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

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Algorithm: MultiStep Generalization of Kantorovich Method (MSGKM)

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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 [1] 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[2] 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[3].

• Purpose of this talk is to present algorithm for generalization of the standard adiabatic ansatz,

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

for the case of multi-channel wave function when all variables treated dynamically [4].

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[1] Born, M., Oppenheimer, J. R.: Ann. Phys. (Leipzig): 84, 457 (1927).

[2] Born, M., Huang, K.: Dynamical Theory of Crystal Lattices. Oxford: Clarendon, 1954

[3] J. Makarewicz, Adiabatic multi-step separation method and its application to coupled oscillators. Theor. Chim. Acta **68**, 321–334 (1985).

[4] V.M. Dubovik, B.L. Markovski, and S.I. Vinitsky, Multistep adiabatic approximation. Preprint JINR E4-87-743, (Dubna, 1987);

• For this reason we are introducing the step-by-step averaging methods for order to eliminate consequently from faster to slower variables ($\vec{x} = \{\vec{x}_f, \vec{x}_s\} = \{x_N \succ x_{N-1} \succ ... \succ x_1\}^T$) and to improve accuracy of calculations of the parametric basis functions and corresponded matrix elements, and to reduce computer resources in multi-dimension case by using MPI technology.

• We present a symbolic-numerical algorithm for reduction of multistep adiabatic equations, corresponding to the MultiStep Generalization Kantorovich Method[5] (MSGKM), for solving multidimensional boundary-value problems[6]:

$$H\psi_{n_1} - 2E_{n_1}\psi_{n_1} = 0,$$

$$\langle n_1'|n_1\rangle = \int dx_N...dx_1\psi^\dagger_{n_1'}(\vec{x})\psi_{n_1}(\vec{x}) = \delta_{n_1'n_1},$$

$$H = \sum_{i=1}^N H_{N+1-i}, \qquad H_i \equiv H_i(x_i; x_{i-1}, ..., x_1).$$

with characterized frequencies $\omega_N > \omega_{N-1}, ..., \omega_1$.

[5] Kantorovich L. V. and Krylov V. I. Approximate Methods of Higher Analysis (New York, Wiley, 1964)

[6] O. Chuluunbaatar, et al, KANTBP: A program for computing energy levels, reaction matrix and radial wave functions in the coupled-channel hyperspherical adia-batic approach. Comput. Phys. Commun. **177**, 649–675 (2007).

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

$R = \sqrt{|\vec{r}_1|^2 + |\vec{r}_2|^2}$,
$\mathrm{tg}\alpha/2 = |\vec{r}_1|/|\vec{r}_2|$,
$\cos\theta = (\frac{\vec{r}_1}{|\vec{r}_1|}, \frac{\vec{r}_2}{|\vec{r}_2|})$.

The Schrödinger equation for a Helium atom with total zero-angular momentum in hyperspherical coordinates[7], $x_3 \succ x_2 \succ x_1$ ($R \equiv x_1 \in [0, +\infty), \alpha \equiv x_2 \in [0, \pi]$, $\theta \equiv x_3 \in [0, \pi]$):

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

[7] A.G. Abrashkevich, et al. J. Comput. Phys., **163**, 328 (2000).

$$H_1(x_1) = \hat{H}_1(x_1),$$

$$\hat{H}_1(x_1) = -\frac{1}{x_1^5}\frac{\partial}{\partial x_1}x_1^5\frac{\partial}{\partial x_1} - \frac{4}{x_1^2}$$

$$H_2(x_2; x_1) = \frac{4}{x_1^2}\hat{H}_2(x_2; x_1),$$

$$\hat{H}_2(x_2; x_1) = -\frac{1}{\sin^2 x_2}\frac{\partial}{\partial x_2}\sin^2 x_2\frac{\partial}{\partial x_2} + \hat{V}_2(x_2, x_1) + 1$$

