

Algorithm for reduction of boundary-value problems in multistep adiabatic approximation¹

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Abstract

The adiabatic approximation is well-known method for effective study of few-body systems in solid, molecular, atomic and nuclear physics, using the idea of separation of "fast" and "slow" variables. The generalization of the standard adiabatic ansatz for the case of multi-channel wave function when all variables treated dynamically is presented. For this reason we are introducing the step-by-step averaging methods in order to eliminate consequently from faster to slower variables. We present a symbolic-numerical algorithm for reduction of multistep adiabatic equations, corresponding to the MultiStep Generalization of Kantorovich Method, for solving multidimensional boundary-value problems by finite element method. An application of the algorithm to calculation of the ground and first excited states of a Helium atom is given.

Key words: Multistep adiabatic approximation, multidimensional boundary-value problems

1 Motivation

The adiabatic approximation is well-known method for effective study of few-body systems in molecular, atomic and nuclear physics. On the base of pioneering work of Born and Oppenheimer [6] the method was applied in various problems of physics, using the idea of separation of "fast" \vec{x}_f and "slow" \vec{x}_s variables [5] in Hamiltonian composed by fast and slow subsystems $H(\vec{x}_f, \vec{x}_s) = H_f(\vec{x}_f; \vec{x}_s) + H_s(\vec{x}_s)$ with characterized frequencies $\omega_f > \omega_s$, for example in Hénon-Heiles model [16] or quantum dot (QD) models [12].

Purpose of this paper is to present algorithm for generalization of the standard adiabatic ansatz [15, 4],

$$\langle \vec{x}_f, \vec{x}_s | n_k \rangle := \sum_{n'_{k+1}} \langle \vec{x}_f | n'_{k+1}, \vec{x}_s \rangle \langle \vec{x}_s, n'_{k+1} | n_k \rangle, \quad (1)$$

for the case of multi-channel wave function when all variables treated dynamically [10] and to give a general scheme and examples of its application to calculation of ground and excited states of Helium atom [11, 3].

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For this reason we are introducing the step-by-step averaging methods in order to eliminate consequently ordered independent variables ($\vec{x} = \{\vec{x}_f, \vec{x}_s\} = \{x_N \succ x_{N-1} \succ \dots \succ x_1\}^T \in \mathbf{X} = \mathbf{X}_N \cup \dots \cup \mathbf{X}_1$ of subspace of coordinate space $\mathbf{X} \subset \mathbf{R}^N$) and to improve accuracy of calculations of the parametric basis functions and corresponded matrix elements, and to have possibility for reducing computer resources in multi-dimension case by using in perspective the MPI technology.

We present a symbolic-numerical algorithm for reduction of multistep adiabatic equations, corresponding to the MultiStep Generalization of Kantorovich Method [14] named below as (MSGKM), for solving multidimensional boundary-value problems with solutions subject to corresponding boundary conditions [7]

$$H\psi_{n_1} - 2E_{n_1}\psi_{n_1} = 0. \quad (2)$$

Here the Hamiltonian $H = \sum_{i=1}^N H_{N+1-i}$ of a quantum system presented by sum of parametric Hamiltonians $H_i \equiv H_i(x_i; x_{i-1}, \dots, x_1)$ of subsystems, depending on subset of independent variable x_i and parameters x_{i-1}, \dots, x_1 , and solutions satisfy to orthogonality and normalizing conditions

$$\langle n'_1 | n_1 \rangle = \int_{\mathbf{X}} dx_N \dots dx_1 \psi_{n'_1}^\dagger(\vec{x}) \psi_{n_1}(\vec{x}) = \delta_{n'_1 n_1}. \quad (3)$$

For solving of problem (2)–(3) we propose multistep generalization of the standard adiabatic ansatz (1) in the following form:

$$\begin{aligned} \psi_{n_1}(\vec{x}) &= \psi_{n_1}^{(1)}(x_N, \dots, x_1) = \sum_{n'_2} \psi_{n'_2}^{(2)}(x_N, \dots, x_2; x_1) \chi_{n'_2 n_1}^{(1)}(x_1) \\ &= \sum_{n'_N \dots n'_2} \psi_{n'_N}^{(N)}(x_N; x_{N-1}, \dots, x_1) \dots \chi_{n'_k+1 n'_k}^{(k)}(x_k; x_{k-1}, \dots, x_1) \dots \chi_{n'_3 n'_2}^{(2)}(x_2; x_1) \chi_{n'_2 n_1}^{(1)}(x_1). \end{aligned} \quad (4)$$

Optimization of a convergence rate of the method is possible at an appropriate choice of characterized frequencies $\omega_N > \omega_{N-1} > \dots > \omega_1$ of subsystems.

2 Algorithm MSGKM

Below we present symbolic algorithm MSGKM for generation of the boundary-value problems realizing multistep adiabatic expansion (4) in solving eigenvalue problem (2) in a symbolic form by using a Maple system. The examples of different versions of the algorithm are given in the next sections.

