UDC 517.958:530.145.6

KANTBP 3.0: New Version of a Program for Computing Energy Levels, Reflection and Transmission Matrices, and Corresponding Wave Functions in the Coupled-Channel Adiabatic Approach

A. A. Gusev*, **O. Chuluunbaatar**†, **S. I. Vinitsky***, **A. G. Abrashkevich**‡

* *Joint Institute for Nuclear Research*
6, Joliot-Curie, Dubna, Moscow region, Russia, 141980
† *School of Mathematics and Computer Science*
National University of Mongolia, Mongolia
‡ *IBM Toronto Lab,*
8200 Warden Avenue, Markham, ON L6G 1C7, Canada

Brief description of a FORTRAN 77 program for calculating energy values, refection and transmission matrices, and corresponding wave functions in a coupled-channel approximation of the adiabatic approach is presented. In this approach, a multidimensional Schrödinger equation is reduced to a system of the coupled second-order ordinary differential equations on a finite interval with the homogeneous boundary conditions of the third type at the left- and right-boundary points for continuous spectrum problem, or a set of first, second and third type boundary conditions for discrete spectrum problem. The resulting system of these equations containing the potential matrix elements and first-derivative coupling terms is solved using high-order accuracy approximations of the finite element method.

Key words and phrases: boundary value problem, multichannel scattering problem, finite element method, Kantorovich method.

1. Introduction

In this work we present a brief description of a KANTBP3 program for calculating with a required accuracy approximate eigensolutions of the continuum spectrum for systems of coupled differential equations on finite intervals of the variable $z \in [z_{\min}, z_{\max}]$ using a general homogeneous boundary condition of the third-type [1]. The third-type boundary conditions are formulated for problems under consideration by using known asymptotics for a set of linear independent asymptotic regular and irregular solutions in the open channels, and a set of linear independent regular asymptotic solutions in the closed channels, respectively [2]. These problems are solved by the finite element method [3, 4]. This approach can be used in calculations of effects of electron screening on low-energy fusion cross sections, channeling processes, threshold phenomena in the formation and ionization of (anti)hydrogen-like atoms and ions in magnetic traps, scattering problem for quantum dots and quantum wires in magnetic field, potential scattering with confinement potentials, penetration through a two-dimensional fission barrier, tunneling from false vacuum of two interacted particles and three-dimensional tunneling of a diatomic molecule incident upon a potential barrier [2, 5].

2. Statement of the Problem

In the Kantorovich method or close-coupling adiabatic approach, the multidimensional Schrödinger equation is reduced to a finite set of N ordinary second-order differential equations on the finite interval $[z_{\min}, z_{\max}]$ for the partial solution

Received 27$^{\text{th}}$ September, 2013.

The work was supported partially by grants 13-602-02 JINR, 11-01-00523 and 13-01-00668 RFBR..

$$\boldsymbol{\chi}^{(j)}(z) = \left(\chi_1^{(j)}(z), \ldots,\ \chi_N^{(j)}(z)\right)^T,$$

$$(\mathbf{L}-2E\,\mathbf{I})\boldsymbol{\chi}^{(j)}(z)=0,\ \mathbf{L}=-\mathbf{I}\frac{1}{z^{d-1}}\frac{\mathrm{d}}{\mathrm{d}z}z^{d-1}\frac{\mathrm{d}}{\mathrm{d}z}+\mathbf{V}(z)+\mathbf{Q}(z)\frac{\mathrm{d}}{\mathrm{d}z}+\frac{1}{z^{d-1}}\frac{\mathrm{d}\,z^{d-1}\,\mathbf{Q}(z)}{\mathrm{d}z}. \quad (1)$$

Here $\mathbf{I}$, $\mathbf{V}(z)$ and $\mathbf{Q}(z)$ are the unit, symmetric and antisymmetric $N \times N$ matrices, respectively. We assume that $\mathbf{V}(z)$ and $\mathbf{Q}(z)$ matrices have the following asymptotic behaviour at large $z = z_\pm \to \pm\infty$

$$V_{ij}(z_\pm) = \left(\epsilon_j + \frac{2Z_j^\pm}{z_\pm}\right)\delta_{ij} + \sum_{l=2}\frac{v_{ij}^{(l,\pm)}}{z_\pm^l}, \quad Q_{ij}(z_\pm) = \sum_{l=1}\frac{q_{ij}^{(l,\pm)}}{z_\pm^l}, \quad (2)$$

where $\epsilon_1 \leqslant \ldots \leqslant \epsilon_N$ are the threshold energy values.