$$\hat{V}_2(x_2, x_1) = \frac{x_1}{2}\left(\frac{Z_a Z_c}{\sin\frac{x_2}{2}} + \frac{Z_b Z_c}{\cos\frac{x_2}{2}}\right),$$

$$H_3(x_3; x_2, x_1) = \frac{4}{x_1^2\sin^2 x_2}\hat{H}_3(x_3; x_2, x_1),$$

$$\hat{H}_3(x_3; x_2, x_1) = -\frac{1}{\sin x_3}\frac{\partial}{\partial x_3}\sin x_3\frac{\partial}{\partial x_3} + \hat{V}_3(x_3, x_2, x_1)$$

$$\hat{V}_3(x_3, x_2, x_1) = \frac{x_1\sin^2 x_2}{2}\frac{Z_a Z_b}{\sqrt{1 - \sin x_2\cos x_3}}$$

Wave functions are orthonormalized

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

and satisfy to the boundary conditions

$$\lim_{x_1\to 0} x_1^5 \frac{\partial \Psi_i(x_3, x_2, x_1)}{\partial x_1} = 0, \quad \lim_{x_1\to\infty} x_1^5 \Psi_i(x_3, x_2, x_1) = 0,$$

$$\lim_{x_2\to 0,\pi} \sin^2 x_2 \frac{\partial \Psi_i(x_3, x_2, x_1)}{\partial x_2} = 0, \quad \lim_{x_3\to 0,\pi} \sin x_3 \frac{\partial \Psi_i(x_3, x_2, x_1)}{\partial x_3} = 0.$$

Algorithm 1. Example of the conventional Kantorovich method.
We consider two boundary-value problems $\vec{x}_f = \{x_3, x_2\}$, $\vec{x}_s = \{x_1\}$

$$(\hat{H}_2(x_2;x_1) + \frac{1}{\sin^2 x_2}\hat{H}_3(x_3;x_2,x_1) - \frac{1}{2}E^{(2)}_{i_2}(x_1))\Psi^{(2)}_{i_2}(x_3,x_2;x_1) = 0, \quad (1)$$

$$\int \sin^2 x_2 dx_2 \sin x_3 dx_3 \Psi^{(2)}_{i_2}(x_3,x_2;x_1)\Psi^{(2)}_{j_2}(x_3,x_2;x_1) = \delta_{i_2 j_2},$$

$$(\hat{H}_1(x_1) + \frac{4}{x_1^2}\hat{H}_2(x_2;x_1) + \frac{4}{x_1^2 \sin^2 x_2}\hat{H}_3(x_3;x_2,x_1) - 2E^{(1)}_{i_1})\Psi^{(1)}_{i_1}(x_3,x_2,x_1) = 0, \quad (2)$$

$$\frac{1}{8}\int x_1^5 dx_1 \sin^2 x_2 dx_2 \sin x_3 dx_3 \Psi^{(1)}_{i_1}(x_3,x_2,x_1)\Psi^{(1)}_{j_1}(x_3,x_2,x_1) = \delta_{i_1 j_1},$$

Algorithm 1.

Step 1 Solving the problem (1)

We find the required solution in the series expansion over the Legendre polynomials $P_{i_1}(\cos x_3)$ for each values of x_1:

$$\Psi^{(2)}_{i_2}(x_3, x_2; x_1) = \sum_{i_1=1}^{i_1^{\max}} P_{i_1}(\cos x_3)\chi^{(2)}_{i_1 i_2}(x_2; x_1). \qquad (3)$$

Algorithm 1.