Algorithm MSGKM

Input:

$H = \sum_{i=1}^N H_{N+1-i}$ is main Hamiltonian dependent on ordered variables $\vec{x} = \{x_N \succ x_{N-1} \succ \dots \succ x_1\}^T$ decomposed to sum of parametric Hamiltonians $H_i \equiv H_i(x_i; x_{i-1}, \dots, x_1)$, dependent on subset independent variable x_i and parameters x_{i-1}, \dots, x_1 ;
 $H\psi_{n_1} - 2E_{n_1}\psi_{n_1} = 0,$

$\langle n'_1 | n_1 \rangle = \int_{\mathbf{X}} dx_N \dots dx_1 \psi_{n'_1}^\dagger(\vec{x}) \psi_{n_1}(\vec{x}) = \delta_{n'_1 n_1}$
 is main eigenvalue problem for calculation of unknowns
 $\psi_{n_1} \equiv |n_1\rangle \leftrightarrow \langle \vec{x} | n_1 \rangle \equiv \psi_{n_1}(\vec{x})$ and $2E_{n_1} = \varepsilon_{n_1}$.

Output:

A set of Eq(k), $k = 1, \dots, N$, is a set of auxiliary parametric eigenvalue problems for calculation of $\psi_{n_k}^{(k)} \equiv \psi_{n_k}^{(k)}(x_N, \dots, x_k; x_{k-1}, \dots, x_1)$ and $\varepsilon_{n_k} \equiv \varepsilon_{n_k}^{(k)}(x_{k-1} \dots x_1)$, where $\psi_{n_1} = \psi_{n_1}^{(1)}$ and $2E_{n_1} = \varepsilon_{n_1}^{(1)}$ are solutions of the main eigenvalue problem.

Local:

$\psi_{n_k}^{(k)} \equiv \psi_{n_k}^{(k)}(x_N, \dots, x_k; x_{k-1}, \dots, x_1)$ and $\varepsilon_{n_k} \equiv \varepsilon_{n_k}^{(k)} \equiv \varepsilon_{n_k}^{(k)}(x_{k-1} \dots x_1)$ are solutions of the auxiliary parametric eigenvalue problems:

$$\left(\sum_{i=N+1-k}^N H_{N+1-i} \right) \psi_{n_k}^{(k)} - \varepsilon_{n_k}^{(k)} \psi_{n_k}^{(k)} = 0,$$

$$\langle n'_k | n_k \rangle = \int_{\mathbf{X}_N \cup \dots \cup \mathbf{X}_{N+1-k}} dx_N \dots dx_{N+1-k} \psi_{n'_k}^{(k)\dagger} \psi_{n_k}^{(k)} = \delta_{n'_k n_k};$$

$\langle n'_{k+1} | n_k \rangle \equiv \chi_{n'_{k+1} n_k}^{(k)}(x_k; x_{k-1}, \dots, x_1)$ are auxiliary parametric solutions defined as:

$$\langle n'_{k+1} | n_k \rangle = \int_{\mathbf{X}_N \cup \dots \cup \mathbf{X}_{k+1}} dx_N \dots dx_{k+1} \psi_{n'_{k+1}}^{(k+1)\dagger} \psi_{n_k}^{(k)},$$

the square brackets $[,]$ means a commutator:

$$\langle n_{k+1} | [H_k, n'_{k+1}] \rangle = \langle n_{k+1} | H_k n'_{k+1} \rangle - \langle n_{k+1} | n'_{k+1} \rangle H_k.$$

1: Eq(N): $= \{ H_{n_N} | n_N \rangle - \varepsilon_{n_N} | n_N \rangle = 0, \quad \langle \psi_{n_N}^{(N)\dagger} | \psi_{n'_N}^{(N)} \rangle = \delta_{n_N n'_N} \}$

2: Eq(N) $\rightarrow \{ |n_N\rangle, \varepsilon_{n_N} \}$

3: for $k:=N-1:1$ step -1

4: Eq(k): $= \{ (H_k + \varepsilon_{n_{k+1}}^{(k+1)} - \varepsilon_{n_k}^{(k)}) \langle n_{k+1} | n_k \rangle + \sum_{n'_{k+1}} \langle n_{k+1} | [H_k, n'_{k+1}] \rangle \langle n'_{k+1} | n_k \rangle = 0 \}$.

5: Eq(k) $\rightarrow \{ \langle n'_{k+1} | n_k \rangle, \varepsilon_{n_k}^{(k)} \}$

6: $|n_k\rangle := \sum_{n'_{k+1}} |n'_{k+1}\rangle \langle n'_{k+1} | n_k \rangle$

7: end for

8: $\psi_{n_1} = |n_1\rangle, 2E_{n_1} = \varepsilon_{n_1}^{(1)}$

3 Statement of the problem for a Helium atom ($N = 3$)

The Schrödinger equation for a Helium atom with total zero-angular momentum in hyperspherical coordinates [3]: $\theta \equiv x_3 \in \mathbf{X}_3 = [0, \pi], \alpha \equiv x_2 \in \mathbf{X}_2 = [0, \pi], R \equiv x_1 \in \mathbf{X}_1 = [0, +\infty), \vec{x} = \{x_3 \succ x_2 \succ x_1\}^T \in \mathbf{X} = \mathbf{X}_3 \cup \mathbf{X}_2 \cup \mathbf{X}_1$ reads as,

$$(H_3(x_3; x_2, x_1) + H_2(x_2; x_1) + H_1(x_1) - 2E_i) \Psi_i(x_3, x_2, x_1) = 0.$$

