Symbolic-Numerical Algorithms to Solve the Quantum Tunneling Problem for a Coupled Pair of Ions

A.A. Gusev, S.I. Vinitsky, O. Chuluunbaatar, V.P. Gerdt, and V.A. Rostovtsev

Joint Institute for Nuclear Research, Dubna, Russia
{gooseff,chuka,gerdt,rost}@jinr.ru, vinitsky@theor.jinr.ru

Abstract. Symbolic-numerical algorithms for solving a boundary value problem (BVP) for the 2D Schrödinger equation with homogeneous third type boundary conditions to study the quantum tunneling model of a coupled pair of nonidentical ions are described. The Kantorovich reduction of the above problem with non-symmetric long-range potentials to the BVPs for sets of the second order ordinary differential equations (ODEs) is given by expanding solution over the one-parametric set of basis functions. Symbolic algorithms for evaluation of asymptotics of the basis functions, effective potentials, and linear independent solutions of the ODEs in the form of inverse power series of independent variable at large values are given by using appropriate etalon equations. Benchmark calculation of quantum tunneling problem of coupled pair of identical ions through Coulomb-like barrier is presented.

1 Introduction

Quantum mechanical treatment on the basis of adiabatic description of penetration through a two-dimensional fission barrier has been studied for a long period of time [1,2]. Current interest is stimulated by the prominent papers in which the model of quantum tunneling problem of coupled pair of ions through truncated Coulomb barrier were investigated for identical mass and charges of ions [3,4]. Study of quantum tunneling problem for a coupled pair of ions with distinct mass and charges for their penetration through a nontruncated Coulomb barrier is an important problem.

The aim of this paper is to develop a symbolic-numerical algorithm (SNA) for solving the 2D boundary value problem (BVP) with homogeneous third type boundary conditions to analyze the above problem. In the framework of Kantorovich method (KM) [5], we search for a solution by means of expansion over the solution to the one-parametric eigenvalue problem calculated by program ODPEVP [6]. This way the BVP is reduced to a set of second order differential equations (ODEs) on the whole axis with homogeneous third type boundary conditions of general type. The main task here is to formulate these boundary conditions which are not invariant under reflection with respect to the x-axis.

V.P. Gerdt et al. (Eds.): CASC 2011, LNCS 6885, pp. 175–191, 2011.

This is because the conventionally used symmetric conditions are applicable only for identical particles. To apply the finite element method (FEM) to solving the BVP on a finite interval we need not only the adaptation of KANTBP 2.0 code [7], but also the elaboration of new symbolic algorithms to evaluate coefficients of the asymptotic expansion of both effective potential and solution to ODEs. These coefficients are needed to match evaluated asymptotic solutions with numerical ones at boundary points and extract the required matrix of transmission and the reflections amplitudes from numerical solutions.

In this paper, we present algorithms for calculation of the asymptotic expansions for solution to the eigenvalue problem with a long-range potential of general type. These asymptotic expansions are applied to evaluate the effective potentials of ODEs. The next step is to design a new algorithm for evaluation of the asymptotic expansion of linear independent solutions to ODEs. This distingue algorithm is substantially different from the previously elaborated one [8]. Instead of applying an expansion over the solution to an etalon equation, we propose to use an appropriate etalon equation with a long-range potential in the form of the inverse power series that provides a more economical and universal way to generate relevant recurrence relations and the corresponding FORTRAN subroutines.

The paper is organized as follows. In Section 2, the problem statement is done. In Section 3, the BVP is formulated for ODEs. Here the symbolic algorithms for the evaluation of asymptotic expansions of solutions to parametric BVP, for calculation of the corresponding integrals, and for the asymptotic expansion of linear independent solutions to ODEs together with their implementation in Maple are described. Section 4 is devoted to the benchmark calculation of the penetration coefficients for tunneling of the identical ions through long-range Coulomb like barriers. In Conclusion, we summarize the results and discuss the future applications of our SNAs.

2 Problem Statement

Wave function $\Psi(x,y)$ of model of heavy ion pair connected with oscillator potential scattering in the center mass coordinate system through Coulomb barriers satisfies the two-dimensional (2D) Schrödinger equation [3]:

$$\left\{-\frac{\partial^2}{\partial y^2}-\frac{\partial^2}{\partial x^2}+x^2+2(U_1(x_1)+U_2(x_2)-E)\right\}\Psi(x,y)=0, \tag{1}$$

where $x_1 = s_2 y + s_1 x$, $x_2 = s_2 y - s_3 x$ are variables in the laboratory coordinate system, parameters $s_2 = \frac{\sqrt{m_1 m_2}}{M}$, $s_1 = \frac{m_2}{M}$, $s_3 = \frac{m_1}{M}$ are defined via masses of ions m_1 and m_2 and total mass $M = m_1 + m_2$ and reduced mass $\mu = \frac{m_1 m_2}{M}$ in the oscillator units of length $x_{osc} = \sqrt{\frac{\hbar}{\mu\omega}}$ and energy $E_{osc} = \hbar\omega$ (ω is oscillator frequency). We choose barrier potential $U_i(x_i)$ of ions labelled by $i = 1, 2$ with charges $\hat{Z}_i > 0$ in the form of the truncated Coulomb potential cut off on small $0 < \bar{x}_{\min} < 1$ and large $\bar{x}_{\max} > 1$ distances from origin,

$$U_i\left(x_i\right)=\left\{\frac{\hat{Z}_i}{\bar{x}_{\min}}-\frac{\hat{Z}_i}{\bar{x}_{\max}},|x_i|\leq\bar{x}_{\min};\frac{\hat{Z}_i}{|x_i|}-\frac{\hat{Z}_i}{\bar{x}_{\max}},\begin{matrix}|x_i|>\bar{x}_{\min}\\|x_i|\leq\bar{x}_{\max}\end{matrix};0,|x_i|>\bar{x}_{\max}\right\}, \quad (2)$$

or the Coulomb-like potentials that depend on the integer parameter $s \geq 2$ and truncation parameter $\bar{x}_{\min} > 0$ and defined as

$$U_i\left(x_i\right) = \hat{Z}_i(|x_i|^s + \bar{x}^s_{\min})^{-1/s}\,. \quad (3)$$

In both cases, the sum of barrier potential functions $U(x,y) = U_1\left(x_1\right) + U_2\left(x_2\right)$ has asymptotic form

$$U(x,y) \to \sigma_y\frac{Z_{12}}{y} + O(y^{-3}), \quad y \to \pm\infty, \quad (4)$$

where $\sigma_y = 1$ if $y > 0$ and $\sigma_y = -1$ if $y < 0$; $Z_{12} = 0$ for Eq. (2) and $Z_{12} = (\hat{Z}_1 + \hat{Z}_2)/s_2$ for Eq. (3).

The asymptotic boundary conditions for the solution $\Psi(y,x)=\{\Psi_{i_o}(y,x)\}_{i_o=1}^{N_o}$ with direction $v =\to$ can be written in the obvious form

$$\begin{aligned}\Psi_{i_o}(y\to-\infty,x) &\to B^{(0)}_{i_o}(x)\frac{\exp\left(\imath\left(p_{i_o}y-\sigma_y\frac{Z_{12}}{p_{i_o}}\ln(2p_{i_o}|y|)\right)\right)}{\sqrt{p_{i_o}}}\\&\quad+\sum_{j=1}^{N_o}B^{(0)}_j(x)\frac{\exp\left(-\imath\left(p_jy-\sigma_y\frac{Z_{12}}{p_j}\ln(2p_j|y|)\right)\right)}{\sqrt{p_j}}R_{ji_o},\\\Psi_{i_o}(y\to+\infty,x) &\to \sum_{j=1}^{N_o}B^{(0)}_j(x)\frac{\exp\left(\imath\left(p_jy-\sigma_y\frac{Z_{12}}{p_j}\ln(2p_j|y|)\right)\right)}{\sqrt{p_j}}T_{ji_o}, \quad (5)\\\Psi_{i_o}(y,x\to\pm\infty) &\to 0.\end{aligned}$$

