
          ------------------------------
```

```
   1.00000     -.497999E-09 -.320749E-07 -.160361E-06 -.466201E-06 -.105346E-05
  0.202460E-08  1.00000     0.722264E-07 0.141761E-06 -.134774E-07 -.153784E-05
  -.512979E-07 0.843397E-07  1.00002     0.907839E-06 0.516355E-07 -.528737E-05
  -.289234E-06 0.190461E-06 0.121896E-05  1.00046     0.399782E-05 -.107733E-04
  -.876239E-06 0.116431E-06 0.602785E-06 0.616311E-05  1.00545     -.838095E-06
  -.203693E-05 -.125993E-05 -.427531E-05 -.816296E-05 0.764553E-05  1.03840

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

          R E A C T I O N   M A T R I X
         -------------------------------
  -.126136     0.500076E-07 0.947352E-08 0.623779E-07 0.254430E-06 0.646967E-06
  0.488556E-07 0.594057     0.329502E-01 0.643311E-02 0.227628E-02 0.102439E-02
  -.731879E-09 0.329500E-01 0.633301     0.416376E-01 0.972776E-02 0.378363E-02
  0.126927E-09 0.643288E-02 0.416358E-01 0.634932     0.430101E-01 0.103123E-01
  0.647861E-08 0.227596E-02 0.972623E-02 0.429971E-01 0.625075     0.422897E-01
  0.163590E-07 0.102391E-02 0.378175E-02 0.103055E-01 0.422177E-01 0.583695

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


 PROBLEM:   Reaction matrix of the 2D problem - II
 ********


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

    NUMBER OF DIFFERENTIAL EQUATIONS..... (MDIM  ) =      6
    NUMBER OF FINITE ELEMENTS............ (NELEM ) =   8000
    NUMBER OF GRID POINTS................ (NGRID ) =  32001
    ORDER OF SHAPE FUNCTIONS............. (NPOL  ) =      4
    ORDER OF GAUSS-LEGENDRE QUADRATURE... (NGQ   ) =      5
    DIMENSION OF ENVELOPE SPACE.......... (IDIM  ) =      2
    BOUNDARY CONDITION CODE.............. (IBOUND) =      8
    DOUBLE ENERGY SPECTRUM............... (SHIFT ) =   0.100000E-01


   SUBDIVISION OF RHO-REGION ON THE FINITE-ELEMENT GROUPS:
   ******************************************************

  NO OF  NUMBER OF  BEGIN OF  LENGTH OF    GRID     END OF
  GROUP  ELEMENTS   INTERVAL   ELEMENT     STEP    INTERVAL
  -----  ---------  --------  ---------  --------  --------
    1      2000        0.000   0.05000   0.01250    100.000
    2      4000      100.000   0.47500   0.11875   2000.000
    3      2000     2000.000   4.50000   1.12500  11000.000


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

    TOTAL NUMBER OF ALGEBRAIC EQUATIONS.... (NN ) =    32001
    TOTAL NUMBER OF MATRIX ELEMENTS........ (NWK) =   112001
    MAXIMUM HALF BANDWIDTH................. (MK ) =        5
    MEAN    HALF BANDWIDTH................. (MMK) =        3


    NDIM, MDIM=         1         6

    NUMBER OF OPEN CHANNELS......... (NOPEN) =      1
```

```
     VALUE OF I-TH MOMENTUM......... (I,QR ) =      1  0.1000E+00

           C H E C K  W R O N S K I A N
          ------------------------------
   1.00000

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

           R E A C T I O N   M A T R I X
          -------------------------------
  -2.56560

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


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

     TOTAL NUMBER OF ALGEBRAIC EQUATIONS.... (NN ) =   192006
     TOTAL NUMBER OF MATRIX ELEMENTS........ (NWK) =  3552021
     MAXIMUM HALF BANDWIDTH................. (MK ) =       30
     MEAN    HALF BANDWIDTH................. (MMK) =       18


     NDIM, MDIM=         6         6

     NUMBER OF OPEN CHANNELS........ (NOPEN) =      6
     VALUE OF I-TH MOMENTUM......... (I,QR ) =      1  0.1000E+00
     VALUE OF I-TH MOMENTUM......... (I,QR ) =      2  0.1000E+00
     VALUE OF I-TH MOMENTUM......... (I,QR ) =      3  0.1000E+00
     VALUE OF I-TH MOMENTUM......... (I,QR ) =      4  0.1000E+00
     VALUE OF I-TH MOMENTUM......... (I,QR ) =      5  0.1000E+00
     VALUE OF I-TH MOMENTUM......... (I,QR ) =      6  0.1000E+00

           C H E C K  W R O N S K I A N
          ------------------------------
   1.00000     0.567061E-08 0.102062E-07 0.138098E-07 0.108079E-07 -.191238E-07
  0.586799E-08  1.00000     0.349612E-07 0.436920E-07 0.312694E-07 -.679934E-07
  0.110412E-07 0.401423E-07  1.00002     0.113035E-06 0.551983E-07 -.152542E-06
  0.160442E-07 0.529045E-07 0.147761E-06  1.00037     0.277508E-06 -.279382E-06
  0.154999E-07 0.479263E-07 0.963258E-07 0.404796E-06  1.00291     0.206195E-06
  -.106373E-07 -.399516E-07 -.946524E-07 -.160079E-06 0.524729E-06  1.01472

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

           R E A C T I O N   M A T R I X
          -------------------------------
  -2.56205     -.615521E-01 -.127812E-01 -.462205E-02 -.218770E-02 -.121841E-02
  -.615521E-01 -2.63648     -.789722E-01 -.196070E-01 -.805618E-02 -.418943E-02
  -.127812E-01 -.789723E-01 -2.64465     -.825942E-01 -.217596E-01 -.945895E-02
  -.462208E-02 -.196071E-01 -.825940E-01 -2.65580     -.850115E-01 -.231961E-01
  -.218774E-02 -.805632E-02 -.217598E-01 -.850074E-01 -2.69374     -.891220E-01
  -.121843E-02 -.418952E-02 -.945904E-02 -.231949E-01 -.890963E-01 -2.80482

*******************************************************************************
```

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