Here the Hamiltonians H_i of subsystems consist of differential operators by independent variables and multiplication operators of the Coulomb potential energy \hat{V}_i of the three interacted particles with charges $Z_a = -1$, $Z_b = -1$, $Z_c = 2$, including appropriate choice of weight factors:

$$\begin{aligned}
H_3(x_3; x_2, x_1) &= \frac{4}{x_1^2 \sin^2 x_2} \hat{H}_3(x_3; x_2, x_1), \\
\hat{H}_3(x_3; x_2, x_1) &= -\frac{1}{\sin x_3} \frac{\partial}{\partial x_3} \sin x_3 \frac{\partial}{\partial x_3} + \hat{V}_3(x_3; x_2, x_1), \\
\hat{V}_3(x_3; x_2, x_1) &= \frac{x_1 \sin^2 x_2}{2} \frac{Z_a Z_b}{\sqrt{1 - \sin x_2 \cos x_3}}, \\
H_2(x_2; x_1) &= \frac{4}{x_1^2} \hat{H}_2(x_2; x_1), \\
\hat{H}_2(x_2; x_1) &= -\frac{1}{\sin^2 x_2} \frac{\partial}{\partial x_2} \sin^2 x_2 \frac{\partial}{\partial x_2} + 1 + \hat{V}_2(x_2; x_1), \\
\hat{V}_2(x_2; x_1) &= \frac{x_1}{2} \left(\frac{Z_a Z_c}{\sin \frac{x_2}{2}} + \frac{Z_b Z_c}{\cos \frac{x_2}{2}} \right), \\
H_1(x_1) &= \hat{H}_1(x_1), \\
\hat{H}_1(x_1) &= -\frac{1}{x_1^5} \frac{\partial}{\partial x_1} x_1^5 \frac{\partial}{\partial x_1} - \frac{4}{x_1^2}.
\end{aligned}$$

Solutions of discrete spectrum satisfy to orthonormalization conditions

$$\frac{1}{8} \int_{\mathbf{X}} \sin x_3 dx_3 \sin^2 x_2 dx_2 x_1^5 dx_1 \Psi_i(x_3, x_2, x_1) \Psi_j(x_3, x_2, x_1) = \delta_{ij}$$

and subject to the boundary conditions

$$\begin{aligned}
\lim_{x_1 \rightarrow 0} x_1^5 \frac{\partial \Psi_i(x_3, x_2, x_1)}{\partial x_1} = 0, \quad \lim_{x_1 \rightarrow \infty} x_1^5 \Psi_i(x_3, x_2, x_1) = 0, \quad (5) \\
\lim_{x_2 \rightarrow 0, \pi} \sin^2 x_2 \frac{\partial \Psi_i(x_3, x_2, x_1)}{\partial x_2} = 0, \quad \lim_{x_3 \rightarrow 0, \pi} \sin x_3 \frac{\partial \Psi_i(x_3, x_2, x_1)}{\partial x_3} = 0.
\end{aligned}$$

4 Algorithm 1. Example of the conventional Kantorovich method.

We consider one-parametric boundary-value problem with respect to fast $\vec{x}_f = \{x_3, x_2\}$ independent variables

$$\left(\frac{\hat{H}_3(x_3; x_2, x_1)}{\sin^2 x_2} + \hat{H}_2(x_2; x_1) - \frac{1}{2} E_{i_2}^{(2)}(x_1) \right) \Psi_{i_2}^{(2)}(x_3, x_2; x_1) = 0, \quad (6)$$

$$\int_{\mathbf{X}_3 \cup \mathbf{X}_2} \sin x_3 dx_3 \sin^2 x_2 dx_2 \Psi_{i_2}^{(2)}(x_3, x_2; x_1) \Psi_{j_2}^{(2)}(x_3, x_2; x_1) = \delta_{i_2 j_2}, \quad (7)$$

and conventional one by independent variables $\vec{x} = \{x_3 \succ x_2 \succ x_1\}$,

$$\left(\frac{4\hat{H}_3(x_3; x_2, x_1)}{x_1^2 \sin^2 x_2} + \frac{4\hat{H}_2(x_2; x_1)}{x_1^2} + \hat{H}_1(x_1) - 2E_{i_1}^{(1)} \right) \Psi_{i_1}^{(1)}(x_3, x_2, x_1) = 0, \quad (8)$$

$$\frac{1}{8} \int_{\mathbf{X}} \sin x_3 dx_3 \sin^2 x_2 dx_2 x_1^5 dx_1 \Psi_{i_1}^{(1)}(x_3, x_2, x_1) \Psi_{j_1}^{(1)}(x_3, x_2, x_1) = \delta_{i_1 j_1}, \quad (9)$$

with boundary conditions following from (5).

In **Step 1** we find the required solution of the problem (6) in the series expansion over the Legendre polynomials $P_{i_1}(\cos x_3)$ for each values of x_1 :

$$\Psi_{i_2}^{(2)}(x_3, x_2; x_1) = \sum_{i_1=1}^{i_1^{\max}} P_{i_1}(\cos x_3) \chi_{i_1 i_2}^{(2)}(x_2; x_1). \quad (10)$$

Substituting expansion (10) into equation (6) and projecting with account of orthonormalization conditions of Legendre polynomials, we arrive to the one-parametric problem for unknown vector eigenfunctions, $\chi_{j_1 i_2}^{(2)}(x_2; x_1)$, and corresponded eigenvalue (potential curve), $E_{i_2}^{(2)}(x_1)$,

$$\left(-\frac{1}{\sin^2 x_2} \frac{\partial}{\partial x_2} \sin^2 x_2 \frac{\partial}{\partial x_2} + 1 + \hat{V}_2(x_2, x_1) + \frac{i_1(i_1 + 1)}{\sin^2 x_2} - \frac{1}{2} E_{i_2}^{(2)}(x_1) \right) \chi_{i_1 i_2}^{(2)}(x_2; x_1) + \frac{1}{\sin^2 x_2} \sum_{j_1=1}^{i_1^{\max}} \hat{V}_{i_1 j_1}^{(3)}(x_2; x_1) \chi_{j_1 i_2}^{(2)}(x_2; x_1) = 0, \quad (11)$$

$$\hat{V}_{i_1 j_1}^{(3)}(x_2; x_1) = \int_{\mathbf{X}_3} \sin x_3 dx_3 P_{i_1}(\cos x_3) \hat{V}_3(x_3, x_2; x_1) P_{j_1}(\cos x_3)$$

with boundary conditions following from (5).