In the present work, scattering problem is solved using the boundary conditions at $d = 1$, $z = z_{\min}$ and $z = z_{\max}$:

$$\left.\frac{\mathrm{d}\boldsymbol{\Phi}(z)}{\mathrm{d}z}\right|_{z=z_{\min}} = \mathcal{R}(z_{\min})\boldsymbol{\Phi}(z_{\min}), \quad \left.\frac{\mathrm{d}\boldsymbol{\Phi}(z)}{\mathrm{d}z}\right|_{z=z_{\max}} = \mathcal{R}(z_{\max})\boldsymbol{\Phi}(z_{\max}), \quad (3)$$

where $\mathcal{R}(z)$ is a unknown $N \times N$ matrix-function, $\boldsymbol{\Phi}(z) = \{\boldsymbol{\chi}^{(j)}(z)\}_{j=1}^{N_o}$ is the required $N \times N_o$ matrix-solution and N_o is the number of open channels, $N_o = \max_{2E \geqslant \epsilon_j} j \leqslant N$.

From this we obtain the quadratic functional at $d = 1$ (similar to Eq. (5) in [3])

$$\boldsymbol{\Xi}(\boldsymbol{\Phi}, E, z_{\min}, z_{\max}) \equiv \int\limits_{z_{\min}}^{z_{\max}} \boldsymbol{\Phi}^T(z)\,(\mathbf{L} - 2E\,\mathbf{I})\,\boldsymbol{\Phi}(z)\mathrm{d}z = \boldsymbol{\Pi}(\boldsymbol{\Phi}, E, z_{\min}, z_{\max}) - \\ - \boldsymbol{\Phi}^T(z_{\max})\mathbf{G}(z_{\max})\boldsymbol{\Phi}(z_{\max}) + \boldsymbol{\Phi}^T(z_{\min})\mathbf{G}(z_{\min})\boldsymbol{\Phi}(z_{\min}), \quad (4)$$

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

$$\boldsymbol{\Pi}(\boldsymbol{\Phi}, E, z_{\min}, z_{\max}) = \int\limits_{z_{\min}}^{z_{\max}} \left[\frac{\mathrm{d}\boldsymbol{\Phi}^T(z)}{\mathrm{d}z}\frac{\mathrm{d}\boldsymbol{\Phi}(z)}{\mathrm{d}z} + \boldsymbol{\Phi}^T(z)\mathbf{V}(z)\boldsymbol{\Phi}(z) + \right. \\ \left. + \boldsymbol{\Phi}^T(z)\mathbf{Q}(z)\frac{\mathrm{d}\boldsymbol{\Phi}(z)}{\mathrm{d}z} - \frac{\mathrm{d}\boldsymbol{\Phi}(z)^T}{\mathrm{d}z}\mathbf{Q}(z)\boldsymbol{\Phi}(z) - 2E\boldsymbol{\Phi}^T(z)\boldsymbol{\Phi}(z)\right]\mathrm{d}z, \quad (5)$$

and $\mathbf{G}(z) = \mathcal{R}(z) - \mathbf{Q}(z)$ is the $N \times N$ matrix-function which should be symmetric according to the conventual $\mathbf{R}$-matrix theory.

3. The Physical Scattering Asymptotic Forms

Matrix-solution $\boldsymbol{\Phi}_v(z) = \boldsymbol{\Phi}(z)$ describing the incidence of the particle and its scattering, which has the asymptotic form "incident wave + outgoing waves" is

$$\boldsymbol{\Phi}_v(z \to \pm\infty) = \begin{cases} \begin{cases} \mathbf{X}^{(+)}(z)\mathbf{T}_v, & z > 0, \\ \mathbf{X}^{(+)}(z) + \mathbf{X}^{(-)}(z)\mathbf{R}_v, & z < 0, \end{cases} & v = \to, \\ \begin{cases} \mathbf{X}^{(-)}(z) + \mathbf{X}^{(+)}(z)\mathbf{R}_v, & z > 0, \\ \mathbf{X}^{(-)}(z)\mathbf{T}_v, & z < 0, \end{cases} & v = \leftarrow, \end{cases} \quad (6)$$