Here N_o is the number of open channels at fixed energy $2E = p^2 + \varepsilon^{(0)}_{i_o} > 0$, T_{ji_o} and R_{ji_o} are unknown transition and reflections amplitudes, $B^{(0)}_j(x)$ are the basis functions of oscillator with energy $\varepsilon^{(0)}_j = 2n+1$ at $n \geq 0$, $j = n+1$

$$\left\{-\frac{\partial^2}{\partial x^2}+x^2-\varepsilon^{(0)}_j\right\}B^{(0)}_j(x)=0, \quad \int_{-\infty}^{+\infty}B^{(0)}_j(x)B^{(0)}_{j'}(x)dx=\delta_{jj'}. \quad (6)$$

3 Formulation of BVP for a Set of the Kantorovich ODEs

We construct a desired solution of the BVP in the form of Kantorovich's expansion:

$$\Psi_{i'}(x,y) = \sum_{j=1}^{N}B_j(x;y)\chi_{ji'}(y). \quad (7)$$

The basis functions $B_j(x;y)$ of the fast variable x and the potential curves $E_i(y)$ that depend continuously on the slow variable y as a parameter are chosen as solutions of the BVPs for the equation on grid $\Omega_x\{x_{\min}(y), x_{\max}(y)\}$

$$\left\{-\frac{d^2}{dx^2} + x^2 + 2U(x,y) - \varepsilon_j(y)\right\} B_j(x;y) = 0, \tag{8}$$

which are subject to the boundary, normalization, and orthogonality conditions

$$B_j(x_{\min}(y);y) = B_j(x_{\max}(y);y) = 0,\ \langle B_i|B_j\rangle = \int_{x_{\min}(y)}^{x_{\max}(y)} B_i(x;y)B_j(x;y)dx = \delta_{ij}. \tag{9}$$

By substituting (7) into (1)–(5) and by taking average over (9), we obtain the BVP for a set of N coupled ODEs that describes the slow subsystem for the partial solutions $\boldsymbol{\chi}^{(i')}(y) = (\chi_1^{(i')}, ..., \chi_N^{(i')})^T$:

$$\{\mathbf{H} - 2E\,\mathbf{I}\}\ \boldsymbol{\chi}^{(i')}(y) = 0, \quad \mathbf{H} = -\mathbf{I}\frac{d^2}{dy^2} + \mathbf{V}(y) + \mathbf{Q}(y)\frac{d}{dy} + \frac{d\mathbf{Q}(y)}{dy}. \tag{10}$$

Here $\mathbf{I}$ is the unit matrix, $\mathbf{V}(y)$ and $\mathbf{Q}(y)$ are the effective potential $N \times N$ matrices:

$$V_{ij}(y) = \varepsilon_j(y)\delta_{ij} + H_{ij}(y), \quad H_{ij}(y) = \int_{x_{\min}(y)}^{x_{\max}(y)} \frac{\partial B_i(x;y)}{\partial y}\frac{\partial B_j(x;y)}{\partial y}dx, \tag{11}$$

$$Q_{ij}(y) = -\int_{x_{\min}(y)}^{x_{\max}(y)} B_i(x;y)\frac{\partial B_j(x;y)}{\partial y}dx.$$

that is calculated numerically by means of program ODPEVP [6]. The boundary conditions at $y = y_{\min} \ll -1$ and $y = y_{\max} \gg 1$ are given by

$$\left.\frac{d\boldsymbol{\Phi}(y)}{dy}\right|_{y=y_{\min}} = \mathcal{R}(y_{\min})\boldsymbol{\Phi}(y_{\min}), \quad \left.\frac{d\boldsymbol{\Phi}(y)}{dy}\right|_{y=y_{\max}} = \mathcal{R}(y_{\max})\boldsymbol{\Phi}(y_{\max}), \tag{12}$$

where $\mathcal{R}(y)$ is an unknown $N \times N$ nonsymmetric matrix-function, $\boldsymbol{\Phi}(y) = \{\boldsymbol{\chi}^{(i_o)}(y)\}_{i_o=1}^{N_o}$ is the required $N \times N_o$ matrix solution, and N_o is the number of open channels, $N_o = \max_{2E\geq\varepsilon_j} j \leq N$ that is calculated numerically by means of the program KANTBP 3.0. It is a modified version of the program KANTBP 2.0 [7] including matching asymptotic solutions evaluated in the next sections with numerical ones at boundary points $y = y_{\min} \ll -1$ and $y = y_{\max} \gg 1$ in (12).

The matrix solution $\boldsymbol{\Phi}_v(y) = \boldsymbol{\Phi}(y)$ that describes the incidence of the particle and its scattering, having the asymptotic form "incident wave + outgoing waves", is

$$\boldsymbol{\Phi}_v(y \to \pm\infty) = \left\{ \begin{array}{ll} \left\{ \begin{array}{ll} \mathbf{X}^{(+)}(y)\mathbf{T}_v, & y > 0, \\ \mathbf{X}^{(+)}(y) + \mathbf{X}^{(-)}(y)\mathbf{R}_v, & y < 0, \end{array} \right. & v = \rightarrow, \\ \left\{ \begin{array}{ll} \mathbf{X}^{(-)}(y) + \mathbf{X}^{(+)}(y)\mathbf{R}_v, & y > 0, \\ \mathbf{X}^{(-)}(y)\mathbf{T}_v, & y < 0, \end{array} \right. & v = \leftarrow, \end{array} \right. \tag{13}$$

with $\mathbf{R}_v$ and $\mathbf{T}_v$ being the reflection and transmission $N_o \times N_o$ matrices, v denotes the initial direction of the particle motion along the y-axis. Here the leading term of the asymptotic rectangle-matrix functions $\mathbf{X}^{(\pm)}(y)$ has the form

$$X^{(\pm)}_{ji_o}(y) \to p_j^{-1/2} \exp\left(\pm\imath\left(p_j y - \sigma_y \frac{Z_{12}}{p_j}\ln(2p_j|y|)\right)\right)\delta_{ji_o}, \tag{14}$$
$$p_{i_o} = \sqrt{2E - \varepsilon_{i_o}}, \quad j = 1,\ldots,N, \quad i_o = 1,\ldots,N_o.$$

The matrix solution $\boldsymbol{\Phi}_v(y,E)$ is normalized so that

$$\int_{-\infty}^{\infty} \boldsymbol{\Phi}^{\dagger}_{v'}(y,E')\boldsymbol{\Phi}_v(y,E)dy = 2\pi\delta(E'-E)\delta_{v'v}\mathbf{I}_{oo}, \tag{15}$$

where $\mathbf{I}_{oo}$ is the identity $N_o \times N_o$ matrix.

Suppose that a set of linear independent regular square-solutions $\boldsymbol{\Phi}^{\rm reg}_v(y) = \{\boldsymbol{\chi}^{(i')}_{\rm reg}(y)\}_{i'=1}^{N}$ for a problem under consideration with components $\boldsymbol{\chi}^{(i')}_{\rm reg}(y) = (\chi^{\rm reg}_{1i'}(y),\ldots,\chi^{\rm reg}_{Ni'}(y))^T$ is known at $y > 0$, $v = \rightarrow$ or $y < 0$, $v = \leftarrow$, i.e.,

$$\boldsymbol{\Phi}^{\rm reg}_{\rightarrow}(y) = \tilde{\mathbf{X}}^{(+)}(y), \quad y > 0, \quad \boldsymbol{\Phi}^{\rm reg}_{\leftarrow}(y) = \tilde{\mathbf{X}}^{(-)}(y), \quad y < 0.$$
$$\tilde{X}^{(\pm)}_{ji_o}(y) = X^{(\pm)}_{ji_o}(y), \quad j = 1,\ldots,N, \quad i_o = 1,\ldots,N_o. \tag{16}$$

In a case of some channels are closed, we must use additional leading terms of regular asymptotic functions correspondingly at $z > 0$ and $z < 0$

$$\tilde{X}^{(\pm)}_{ji_c}(y) \to q_j^{-1/2} \exp\left(\mp\left(q_j y + \sigma_y \frac{Z_{12}}{q_j}\ln(2q_j|y|)\right)\right)\delta_{ji_c}, \tag{17}$$
$$q_{i_c} = \sqrt{\epsilon_{i_c} - 2E}, \quad j = 1,\ldots,N, \quad i_c = N_o+1,\ldots,N.$$

In this case, the required part of $\mathcal{R}_{\rightarrow}(y)$ at $y = y_{\max} > 0$ and $\mathcal{R}_{\rightarrow}(y)$ matrix $y = y_{\min} < 0$ can be found via the known set of linear independent regular solutions $\boldsymbol{\Phi}^{\rm reg}_v(y)$

$$\mathcal{R}_v(y) = \frac{d\boldsymbol{\Phi}^{\rm reg}_v(y)}{dy}\left(\boldsymbol{\Phi}^{\rm reg}_v(y)\right)^{-1}. \tag{18}$$

These matrix-functions $\mathcal{R}_v(y)$ by dimension of $N \times N$ are used for calculating numerical solutions $\boldsymbol{\Phi}^h_v(y)$ of BVP (10)–(12).

