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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 [☆]

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ARTICLE INFO

Article history:

Received 28 December 2007
 Received in revised form 6 June 2008
 Accepted 12 June 2008
 Available online 17 June 2008

PACS:

02.30.Hq
 02.60.Jh
 02.60.Lj
 03.65.Nk
 31.15.Ja
 31.15.Pf
 34.50.-s
 34.80.Bm

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

ABSTRACT

A FORTRAN 77 program for calculating energy values, reaction matrix and corresponding radial wave functions in a coupled-channel approximation of the hyperspherical adiabatic approach is presented. In this approach, a multi-dimensional Schrödinger equation is reduced to a system of the coupled second-order ordinary differential equations on a finite interval with homogeneous boundary conditions: (i) the Dirichlet, Neumann and third type at the left and right boundary points for continuous spectrum problem, (ii) the Dirichlet and Neumann type conditions at left boundary point and Dirichlet, Neumann and third type at the right boundary point for the discrete spectrum problem. The resulting system of radial equations containing 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 reaction matrix and radial wave functions for 3D-model of a hydrogen-like atom in a homogeneous magnetic field. This version extends the previous version 1.0 of the KANTBP program [O. Chuluunbaatar, A.A. Gusev, A.G. Abrashkevich, A. Amaya-Tapia, M.S. Kaschiev, S.Y. Larsen, S.I. Vinitzky, Comput. Phys. Commun. 177 (2007) 649–675].

Program summary

Program title: KANTBP

Catalogue identifier: ADZH_v2_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADZH_v2_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.: 20 403

No. of bytes in distributed program, including test data, etc.: 147 563

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: This depends on

1. the number of differential equations;
2. the number and order of finite elements;
3. the number of hyperradial points; and
4. the number of eigensolutions required.

The test run requires 2 MB

Classification: 2.1, 2.4

External routines: GAULEG and GAUSSJ [2]

Nature of problem: In the hyperspherical adiabatic approach [3–5], a multidimensional Schrödinger equation for a two-electron system [6] or a hydrogen atom in magnetic field [7–9] is reduced by

[☆] 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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separating radial coordinate ρ from the angular variables to a system of the second-order ordinary differential equations containing the 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 of the continuum spectrum for such systems of coupled differential equations on finite intervals of the radial variable $\rho \in [\rho_{\min}, \rho_{\max}]$. This approach can be used in the calculations of effects of electron screening on low-energy fusion cross sections [10–12].

Solution method: The boundary problems for the coupled second-order differential equations are solved by the finite element method using high-order accuracy approximations [13]. The generalized algebraic eigenvalue problem $\mathbf{A}\mathbf{F} = \mathbf{E}\mathbf{B}\mathbf{F}$ 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 [14]. The generalized algebraic eigenvalue problem $(\mathbf{A} - \mathbf{E}\mathbf{B})\mathbf{F} = \lambda\mathbf{D}\mathbf{F}$ with respect to pair unknowns (λ, \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}^T factorization of symmetric matrix and back-substitution methods using the DECOMP and REDBAK programs, respectively [14]. As a test desk, the program is applied to the calculation of the reaction matrix and corresponding radial wave functions for 3D-model of a hydrogen-like atom in a homogeneous magnetic field described in [9] on finite intervals of the radial variable $\rho \in [\rho_{\min}, \rho_{\max}]$. For this benchmark model the required analytical expressions for asymptotics of the potential matrix elements and first-derivative coupling terms, and also 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:

1. the number of differential equations;
2. the number and order of finite elements;
3. the total number of hyperradial points; and
4. the number of eigensolutions required.

Restrictions due to dimension sizes may be easily alleviated by altering PARAMETER statements (see Section 3 and [1] for details). The user must also supply subroutine POTCAL for evaluating potential matrix elements. The user should also supply subroutines ASYMEV (when solving the eigenvalue problem) or ASYMSO and ASYMSC (when solving the scattering problem) which evaluate asymptotics of the radial wave functions at left and right boundary points in case of a boundary condition of the third type for the above problems.