where $\mathbf{R}_v$ and $\mathbf{T}_v$ are the reflection and transmission $N_o \times N_o$ matrices, $v =\rightarrow$ and $v =\leftarrow$ denote the initial direction of the particle motion along the z axis. Here the leading term of the asymptotic rectangle-matrix functions $\mathbf{X}^{(\pm)}(z)$ has the form [2]

$$X_{ij}^{(\pm)}(z) \to p_j^{-1/2} \exp\left(\pm\imath\left(p_j z - \frac{Z_j}{p_j}\ln(2p_j|z|)\right)\right)\delta_{ij}, \tag{7}$$

$$p_j = \sqrt{2E - \epsilon_j} \quad i = 1,\ldots,N, \quad j = 1,\ldots,N_o,$$

where $Z_j = Z_j^+$ at $z > 0$ and $Z_j = Z_j^-$ at $z < 0$.

The matrix-solution $\mathbf{\Phi}_v(z,E)$ is normalized by

$$\int\limits_{-\infty}^{\infty} \mathbf{\Phi}_{v'}^{\dagger}(z,E')\mathbf{\Phi}_v(z,E)\mathrm{d}z = 2\pi\delta(E'-E)\delta_{v'v}\mathbf{I}_{oo}, \tag{8}$$

where $\mathbf{I}_{oo}$ is the unit $N_o \times N_o$ matrix. Let us rewrite Eq. (6) in the matrix form at $z_+ \to +\infty$ and $z_- \to -\infty$ as

$$\begin{pmatrix} \mathbf{\Phi}_{\rightarrow}(z_+) & \mathbf{\Phi}_{\leftarrow}(z_+) \\ \mathbf{\Phi}_{\rightarrow}(z_-) & \mathbf{\Phi}_{\leftarrow}(z_-) \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \mathbf{X}^{(-)}(z_+) \\ \mathbf{X}^{(+)}(z_-) & \mathbf{0} \end{pmatrix} + \begin{pmatrix} \mathbf{0} & \mathbf{X}^{(+)}(z_+) \\ \mathbf{X}^{(-)}(z_-) & \mathbf{0} \end{pmatrix}\mathbf{S}, \tag{9}$$

where the scattering matrix $\mathbf{S}$

$$\mathbf{S} = \begin{pmatrix} \mathbf{R}_{\rightarrow} & \mathbf{T}_{\leftarrow} \\ \mathbf{T}_{\rightarrow} & \mathbf{R}_{\leftarrow} \end{pmatrix} \tag{10}$$

is composed of the reflection and transmission matrices.

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

$$\mathbf{Wr}(\mathbf{Q}(z);\mathbf{X}^{(\mp)}(z),\mathbf{X}^{(\pm)}(z)) = \pm 2\imath\mathbf{I}_{oo}, \ \mathbf{Wr}(\mathbf{Q}(z);\mathbf{X}^{(\pm)}(z),\mathbf{X}^{(\pm)}(z)) = \mathbf{0}, \tag{11}$$

where

$$\mathbf{Wr}(\bullet;\mathbf{a}(z),\mathbf{b}(z)) = \mathbf{a}^T(z)\left(\frac{\mathrm{d}\mathbf{b}(z)}{\mathrm{d}z} - \bullet\mathbf{b}(z)\right) - \left(\frac{\mathrm{d}\mathbf{a}(z)}{\mathrm{d}z} - \bullet\mathbf{a}(z)\right)^T\mathbf{b}(z). \tag{12}$$

This Wronskian is used to estimate a desirable accuracy of the above expansion.

Note, using a wronskian, we obtain the following properties of the reflection and transmission matrices:

$$\begin{gathered} \mathbf{T}_{\rightarrow}^{\dagger}\mathbf{T}_{\rightarrow} + \mathbf{R}_{\rightarrow}^{\dagger}\mathbf{R}_{\rightarrow} = \mathbf{I}_{oo} = \mathbf{T}_{\leftarrow}^{\dagger}\mathbf{T}_{\leftarrow} + \mathbf{R}_{\leftarrow}^{\dagger}\mathbf{R}_{\leftarrow}, \\ \mathbf{T}_{\rightarrow}^{\dagger}\mathbf{R}_{\leftarrow} + \mathbf{R}_{\rightarrow}^{\dagger}\mathbf{T}_{\leftarrow} = \mathbf{0} = \mathbf{R}_{\leftarrow}^{\dagger}\mathbf{T}_{\rightarrow} + \mathbf{T}_{\leftarrow}^{\dagger}\mathbf{R}_{\rightarrow}, \\ \mathbf{T}_{\rightarrow}^{T} = \mathbf{T}_{\leftarrow}, \quad \mathbf{R}_{\rightarrow}^{T} = \mathbf{R}_{\rightarrow}, \quad \mathbf{R}_{\leftarrow}^{T} = \mathbf{R}_{\leftarrow}. \end{gathered} \tag{13}$$

This means that the scattering matrix (10) is symmetric and unitary.