By using $\boldsymbol{\Phi}^h_{\rightarrow}(y_{\max})$ and $\mathcal{R}_{\rightarrow}(y)$ numerically calculated with KANTBP 3.0, we obtain the following matrix equations for the reflection $\mathbf{R}_{\rightarrow}$ and transmission $\mathbf{T}_{\rightarrow}$ matrices

$$\mathbf{Y}_{\rightarrow}^{(-)}(y_{\min})\mathbf{R}_{\rightarrow} = -\mathbf{Y}_{\rightarrow}^{(+)}(y_{\min}), \quad \mathbf{X}^{(+)}(y_{\max})\mathbf{T}_{\rightarrow} = \boldsymbol{\Phi}_{\rightarrow}^{h}(y_{\max}), \tag{19}$$
$$\mathbf{Y}_{\rightarrow}^{(\pm)}(y) = \frac{d\mathbf{X}^{(\pm)}(y)}{dy} - \mathcal{R}_{\rightarrow}(y)\mathbf{X}^{(\pm)}(y).$$

Note that, when some channels are closed, the $\mathbf{Y}_{\leftarrow}^{(\pm)}(y)$ and $\mathbf{X}^{(-)}(y)$ are rectangular $N \times N_o$ matrices. The reflection $\mathbf{R}_{\rightarrow}$ and transmission $\mathbf{T}_{\rightarrow}$ matrices are evaluated in terms of the pseudoinverse matrices of $\mathbf{Y}_{\rightarrow}^{(-)}(y_{\min})$ and $\mathbf{X}^{(+)}(y_{\max})$

$$\mathbf{R}_{\rightarrow} = -\left(\left(\mathbf{Y}_{\rightarrow}^{(-)}(y_{\min})\right)^{T}\mathbf{Y}_{\rightarrow}^{(-)}(y_{\min})\right)^{-1}\left(\mathbf{Y}_{\rightarrow}^{(-)}(y_{\min})\right)^{T}\mathbf{Y}_{\rightarrow}^{(+)}(y_{\min}), \tag{20}$$
$$\mathbf{T}_{\rightarrow} = \left(\left(\mathbf{X}^{(+)}(y_{\max})\right)^{T}\mathbf{X}^{(+)}(y_{\max})\right)^{-1}\left(\mathbf{X}^{(+)}(y_{\max})\right)^{T}\boldsymbol{\Phi}_{\rightarrow}^{h}(y_{\max}).$$

Having $\boldsymbol{\Phi}_{\leftarrow}^{h}(y_{\min})$ and $\mathcal{R}_{\leftarrow}(y)$ numerically calculated with KANTBP 3.0, we obtain the following matrix equations for the reflection $\mathbf{R}_{\leftarrow}$ and transmission $\mathbf{T}_{\leftarrow}$ matrices:

$$\mathbf{Y}_{\leftarrow}^{(+)}(y_{\max})\mathbf{R}_{\leftarrow} = -\mathbf{Y}_{\leftarrow}^{(-)}(y_{\max}), \quad \mathbf{X}^{(-)}(y_{\min})\mathbf{T}_{\leftarrow} = \boldsymbol{\Phi}_{\leftarrow}^{h}(y_{\min}), \tag{21}$$
$$\mathbf{Y}_{\leftarrow}^{(\pm)}(y) = \frac{d\mathbf{X}^{(\pm)}(y)}{dy} - \mathcal{R}_{\leftarrow}(y)\mathbf{X}^{(\pm)}(y).$$

Therefore, using the pseudoinverse matrices of $\mathbf{Y}_{\leftarrow}^{(+)}(y)$ and $\mathbf{X}^{(-)}(y)$, we obtain the following formulae:

$$\mathbf{R}_{\leftarrow} = -\left(\left(\mathbf{Y}_{\leftarrow}^{(+)}(y_{\max})\right)^{T}\mathbf{Y}_{\leftarrow}^{(+)}(y_{\max})\right)^{-1}\left(\mathbf{Y}_{\leftarrow}^{(+)}(y_{\max})\right)^{T}\mathbf{Y}_{\leftarrow}^{(-)}(y_{\max}), \tag{22}$$
$$\mathbf{T}_{\leftarrow} = \left(\left(\mathbf{X}^{(-)}(y_{\min})\right)^{T}\mathbf{X}^{(-)}(y_{\min})\right)^{-1}\left(\mathbf{X}^{(-)}(y_{\min})\right)^{T}\boldsymbol{\Phi}_{\leftarrow}^{h}(y_{\min}).$$

Let us now rewrite Eq. (13) in the matrix form at $y_{\pm} \to \pm\infty$

$$\begin{pmatrix} \boldsymbol{\Phi}_{\rightarrow}(y_+) & \boldsymbol{\Phi}_{\leftarrow}(y_+) \\ \boldsymbol{\Phi}_{\rightarrow}(y_-) & \boldsymbol{\Phi}_{\leftarrow}(y_-) \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{X}^{(-)}(y_+) \\ \mathbf{X}^{(+)}(y_-) & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \mathbf{X}^{(+)}(y_+) \\ \mathbf{X}^{(-)}(y_-) & \mathbf{0} \end{pmatrix} \mathbf{S}, \tag{23}$$

where the symmetric and unitary scattering matrix $\mathbf{S}$ is composed of the transmission and reflection matrices from (20) and (22)

$$\mathbf{S} = \begin{pmatrix} \mathbf{R}_{\rightarrow} & \mathbf{T}_{\leftarrow} \\ \mathbf{T}_{\rightarrow} & \mathbf{R}_{\leftarrow} \end{pmatrix}, \quad \mathbf{S}\mathbf{S}^{\dagger} = \mathbf{S}^{\dagger}\mathbf{S} = \mathbf{I}. \tag{24}$$

In addition, it should be noted that the functions $\mathbf{X}^{(\pm)}(y)$ satisfy relations

$$\mathbf{Wr}(\mathbf{Q}(y); \mathbf{X}^{(\mp)}(y), \mathbf{X}^{(\pm)}(y)) = \pm 2\imath \mathbf{I}_{oo}, \; \mathbf{Wr}(\mathbf{Q}(y); \mathbf{X}^{(\pm)}(y), \mathbf{X}^{(\pm)}(y)) = 0, \tag{25}$$

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

$$\mathbf{Wr}(\bullet;\mathbf{a}(y),\mathbf{b}(y)) = \mathbf{a}^T(y)\left(\frac{d\mathbf{b}(y)}{dy} - \bullet\mathbf{b}(y)\right) - \left(\frac{d\mathbf{a}(y)}{dy} - \bullet\mathbf{a}(y)\right)^T \mathbf{b}(y). \quad (26)$$

Remark 1. This Wronskian will be used below to estimate a desirable precision of the above expansion as well as the symmetry and unitarity properties of the scattering matrix $\mathbf{S}$ in (24).