Substituting expansion (10) into (7), we have orthonormation conditions

$$\sum_{i_2=1}^{i_2^{\max}} \int_{\mathbf{X}_2} \sin^2 x_2 dx_2 \chi_{i_1 i_2}^{(2)}(x_2; x_1) \chi_{j_1 i_2}^{(2)}(x_2; x_1) = \delta_{i_1 j_1}. \quad (12)$$

This one-parametric problem is solved with help of the adaptation of KANTBP program [7], named here as KANTBP 3.0.

In **Step 2** we find the solution of the problem (8) in the series expansion over solutions of problem (6) solved in the **Step 1**,

$$\Psi_{i_1}^{(1)}(x_3, x_2, x_1) = \sum_{i_2=1}^{i_2^{\max}} \Psi_{i_2}^{(2)}(x_3, x_2; x_1) \chi_{i_2 i_1}^{(1)}(x_1). \quad (13)$$

Substituting expansion (13) into equation (8) and projecting with account of orthonormalization conditions (7) of parametric basis functions $\Psi_{i_2}^{(2)}(x_3, x_2; x_1)$

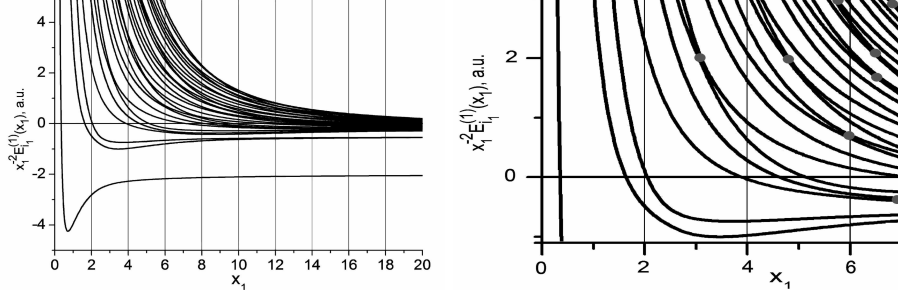


Figure 1: Calculated potential curves in step 1 of equation in step 2. Circles on right panel note avoiding crossing points.

from (10) calculated in **Step 1**, we arrive to the problem for unknown vector functions, $\chi_{i_2 i_1}^{(1)}(x_1)$, and corresponding eigenenergy, $E_{i_1}^{(1)}$,

$$\left(-\frac{1}{x_1^5} \frac{\partial}{\partial x_1} x_1^5 \frac{\partial}{\partial x_1} + \frac{2E_{i_2}^{(2)}(x_1) - 4}{x_1^2} - 2E_{i_1}^{(1)} \right) \chi_{i_2 i_1}^{(1)}(x_1) + \sum_{j_2=1}^{i_2^{\max}} \langle i_2 | [H_1, j_2] \rangle \chi_{j_2 i_1}^{(1)}(x_1) = 0, \quad (14)$$

$$\langle i_2 | [H_1, j_2] \rangle = \left(A_{i_2 j_2}^{1;1;1}(x_1) - \frac{1}{x_1^5} \frac{\partial}{\partial x_1} x_1^5 A_{i_2 j_2}^{1;0;1}(x_1) - A_{i_2 j_2}^{1;0;1}(x_1) \frac{\partial}{\partial x_1} \right)$$

with boundary conditions following from (5). Substituting expansion (13) into (9), we have orthonormation conditions

$$\sum_{j_2=1}^{i_2^{\max}} \frac{1}{8} \int_{\mathbf{X}_1} x_1^5 dx_1 \chi_{j_2 i_1}^{(1)}(x_1) \chi_{j_2 j_1}^{(1)}(x_1) = \delta_{i_1 j_1}. \quad (15)$$

In (14) we have definitions of elements of matrix of effective potentials ($l_1 = 0, 1$):

$$A_{i_2 j_2}^{1; l_1; r_1}(x_1) = \int_{\mathbf{X}_3 \cup \mathbf{X}_2} \sin x_3 dx_3 \sin^2 x_2 dx_2 \frac{\partial^{l_1} \Psi_{i_2}^{(2)}(x_3, x_2; x_1)}{\partial x_1^{l_1}} \frac{\partial^{r_1} \Psi_{j_2}^{(2)}(x_3, x_2; x_1)}{\partial x_1^{r_1}}, \quad (16)$$

$$\frac{\partial^0}{\partial x_1^0 \Psi_{i_2}^{(2)}(x_3, x_2; x_1)} \equiv \Psi_{i_2}^{(2)}(x_3, x_2; x_1).$$

A parametric derivatives of eigenfunction $\Psi_{j_2}^{(2)}(x_3, x_2; x_1)$ in (16) are calculated with help of KANTBP 3.0 program together with corresponding integrals, where integration by variable x_3 perform analytically by using of orthonormalization conditions of Legendre polynomials. As an example, some potential curves and matrix elements of effective potential matrix are shown in Figs. 1 and 2. One can