4. Test Desk

We consider the boundary problem (1)–(3) with parameters $d = 1$, $\hat{Z}_1 = \hat{Z}_2 = 0.1$, $m_1 = 1$, $m_2 = 3$, $s = 8$, $\bar{x}_{\min} = 0.1$. This problem is followed from Kantorovich expansion of the 2D BVP described the tunneling problem of transmission of two ions through repulsive barrier (for details, see [2])

$$\left(-\frac{\partial^2}{\partial y^2}-\frac{\partial^2}{\partial x^2}+x^2+U_1(x_1)+U_2(x_2)-\mathcal{E}\right)\Psi(x,y)=0, \qquad (14)$$

where $U_i(x_i)=2\hat{Z}_i/\sqrt[s]{|x_i|^s+\bar{x}^s_{\min}}$ are Coulomb-like barrier potentials, $x_1=s_2y+s_1x$ and $x_2=s_2y-s_3x$ are Jacobi coordinates with $s_1=m_1/M$, $s_3=m_2/M$, $s_2=\sqrt{m_1m_2}/M$, $s_2=\sqrt{\dfrac{\mu}{M}}$, $M=m_1+m_2$.

The required asymptotics of regular and irregular solutions given in [2]. The following values of numerical parameters and characters described in [1] have been used in the test run via the supplied input file SQRTBT.INP

```
&PARAS TITLE='  REFLECTION AND TRANSMISSION MATRICES  ',
       IPTYPE=1,NROOT=1,MDIM=4,IDIM=1,NPOL=4,
       SHIFT= 4D0,IPRINT=1,IPRSTP=120,
       NMESH=7,RMESH=-25D0,100D0,-6D0,100D0,6D0,100D0,25D0,
       NDIR=1, NDIL=4, NMDIL=0,THRSHL= 1.D0,3D0,5D0,7D0,IBOUND=8,
       FNOUT='KANTBP.LPR',IOUT=7,POTEN='ODPEVP.PTN',IOUP=10,
       FMATR='KANTBP.MAT',IOUM=11,EVWFN='KANTBP.WFN',IOUF=0
&END
```

Boundary problem (14) and the corresponding matrix elements $\mathbf{V}(y)$, $\mathbf{Q}(y)$ have been solved by the ODPEVP program [6] on grids $\Omega_x\{x_{\min},x_{\max}\}=\{-x_{\min}(64)x_{\max}\}$ with accuracy $eps=10^{-10}$. Boundary points are $x_{\max}=-x_{\min}=8.1$. All calculation details of this problem were written into file ODPEVP.LPR.