Algorithm 1. Evaluating Effective Potential Asymptotics

Input. We evaluate the asymptotics of effective potentials (11) at large $|y|$ via the asymptotics of solutions to the eigenvalue problem (8), (9) at $|y/x| \gg 1$,

$$\left(\frac{d^2}{dx^2} + x^2 + 2U(x,y) - \varepsilon_j(y)\right) B_j(x;y) = 0, \int\limits_{x_{\min}(y)}^{x_{\max}(y)} B_i(x;y)B_j(x;y)dx = \delta_{ij}. (27)$$

with the Coulomb-like potential

$$2U(x,y) = 2\hat{Z}_1/\sqrt[s]{(s_2y + s_1x)^s + \bar{x}^s_{\min}} + 2\hat{Z}_2/\sqrt[s]{(s_2y - s_3x)^s + \bar{x}^s_{\min}}. \quad (28)$$

At **step 1** we find $B_j(x;y)$ and $\varepsilon_j(y)$ as a series expansion with $j = n+1$

$$B_j(x;y) = \sum_{k=0}^{k_{\max}} \frac{B_n^{(k)}(x)}{y^k}, \ \varepsilon_j(y) = \sum_{k=0}^{k_{\max}} \frac{\varepsilon_n^{(k)}}{y^k}. \quad (29)$$

Substituting (29) to (27) and equating coefficients of the same powers of y, we arrive at a system of recurrence differential equations for evaluating coefficients $B_n^{(k)}(x)$ and $\varepsilon_n^{(k)}$, $k = 1,\ldots,k_{\max}$:

$$L(n)B_n^{(k)}(x) = f_n^{(k)}(x), \qquad L(n) = -\frac{d^2}{dx^2} - (2n+1) + x^2, \quad (30)$$

with the initial data $\varepsilon_n^{(0)} = 2n+1$ and with $B_n^{(0)}(x)$ as the known solution of the problem

$$\text{Ł}(n)B_n^{(0)}(x) = 0, \quad \int_{-\infty}^{+\infty} B_n^{(0)}(x)B_{n'}^{(0)}(x)dx = \delta_{nn'}. \quad (31)$$

In Eqs. (30), the right-hand sides $f_n^{(k)}(x)$ are defined by relations

$$f_n^{(k)}(x) = \sum_{p=1}^{k}(U^{(p)}(x) - \varepsilon_n^{(p)})B^{(k-p)}(x),$$

Table 1. Values of the partial sums (41) for $V_{jj} \equiv V_{jj}(y)$ from (11) depending on $k_{\max}$ for $s_1 = s_2 = s_3 = 1/2$, $\bar{x}_{\min} = 0.1$, $s = 8$, $\hat{Z}_1 = \hat{Z}_2 = 1$, $y = y_2^{match} = 12.5$. The last row contains the corresponding numerical values (n.v.).

$k_{\max}$	V_{11}	V_{22}	V_{33}	V_{44}	V_{55}	V_{66}
0	1.000000000	3.000000000	5.000000000	7.000000000	9.000000000	11.00000000
1	1.640000000	3.640000000	5.640000000	7.640000000	9.640000000	11.64000000
2	1.640000000	3.640000000	5.640000000	7.640000000	9.640000000	11.64000000
3	1.642048000	3.646144000	5.650240000	7.654336000	9.658432000	11.66252800
4	1.642048000	3.646144000	5.650240000	7.654336000	9.658432000	11.66252800
5	1.642067661	3.646242304	5.650495590	7.654827520	9.659238093	11.66372731
6	1.642065564	3.646236013	5.650485105	7.654812840	9.659219218	11.66370424
7	1.642065878	3.646238215	5.650492969	7.654832658	9.659259798	11.66377691
8	1.642065798	3.646237812	5.650491922	7.654830645	9.659256497	11.66377199
9	1.642065809	3.646237888	5.650492232	7.654831584	9.659258797	11.66377684
10	1.642065806	3.646237868	5.650492158	7.654831394	9.659258408	11.66377614
11	1.642065807	3.646237871	5.650492174	7.654831450	9.659258560	11.66377650
12	1.642065807	3.646237870	5.650492169	7.654831434	9.659258520	11.66377642
nv	1.642065807	3.646237871	5.650492170	7.654831437	9.659258529	11.66377644

where the coefficients $U^{(j)}(x)$ are determined by Taylor expansion of (28) at large y

$$2U(x,y) = \sum_{k=1}^{k_{\max}} \frac{U^{(k)}(x)}{y^k}, \tag{32}$$

$$\begin{aligned}
&U^{(1)}(x) = \sigma_y 2(\hat{Z}_1 + \hat{Z}_2)/s_2, && U^{(2)}(x) = \sigma_y 2x(\hat{Z}_1 s_1 - \hat{Z}_2 s_3)/s_2^2,\\
&U^{(3)}(x) = \sigma_y 2x^2(\hat{Z}_1 s_1^2 + \hat{Z}_2 s_3^2)/s_2^3, && U^{(4)}(x) = \sigma_y 2x^3(\hat{Z}_1 s_1^3 - \hat{Z}_2 s_3^3)/s_2^4,\\
&U^{(5)}(x) = \sigma_y 2x^4(\hat{Z}_1 s_1^4 + \hat{Z}_2 s_3^4)/s_2^5, && U^{(6)}(x) = \sigma_y 2x^5(\hat{Z}_1 s_1^5 - \hat{Z}_2 s_3^5)/s_2^6,\\
&U^{(7)}(x) = \sigma_y 2x^6(\hat{Z}_1 s_1^6 + \hat{Z}_2 s_3^6)/s_2^7, && U^{(8)}(x) = \sigma_y 2x^7(\hat{Z}_1 s_1^7 - \hat{Z}_2 s_3^7)/s_2^8,\\
&U^{(9)}(x) = \sigma_y 2x^8(\hat{Z}_1 s_1^8 + \hat{Z}_2 s_3^8)/s_2^9 - \sigma_y \bar{x}_{\min}^8(\hat{Z}_1 + \hat{Z}_2)/(4s_2^9), &&\\
&U^{(10)}(x) = \sigma_y 2x^9(\hat{Z}_1 s_1^9 - \hat{Z}_2 s_3^9)/s_2^{10} - \sigma_y 9x\bar{x}_{\min}^8(\hat{Z}_1 - \hat{Z}_2)/(8s_2^{10}). &&
\end{aligned}$$

The orthogonality and normalization conditions follow from (27) and (29)

$$I_{jj'}^{(k)} = \sum_{l=0}^{k} \int_{-\infty}^{\infty} B_{n_l}^{(l)}(x) B_{n_r}^{(k-l)}(x) dx = \delta_{k0}\delta_{n_l n_r} \tag{33}$$

where $n_l = j - 1$, $n_r = j' - 1$.

We find the asymptotics of matrix elements $H_{jj'}(y)$ and $Q_{jj'}(y)$ from (11) in the form of expansions

$$Q_{jj'}(y) = \sum_{k=1}^{k_{\max}} \frac{Q_{jj'}^{(k)}}{y^k}, \quad H_{jj'}(y) = \sum_{k=2}^{k_{\max}} \frac{H_{jj'}^{(k)}}{y^k}. \tag{34}$$

Table 2. The same as in Table 1, but for $Q_{jj'} \equiv Q_{jj'}(y)$ at $j \neq j'$

$k_{\max}$	$Q_{13}, 10^{-4}$	$Q_{15}, 10^{-6}$	$Q_{24}, 10^{-4}$	$Q_{26}, 10^{-6}$	$Q_{35}, 10^{-4}$	$Q_{46}, 10^{-4}$
3	0.00000000	0.000000	0.00000000	0.000000	0.00000000	0.00000000
4	1.73778562	0.000000	3.00993299	0.000000	4.25668806	5.49536066
5	1.73778562	0.000000	3.00993299	0.000000	4.25668806	5.49536066
6	1.79339476	1.605297	3.17046275	3.589554	4.57452077	6.02291528
7	1.78627679	1.605297	3.15813407	3.589554	4.55708537	6.00040628
8	1.78814526	1.713173	3.16568539	3.927259	4.57691814	6.04176657
9	1.78761568	1.705283	3.16415663	3.909616	4.57389135	6.03674256
10	1.78771659	1.711496	3.16457995	3.934625	4.57519301	6.03996585
11	1.78768515	1.710423	3.16444912	3.931266	4.57484597	6.03923893
12	1.78769198	1.710818	3.16447978	3.933127	4.57494688	6.03951537
nv	1.78769041	1.710734	3.16447143	3.932815	4.57491909	6.03944626

Here the coefficients $Q_{jj'}^{(k)}$ and $H_{jj'}^{(k)}$ are defined by the relations

$$Q_{jj'}^{(k)} = -\sum_{l=0}^{k-1} \int_{-\infty}^{+\infty} B_{n_l}^{(l)}(x) \hat{Q} B_{n_r}^{(k-1-l)}(x) dx, \quad \hat{Q} B_{n_l}^{(l)}(x) = l B_{n_l}^{(l)}(x),$$

$$H_{jj'}^{(k)} = \sum_{l=0}^{k-2} \int_{-\infty}^{+\infty} \hat{Q} B_{n_l}^{(l)}(x) \hat{Q} B_{n_r}^{(k-2-l)}(x) dx. \tag{35}$$