Step 1

Substituting expansion (4) into equation (2) and projecting with account of orthonormalization conditions Legendre polynomials, we arrive to the problem for unknown vector functions $\chi^{(2)}_{j_1 i_2}(x_2; x_1)$:

$$\left(-\frac{1}{\sin^2 x_2}\frac{\partial}{\partial x_2}\sin^2 x_2\frac{\partial}{\partial x_2} + \frac{i_1(i_1+1)}{\sin^2 x_2} + 1 + \hat{V}_2(x_2, x_1)\right)\chi^{(2)}_{i_1 i_2}(x_2; x_1)$$
$$+\frac{1}{\sin^2 x_2}\sum_{j_1=1}^{i_1^{\max}}\int P_{i_1}(\cos x_3)\hat{V}_3(x_3, x_2, x_1)P_{j_1}(\cos x_3)\chi^{(2)}_{j_1 i_2}(x_2; x_1)$$
$$-\frac{1}{2}E^{(2)}_{i_2}(x_1)\chi^{(2)}_{i_1 i_2}(x_2; x_1) = 0,$$

Substituting expansion (3) into orthonormation conditions (1), we have

$$\sum_{i_2=1}^{i_2^{\max}}\int \sin^2 x_2 dx_2 \chi^{(2)}_{i_1 i_2}(x_2; x_1)\chi^{(2)}_{j_1 i_2}(x_2; x_1) = \delta_{i_1 j_1}.$$

This problem is solved with help of the KANTBP 3.0 program.

Step 2 Solution of the problem (2)

We find the solution of the problem (2) in the series expansion over solutions of problem (1) solved in the step 1,

$$\Psi^{(1)}_{i_1}(x_3, x_2, x_1) = \sum_{i_2=1}^{i_2^{\max}} \Psi^{(2)}_{i_2}(x_3, x_2; x_1)\chi^{(1)}_{i_2 i_1}(x_1), \quad (4)$$

Step 2

Substituting expansion (4) into equation (2) and projecting with account of orthonormalization conditions of parametric basis functions from Step 1, we arrive to the problem for unknown vector functions $\chi_{ll}^{(1)}(x_1)$:

$$\left(-\frac{1}{x_1^5}\frac{\partial}{\partial x_1}x_1^5\frac{\partial}{\partial x_1}+\frac{2E_{i_2}^{(2)}(x_1)-4}{x_1^2}\right)\chi_{i_2i_1}^{(1)}(x_1)$$

$$+\sum_{j_2=1}^{i_2^{\max}}\langle i_2|\Big[H_1,j_2\rangle\Big]\chi_{j_2i_1}^{(1)}(x_1)-2E_{i_1}^{(1)}\chi_{i_2i_1}^{(1)}(x_1)=0,$$

$$\langle i_2|\Big[H_1,j_2\rangle\Big]=\left(A_{i_2j_2}^{1;1;1}(x_1)-\frac{1}{x_1^5}\frac{\partial}{\partial x_1}x_1^5A_{i_2j_2}^{1;0;1}(x_1)-A_{i_2j_2}^{1;0;1}(x_1)\frac{\partial}{\partial x_1}\right)$$

Substituting expansion (4) into orthonormation conditions (2), we have

$$\sum_{j_2=1}^{i_2^{\max}}\frac{1}{8}\int x_1^5dx_1\chi_{j_2i_1}^{(1)}(x_1)\chi_{j_2j_1}^{(1)}(x_1)=\delta_{i_1j_1}.$$

Algorithm 1.

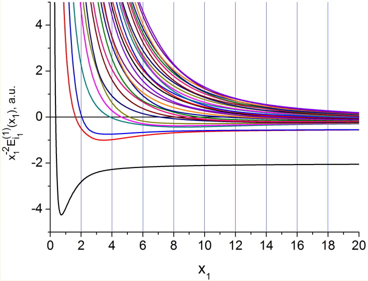
Step 2

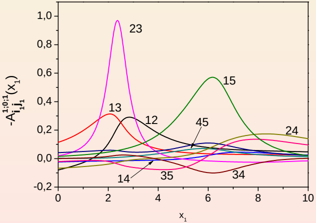
Here we introduce notations $(l_1 = 0, 1)$:

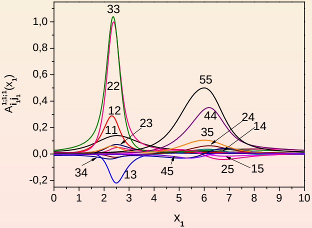
$$A_{i_2 j_2}^{1;l_1;r_1}(x_1) = \int \sin^2 x_2 dx_2 \sin x_3 dx_3 \frac{\partial^{l_1}}{\partial x_1^{l_1}} \Psi_{i_2}^{(2)}(x_3, x_2; x_1) \frac{\partial^{r_1}}{\partial x_1^{r_1}} \Psi_{j_2}^{(2)}(x_3, x_2; x_1)$$

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

Step 2 Calculated eigenvalues and matrix elements at step 1 of equation at step 2







Results of step 2

Ground state 1s1s energy $E_2^{(1)}$ of Helium atom (in a.u.) versus number n of basis functions and number $i_1^{\max}$ of the Legengre polynomials

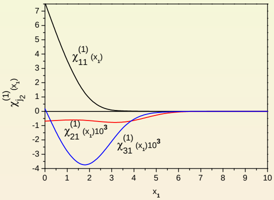
$i_2^{\max}$	ref^A $i_1^{\max}=12$	$i_1^{\max}=12$	$i_1^{\max}=21$	$i_1^{\max}=28$
1	−2.887 911 68	−2.895 539 01	−2.895 551 19	−2.895 552 76
2	−2.891 379 91	−2.898 631 39	−2.898 643 21	−2.898 644 74
6	−2.903 004 48	−2.903 643 86	−2.903 655 95	−2.903 657 51
10	−2.903 636 13	−2.903 702 68	−2.903 714 86	−2.903 716 36
15	−2.903 705 49	−2.903 708 49	−2.903 720 68	−2.903 722 17
21	−2.903 722 64	−2.903 709 31	−2.903 721 50	−2.903 722 994
28	−2.903 722 66	−2.903 709 31		−2.903 722 997
ref^B				−2.903 722 998
ref^V				−2.903 724 377

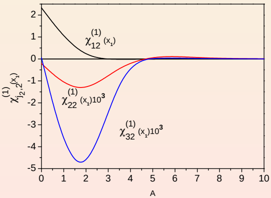
ref^A: Abrashkevich A.G. et al J. Comput. Phys., **163**, 328 (2000).
ref^B: J.J. De Groote et al, J. Phys. B **31** 4755 (1998).
ref^V: Chuluunbaatar et al, J. Phys. B **34** L425 (2001).

One can see that convergence start from $i_2^{\max}=21$ is slow with respect to upper variational estimation ref^V. So, to improve convergence of calculation of the parametric basis functions by number $i_1^{\max}>28$ we introduce below the step-by-step averaging method for improved calculation with a more high accuracy.

Results of step 2

Radial eigenfunctions of ground and first exited states.





First exited state 1s2s energy $E_2^{(1)}$ of Helium atom (in a.u.) versus number $i_2^{\max}$ of basis functions

$i_2^{\max}$	$i_1^{max} = 28$
1	−2.139 935 68
2	−2.141 664 33
6	−2.145 700 22
10	−2.145 915 09
15	−2.145 957 35
21	−2.145 968 77
28	−2.145 970 28
ref^B	−2.145 956 975
ref^V	−2.145 974 046

ref^B: J.J. De Groote et al, J. Phys. B **31** 4755 (1998)

ref^V: G.W.F. Drake et al, Chem. Phys. Lett. **229** 486 (1994)

One can see that our upper estimation at $i_2^{\max} = 28$ is lowing than result of ref^B and upper then vartiational ref^V.