TEST RUN OUTPUT

```
 PROBLEM:   REFLECTION AND TRANSMISSION MATRICES
 ********
              C O N T R O L   I N F O R M A T I O N
              ------------------------------------

     NUMBER OF DIFFERENTIAL EQUATIONS. . . . . (MDIM  ) =      4
     NUMBER OF FINITE ELEMENTS . . . . . . . . (NELEM ) =    300
     NUMBER OF GRID POINTS . . . . . . . . . . (NGRID ) =   1201
     ORDER OF SHAPE FUNCTIONS. . . . . . . . . (NPOL  ) =      4
     ORDER OF GAUSS-LEGENDRE QUADRATURE. . . . (NGQ   ) =      5
     DIMENSION OF ENVELOPE SPACE . . . . . . . (IDIM  ) =      1
     BOUNDARY CONDITION CODE . . . . . . . . . (IBOUND) =      8
     DOUBLE ENERGY SPECTRUM. . . . . . . . . . (SHIFT ) =    4.00000

    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      -25.000   0.19000   0.04750    -6.000
     2       100       -6.000   0.12000   0.03000     6.000
     3       100        6.000   0.19000   0.04750    25.000

              T O T A L   S Y S T E M   D A T A
              -------------------------------
     TOTAL NUMBER OF ALGEBRAIC EQUATIONS. . . . (NN ) =     4804
     TOTAL NUMBER OF MATRIX ELEMENTS. . . . . . (NWK) =    60010
     MAXIMUM HALF BANDWIDTH . . . . . . . . . . (MK ) =       20
     MEAN    HALF BANDWIDTH . . . . . . . . . . (MMK) =       12
```

```
     NDIM, MDIM=         4         4
********************************************************************************

     CALCULATION OF WAVE FUNCTION WITH DIRECTION <--

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

     NUMBER OF OPEN CHANNELS. . . . . . . . . (NOPEN) =      2
     VALUE OF I-TH MOMENTUM . . . . . . . . . (I,QR ) =      1  0.1732E+01
     VALUE OF I-TH MOMENTUM . . . . . . . . . (I,QR ) =      2  0.1000E+01

           I M  P A R T:  W R O N S K I A N
         ---------------------------------
  -2.00000     -.168196E-08
  -.168196E-08 -2.00000

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

            R E  P A R T:  RR M A T R I X
          -----------------------------------
  -.194759     -.590855E-03
  -.590855E-03 -.485377E-01

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

            I M  P A R T:  RR M A T R I X
          -----------------------------------
  -.124681     0.172716
  0.172716     0.931470

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

            R E  P A R T:  TT M A T R I X
          -----------------------------------
  0.600459     -.317924E-01
  0.317924E-01 -.276468

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

            I M  P A R T:  TT M A T R I X
          -----------------------------------
  -.729781     0.150166
  -.150166     0.134581E-01

********************************************************************************
      Z       R E  P A R T:   F U N C T I O N S
      -       --------------------------------

  -25.0000  0.6664D+00 -.1165D+00 0.1531D+00 -.1120D+00 0.7601D-06 0.8680D-05 0.2445D-07 0.4751D-06
  -13.6000  0.6802D+00 -.7978D-01 0.4223D-01 0.2431D+00 -.2701D-04 0.3867D-04 -.2948D-05 0.3128D-05
   -3.6000  0.1490D-01 -.5461D-01 -.3718D-01 -.2780D+00 -.9230D-02 0.2404D-02 -.1299D-02 -.2425D-03
    0.0000  -.8416D+00 0.7861D-01 0.9335D-02 0.4446D+00 0.5115D-01 -.1732D-01 -.2247D-02 -.6850D-02
    3.6000  -.4115D+00 -.6691D-01 0.8351D-01 0.1351D+01 -.4630D-02 0.2048D-01 -.2890D-04 -.9308D-04
   13.6000  0.5769D+00 -.6829D-01 -.8088D-01 -.1298D+01 -.3777D-04 -.5932D-04 0.3999D-05 0.9632D-05
   25.0000  0.2716D+00 -.1259D+00 -.1631D+00 -.5370D+00 0.1506D-05 0.4406D-04 -.6915D-07 -.2284D-05

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

      Z       I M  P A R T:   F U N C T I O N S
      -       --------------------------------

  -25.0000  0.2735D+00 0.1055D-01 -.2391D-01 -.2560D+00 0.6563D-05 -.4645D-05 0.3403D-06 -.2162D-06
  -13.6000  -.2428D+00 0.8603D-01 0.1506D+00 -.1425D+00 0.2784D-04 0.5248D-04 0.2187D-05 0.5597D-05
   -3.6000  0.7372D+00 -.1083D+00 -.1518D+00 0.1221D+00 0.1107D-02 -.5541D-02 -.1592D-02 -.3799D-03
    0.0000  0.5262D+00 -.1487D+00 -.1846D-01 0.6235D+00 -.3508D-01 -.4223D-03 -.5965D-02 -.9388D-02
    3.6000  -.5284D+00 -.8131D-01 0.1780D+00 0.1380D+01 0.1289D-01 0.1938D-01 -.2320D-02 0.4662D-04
   13.6000  -.5507D+00 0.1129D+00 -.1559D+00 -.1335D+01 0.6059D-05 -.8405D-04 -.3894D-06 0.1222D-04
   25.0000  -.8982D+00 0.3837D-01 0.6149D-01 -.6546D+00 0.5103D-05 0.4498D-04 -.2851D-06 -.2320D-05

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