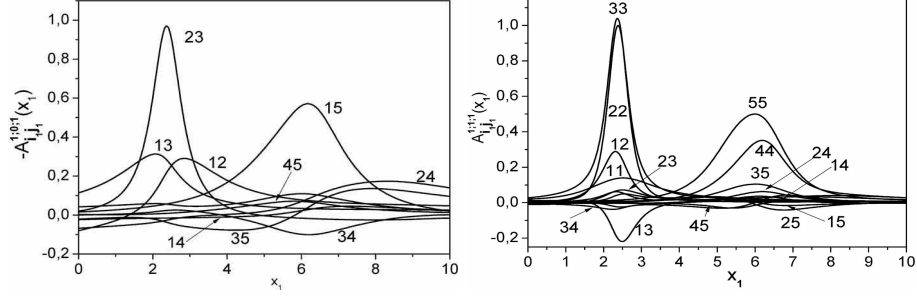


Figure 2: Calculated matrix elements in step 1 of equation in step 2.

Table 1: Ground state 1s1s energy $E_2^{(1)}$ and first excited state 1s2s energy $E_2^{(1)}$ of Helium atom (in a.u.) versus number i_2^{\max} of basis functions and number i_1^{\max} of the Legendre polynomials

i_2^{\max}	1s1s: $i_1^{\max} = 12$	1s1s: $i_1^{\max} = 21$	1s1s: $i_1^{\max} = 28$	1s2s: $i_1^{\max} = 28$
1	-2.895 539 01	-2.895 551 19	-2.895 552 76	-2.139 935 68
2	-2.898 631 39	-2.898 643 21	-2.898 644 74	-2.141 664 33
6	-2.903 643 86	-2.903 655 95	-2.903 657 51	-2.145 700 22
10	-2.903 702 68	-2.903 714 86	-2.903 716 36	-2.145 915 09
15	-2.903 708 49	-2.903 720 68	-2.903 722 17	-2.145 957 35
21	-2.903 709 31	-2.903 721 50	-2.903 722 994	-2.145 968 77
28	-2.903 709 31		-2.903 722 997	-2.145 970 28
[11]			-2.903 722 998	-2.145 956 975
[9]			-2.903 724 377	-2.145 974 046

see that these matrix elements have smooth behavior with respect to parameter x_1 that achieve by imposing conditions of continuity of eigenfunctions with respect to parameter x_1 in avoiding crossing points of potential curves $E_{i_2}^{(2)}(x_1)$, shown by circles in Fig. 1, where change number of zeros of corresponding pair of eigenfunctions by each of independent variables x_2 and x_3 occurs after passing these points, as discussed in [3, 2]. As we show in Table 1, such continuation via these points leads to increase of the convergence rate of expansion (13) of total solution in calculation of ground and first excited states energy $E_{i_1}^{(1)}$ with respect to previous one [3]. One can see from the Table 1 that convergence start from $i_2^{\max} = 21$ is slow with respect to upper variational estimation [9]. So, to improve convergence of calculation of the parametric basis functions from expansion (10) by number $i_1^{\max} > 28$, we begin to study in the next section the step-by-step averaging method for realizing calculation with a more high accuracy with help of Algorithm 2. Meanwhile, our upper estimation at $i_2^{\max} = 28$ for first excited state is lowering than result of [11]. On Fig. 3 we show the radial eigenfunctions of ground and first excited states. Note that, as following from asymptotic effective potentials (see Fig. 2) the ground state solution has asymptotic in a vicinity

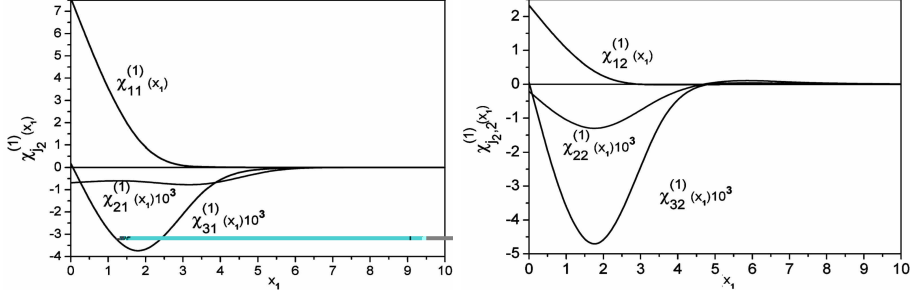


Figure 3: Radial eigenfunctions of ground and first excited states.

triple-collision point $R \rightarrow 0$ including logarithmic terms that corresponding to Fock expansion [2, 13].

5 Algorithm 2. Example of MultiStep Generalization of Kantorovich Method (MSGKM)

We examine a split sequence of boundary-value problems consists of the two-parametric problem by one of fast independent variables, $\vec{x}_f = \{x_3\}$,

$$\begin{aligned} (\hat{H}_3(x_3; x_2, x_1) - \frac{1}{2}E_{i_3}^{(3)}(x_2, x_1))\Psi_{i_3}^{(3)}(x_3; x_2, x_1) &= 0, \\ \int_{\mathbf{x}_3} \sin x_3 dx_3 \Psi_{i_3}^{(3)}(x_3; x_2, x_1) \Psi_{j_3}^{(3)}(x_3; x_2, x_1) &= \delta_{i_3 j_3}, \end{aligned} \quad (17)$$

the one-parametric problem (6)–(7) by fast independent variables $\vec{x}_f = \{x_3 \succ x_2\}$ and conventional problem (8)–(9) by independent variables $\vec{x} = \{x_3 \succ x_2 \succ x_1\}$ with corresponding boundary conditions following from (5).