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

We consider sequence of parametric boundary-value problems (with ordering from fast to slow independent variables $x_3 \succ x_2 \succ x_1$):

$$(\hat{H}_3(x_3; x_2, x_1) - \frac{1}{2} E_{i_3}^{(3)}(x_2, x_1))\Psi_{i_3}^{(3)}(x_3; x_2, x_1) = 0, \quad (1)$$

$$\int \sin x_3 dx_3 \Psi_{i_3}^{(3)}(x_3; x_2, x_1)\Psi_{j_3}^{(3)}(x_3; x_2, x_1) = \delta_{i_3 j_3}.$$

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

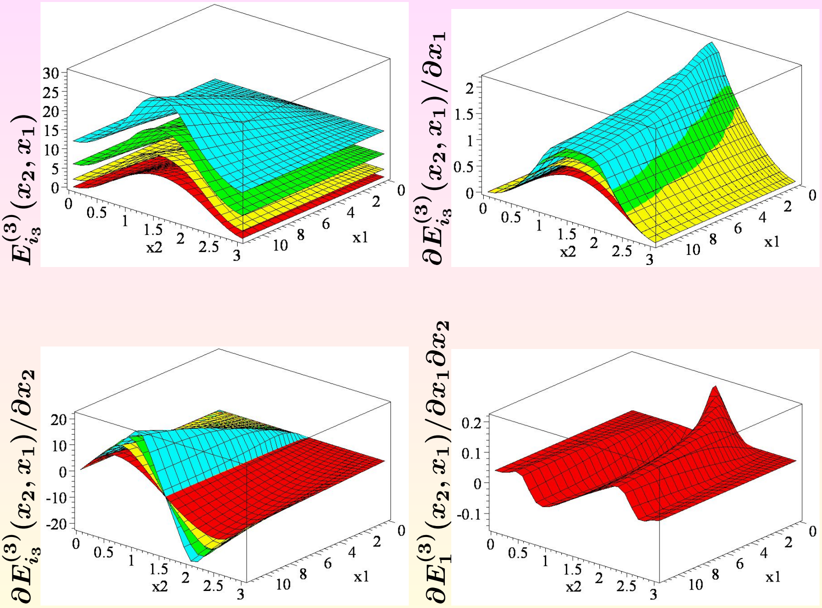
$$\int \sin^2 x_2 dx_2 \sin x_3 dx_3 \Psi_{i_2}^{(2)}(x_3, x_2; x_1)\Psi_{j_2}^{(2)}(x_3, x_2; x_1) = \delta_{i_2 j_2},$$

$$(\hat{H}_1(x_1) + \frac{4}{x_1^2}\hat{H}_2(x_2; x_1) + \frac{4}{x_1^2 \sin^2 x_2}\hat{H}_3(x_3; x_2, x_1) - 2E_{i_1}^{(1)})\Psi_{i_1}^{(1)}(x_3, x_2, x_1) = 0, \quad (3)$$

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

Step 1. Solving the problem (1)

The problem (1) is solved with help of the ODPEVP 2.0 program. for each values of x_1 and x_2:


$E_{i_3}^{(3)}(x_2, x_1)$
$\partial E_{i_3}^{(3)}(x_2, x_1)/\partial x_1$
$\partial E_{i_3}^{(3)}(x_2, x_1)/\partial x_2$
$\partial E_1^{(3)}(x_2, x_1)/\partial x_1 \partial x_2$
x2
x1

Algorithm 2.

Step 2. Solving the problem (2)

We find the solution of the problem (2) in the series expansion over solutions of problem (1) solved in the step 1:

$$\Psi^{(2)}_{i_2}(x_3, x_2; x_1) = \sum_{i_3=1}^{i_3^{\max}} \Psi^{(3)}_{i_3}(x_3; x_2, x_1)\chi^{(2)}_{i_3 i_2}(x_2; x_1), \quad (4)$$

Step 2.
Substituting expansion (4) into equation (2) and projecting with account of orthonormalization conditions of parametric basis functions from Step 1, we arrive to the problem for unknown vector functions $\chi^{(2)}_{i_3 i_2}(x_2; x_1)$:

$$\left(-\frac{1}{\sin^2 x_2}\frac{\partial}{\partial x_2}\sin^2 x_2\frac{\partial}{\partial x_2}+\hat{V}_2(x_2,x_1)+\frac{E^{(3)}_{i_3}(x_2,x_1)}{2\sin^2 x_2}\right)\chi^{(2)}_{i_3 i_2}(x_2;x_1)$$