```
     CALCULATION OF WAVE FUNCTION WITH DIRECTION -->

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

     NUMBER OF OPEN CHANNELS. . . . . . . . . (NOPEN) =      2
     VALUE OF I-TH MOMENTUM . . . . . . . . . (I,QR ) =      1  0.1732E+01
     VALUE OF I-TH MOMENTUM . . . . . . . . . (I,QR ) =      2  0.1000E+01

           I M  P A R T:  W R O N S K I A N
          ----------------------------------
   2.00000     -.168196E-08
  -.168196E-08  2.00000

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

            R E  P A R T:  RR M A T R I X
          ------------------------------------
  -.194759     0.590855E-03
  0.590855E-03 -.485377E-01

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

            I M  P A R T:  RR M A T R I X
          ------------------------------------
  -.124681     -.172716
  -.172716     0.931470

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

            R E  P A R T:  TT M A T R I X
          ------------------------------------
  0.600459     0.317924E-01
  -.317924E-01 -.276468

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

            I M  P A R T:  TT M A T R I X
          ------------------------------------
  -.729781     -.150166
  0.150166     0.134581E-01

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

      Z       R E  P A R T:   F U N C T I O N S
      -       --------------------------------

   -25.0000  0.2716D+00 0.1259D+00 0.1631D+00 -.5370D+00 0.1506D-05 -.4406D-04 0.6915D-07 -.2284D-05
   -13.6000  0.5769D+00 0.6829D-01 0.8088D-01 -.1298D+01 -.3777D-04 0.5932D-04 -.3999D-05 0.9632D-05
    -3.6000  -.4115D+00 0.6691D-01 -.8351D-01 0.1351D+01 -.4630D-02 -.2048D-01 0.2890D-04 -.9308D-04
     0.0000  -.8416D+00 -.7861D-01 -.9335D-02 0.4446D+00 0.5115D-01 0.1732D-01 0.2247D-02 -.6850D-02
     3.6000  0.1490D-01 0.5461D-01 0.3718D-01 -.2780D+00 -.9230D-02 -.2404D-02 0.1299D-02 -.2425D-03
    13.6000  0.6802D+00 0.7978D-01 -.4223D-01 0.2431D+00 -.2701D-04 -.3867D-04 0.2948D-05 0.3128D-05
    25.0000  0.6664D+00 0.1165D+00 -.1531D+00 -.1120D+00 0.7601D-06 -.8680D-05 -.2445D-07 0.4751D-06

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

      Z       I M  P A R T:   F U N C T I O N S
      -       --------------------------------

   -25.0000  -.8982D+00 -.3837D-01 -.6149D-01 -.6546D+00 0.5103D-05 -.4498D-04 0.2851D-06 -.2320D-05
   -13.6000  -.5507D+00 -.1129D+00 0.1559D+00 -.1335D+01 0.6059D-05 0.8405D-04 0.3894D-06 0.1222D-04
    -3.6000  -.5284D+00 0.8131D-01 -.1780D+00 0.1380D+01 0.1289D-01 -.1938D-01 0.2320D-02 0.4662D-04
     0.0000  0.5262D+00 0.1487D+00 0.1846D-01 0.6235D+00 -.3508D-01 0.4223D-03 0.5965D-02 -.9388D-02
     3.6000  0.7372D+00 0.1083D+00 0.1518D+00 0.1221D+00 0.1107D-02 0.5541D-02 0.1592D-02 -.3799D-03
    13.6000  -.2428D+00 -.8603D-01 -.1506D+00 -.1425D+00 0.2784D-04 -.5248D-04 -.2187D-05 0.5597D-05
    25.0000  0.2735D+00 -.1055D-01 0.2391D-01 -.2560D+00 0.6563D-05 0.4645D-05 -.3403D-06 -.2162D-06

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

              C H E C K   P R O P E R T I E S
```

```
          ----------------------------------------
********************************************************************************

             C H E C K |RR_<-|^2 + |TT_<-|^2
          -------------------------------------
   1.00000      0.242339E-09
  0.242339E-09  1.00000

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

             C H E C K |RR_->|^2 + |TT_->|^2
          -------------------------------------
   1.00000      -.407011E-09
  -.407011E-09  1.00000

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

            R E  P A R T:  TT_->^1 * RR_<- + RR_->^1 * TT_<-
          ----------------------------------------------------
  0.185469E-09 0.420999E-09
  -.476236E-09 0.157399E-09

            I M  P A R T:  TT_->^1 * RR_<- + RR_->^1 * TT_<-
          ----------------------------------------------------
  0.219235E-11 -.125379E-09
  -.197244E-09 0.129723E-10