At **step 2**, we construct $B_n^{(k)}(x)$ as the expansion with unknown coefficients $b_{n;s}^{(k)}$

$$B_n^{(k)}(x) = \sum_{s=-M(k)}^{M(k)} b_{n;s}^{(k)} B_{n+s}^{(0)}(y). \tag{36}$$

Here $B_v^{(0)}(x)$ are solutions to (31) in terms of the Hermite polynomials [9]

$$B_v^{(0)}(x) = \frac{H_v(x) \exp(-x^2/2)}{\sqrt[4]{\pi}\sqrt{2^v}\sqrt{v!}}.$$

By means of the well-known recurrence relation for Hermite polynomials $H_v(x)$ we obtain the recurrence relations for basis functions $B_v^{(0)}(x)$:

$$xB_v^{(0)}(x) = +\frac{\sqrt{v+1}}{\sqrt{2}} B_{v+1}^{(0)}(x) + \frac{\sqrt{v}}{\sqrt{2}} B_{v-1}^{(0)}(x),$$

$$L(n) B_{n+s}^{(0)}(x) \equiv \left(-\frac{d^2}{dx^2} - (2n+1) + x^2 \right) B_{n+s}^{(0)}(x) = 2s B_{n+s}^{(0)}(x). \tag{37}$$

From (30), (32), and (37) we have the needed value of $M(k) = 2k+1$ in expansion (36) to provide calculation of nonzero terms only.

Substituting (36) to (30), taking into account (37), and equating coefficients of the identical powers of y, we arrive at a set of recurrence relations for evaluation of coefficients $E_n^{(k)}$ and $b_{n;s}^{(k)}$

$$2sb^{(k)}_{n;s} = f^{(k)}_{n;s}, \quad I^{(k)}_{jj'} = \sum_{l=0}^{k} \sum_{s=-2k-1}^{2k+1} b^{(l)}_{n_l;s} b^{(k-l)}_{n_r;s+n_l-n_r} = \delta_{k0}\delta_{n_l n_r}, \qquad (38)$$

with initial data $\varepsilon^{(0)}_n = 2n+1$ and $b^{(0)}_{n;s} = \delta_{s0}$.

The corresponding coefficients $Q^{(k)}_{jj'}$ and $H^{(k)}_{jj'}$ in (35) have the following explicit form:

$$Q^{(k)}_{jj+t}(y) = -\sum_{k'=0}^{k-1} \sum_{s=\max(-k+1,k'-k+1-t)}^{\min(k-1,k-1-k'-t)} (k-1-k') b^{(k')}_{n;n+s} b^{(k-1-k')}_{n+t;n+s},$$
$$H^{(k)}_{jj+t}(y) = \sum_{k'=0}^{k-2} \sum_{s=\max(-k+2,k'-k+2-t)}^{\min(k-2,k-2-k'-t)} k'(k-2-k') b^{(k')}_{n;n+s} b^{(k-2-k')}_{n+t;n+s}. \qquad (39)$$

At **step 3**, we evaluate sequentially the solutions $b^{(k)}_{n;s}$ and $\varepsilon^{(k)}_n$ to the set of recurrence relations (38) for each kth order ($k = 1, \ldots, k_{\max}$):

$$f^{(k)}_{n;0} = 0 \to \varepsilon^{(k)}_n; \quad b^{(k)}_{n;s\neq 0} = f^{(k)}_{n;s}/(s); I^{(k)}_{ii} = \delta_{k0} \to b^{(k)}_{n;0}. \qquad (40)$$

At **step 4**, we substitute coefficients $b^{(k)}_{n;s}$ calculated in (40) into the expressions for the matrix elements (34), (39) evaluated at **step 2** and taking into account coefficients $\varepsilon^{(k)}_j$ calculated in (40). In doing so we produce the **output** containing the matrix elements as a series expansion of inverse powers of y for $k = 0, 1, \ldots, k_{\max}$ at $j, j' = 1, \ldots, N$ ($\varepsilon^{(k<0)}_j = H^{(k<2)}_{jj'} = Q^{(k<1)}_{jj'} = 0$):

$$\varepsilon_j(y) = \sum_{k=0}^{k_{\max}} \frac{\varepsilon^{(k)}_j}{y^k}, \quad H_{jj'}(y) = \sum_{k=2}^{k_{\max}} \frac{H^{(k)}_{jj'}}{y^k}, \quad Q_{jj'}(y) = \sum_{k=1}^{k_{\max}} \frac{Q^{(k)}_{jj'}}{y^k}. \qquad (41)$$

The above described calculation was performed by the algorithm implemented in MAPLE up to $k_{\max} = 12$. For example, the explicit expression of the desirable nonzero coefficients $\varepsilon^{(k)}_j$, $H^{(k)}_{ij} = H^{(k)}_{ji}$ and $Q^{(k)}_{ij} = -Q^{(k)}_{ji}$ reads as ($j = n+1$):

$$\begin{aligned}
\varepsilon^{(0)}_j &= (2n+1), \quad \varepsilon^{(1)}_j = \sigma_y \frac{2(\hat{Z}_2 + \hat{Z}_1)}{s_2}, \quad \varepsilon^{(3)}_j = \sigma_y \frac{(2n+1)(\hat{Z}_2 s_3^2 + \hat{Z}_1 s_1^2)}{s_2^3},\\
\varepsilon^{(4)}_j &= -\frac{(\hat{Z}_2 s_3 - \hat{Z}_1 s_1)^2}{s_2^4}, \quad \varepsilon^{(5)}_j = \sigma_y \frac{3(2n^2+2n+1)(\hat{Z}_2 s_3^4 + \hat{Z}_1 s_1^4)}{2 s_2^5},\\
Q^{(5)}_{jj-3} &= -\sigma_y \frac{\sqrt{n-2}\sqrt{n-1}\sqrt{2}\sqrt{n}(\hat{Z}_2 s_3^3 - \hat{Z}_1 s_1^3)}{3 s_2^4}, \qquad (42)\\
Q^{(4)}_{jj-2} &= -\sigma_y \frac{3\sqrt{n-1}\sqrt{n}(\hat{Z}_2 s_3^2 + \hat{Z}_1 s_1^2)}{4 s_2^3},
\end{aligned}$$

Table 3. The same as in Table 1, but for $H_{jj'} \equiv H_{jj'}(y)$ at $j \neq j'$

$k_{\max}$	$H_{13}, 10^{-10}$	$H_{15}, 10^{-8}$	$H_{24}, 10^{-9}$	$H_{26}, 10^{-6}$	$H_{35}, 10^{-9}$	$H_{46}, 10^{-8}$
8	0.000	-7.3972	0.000	-1.65406	0.000	0.0000
9	0.000	-7.3972	0.000	-1.65406	0.000	0.0000
10	0.683	-8.1862	1.972	-1.90107	4.463	0.8643
11	0.683	-8.1256	1.972	-1.88752	4.463	0.8643
12	0.780	-8.1839	2.347	-1.91203	5.488	1.0969
nv	0.782	-8.1763	2.376	-1.91042	5.608	1.1334

$$
\begin{aligned}
Q^{(3)}_{jj-1} &= -\sigma_y \frac{\sqrt{2}\sqrt{n}(-\hat{Z}_1 s_1 + \hat{Z}_2 s_3)}{s_2^2}, \quad Q^{(5)}_{jj-1} = -\sigma_y \frac{3\sqrt{2}n\sqrt{n}(\hat{Z}_2 s_3^3 - \hat{Z}_1 s_1^3)}{s_2^4},\\
H^{(7)}_{jj-3} &= -\frac{3\sqrt{2}\sqrt{n}\sqrt{n-1}\sqrt{n-2}(\hat{Z}_2 s_3^2 + \hat{Z}_1 s_1^2)(-\hat{Z}_1 s_1 + \hat{Z}_2 s_3)}{2 s_2^5},\\
H^{(6)}_{jj-2} &= -\frac{2\sqrt{n}\sqrt{n-1}(\hat{Z}_2 s_3 - \hat{Z}_1 s_1)^2}{s_2^4},\\
H^{(7)}_{jj-1} &= \frac{3n\sqrt{2}\sqrt{n}(\hat{Z}_2 s_3^2 + \hat{Z}_1 s_1^2)(\hat{Z}_2 s_3 - \hat{Z}_1 s_1)}{2 s_2^5},\\
H^{(6)}_{jj} &= \frac{2(2n+1)(\hat{Z}_2 s_3 - \hat{Z}_1 s_1)^2}{s_2^4}.
\end{aligned}
$$

Remark 2. In the case of $\hat{Z}_1 = \hat{Z}_2$, $s_1 = s_3$ (i.e., for equal masses and charges), the set of equations (10) has even and odd parity solutions that are calculated separately: for the even solutions $n = 2j-2$ and for the odd solutions $n = 2j-1$. In this case, the above coefficients which contain terms like $(-\hat{Z}_1 s_1 + \hat{Z}_2 s_3)$ vanish when they have no terms $(\hat{Z}_1 s_1 + \hat{Z}_2 s_3)$.