Running time: The running time depends critically upon:

1. the number of differential equations;
2. the number and order of finite elements;
3. the total number of hyperradial points on interval $[\rho_{\min}, \rho_{\max}]$; and
4. the number of eigensolutions required.

The test run which accompanies this paper took 2 s without calculation of matrix potentials on the Intel Pentium IV 2.4 GHz.

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1. Introduction

In our previous paper [1] we have described the finite element method procedure based on the use of high-order accuracy approximations for calculating approximate eigensolutions of the discrete and continuum spectrum for systems of coupled differential equations on

a finite interval of the radial variable $\rho \in [\rho_{\min}, \rho_{\max}]$ with homogeneous boundary conditions: the Dirichlet, Neumann type at $\rho = \rho_{\min}$; the Dirichlet, Neumann and third type at $\rho = \rho_{\max}$.

The purpose of this paper is to extend the framework of work [1] for calculating approximate eigensolutions of the continuum spectrum for systems of coupled differential equations on finite intervals of the radial variable $\rho \in [\rho_{\min}, \rho_{\max}]$ using a general homogeneous boundary condition of the third type at $\rho = \rho_{\min}$. The third-type boundary conditions at $\rho = \rho_{\min}$ are formulated by using known asymptotics for a set of linear independent regular solutions for problems under consideration [2–9]. This approach can be used in calculations of effects of electron screening on low-energy fusion cross sections [10–13], channeling processes [14,15], threshold phenomena in the formation and ionization of (anti)hydrogen-like atoms and ions in magnetic traps [16], quantum dots in magnetic field [17–19] and potential scattering with confinement potentials [20].

The paper is organized as follows. In Section 2 we give a brief overview of the problem. A description of the new version of the KANTBP program is given in Section 3. Example of the asymptotic expansions of matrix elements and regular solutions at small ρ together with Test desk are discussed in Section 4.

2. Statement of the problem

In the Kantorovich approach [21], the d -dimensional Schrödinger equation is reduced to a finite set of N ordinary second-order differential equations on the finite interval $[\rho_{\min}, \rho_{\max}]$ for the partial solution $\chi(\rho) \equiv \chi^{(i)}(\rho) = (\chi_1^{(i)}(\rho), \dots, \chi_N^{(i)}(\rho))^T$

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

Here \mathbf{I} , $\mathbf{V}(\rho)$ and $\mathbf{Q}(\rho)$ are the unit, symmetric and antisymmetric matrices of dimension $N \times N$, respectively.

In the present work, scattering problem is solved using the homogeneous third type boundary conditions at $\rho = \rho_{\min} > 0$ and $\rho = \rho_{\max} \gg 1$:

$$\frac{d\Phi(\rho)}{d\rho} = \mathbf{R}(\rho)\Phi(\rho), \quad (2)$$

where $\Phi(\rho) = \{\chi^{(i)}(\rho)\}_{i=1}^{N_0}$ is the required matrix-solution of dimension $N \times N_0$ and N_0 is the number of open channels. Suppose that a set of linear independent regular solutions $\tilde{\Phi}_{\text{reg}}(\rho) = \{\tilde{\chi}_{\text{reg}}^{(i)}(\rho)\}_{i=1}^N$ for a problem under consideration with components $\tilde{\chi}_{\text{reg}}^{(i)}(\rho) = (\tilde{\chi}_{1i}^{\text{reg}}(\rho), \dots, \tilde{\chi}_{Ni}^{\text{reg}}(\rho))^T$ is known at small ρ (see, e.g., [2–9,16,22]).

Using a linear combination of these regular solutions, $\tilde{\chi}_{\text{reg}}^{(i)}(\rho)$, we can find required matrix solution $\Phi(\rho)$ at $\rho = \rho_{\min} > 0$:

$$\Phi(\rho) = \tilde{\Phi}_{\text{reg}}(\rho)\mathbf{C}, \quad (3)$$

where \mathbf{C} is the unknown nonzero constant matrix of dimension $N \times N_0$. Using identity $\mathbf{C}\mathbf{C}^{-1} = \mathbf{I}$, the $\mathbf{R}(\rho)$ matrix at $\rho = \rho_{\min}$ can be easily found via the known set of linear independent regular solutions $\tilde{\Phi}_{\text{reg}}(\rho)$

$$\mathbf{R}(\rho) \equiv \frac{d\tilde{\Phi}_{\text{reg}}(\rho)}{d\rho} \tilde{\Phi}_{\text{reg}}^{-1}(\rho) = \frac{d\Phi(\rho)}{d\rho} \Phi^{-1}(\rho). \quad (4)$$

