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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 [a], O. Chuluunbaatar [a,b,*], S.I. Vinitsky [a], A.G. Abrashkevich [c]

[a] Joint Institute for Nuclear Research, Dubna, 141980 Moscow region, Russia

[b] National University of Mongolia, Ulaanbaatar, Mongolia

[c] IBM Toronto Lab, 8200 Warden Avenue, Markham, ON L6G 1C7, Canada

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ABSTRACT

A FORTRAN program for calculating energy values, reflection 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. 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. As a test desk, the program is applied to the calculation of the reflection and transmission matrices and corresponding wave functions for the two-dimensional problem with different barrier potentials.

Program summary

Program title: KANTBP

Catalogue identifier: ADZH_v3_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADZH_v3_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.: 81813

No. of bytes in distributed program, including test data, etc.: 276779

Distribution format: tar.gz

Programming language: FORTRAN 90/95. Compilers: Intel Fortran 8.0+, GNU Fortran 95 4.4.5+.

Computer: Personal computer.

Operating system: Unix/Linux, Window.

RAM: Depends on

(a) the number of differential equations
(b) the number and order of finite elements
(c) the number of longitudinal points
(d) the number of eigensolutions required.

Classification: 2.7.

Does the new version supersede the previous version?: No

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

* Corresponding author at: Joint Institute for Nuclear Research, Dubna, 141980 Moscow region, Russia. Tel.: +7 4962162529; fax: +7 4962165084.
E-mail addresses: gooseff@jinr.ru (A.A. Gusev), chuka@jinr.ru (O. Chuluunbaatar), vinitky2008@gmail.com (S.I. Vinitsky), aabrashk@ca.ibm.com (A.G. Abrashkevich).

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Catalogue identifier of previous version: ADZH_v2_0

Journal reference of previous version: Comput. Phys. Comm. 179 (2008) 685

Nature of problem:
In the adiabatic approach [1], a multidimensional Schrödinger equation for quantum reflection [2], three-dimensional tunneling of a diatomic molecule incident upon a potential barrier [3], fission model of collision of heavy ions [4] or the photoionization of a hydrogen atom in magnetic field [5] is reduced by separating the longitudinal coordinate, labeled as z, from the transversal 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 new version of the program based on the use of the finite element method of high-order accuracy approximations for calculating reflection and transmission matrices and wave functions for such systems of coupled differential equations on finite intervals of the variable $z \in [z_{min}, z_{max}]$ with homogeneous boundary conditions of the third-type at the left- and right-boundary points following from the above scattering problems.

Solution method:
The boundary-value problems for the coupled second-order differential equations are solved by the finite element method using high-order accuracy approximations [6–8]. The generalized algebraic eigenvalue problem $\mathbf{A}\,\mathbf{F} = E\,\mathbf{B}\,\mathbf{F}$ with respect to pair unknowns $(E, \mathbf{F})$ arising after the replacement of the differential eigenvalue problem by the finite-element approximation is solved by the subspace iteration method [6]. The generalized algebraic eigenvalue problem $(\mathbf{A} - E\,\mathbf{B})\,\mathbf{F} = \mathbf{D}\,\mathbf{F}$ with respect to pair unknowns $(\mathbf{D}, \mathbf{F})$ arising after the corresponding replacement of the scattering boundary problem in open channels at fixed energy value, E, is solved by the $\mathbf{L}\,\mathbf{D}\,\mathbf{L}^{\mathbf{T}}$ factorization of symmetric matrix and back-substitution methods [6].

Reasons for new version:
The previous versions of KANTBP were intended only to calculate the energy levels, reaction matrix and radial wave functions of the bound state problem and scattering problem in the coupled-channel hyperspherical adiabatic approach, in which original problems were reduced to a set of coupled-channel second order differential equations with respect to radial variable in a semi-axis. However a wider range of physical scattering problems are reduced to a set of coupled-channel second order differential equations with respect to the longitudinal variable on the whole axis. In this case one needs to formulate the third-type boundary conditions for systems of coupled differential equations on a finite interval and calculate a desirable scattering matrix which is expressed via unknown reflection and transmission amplitude matrices of asymptotes of solutions in the open channels. The purpose of this new version is to provide a program for calculating the reflection and transmission amplitude matrices and corresponding wave functions of the continuous spectrum problem thus covering a wider range of physical scattering problems.

Summary of revisions:
The KANTBP 3.0 extends the framework of the previous versions, KANTBP 1.0 and KANTBP 2.0. It calculates the reflection and transmission amplitude matrices and corresponding wave functions of the continuous 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 at $z = z_{min} < 0$ and $z = z_{max} > 0$. The third-type boundary conditions are formulated for the continuous problems under consideration by using known asymptotes 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. The program is applied to the computation of the penetration coefficient for 2D-model of pair particles connected by the oscillator interaction potential (throughout symmetric or nonsymmetric) as well as the Coulomb-like barriers.

Restrictions:
The computer memory requirements depend on:

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

The user must supply subroutine POTCAL for evaluating potential matrix elements. The user should also supply subroutine ASYMEV (when solving the eigenvalue problem) or ASYMSL and ASYMSR (when solving the scattering problem) which evaluate asymptotics of the wave functions at boundary points in case of a boundary condition of the third-type for the above problems.

Running time:
The running time depends critically upon:

(a) the number of differential equations
(b) the number and order of finite elements
(c) the total number of longitudinal points on interval $[z_{min}, z_{max}]$
(d) the number of eigensolutions required.

As a test desk, the program is applied to the calculation of the reflection and transmission matrices and corresponding wave functions of the boundary-value problem for a set of N coupled-channel ordinary second order differential equations which follows from the two-dimensional problem describing a quantum tunneling of two particles $i = 1, 2$ with masses m_i and effective charges Z_i, interacted by a harmonic oscillator potential through the repulsive Coulomb-like barrier potential $U_i(x_i) = Z_i(x_i^s + \bar{x}_{min}^s)^{-1/s}$ [8]. The following values of parameters were used: $m_1 = 1, m_2 = 3, \bar{x}_{min} = 0.1, Z_1 = Z_2 = 0.1,$

$s = 8$, $N = 4$. The test run took 25 s with calculation of matrix potentials on the Intel Core i5 CPU 3.33 GHz, 4 GB RAM, Windows 7. This test run requires 5 MB of disk storage. The program KANTBP was tested on the JINR Central Information and Computer Complex.

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