$$+\sum_{j_3=1}^{i_3^{\max}}\langle i_3|\Big[H_2,j_3\rangle\Big]\chi^{(2)}_{j_3 i_2}(x_2;x_1)-\frac{1}{2}E^{(2)}_{i_2}(x_1)\chi^{(2)}_{i_3 i_2}(x_2;x_1)=0,$$

$$\langle i_3|\Big[H_2,j_3\rangle\Big]=\left(A^{2;10;10}_{i_3 j_3}(x_2,x_1)-\frac{1}{\sin^2 x_2}\frac{\partial}{\partial x_2}\sin^2 x_2 A^{2;00;10}_{i_3 j_3}(x_2,x_1)\right.$$
$$\left.-A^{2;00;10}_{i_3 j_3}(x_2,x_1)\frac{\partial}{\partial x_2}\right)$$

Substituting expansion (4) into orthonormation conditions (2), we have

$$\sum_{j_3=1}^{i_3^{\max}}\int\sin^2 x_2 dx_2\chi^{(2)}_{j_3 i_2}(x_2;x_1)\chi^{(2)}_{j_3 j_2}(x_2;x_1)=\delta_{i_2 j_2}.$$

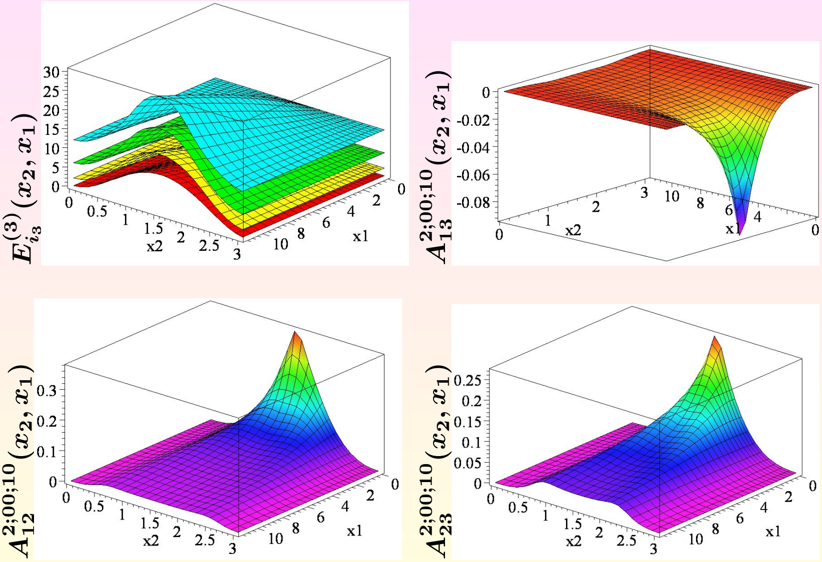
Step 2.
Here we introduce notations:

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

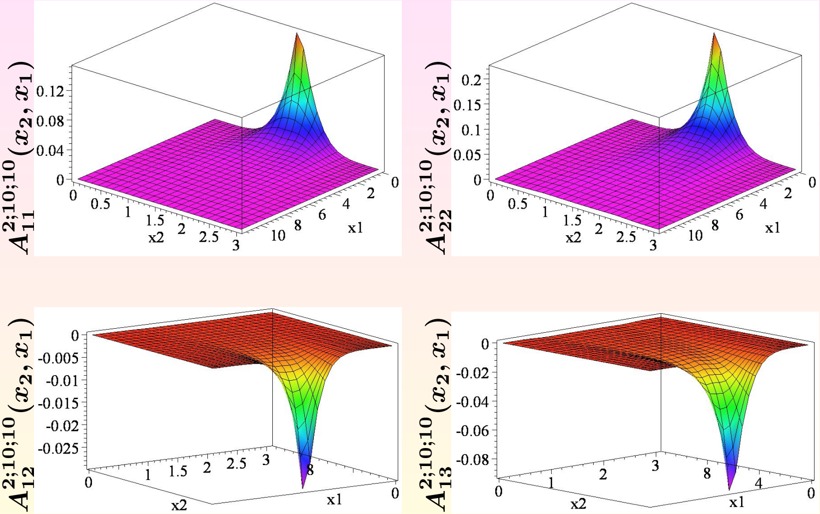
$$\frac{\partial^0}{\partial x_2^0 \partial x_1^0} \Psi_{i_3}^{(3)}(x_3;x_2,x_1) \equiv \Psi_{i_3}^{(3)}(x_3;x_2,x_1)$$