From this we obtain the quadratic functional (compare with Eq. (23) in [1])

$$\begin{aligned} \Xi(\Phi, E, \rho_{\min}, \rho_{\max}) &\equiv \int_{\rho_{\min}}^{\rho_{\max}} \Phi^T(\rho) (\mathbf{L} - 2E\mathbf{I}) \Phi(\rho) \rho^{d-1} d\rho \\ &= \Pi(\Phi, E, \rho_{\min}, \rho_{\max}) - \rho_{\max}^{d-1} \Phi^T(\rho_{\max}) \mathbf{G}(\rho_{\max}) \Phi(\rho_{\max}), \end{aligned} \quad (5)$$

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

$$\begin{aligned} \Pi(\Phi, E, \rho_{\min}, \rho_{\max}) &= \int_{\rho_{\min}}^{\rho_{\max}} \left[\frac{d\Phi^T(\rho)}{d\rho} \frac{d\Phi(\rho)}{d\rho} + \Phi^T(\rho) \mathbf{V}(\rho) \Phi(\rho) \right. \\ &\quad \left. + \Phi^T(\rho) \mathbf{Q}(\rho) \frac{d\Phi(\rho)}{d\rho} - \frac{d\Phi(\rho)^T}{d\rho} \mathbf{Q}(\rho) \Phi(\rho) - 2E\Phi^T(\rho) \Phi(\rho) \right] \rho^{d-1} d\rho \\ &\quad + \rho_{\min}^{d-1} \Phi^T(\rho_{\min}) \mathbf{G}(\rho_{\min}) \Phi(\rho_{\min}), \end{aligned} \quad (6)$$

and $\mathbf{G}(\rho) = \mathbf{R}(\rho) - \mathbf{Q}(\rho)$ is the matrix of dimension $N \times N$ which should be symmetric according to the conventional \mathbf{R} -matrix theory. The matrix $\mathbf{G}(\rho_{\max})$ is calculated by a procedure in the framework of the FEM described in our previous paper [1].

After numerical calculation of solution $\Phi(\rho)$ in the nodes of the finite element grid Ω on interval $[\rho_{\min}, \rho_{\max}]$ using scheme implemented in [1] which takes into account Eqs. (2)–(6), matrix \mathbf{C} can be evaluated by the formula

$$\mathbf{C} = \tilde{\Phi}_{\text{reg}}^{-1}(\rho_{\min}) \Phi(\rho_{\min}). \quad (7)$$

The matrix \mathbf{C} is applied for analysis of the matrix-solution $\Phi(\rho)$ in the vicinity of $\rho = 0$. For example, constant matrix \mathbf{C} satisfies ratio $\tilde{\Phi}_{\text{reg}}^{-1}(0)\Phi(0)$ even if $\Phi(0) \equiv \mathbf{0}$ or is very close to zero. To extract required matrix \mathbf{C} in later case, a user can use known asymptotics of the regular solutions at ρ_{\min} . Value ρ_{\min} is defined on the asymptotic domain of the $\tilde{\Phi}_{\text{reg}}(\rho)$.