Algorithm 2. Evaluation of the Asymptotic Solutions

Input. We calculate the asymptotic solution to the set of N ODEs at large values of the independent variable $|y| \gg 1$

$$
\begin{aligned}
&\left[-\frac{1}{y^{d-1}}\frac{d}{dy}y^{d-1}\frac{d}{dy} + \varepsilon_i(y) + H_{ii}(y) - 2E\right]\chi_{ii'}(y) \\
&= \sum_{j=1, j\neq i}^{N}\left[-Q_{ij}(y)\frac{d}{dy} - \frac{1}{y^{d-1}}\frac{d}{dy}y^{d-1}Q_{ij}(y) - H_{ij}(y)\right]\chi_{ji'}(y).
\end{aligned}
\tag{43}
$$

Here $d \geq 1$ is the dimension of configuration space of a general scattering problem [7] while in the considered case (10), we put $d = 1$ and calculate asymptotic solution on two intervals $-\infty < y \leq y_{\min}$ and $y_{\max} \leq y < \infty$. We suppose that coefficients of Eqs. (43) are present in the general form (41) and, in particular, in the form (42).

Step 1. We construct the solution to Eqs. (43) in the form:

$$\chi_{ji'}(y) = \left(\phi_{ji'}(y) + \psi_{ji'}(y)\frac{d}{dy}\right) R_{i'}(y), \tag{44}$$

where $\phi_{ji'}(y)$ and $\psi_{ji'}(y)$ are unknown functions, $R_{i'}(y)$ is known function. We choose $R_{i'}(y)$ as solutions of the auxiliary problem treated like etalon equation ($Z_{i'}^{(k<1)} = Z_{i'}^{(k>k'_{\max})} = 0$):

$$\left[-\frac{1}{y^{d-1}}\frac{d}{dy}y^{d-1}\frac{d}{dy} + \sum_{k=1}^{k'_{\max}}\frac{Z_{i'}^{(k)}}{y^k} - p_{i'}^2\right] R_{i'}(y) = 0. \tag{45}$$

Remark 3. If $Z_{i'}^{(k\geq 3)} = 0$ then solutions to the last equation are presented via hypergeometric functions, exponential, trigonometric, Bessel, Coulomb functions, etc. For example, if the leading terms of the asymptotic solutions are given by formula

$$R_{i'}(y) = \frac{1}{\sqrt{p_{i'}y^{d-1}}}\exp\left(\pm\imath\left(p_{i'}y - \frac{Z_{i'}^{(1)}}{2p_{i'}}\ln(2p_{i'}|y|)\right)\right), \tag{46}$$

the coefficient $Z_{i'}^{(2)}$ of potential in the etalon equation (45) has the form:

$$Z_{i'}^{(2)} = -\frac{(d-3)(d-1)}{4} \pm \imath\frac{Z_{i'}^{(1)}}{p_{i'}} - \frac{(Z_{i'}^{(1)})^2}{p_{i'}^2}. \tag{47}$$

Step 2. At this step, we compute the coefficients $\phi_{i'}(y)$ and $\psi_{i'}(y)$ of the expansion (44) in the form of series by inverse powers of y ($\phi_{ji'}^{(k'<0)} = \psi_{ji'}^{(k'<0)} = 0$):

$$\phi_{ji'}(y) = \phi_{ji'}^{(0)} + \sum_{k'=1}^{k_{\max}}\frac{\phi_{ji'}^{(k')}}{y^{k'}}, \quad \psi_{ji'}(y) = \psi_{ji'}^{(0)} + \sum_{k'=1}^{k_{\max}}\frac{\psi_{ji'}^{(k')}}{y^{k'}}. \tag{48}$$

After substitution of (44),(48) into (43) with the use of Eq. (45), we arrive at the set of recurrence relations at $k' \leq k_{\max}$:

$$\begin{aligned} &\left(\varepsilon_i^{(0)} - 2E + p_{i'}^2\right)\phi_{ii'}^{(k')} + \left(\varepsilon_i^{(1)} - Z_{i'}^{(1)}\right)\phi_{ii'}^{(k'-1)} - 2p_{i'}^2(k'-1)\psi_{ii'}^{(k'-1)} = -f_{ii'}^{(k')}, \\ &\left(\varepsilon_i^{(0)} - 2E + p_{i'}^2\right)\psi_{ii'}^{(k')} + 2(k'-1)\phi_{ii'}^{(k'-1)} + \left(\varepsilon_i^{(1)} - Z_{i'}^{(1)}\right)\psi_{ii'}^{(k'-1)} = -g_{ii'}^{(k')}, \end{aligned} \tag{49}$$

where the right-hand sides $f_{ii'}^{(k)}$ and $g_{ii'}^{(k)}$ are defined by relations

$$f_{ii'}^{(k')} = -(k'-2)(k'-d)\phi_{ii'}^{(k'-2)} + \sum_{k=2}^{k'}\left(V_{ii}^{(k)} - Z_{i'}^{(k)}\right)\phi_{ii'}^{(k'-k)}$$

$$+\sum_{k=1}^{k'}\Big(Z_{i'}^{(k)}(2k'-2-k)\psi_{ii'}^{(k'-k-1)}+\sum_{j=1,j\neq i}^{N}\Big(\sum_{k''=1}^{k'}2Q_{ij}^{(k)}Z_{i'}^{(k'')}\psi_{ji'}^{(k'-k-k'')}$$

$$-2p_{i'}^2Q_{ij}^{(k)}\psi_{ji'}^{(k'-k)}+Q_{ij}^{(k)}(-2k'+k+d+1)\phi_{ji'}^{(k'-k-1)}+V_{ij}^{(k)}\phi_{ji'}^{(k'-k)}\Big)\Big); \quad (50)$$

$$g_{ii'}^{(k)}=-(k'-1)(k'-3+d)\psi_{ii'}^{(k'-2)}+\sum_{k=2}^{k'}\left(V_{ii}^{(k)}-Z_{i'}^{(k)}\right)\psi_{ii'}^{(k'-k)}$$

$$+\sum_{j=1,j\neq i}^{N}\sum_{k=1}^{k'}\Big(2Q_{ij}^{(k)}\phi_{ji'}^{(k'-k)}-Q_{ij}^{(k)}(2k'+d-3-k)\psi_{ji'}^{(k'-k-1)}+V_{ij}^{(k)}\psi_{ji'}^{(k'-k)}\Big)$$

with initial conditions $p_{i'}^2=2E-\varepsilon_{i'}^{(0)}$, $\phi_{ii'}^{(0)}=\delta_{ii'}$, $\psi_{ii'}^{(0)}=0$, at $i'=i_o$ run the open channels $i_o=1,...,N_o$ and $p_{i'}=\imath q_{i'}$, $q_{i'}>0$, $q_{i'}^2=\varepsilon_{i'}^{(0)}-2E$ at $i'=i_c$ run the closed channels $i_c=N_o+1,...,N$ that follow from (14) and (17). Also from Eq. (49) at $k'=1$ and $i=i'$,

$$\left(\varepsilon_{i'}^{(1)}-Z_{i'}^{(1)}\right)\phi_{i'i'}^{(0)}=0,\quad \left(\varepsilon_{i'}^{(1)}-Z_{i'}^{(1)}\right)\psi_{i'i'}^{(0)}=0, \quad (51)$$

we obtain condition $Z_{i'}^{(1)}=\varepsilon_{i'}^{(1)}$.