A parametric derivatives are calculated with help of KANTBP 3.0 program.

Step 2. Calculated eigenvalues and matrix elements at step 1 of equation at step 2



Step 2. Calculated eigenvalues and matrix elements at step 1 of equation at step 2



Step 3. Solving the problem (3)

We find the solution of the problem (3) in the series expansion over solutions of problem (2) solved in the step 2:

$$\Psi_{i_1}^{(1)}(x_3, x_2, x_1) = \sum_{i_2=1}^{i_2^{\max}} \Psi_{i_2}^{(2)}(x_3, x_2; x_1)\chi_{i_2 i_1}^{(1)}(x_1), \quad (5)$$

Step 3.

Substituting expansion (5) into equation (3) and projecting with account of orthonormalization conditions of parametric basis functions from Step 2, we arrive to the problem for unknown vector functions $\chi^{(1)}_{i_2 i_1}(x_1)$:

$$\left(-\frac{1}{x_1^5}\frac{\partial}{\partial x_1}x_1^5\frac{\partial}{\partial x_1}+\frac{2E^{(2)}_{i_2}(x_1)-4}{x_1^2}\right)\chi^{(1)}_{i_2 i_1}(x_1)$$

$$+\sum_{j_2=1}^{i_2^{\max}}\langle i_2|\Big[H_1,j_2\rangle\Big]\chi^{(1)}_{j_2 i_1}(x_1)-2E^{(1)}_{i_1}\chi^{(1)}_{i_2 i_1}(x_1)=0,$$

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

Substituting expansion (5) into orthonormation conditions (3), we have

$$\sum_{j_2=1}^{i_2^{\max}}\frac{1}{8}\int x_1^5 dx_1\chi^{(1)}_{j_2 i_1}(x_1)\chi^{(1)}_{j_2 j_1}(x_1)=\delta_{i_1 j_1}.$$

Step 3.

Here we introduce notations:

$$A^{1;l_1;r_1}_{i_2 j_2}(x_1)=\int \sin^2 x_2 dx_2 \sin x_3 dx_3 \frac{\partial^{l_1}}{\partial x_1^{l_1}} \Psi^{(2)}_{i_2}(x_3,x_2;x_1) \frac{\partial^{r_1}}{\partial x_1^{r_1}} \Psi^{(2)}_{j_2}(x_3,x_2;x_1)$$

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

Substituting expansion (4) we find matrix elements $A^{1;l_1;r_1}_{i_2 j_2}(x_1)$ via matrix elements $A^{2;l_1 l_2;r_1 r_2}_{i_3 j_3}(x_2,x_1)$ calculated with help of improved parametric basis functions from Step 2:

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

$$\times \int \sin^2 x_2 dx_2 \sin x_3 dx_3 \frac{\partial^{k_l}}{\partial x_1^{k_l}} \Psi^{(3)}_{i_3}(x_3;x_2,x_1) \frac{\partial^{l_1-k_l}}{\partial x_1^{l_1-k_l}} \chi^{(2)}_{i_3 i_2}(x_2;x_1)$$

$$\times \frac{\partial^{k_r}}{\partial x_1^{k_r}} \Psi^{(3)}_{j_3}(x_3;x_2,x_1) \frac{\partial^{r_1-k_r}}{\partial x_1^{r_1-k_r}} \chi^{(2)}_{j_3 j_2}(x_2;x_1)$$