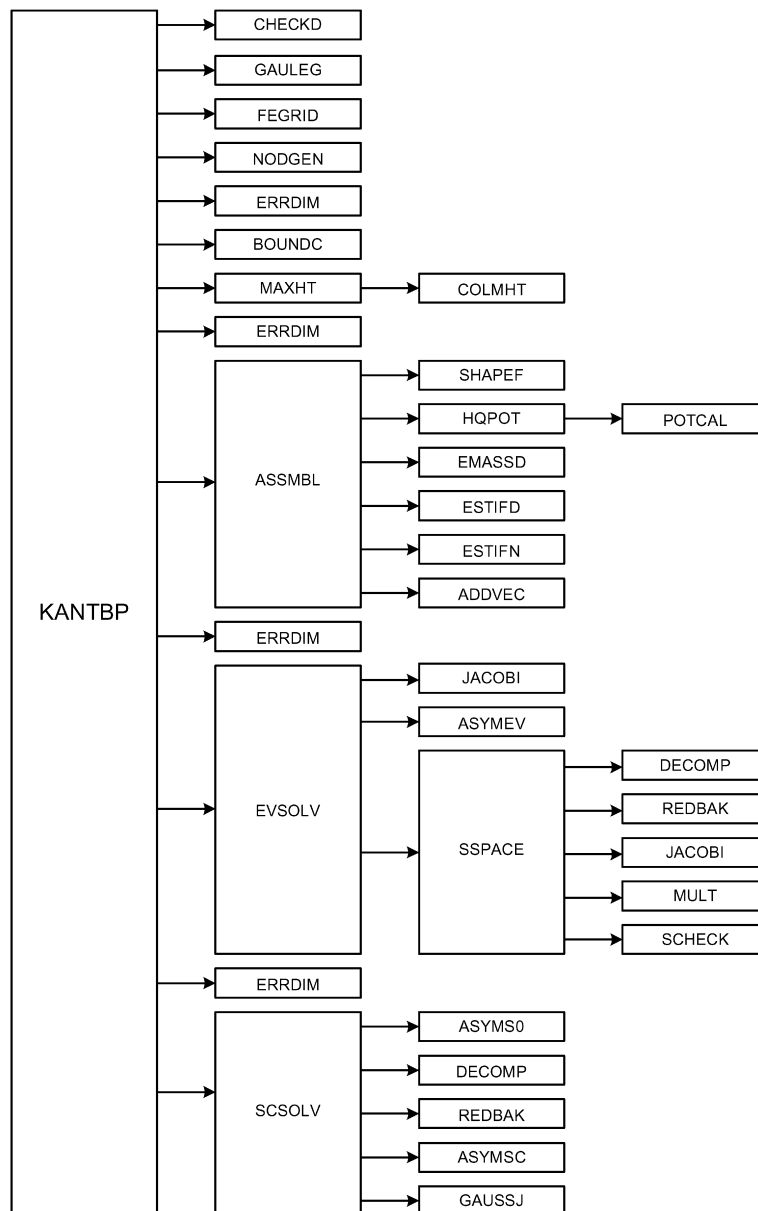


Fig. 1. Flow diagram of the new version of the KANTBP program.

3. Description of the program

Fig. 1 presents a flow diagram for the new version of the KANTBP program. The function of each subroutine except for a new user-supplied subroutine ASYMS0 is described in [1]. 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 ≥ 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, FNOU, IOU, POTEN, IOUP, FMATR, IOUM,
3          EVWFN, IOUF, TOT, ITOT, MTOT, MITOT)
```

A new user-supplied subroutine ASYMSO for calculating the regular asymptotic matrix-solution and its derivative at $\rho = \rho_{\min}$ has been added to the scattering problem solver program. It should be written as follows:

```
SUBROUTINE ASYMSO (RMIN, NDIM, SHIFT, NOPEN, QR, PREG, DREG, IOU)
C . . . . .
C .
C .   P R O G R A M
C .
C .   TO CALCULATE THE REGULAR ASYMPTOTIC MATRIX
C .   SOLUTION PREG AND ITS DERIVATIVE DREG
C .   AT RMIN
C .
C .
C . . . . .
IMPLICIT REAL*8 (A-H, O-Z)
DIMENSION QR (NOPEN), PREG (NDIM, NDIM), DREG (NDIM, NDIM)
RETURN
END
```

Here array QR contains a set of momentum values, SHIFT contains the given double energy spectrum value, and NOPEN is the number of open channels. To set the third type boundary conditions at both points ρ_{\min} and ρ_{\max} , flag IBOUND always should be 8. Other parameters used in the ASYMSO and also input and output data for the KANTBP program are described in [1].

4. Test desk

4.1. Asymptotic expansions of the matrix elements at small ρ

The test run which accompanies the KANTBP program computes the reaction matrix and corresponding radial wave functions for 3D-model of a hydrogen-like atom in a homogeneous magnetic field [22]. According to [16], asymptotic values of the potential curves $E_j(\rho)$, radial matrix elements $H_{jj'}(\rho)$ and $Q_{jj'}(\rho)$ at small ρ in Eq. (1) describing a hydrogen atom in a homogeneous magnetic field characterized by $l = 2j - 2 + |m|$ for even states ($\sigma = +1$) and $l = 2j - 1 + |m|$ for odd states ($\sigma = -1$) are given by expansion in powers of ρ with finite l, l'

$$E_j(\rho) = \bar{E}_j^{(0)} + \bar{E}_j^{(2)}\rho^2 + \sum_{k=1}^{[k_{\max}/4]} \rho^{4k} \bar{E}_j^{(4k)}, \quad H_{jj'}(\rho) = \sum_{k=2}^{[k_{\max}/4]} \rho^{4k-2} \bar{H}_{jj'}^{(4k-2)},$$

$$Q_{jj'}(\rho) = \sum_{k=1}^{[k_{\max}/4]} \rho^{4k-1} \bar{Q}_{jj'}^{(4k-1)}, \quad \rho \ll \min(l, l')/\sqrt{4\gamma}. \tag{8}$$

Note, that all

$$\bar{Q}_{jj'}^{(4k-1)} \equiv 0 \quad \text{and} \quad \bar{H}_{jj'}^{(4k-2)} \equiv 0 \quad \text{if} \quad |j - j'| > 2k. \tag{9}$$

In this work, the calculations of the above matrix elements were performed using algorithm implemented in MAPLE up to $k_{\max} = 16$. Below we present the first several coefficients of the matrix elements expansions:

$$\bar{E}_j^{(0)} = l(l+1), \quad \bar{E}_j^{(2)} = \gamma m, \quad \bar{E}_j^{(4)} = \frac{\gamma^2}{2} \frac{l^2 + l - 1 + m^2}{(2l-1)(2l+3)},$$

$$\bar{Q}_{jj+2}^{(3)} = \frac{\gamma^2}{2} \frac{\sqrt{(l+1)^2 - m^2} \sqrt{(l+2)^2 - m^2}}{\sqrt{2l+1}(2l+3)^2 \sqrt{2l+5}},$$

$$\bar{H}_{jj}^{(6)} = \frac{\gamma^4}{2} ((16l^4 + 32l^3 + 248l^2 + 232l + 201)m^4 + (-10l^2 - 224l^4 - 96l^5 + 118l - 288l^3 - 32l^6 - 195)m^2 + 16l^8 + 64l^7 + 46l + 40l^6 - 127l^4 - 104l^5 + 71l^2 - 6l^3 - 6) / ((2l-3)(2l-1)^4(2l+3)^4(2l+5)),$$

$$\bar{H}_{jj+4}^{(6)} = \frac{-\gamma^4 \sqrt{(l+1)^2 - m^2} \sqrt{(l+2)^2 - m^2} \sqrt{(l+3)^2 - m^2} \sqrt{(l+4)^2 - m^2}}{4\sqrt{2l+1}(2l+3)^2(2l+5)(2l+7)^2 \sqrt{2l+9}}. \tag{10}$$

Such asymptotic behavior of the effective potentials on the interval $\rho \in [0, \rho_{\min}]$ allows us to find regular and bound solutions at $\rho \rightarrow 0$ that satisfy the homogeneous third type boundary conditions (2) at $\rho = \rho_{\min} > 0$.

4.2. Asymptotic expansions of the regular solutions at small ρ

The asymptotics of the regular solutions $\tilde{\chi}_{j_i, \text{reg}}^{(i_0)}(\rho) \equiv \tilde{\chi}_{j_i_0}(\rho)$, $j = 1, \dots, N$, $i_0 = 1, \dots, N$, of Eq. (1) are sought as expansions in powers of ρ up to the finite order k_{max}

$$\tilde{\chi}_{j_i, \text{reg}}(\rho) = \sum_{k=0}^{k_{\text{max}}} \tilde{\chi}_{j_i}^{(k)} \rho^{\mu_{i_0} + k}, \quad \tilde{\chi}_{j_i}^{(0)} = \delta_{ji}, \quad \tilde{\chi}_{j_i}^{(k < 0)} \equiv 0, \tag{11}$$