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

            R E  P A R T:  RR_<-^T - RR_<-
          ----------------------------------
   0.00000      -.185546E-09
  0.185546E-09  0.00000

            I M  P A R T:  RR_<-^T - RR_<-
          ----------------------------------
   0.00000      0.356981E-09
  -.356981E-09  0.00000

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

            R E  P A R T:  RR_->^T - RR_->
          ----------------------------------
   0.00000      0.103188E-09
  -.103188E-09  0.00000

           I M  P A R T:  RR_->^T - RR_->
          ----------------------------------
   0.00000      -.533526E-09
  0.533526E-09  0.00000

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

            R E  P A R T:  TT_->^T - TT_<-
          ----------------------------------
  0.231348E-10 0.847061E-10
  -.952086E-13 0.142655E-10

            I M  P A R T:  TT_->^T - TT_<-
          ----------------------------------
  0.186473E-11 0.452252E-09
  0.511466E-09 -.116038E-10
********************************************************************************
```

References

1. A Program Package for Solution of Two-Dimensional Discrete and Continuum Spectra Boundary-Value Problems in Kantorovich (Adiabatic) Approach / O. Chuluunbaatar, A. A. Gusev, S. I. Vinitsky, A. G. Abrashkevich // JINR Lib. — 2013. — http://wwwinfo.jinr.ru/programs/jinrlib/kantbp/indexe.html.
2. Symbolic-Numerical Algorithms to Solve the Quantum Tunneling Problem for a Coupled Pair of Ions / A. A. Gusev, S. I. Vinitsky, O. Chuluunbaatar et al. // Lecture Notes in Computer Science. — 2011. — Vol. 6885. — Pp. 175–191.
3. KANTBP: A Program for Computing Energy Levels, Reaction Matrix and Radial Wave Functions in the Coupled-Channel Hyperspherical Adiabatic Approach / O. Chuluunbaatar, A. A. Gusev, A. G. Abrashkevich et al. // Comput. Phys. Commun. — 2007. — Vol. 177. — Pp. 649–675.
4. 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 / O. Chuluunbaatar, A. A. Gusev, S. I. Vinitsky, A. G. Abrashkevich // Comput. Phys. Commun. — 2008. — Vol. 179. — Pp. 685–693.
5. Symbolic-Numerical Algorithm for Generating Cluster Eigenfunctions: Tunneling of Clusters Through Repulsive Barriers / A. A. Gusev, S. I. Vinitsky, O. Chuluunbaatar et al. // Lecture Notes in Computer Science. — 2013. — Vol. 8136. — Pp. 427–442.
6. 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 / O. Chuluunbaatar, A. A. Gusev, S. I. Vinitsky, A. G. Abrashkevich // Comput. Phys. Commun. — 2009. — Vol. 180, No 8. — Pp. 1358–1375.

УДК 517.958:530.145.6

KANTBP 3.0: новая версия программы для вычисления энергетических уровней, матриц амплитуд отражения и прохождения и соответствующих волновых функций в адиабатическом подходе со связанными каналами

А. А. Гусев*, О. Чулуунбаатар†, С. И. Виницкий*, А. Г. Абрашкевич‡

* *Объединённый институт ядерных исследований*
ул. Жолио-Кюри, д. 6, г. Дубна, Московская область, Россия, 141980
† *Факультет математики и компьютерных наук*
Монгольский государственный университет, Монголия
‡ *Лаборатории IBM в Торонто*
8200 Ворден авеню, Маркхэм, ON L6G 1C7, Канада

Представлено краткое описание программ на языке Фортран 77 для вычисления энергетических уровней, матриц амплитуд отражения и прохождения и соответствующих волновых функций в адиабатическом подходе со связанными каналами. В этом подходе многомерное уравнение Шрёдингера сводится к системе связанных обыкновенных дифференциальных уравнений второго порядка на конечном интервале с однородными граничными условиями третьего рода на левой и правой граничных точках для задачи непрерывного спектра или набора граничных условий первого, второго и третьего рода для задачи дискретного спектра. Полученная система уравнений, содержащая матричные потенциалы, а также связанная слагаемыми, содержащими первые производные, решается в приближении высокого порядка точности методом конечных элементов.

Ключевые слова: краевая задача, многоканальная задача рассеяния, метод конечных элементов, метод Канторовича.