$$\equiv \sum_{i_3,j_3} \sum_{k_l=0}^{l_1} \sum_{k_r=0}^{r_1} \frac{l_1!}{k_l!(l_1-k_l)!} \frac{r_1!}{k_r!(r_1-k_r)!}$$

$$\times \int \sin^2 x_2 dx_2 A^{2;0k_l;0k_r}_{i_3 j_3}(x_2,x_1) \frac{\partial^{l_1-k_l}}{\partial x_1^{l_1-k_l}} \chi^{(2)}_{i_3 i_2}(x_2;x_1) \frac{\partial^{r_1-k_r}}{\partial x_1^{r_1-k_r}} \chi^{(2)}_{j_3 j_2}(x_2;x_1).$$

Current status of the work

• In the present time we are adapting program KANTBP 3.0 for solving the problem with respect to unknowns (i.e. calculation of improved parametric basis functions) from Steps 2–(n-1), with matrices of variable coefficients calculated and presented above.

• In conclusion on the talk we present a symbolic-numerical algorithm for reduction of multistep adiabatic equations, corresponding to the MultiStep Generalization of Kantorovich Method (MSGKM), for solving multidimensional boundary-value problems.

Algorithm MSGKM

Input:
$H=\sum_{i=1}^{N} H_{N+1-i}$ is initial Hamiltonian dependent on ordered variables $\vec{x}=\{x_N \succ x_{N-1} \succ ... \succ x_1\}^T$ decomposed to sum of partial Hamiltonians $H_i \equiv H_i(x_i; x_{i-1}, ..., x_1)$, dependent on subset "faster" x_i and "slower" $x_{i-1}, ..., x_1$ variables;
$H\psi_{n_1} - 2E_{n_1}\psi_{n_1} = 0, \qquad \langle n_1' | n_1 \rangle = \int dx_N ... dx_1 \psi^{\dagger}_{n_1'}(\vec{x})\psi_{n_1}(\vec{x}) = \delta_{n_1' n_1}$
is main eigenvalue problem for calculation of $\langle \vec{x} | n_1 \rangle \equiv \psi_{n_1}(\vec{x})$ and $E_{n_1} = \varepsilon_{n_1}$.

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

Local:

$\psi_{n_k}^{(k)} \equiv \psi_{n_k}^{(k)}(x_N, ..., x_k; x_{k-1}, ..., x_1)$ and

$\varepsilon_{n_k} \equiv \varepsilon_{n_k}^{(k)} \equiv \varepsilon_{n_k}^{(k)}(x_{k-1}...x_1)$ are solutions of the auxiliary parametric eigenvalue problems

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

$\langle n'_k|n_k\rangle \equiv \int dx_N...dx_{N+1-k}\psi^{\dagger}_{n'_k}\psi_{n_k}$

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

$\langle n'_{k+1}|n_k\rangle = \int dx_N...dx_{k+1}\psi^{(k+1)}_{n'_{k+1}}\psi^{(k)}_{n_k}$.

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

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

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

4: Eq(k):=$\{(\varepsilon^{(k+1)}_{n_{k+1}} - \varepsilon^{(k)}_{n_k} + H_k)\langle n_{k+1}|n_k\rangle$

$$+\sum_{n'_{k+1}}\langle n_{k+1}|\left[H_k, n'_{k+1}\rangle\right]\langle n'_{k+1}|n_k\rangle = 0\}.$$

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

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

7: **end for**

8: $\Psi = |n_1\rangle$, $2E_{n_1} = \varepsilon^{(1)}_{n_1}$

Perspectives:

For example, for three-body problem with $N = 6$ independent variables in framework of the conventional Kantorovich method one has series expansion of required solutions over one-parametric basis functions of N-1=5 fast variables. Then such Kantorovich reduction leads to eigenvalue problem for set of $\sim 10^{N-1} =\sim 10^5$ ordinary second-order differential equations.

Generalization of MultiStep Kantorovich method presented below 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 $N - 1$, $N - 2$,..., 1, 0 independent parameter using MPI and/or GRID technology.