where μ_{i_0} is the unknown characteristic parameter. Substituting expansion (11) into (1) and taking into account Eqs. (8)–(10), we obtain the following system of recurrence relations for the set of the unknown coefficients $\tilde{\chi}_{j_i}^{(k)}$

$$\begin{aligned} & -(l' + 1 + \mu_{i_0} + k)(\mu_{i_0} - l' + k) \tilde{\chi}_{j_i}^{(k)} \\ & = 2Z \tilde{\chi}_{j_i}^{(k-1)} - (m\gamma - \epsilon) \tilde{\chi}_{j_i}^{(k-2)} - \sum_{s=4}^k \bar{E}_j^{(s)} \tilde{\chi}_{j_i}^{(k-s)} - \sum_{s=4}^{k-2} \bar{H}_{jj}^{(s)} \tilde{\chi}_{j_i}^{(k-s-2)} \\ & - \sum_{s=3}^{k-1} \sum_{j'=\max(1, i-[s/4]), j' \neq j}^{\min(j_{\text{max}}, i+[s/4])} (2l + 2k - s) \bar{Q}_{jj'}^{(s)} \tilde{\chi}_{j_i}^{(k-s-1)} - \sum_{s=4}^{k-2} \sum_{j'=\max(1, i-[s/4]), j' \neq j}^{\min(j_{\text{max}}, i+[s/4])} \bar{H}_{jj'}^{(s)} \tilde{\chi}_{j_i}^{(k-s-2)}, \end{aligned} \tag{12}$$

where indices l' and l are defined as

$$l' = 2(j - 1) + |m| + (1 - \sigma)/2, \quad l = 2(i - 1) + |m| + (1 - \sigma)/2. \tag{13}$$

As follows from Eqs. (11) and (12) at $k = 0$, the conventional characteristic equation gives two roots for the unknown μ_{i_0} : $\mu_{i_0} = -l - 1$ and $\mu_{i_0} = l$. Value $\mu_{i_0} = -l - 1$ corresponds to irregular unbound solutions and is not considered here. Value $\mu_{i_0} = l$ corresponds to the required regular and bound solutions and is the one we have used in our calculations.

Note that components of vector $\{\tilde{\chi}_{j_i}^{(k)}\}_{j=1}^N$ at fixed i in the left-hand side of Eq. (12) equal to zero if $2(j - i) = k$. In this case we can put $\tilde{\chi}_{i+k/2, i}^{(k)} = 0$ because this term will be determined as the leading term of the asymptotic form of the $(i + k/2)$ th solution. A more detailed analysis of (12) with the account of (9) shows that the right-hand side of Eq. (12) is equal to zero and all $\tilde{\chi}_{j_i}^{(k)}$ are equal to zero if $|j - i| > k/2$.

Thus, the system (12) can be solved sequentially for $k = 1, 2, \dots, k_{\text{max}}$. The calculation was performed using the algorithm implemented in MAPLE up to $k_{\text{max}} = 16$. Below we display the first several non-zero coefficients of the regular solutions expansions:

$$\begin{aligned} \tilde{\chi}_{ii}^{(0)} &= 1, \quad \tilde{\chi}_{ii}^{(1)} = -\frac{Z}{l+1}, \quad \tilde{\chi}_{ii}^{(2)} = -\frac{-2Z^2 + (\epsilon - m\gamma)(l+1)}{2(l+1)(2l+3)}, \\ \tilde{\chi}_{ii}^{(3)} &= \frac{Z(-2Z^2 + (\epsilon - m\gamma)(3l+4))}{6(l+1)(l+2)(2l+3)}, \\ \tilde{\chi}_{i-1i}^{(4)} &= \frac{\bar{Q}_{i-1i}^{(3)}(2l+5)}{6(2l+3)}, \\ \tilde{\chi}_{ii}^{(4)} &= \frac{\bar{E}_i^{(4)}}{4(2l+5)} + \frac{(\epsilon - m\gamma)^2}{8(2l+3)(2l+5)} + \frac{Z^4 - Z^2(\epsilon - m\gamma)(3l+5)}{6(l+1)(l+2)(2l+3)(2l+5)}, \\ \tilde{\chi}_{i+1i}^{(4)} &= \frac{\bar{Q}_{i+1i}^{(3)}(2l+5)}{2(2l+7)}. \end{aligned} \tag{14}$$

The test run which accompanies the KANTBP program computes the reaction matrix and corresponding radial wave functions for 3D-model of a hydrogen-like atom in a homogeneous magnetic field with $\sigma = -1$, $Z = 1$, $\gamma = 1$ and $m = 0$ on the finite intervals of the radial variable $\rho \in [\rho_{\text{min}} = 0.3, \rho_{\text{max}} = 100]$. All needed potential elements are calculated with the help of the POTHMF program [22]. The asymptotics from Eq. (11) and needed coefficients of the matrix elements (8) are included in the subroutine ASYMS0 up to $k_{\text{max}} = 16$.

File 'INPUT2.INP' contains the initial data NAMELIST POTDAT for the calculation of the potential matrix elements for the given atomic state by the POTHMF program. Also this file contains the initial data NAMELIST PARSCP for the calculation of the reaction matrix and corresponding radial wave functions for the KANTBP program. File 'INPUT2.INP' contains the following data:

```
&POTDAT TITLE=' Potential and dipole matrices elements ',
IMATRX=1, IDIPOL=0, IFUNAS=15, WC=0.1D1, CHARGE=1.D0, MDIM=6,
NPOL=4, SHIFTS=3.4D0, IPRINT=1, IPRSTP=1501,
RMESH=0.3D0, 180.D0, 3.D0, 200.D0, 20.D0, 200.D0, 100.D0,
FNOUTP=' FNOUTP.LPR ', IOUPL=7, NMESH=7, NMESH=7,
IPARTL=1, MQNL=0, POTENL=' POTENL.PTN ', IOUPL=8,
WFUNAS=' WFUNAS.PTN ', IOUWF=0
&END
&PARSCP TITLE2=' Reaction matrix ',
IPTYPE=1, NROOT=1, IDIM=3, SHIFTS=3.4D0, IPRINT=2, IPRSTP=400,
IBOUND=8, NDIR=1, NDIL=6, NMDIL=1,
```

```
THRSHL=1.D0,3.D0,5.D0,7.D0,9.D0,11.D0,
FNOU TL='3DNSSC.LPR',NOU T=14,FMATRL='3DNSSC.MAT',NOUM=15,
EVWFNL='3DNSSC.WFN',NOUF=2
```

&END

Physical parameters CHARGE, WC, MQNL, IPARTL and order of asymptotic solutions IFUNAS are accessed via general common block COMMON /CHARGE/ CHARGE, WC, MQNL, IPARTL, IFUNAS. As an example, calculation of matrix **C** is performed by means of Eq. (7) and presented in output file. Note, that values of the partial solutions $\chi_j^{(i)}(\rho)$ at $\rho = 0.3$ presented in the TEST RUN OUTPUT are equal to the corresponding results presented in the TEST RUN OUTPUT of [22] which verifies and confirms the accuracy of the developed calculation scheme.

Acknowledgements

The authors thank Profs. V.S. Melezhhik, V.V. Pupyshv, F.M. Pen'kov, M. Shapiro and Dr. P.M. Krassovitskiy for useful discussions. OC, SIV and AAG acknowledge financial support from a grant I-1402/2004-2007 of the Bulgarian Foundation for Scientific Investigations, grants RFBR 07-01-00660, RFBR 08-01-00604-a and the theme 09-6-1060-2005/2010 "Mathematical support of experimental and theoretical studies conducted by JINR".

Appendix A. TEST RUN OUTPUT