In **Step 1** the two-parametric problem (17) with boundary conditions following from (5) is solved for each values of x_1 and x_2 with help of the adaptation of ODPEVP program [8], named here as ODPEVP 2.0. The eigenvalues (potentials surfaces) $E_{i_3}^{(3)}(x_2; x_1) \equiv E_{i_3}^{(3)}(x_2, x_1)$ and their parametric derivatives are presented on Fig. 4. One can see from Fig. 4, the potential surfaces are symmetric with respect to axis $x_2 = \pi/2$, then the partial derivative $\partial E_{i_3}^{(3)}(x_2, x_1)/\partial x_2 = 0$ for $i_3 = 1, 2, \dots$

In **Step 2** we find the solution of the one-parametric problem (6) in the series expansion over solutions of the problem (17) solved in the **Step 1**:

$$\Psi_{i_2}^{(2)}(x_3, x_2; x_1) = \sum_{i_3=1}^{i_3^{\max}} \Psi_{i_3}^{(3)}(x_3; x_2, x_1) \chi_{i_3 i_2}^{(2)}(x_2; x_1). \quad (18)$$

Substituting expansion (18) into equation (6) and projecting with account of orthonormalization conditions (17) of parametric basis functions from **Step 1**, we

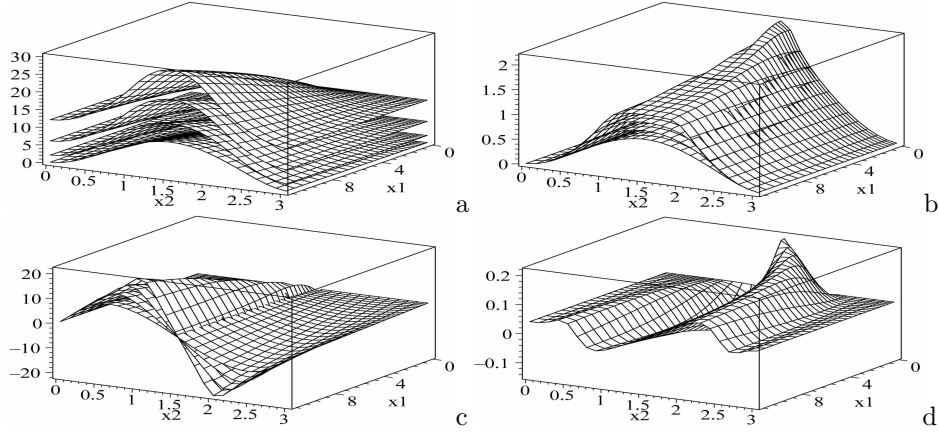


Figure 4: a. The eigenvalues (potentials surfaces) $E_{i_3}^{(3)}(x_2, x_1)$, $i_3 = 1, 2, 3, 4$ of the problem (17). b-c. their parametric derivatives $\partial E_{i_3}^{(3)}(x_2, x_1)/\partial x_1$ and $\partial E_{i_3}^{(3)}(x_2, x_1)/\partial x_2$, $i_3 = 1, 2, 3, 4$. d. their mixed parametric derivative $\partial E_{i_3}^{(3)}(x_2, x_1)/\partial x_1 \partial x_2$

arrive to the one-parametric problem for unknown vector functions $\chi_{i_3 i_2}^{(2)}(x_2; x_1)$ and eigenvalues (potentials curves) $E_{i_2}^{(2)}(x_1)$:

$$\begin{aligned} & \left(-\frac{1}{\sin^2 x_2} \frac{\partial}{\partial x_2} \sin^2 x_2 \frac{\partial}{\partial x_2} + \hat{V}_2(x_2, x_1) + \frac{E_{i_3}^{(3)}(x_2; x_1)}{2 \sin^2 x_2} \right. \\ & \left. - \frac{1}{2} E_{i_2}^{(2)}(x_1) \right) \chi_{i_3 i_2}^{(2)}(x_2; x_1) + \sum_{j_3=1}^{i_3^{\max}} \langle i_3 | [H_2, j_3] \rangle \chi_{j_3 i_2}^{(2)}(x_2; x_1) = 0, \\ \langle i_3 | [H_2, j_3] \rangle & = \left(A_{i_3 j_3}^{2;10;10}(x_2; x_1) - \frac{1}{\sin^2 x_2} \frac{\partial}{\partial x_2} \sin^2 x_2 A_{i_3 j_3}^{2;00;10}(x_2; x_1) \right. \\ & \left. - A_{i_3 j_3}^{2;00;10}(x_2; x_1) \frac{\partial}{\partial x_2} \right). \end{aligned} \quad (19)$$

with boundary conditions following from (5). Substituting expansion (18) into (7), we have orthonormalization conditions

$$\sum_{j_3=1}^{i_3^{\max}} \int_{\mathbf{X}_2} \sin^2 x_2 dx_2 \chi_{j_3 i_2}^{(2)}(x_2; x_1) \chi_{j_3 i_2}^{(2)}(x_2; x_1) = \delta_{i_2 j_2}. \quad (20)$$

In (19) we have definitions of elements of matrix of effective potentials:

$$A_{i_3 j_3}^{2;l_2 l_1; r_2 r_1}(x_2; x_1) = \int_{\mathbf{X}_3} \sin x_3 dx_3 \frac{\partial^{l_2+l_1} \Psi_{i_3}^{(3)}(x_3; x_2, x_1)}{\partial x_2^{l_2} \partial x_1^{l_1}} \frac{\partial^{r_2+r_1} \Psi_{j_3}^{(3)}(x_3; x_2, x_1)}{\partial x_2^{r_2} \partial x_1^{r_1}},$$