Step 3. Here we perform calculation of the coefficients $\phi_{ii'}^{(k')}$ and $\psi_{ii'}^{(k')}$ by a step–by–step procedure of solving Eqs. (49) for $2E\neq\varepsilon_{i'}^{(0)}$, $i\neq i'$ and $k'=2,\ldots,k_{\max}$:

$$\begin{aligned}
\phi_{ii'}^{(k')}&=\left[\varepsilon_i^{(0)}-\varepsilon_{i'}^{(0)}\right]^{-1}\left[-f_{ii'}^{(k')}-\left(\varepsilon_i^{(1)}-Z_{i'}^{(1)}\right)\phi_{ii'}^{(k'-1)}+2p_{i'}^2(k'-1)\psi_{ii'}^{(k'-1)}\right],\\
\psi_{ii'}^{(k')}&=\left[\varepsilon_i^{(0)}-\varepsilon_{i'}^{(0)}\right]^{-1}\left[-g_{ii'}^{(k')}-2(k'-1)\phi_{ii'}^{(k'-1)}-\left(\varepsilon_i^{(1)}-Z_{i'}^{(1)}\right)\psi_{ii'}^{(k'-1)}\right],\\
\phi_{i'i'}^{(k'-1)}&=-\left[2(k'-1)\right]^{-1}g_{i'i'}^{(k)}, \quad (52)\\
\psi_{i'i'}^{(k'-1)}&=\left[2(k'-1)\left(2E-\varepsilon_{i'}^{(0)}\right)\right]^{-1}f_{i'i'}^{(k)}.
\end{aligned}$$

The above described algorithm has been implemented in MAPLE and FORTRAN to calculate the desirable $\phi_{ii'}^{(k')}$ and $\psi_{ii'}^{(k')}$ in the **output** up to $k_{\max}-1=11$ order.

Remark 4. The choice of appropriate values $y_{\min}$ and $y_{\max}$ for the constructed expansions of the linearly independent solutions for $p_{i_o}>0$ is controlled by the fulfillment of the Wronskian condition (26)

$$y^{d-1}Wr(\mathbf{Q}(y);\boldsymbol{\chi}^*(y),\boldsymbol{\chi}(y))=\pm2\imath\mathbf{I}_{oo} \quad (53)$$

up to the prescribed precision ε_{Wr}.

As a result, Algorithms 1 and 2 generate required asymptotic solution (5) up to the order $O(|y|^{-k_{\max}})$ at $|y|/|x|\gg1$ that reduce the BVP (1) from plane $\mathbf{R^2}$

$$\psi_{i'}^{as}(x,y)=\sum_{j=1}^{N}\sum_{k=0}^{k_{\max}}y^{-k}\sum_{s=\min(1-j,-M(k))}^{M(k)}B_{j-1+s}^{(0)}(x)b_{j-1;s}^{(k)}\left(\phi_{ji'}^{(k-p)}+\psi_{ji'}^{(k-p)}\frac{d}{dy}\right)R_{i'}(y) \quad (54)$$

to a finite domain $\Omega_{xy}=[\Omega_x\{x_{\min},x_{\max}\}\times\Omega_y\{y_{\min},y_{\max}\}]$.

4 Benchmark Calculation of Penetration Coefficient

As a benchmark calculation we consider the BVPs (1)–(6) that model the quantum tunneling problem for a coupled pair of identical ions with the following values of parameters: $\bar{x}_{\max} = 5$ for Eq. (2) and $s = 8$ for Eq. (3), $s_1 = s_2 = s_3 = 1/2$, $\bar{x}_{\min} = 0.1$, $\hat{Z}_1 = \hat{Z}_2 = 0.5$ and $\hat{Z}_1 = \hat{Z}_2 = 1$ in oscillator units. For given number N of ODES (10), the values $x_{\min}$ and $x_{\max}$ of grid $\Omega_x\{x_{\min}, x_{\max}\}$ are chosen in the region $|x| > x_0 = \sqrt{2N+1}$ where the Hermite polynomial [9] (or of wave function in a general case) has none zeros. These values are computed with prescribed precision $eps > 0$ from the condition

$$\exp\left(\int_{x_0}^{x} dx\sqrt{x^2 - x_0^2}\right) \le eps,$$

which in the given case leads to inequality

$$\exp\left(-x\sqrt{x^2 - x_0^2}/2\right)\left(x + \sqrt{x^2 - x_0^2}\right)^{x_0^2/2} x_0^{-x_0^2/2} \le eps. \tag{55}$$

To find an approximate solution, at the first step we choose the initial approximation $x_{\max} = x_0$, after that it is increased with step equal 1 until (55) is satisfied. Values $y_{\min} < x_{\min}$ and $y_{\max} > x_{\max}$ were chosen from the condition that potential (2) or (3) is negligible on the interval $x_{\min} < x < x_{\max}$.

The matching points y_1^{match} and y_2^{match} of the numerical (11) and asymptotic (41) effective potential were calculated as follows:

$$y_1^{match} = \min\{y_1^E, y_1^Q, y_1^H\}, \quad y_2^{match} = \max\{y_2^E, y_2^Q, y_2^H\},$$
$$y_t^E = \sigma_y \sqrt[k_{\max}]{\frac{|E_N^{(k_{\max})}|}{eps}}, \quad y_t^Q = \sigma_y \sqrt[k_{\max}]{\frac{|Q_{NN-1}^{(k_{\max})}|}{eps}}, \quad y_t^H = \sigma_y \sqrt[k_{\max}]{\frac{|H_{NN}^{(k_{\max})}|}{eps}},$$

since $|E_j^{(k_{\max})}| < |E_N^{(k_{\max})}|$, $|Q_{jj'}^{(k_{\max})}| < |Q_{NN-1}^{(k_{\max})}|$, $|H_{jj'}^{(k_{\max})}| < |H_{NN}^{(k_{\max})}|$. So, the values $y_{\min}$ and $y_{\max}$ are chosen from the inequalities $y_{\min} < y_1^{match} < x_{\min}$ and $y_{\max} > y_2^{match} > x_{\max}$ taking into account. This gives

$$y_{\min} = \min\left[y_1^{match}, \min_j\left(-\sqrt[k_{\max}]{\frac{|\phi_{ji_o}^{(k_{\max})}|}{eps}}\right), \min_j\left(-\sqrt[k_{\max}]{\frac{|\psi_{ji_o}^{(k_{\max})}|}{eps}}\right)\right],$$
$$y_{\max} = \max\left[y_2^{match}, \max_j\left(\sqrt[k_{\max}]{\frac{|\phi_{ji_o}^{(k_{\max})}|}{eps}}\right), \max_j\left(\sqrt[k_{\max}]{\frac{|\psi_{ji_o}^{(k_{\max})}|}{eps}}\right)\right]. \tag{56}$$

In the considered examples, we used the grids $\Omega_x\{x_{\min}, x_{\max}\} = \{-10(768)10\}$ and $\Omega_y\{y_{\min}, y_{\max}\} = \{-125(200)-25(100)-6(200)6(100)25(200)125\}$ with the Lagrange elements of the order $p = 4$ between the nodes. In the above grids Ω_x and Ω_y, the number of grid elements is shown in the parentheses.

To illustrate Remark 2 by an example, we can point out the lines for $k_{\max} = 3$ (containing only zero values) in Table 2. Other zero values in Tables 2 and 3 point out different leading terms in the inverse power series expansion of matrix elements between various eigenfunctions. The numerical values of effective potentials calculated by ODPEVP [6] with a given precision *eps* of order of 10^{-10} in the last line of the Tables 1, 2 and 3 are in a good agreement with the asymptotic values from (41) in the matching points $y = y_t^{match}$.

In the calculation of solutions, we used the etalon equation (45) at $d = 1$ with the two sets of parameters taken in the first case as in Remark 3 and in second case as $k'_{\max} = 1$, $Z_{i'}^{(1)} = 2\sigma_y Z_{12}$, that corresponds to the known solutions on the open channels

$$R_{i_o}^{\pm}(p_{i_o}, y) = p_{i_o}^{-1/2} \begin{cases} (G_0(p_{i_o}, +y) \pm \imath F_0(p_{i_o}, +y)) \exp(\mp \imath \sigma_{i_o})/2, \; y > 0, \\ (G_0(p_{i_o}, -y) \mp \imath F_0(p_{i_o}, -y)) \exp(\pm \imath \sigma_{i_o})/2, \; y < 0, \end{cases} \quad (57)$$

and on the closed channels

$$R_{i_c}(q_{i_c}, y) = q_{i_c}^{-1/2} t \exp(-t/2)\, U(1 + Z_{12}/q_{i_c}, 2, t), \quad t = 2q_{i_c}|y|. \quad (58)$$

Here $F_0(p_{i_o}, y)$ and $G_0(p_{i_o}, y)$ are regular and irregular continuum zero order Coulomb functions; $\sigma_{i_o} = \arg \Gamma(1 + \imath Z_{12}/p_{i_o})$ is the Coulomb phase shift [9]; and $U(a, b, c)$ is the confluent hypergeometric function of second kind.