```
PROBLEM:      Reaction matrix
*****
```

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 ) =     580
NUMBER OF GRID POINTS . . . . . (NGRID ) =    2321
ORDER OF SHAPE FUNCTIONS. . . . . (NPOL ) =      4
ORDER OF GAUSS-LEGENDRE QUADRATURE. . . . (NGQ ) =      5
DIMENSION OF ENVELOPE SPACE . . . . . (IDIM ) =      3
BOUNDARY CONDITION CODE . . . . . (IBOUND) =      8
DOUBLE ENERGY SPECTRUM. . . . . (SHIFT ) =    3.40000
```

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

NO OF GROUP	NUMBER OF ELEMENTS	BEGIN OF INTERVAL	LENGTH OF ELEMENT	GRID STEP	END OF INTERVAL
1	180	0.300	0.01500	0.00375	3.000
2	200	3.000	0.08500	0.02125	20.000
3	200	20.000	0.40000	0.10000	100.000

```
LAST ADDRESS OF ARRAY ITOT USED =      62082
```

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

```
-----
TOTAL NUMBER OF ALGEBRAIC EQUATIONS. . . . (NN ) =    13926
TOTAL NUMBER OF MATRIX ELEMENTS. . . . . (NWK ) =   257541
MAXIMUM HALF BANDWIDTH . . . . . (MK ) =      30
MEAN HALF BANDWIDTH . . . . . (MMK ) =      18
```

```
LAST ADDRESS OF ARRAY TOT USED =    263150
```

```
NDIM, MDIM=      6      6
```

```
LAST ADDRESS OF ARRAY TOT USED =    371869
```


NUMBER OF OPEN CHANNELS (NOPEN) = 2
 VALUE OF I-TH MOMENTUM (I, QR) = 1 0.1549E+01
 VALUE OF I-TH MOMENTUM (I, QR) = 2 0.6325E+00

TO HAVE REQUIRED EPSC=1.D-14
 VALUE OF MATCHING POINT (RMATCH) = 31.6417
 RECOMMENDED RIGHT BOUND OF
 INTERVAL IS NOT LESS THAN (RMAX) = 33

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

 1.00000 - .102478E-17
 0.197052E-17 1.00000

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

 -1.46347 2.19626
 2.19626 -8.72933

R R A D I A L E I G E N F U N C T I O N S

 0.3000 0.6533D-01 0.1740D+01 -.1153D-01 0.3368D-01 -.1256D-04 0.3139D-04
 0.2082D-07 -.8510D-07 0.7188D-10 -.2697D-09 0.1034D-12 -.3923D-12
 1.8000 -.2666D-01 0.6352D+00 -.8888D+00 0.2455D+01 0.1111D-01 -.4781D-01
 0.4547D-02 -.1653D-01 0.3372D-03 -.1260D-02 0.1491D-04 -.5729D-04
 4.7000 0.2964D+00 -.3511D+00 0.4099D+00 -.1755D+01 0.1383D+00 -.5735D+00
 -.4163D-01 0.1528D+00 0.8703D-02 -.2809D-01 -.8857D-03 0.4631D-02
 13.2000 -.1068D-01 -.4437D-01 0.1694D+00 -.6822D+00 -.7173D-02 0.3852D-01
 -.1107D-03 0.5968D-03 -.3290D-04 0.2413D-03 -.2221D-04 0.8926D-04
 28.0000 0.5274D-01 -.5965D-01 -.8324D-02 -.1117D-01 0.4526D-02 -.1857D-01
 -.1015D-04 0.3768D-04 0.1217D-04 -.4945D-04 0.2971D-07 0.4214D-07
 68.0000 0.2000D-01 -.1611D-01 0.3989D-01 -.1601D+00 0.6037D-04 0.8285D-04
 0.1750D-05 -.7186D-05 0.4147D-07 -.5194D-08 -.3349D-08 0.1340D-07

C M A T R I X

 0.261805 6.97335
 -.468245 1.37416
 -.574532E-02 0.144615E-01
 0.976111E-04 -.402277E-03
 0.382014E-05 -.143464E-04
 0.611522E-07 -.231952E-06

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