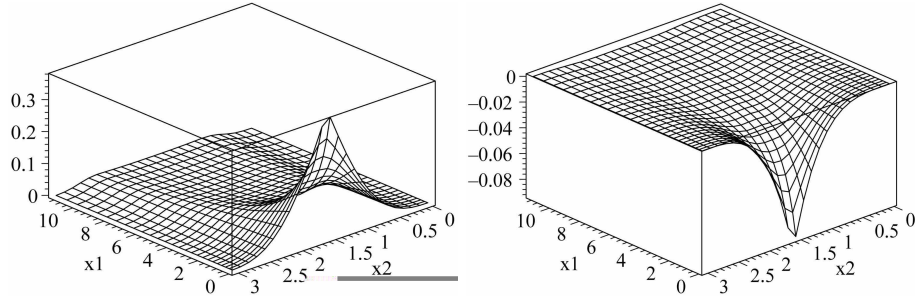


Figure 5: Calculated elements $A_{12}^{2;00;10}(x_2; x_1)$ and $A_{13}^{2;00;10}(x_2; x_1)$ of matrix of effective potentials of Eqs. (19).

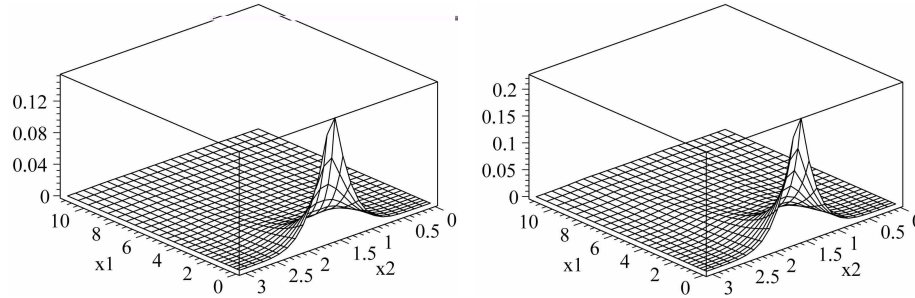


Figure 6: Calculated elements $A_{11}^{2;10;10}(x_2; x_1)$ and $A_{22}^{2;10;10}(x_2; x_1)$ of matrix of effective potentials of Eqs. (19).

$$\frac{\partial^0}{\partial x_2^0 \partial x_1^0} \Psi_{i_3}^{(3)}(x_3; x_2, x_1) \equiv \Psi_{i_3}^{(3)}(x_3; x_2, x_1). \quad (21)$$

Note that this problem is similar to problem (14) from Algorithm 1, but elements of matrix of effective potentials are calculated here with eigenfunctions (17) and their derivatives by parameters x_2 , x_1 by program ODPEVP 2.0 with accuracy $O(h^{2p})$, where p is degree of approximation in a finite element grid [8]. As an example, some elements of effective potential matrix are shown in Figs. 5, 6 and 7. The eigenvalues (potential curves) $E_{i_2}^{(2)}(x_1)$ of (19) calculated here by program KANTBP 3.0 look as the same as in Figs. 1 calculated by Algorithm 1.

In **Step 3** we find the solution of the problem (8) in the series expansion over solutions of problem (6)–(7) solved in the **Step 2**:

$$\Psi_{i_1}^{(1)}(x_3, x_2, x_1) = \sum_{i_2=1}^{i_2^{\max}} \Psi_{i_2}^{(2)}(x_3, x_2; x_1) \chi_{i_2 i_1}^{(1)}(x_1). \quad (22)$$

Substituting expansion (22) into equation (8) and projecting with account of orthonormalization conditions (7) of parametric basis functions from **Step 2**,

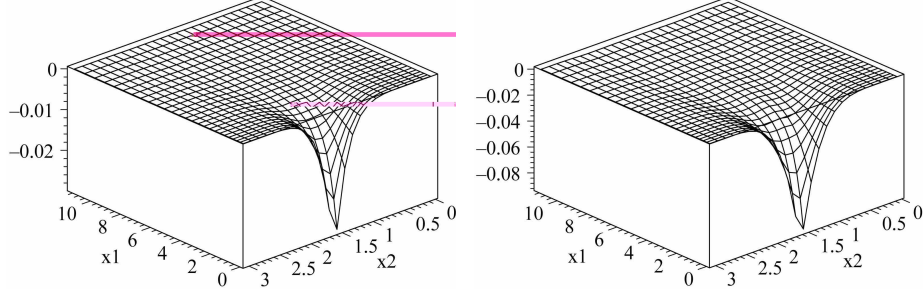


Figure 7: Calculated elements $A_{12}^{2;10;10}(x_2; x_1)$ and $A_{13}^{2;10;10}(x_2; x_1)$ of matrix of effective potentials of Eqs. (19).