Remark 5. In the numerical calculation, the exponential small factor $\exp(-t/2)$ in $R_{i_c}(q_{i_c}, y)$ and its first derivative was neglected since this factor is canceled during evaluation of $\mathcal{R}(y)$ matrix in Eq. (18).

Required reflection $\mathbf{R}_{\rightarrow}$ and transmission $\mathbf{T}_{\rightarrow}$ matrixes calculated by formulas (20) via matrix of logarithmic derivatives $\mathcal{R}_{\rightarrow}(y)$ and solution $\boldsymbol{\Phi}^h_{\rightarrow}(y_{\max})$ calculated numerically on the above grid $\Omega_y\{y_{\min}, y_{\max}\}$ by means of the program KANTBP 3.0, including matching in the boundary points $y_{\min}$ and $y_{\max}$ of (12) with asymptotic solution evaluated in first case has the error of order 0.1% in comparison with a more accurate result obtained with asymptotic solution evaluated in the second case.

According to Remarks 1 and 4, the Wronskian condition depends on the number N of ODEs, on the value of threshold energy, on the type of etalon equation, etc. At the boundary points $y_{\min}$ and $y_{\max}$ of the above grid $\Omega_y\{y_{\min}, y_{\max}\}$, the absolute values ε_{Wr} of components of difference between the calculated Wronskian and its theoretical value (53) are less then 10^{-11}.

The total probabilities $T \equiv T_{11} = \sum_{j=1}^{N_o} |T_{1j}|^2$ of penetration through Truncated Coulomb (2) and Coulomb-like (3) potential barriers are shown in Fig. 1. The first of them is in a good agrement with results obtained by solving the BVP (1), (2), (5), and (6) in the 2D domain using Numerov method in papers [3,4]. These pictures illustrate the important peculiarity that a more realistic nontruncated Coulomb-like barrier having a more wide than truncated one, leads to a set of the probability maximums having a bigger half-width. It can be used for verification of the models and quantum transparency effect.

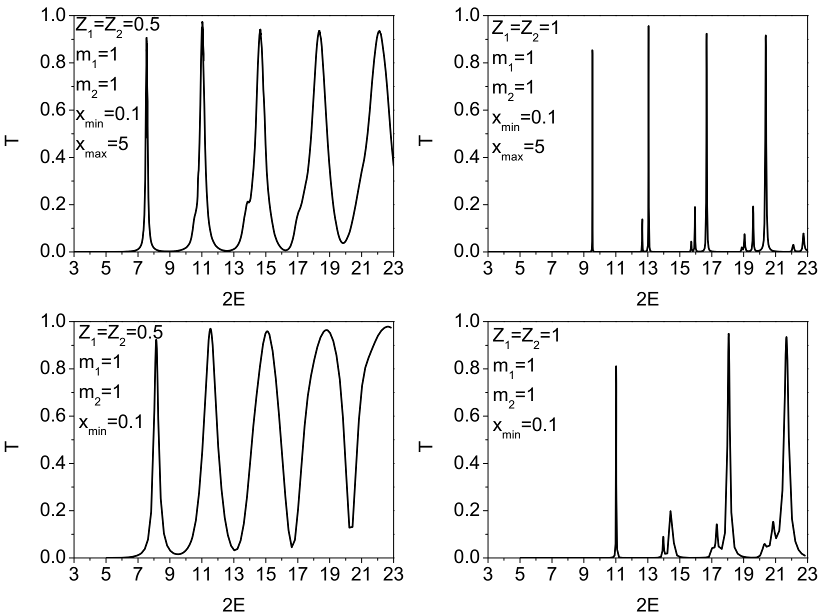

Fig. 1. The total probabilities $T \equiv T_{11} = \sum_{j=1}^{N_o} |T_{1j}|^2$ of penetration through Truncated Coulomb (2) at $x_{\max} = 5$ (upper panel), and Coulomb-like (3) (lower panel), potential barriers: $x_{\min} = 0.1$, $m_1 = m_2 = 1$, left panel: $\hat{Z}_1 = \hat{Z}_2 = 0.5$, right panel: $\hat{Z}_1 = \hat{Z}_2 = 1$.

5 Conclusion

The BVP for the 2D Schrödinger equation with long-range potentials from the 2D plane is reduced to sets of the BVPs for the ODEs in a finite 2D domain with help of the presented symbolic algorithms for evaluation of asymptotics of solutions and effective potentials of the ODEs. The BVPs for the resulting system of equations containing effective potentials, which are calculated by program ODPEVP [6], are solved by the new version of program KANTBP 2.0 using high-order precision approximations of the FEM [7]. The computational efficiency of the SNAs proposed is demonstrated by the benchmark calculation of quantum transmittance of long-range barriers for composite particles. The further development of the SNAs and software for solving the BVPs of the Schrödinger equation with long-range potentials can serve as a useful tool to study quantum transparency effects not only in heavy ion physics but also in quantum chemistry [11] and atomic physics [12].

Authors thank Profs. F.M. Pen'kov and P.M. Krassovitskiy for useful discussion. This work was done within the framework of the Protocols No. 4028-3-10/12 of collaboration between JINR and INP (Almaty) in dynamics of few-body systems and quantum transparency of barriers for structure particles and ions. The work was supported partially by RFBR (grants 10-01-00200 and 11-01-00523).

References

1. Hofmann, H.: Quantum mechanical treatment of the penetration through a two-dimensional fission barrier. Nucl. Phys. A 224, 116–139 (1974)
2. Hagino, K., Rowley, N., Kruppa, A.T.: A program for coupled-channel calculations with all order couplings for heavy-ion fusion reactions. Comput. Phys. Commun. 123, 143–152 (1999)
3. Pen'kov, F.M.: Metastable states of a coupled pair on a repulsive barrier. Phys. Rev. A 62, 044701-1-4 (2000)
4. Pen'kov, F.M.: Quantum Transmittance of Barriers for Composite Particles. JETP 91, 698–705 (2000)
5. Kantorovich, L.V., Krylov, V.I.: Approximate Methods of Higher Analysis. Wiley, New York (1964)
6. Chuluunbaatar, O., Gusev, A.A., Vinitsky, S.I., Abrashkevich, A.G.: ODPEVP: A program for computing eigenvalues and eigenfunctions and their first derivatives with respect to the parameter of the parametric self-adjoined Sturm–Liouville problem. Comput. Phys. Commun. 180, 1358–1375 (2009)
7. Chuluunbaatar, O., Gusev, A.A., Vinitsky, S.I., Abrashkevich, A.G.: KANTBP 2. 0: New version of a program for computing energy levels, reaction matrix and radial wave functions in the coupled-channel hyperspherical adiabatic approach. Comput. Phys. Commun. 179, 685–693 (2008)
8. Chuluunbaatar, O., Gusev, A., Gerdt, V., Kaschiev, M., Rostovtsev, V., Samoylov, V., Tupikova, T., Vinitsky, S.: A Symbolic-numerical algorithm for solving the eigenvalue problem for a hydrogen atom in the magnetic field: cylindrical coordinates. In: Ganzha, V.G., Mayr, E.W., Vorozhtsov, E.V. (eds.) CASC 2007. LNCS, vol. 4770, pp. 118–133. Springer, Heidelberg (2007)
9. Abramowitz, M., Stegun, I.A.: Handbook of Mathematical Functions. Dover, New York (1965)
10. Barnett, A.R., Feng, D.H., Steed, J.W., Goldfarb, L.J.B.: Coulomb wave functions for all real η and ρ. Comput. Phys. Comm. 8, 377–395 (1974)
11. Goodvin, G.L., Shegelski, M.R.A.: Three-dimensional tunneling of a diatomic molecule incident upon a potential barrier. Phys. Rev. A 72, 042713-1-7 (2005)
12. Giannakeas, P., Melezhik, V.S., Schmelcher, P.: D-wave confinement-induced resonances in harmonic waveguides. arXiv:1102.5686v1 (2011)