we arrive to the problem for unknown vector functions $\chi_{i_2 i_1}^{(1)}(x_1)$:

$$\left(-\frac{1}{x_1^5} \frac{\partial}{\partial x_1} x_1^5 \frac{\partial}{\partial x_1} + \frac{2E_{i_2}^{(2)}(x_1) - 4}{x_1^2} - 2E_{i_1}^{(1)} \right) \chi_{i_2 i_1}^{(1)}(x_1) \quad (23)$$

$$+ \sum_{j_2=1}^{i_2^{\max}} \langle i_2 | [H_1, j_2] \rangle \chi_{j_2 i_1}^{(1)}(x_1) = 0,$$

$$\langle i_2 | [H_1, j_2] \rangle = \left(A_{i_2 j_2}^{1;1;1}(x_1) - \frac{1}{x_1^5} \frac{\partial}{\partial x_1} x_1^5 A_{i_2 j_2}^{1;0;1}(x_1) - A_{i_2 j_2}^{1;0;1}(x_1) \frac{\partial}{\partial x_1} \right).$$

with boundary conditions following from (5). Substituting expansion (22) into (9), we have required orthonormation conditions

$$\sum_{j_2=1}^{i_2^{\max}} \frac{1}{8} \int_{\mathbf{X}_1} x_1^5 dx_1 \chi_{j_2 i_1}^{(1)}(x_1) \chi_{j_2 j_1}^{(1)}(x_1) = \delta_{i_1 j_1}. \quad (24)$$

In (23) we have definitions of elements of matrix of effective potentials:

$$A_{i_2 j_2}^{1;l_1;r_1}(x_1) = \int_{\mathbf{X}_3 \cup \mathbf{X}_2} \sin x_3 dx_3 \sin^2 x_2 dx_2 \frac{\partial^{l_1} \Psi_{i_2}^{(2)}(x_3, x_2; x_1)}{\partial x_1^{l_1}} \frac{\partial^{r_1} \Psi_{j_2}^{(2)}(x_3, x_2; x_1)}{\partial x_1^{r_1}},$$

$$\frac{\partial^0 \Psi_{i_2}^{(2)}(x_3, x_2; x_1)}{\partial x_1^0} \equiv \Psi_{i_2}^{(2)}(x_3, x_2; x_1).$$

Substituting expansion (18), we reduce matrix elements $A_{i_2 j_2}^{1;l_1;r_1}(x_1)$ to integrals by variable x_2 only via matrix elements $A_{i_3 j_3}^{2;l_1 l_2; r_1 r_2}(x_2; x_1)$ calculated with help of improved parametric basis functions (18) from **Step 2**:

$$A_{i_2 j_2}^{1;l_1;r_1}(x_1) = \sum_{i_3, j_3} \sum_{k_l=0}^{l_1} \sum_{k_r=0}^{r_1} \frac{l_1!}{k_l!(l_1 - k_l)!} \frac{r_1!}{k_r!(r_1 - k_r)!} \quad (25)$$

$$\times \int_{\mathbf{X}_2} \sin^2 x_2 dx_2 A_{i_3 j_3}^{2;0 k_l; 0 k_r}(x_2; x_1) \frac{\partial^{l_1 - k_l} \chi_{i_3 i_2}^{(2)}(x_2; x_1)}{\partial x_1^{l_1 - k_l}} \frac{\partial^{r_1 - k_r} \chi_{j_3 j_2}^{(2)}(x_2; x_1)}{\partial x_1^{r_1 - k_r}}.$$

Note that set of Eqs. (23) is similar to Eqs. (14) from Algorithm 1, and the potential curves $E_{i_2}^{(2)}(x_1)$ and elements of matrices $A_{i_2 j_2}^{1;l_1;r_1}(x_1)$ calculated by Algorithm 2 look as the same as in Figs. 1 and 2 calculated by Algorithm 1. We can wait that using expansion (18) over the two-parametric basis functions (17) will have a higher rate of convergence and give corresponding elements of matrices of effective potentials (25) with better accuracy in comparison with expansion (10) over the Legendre polynomials. However, matrix elements have a more complicate structure and additional numerical integration by variable x_3 performed in **Step 2** is needed in comparison with (16).

6 Conclusions

In this paper we presented a symbolic algorithm for reduction of multistep adiabatic equations, corresponding to the MultiStep Generalization of Kantorovich Method, for solving multidimensional boundary-value problems and consider examples of its application to Helium atom calculation. Achievement of this approach consist in facts that, on each step solution subject to boundary conditions, elements of matrix of effective potentials calculated with controllable accuracy have smooth behavior with respect to parameters like that in spheroidal coordinates [1]. These facts together with consistency of Kantorovich expansion in a vicinity triple-collision point $R \rightarrow 0$ including logarithmic terms corresponding to Fock expansion [2, 13] provide as shown above a reasonable rate of convergence of these expansions and upper estimations of energy eigenvalues [16] Moreover, asymptotics of these expansions at large value $R \rightarrow \infty$ in vicinities of pair collision points of limit of separated atom are compatible with asymptotic states needed for solving a scattering problem below three body threshold, as shown in papers [2, 13].

Elaboration final version of Program KANTBP 3.0 for solving the problem with respect to unknowns (i.e. calculation of improved parametric basis functions in Algorithm 2) from **Steps 2–(n-1)**, with matrices of variable coefficients calculated and presented above is in progress.

Generalization of MultiStep Kantorovich method presented above reduce to the set of $2N - 1$ of multiparametric eigenvalue problem for set of ~ 10 ordinary second-order differential equations that can solve naturally by each of $N - 1, N - 2, \dots, 1, 0$ independent parameter using MPI and/or GRID technology that will be elaborated in our further investigations.

The computational scheme, the SNA, and the complex of programs allow extension for the analysis of spectral characteristics of both electron(hole), impurity and excitonic states in nanoscale quantum-dimensional models like QWs [17], QWrS[18], QDs [12] with different geometry of structure and spatial form of confining potential and external fields.

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