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

A.A. Gusev*, O. Chuluunbaatar, V.P. Gerdt, B.L. Markovski, V.V. Serov, and S.I. Vinitsky
Joint Institute for Nuclear Research, Dubna, Moscow Region 141980, Russia
aSaratov State University, Saratov, 4100012, Russia

Abstract

The adiabatic approximation is a 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 (1927) the method was applied in various problems of physics, using the idea of separation of “fast” and “slow” variables.

Purpose of this talk is to present algorithm for generalization of the standard adiabatic ansatz for the case of multi-channel wave function when all variables treated dynamically [1, 2]. For this reason we are introducing the step-by-step averaging methods for order to eliminate consequently from faster to slower variables.

We present a symbolic algorithm for reduction of multistep adiabatic equations, corresponding to the MultiStep Generalization Kantorovich Method (MSGKM), for solving multidimensional boundary-value problems [3].

Algorithm MSGKM

Input:

\[ H = \sum_{i=1}^{N} H_{N+1-i} \] is initial Hamiltonian dependent on ordered variables \( \vec{x} = \{x_N > x_{N-1} > ... > x_1\}^T \) 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;

\*gooseff@jinr.ru
\[ H \psi_n - E_n \psi_n = 0, \quad \langle n'_1 | n_1 \rangle = \int dx_N ... dx_1 \psi_{n'_1}^\dagger (\vec{x}) \psi_n (\vec{x}) = \delta_{n'_1 n_1} \]

is main eigenvalue problem for calculation of \( \langle \vec{x} | n_1 \rangle \equiv \psi_n (\vec{x}) \) and \( E_n = \varepsilon_n \).

**Output:**

A set Eq(k) \( k = 1, ..., N \) is a set of auxiliary parametric eigenvalue problems for calculation of \( \psi_{n_k} \equiv \psi_{n_k}^{(k)} (x_N, ..., x_k; x_{k-1}, ..., x_1) \) and \( \varepsilon_{n_k} \equiv \varepsilon_{n_k}^{(k)} (x_{k-1}...x_1) \), where \( \Psi = \psi_n^{(1)} \) and \( E_n = \varepsilon_n^{(1)} \) 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 \( \varepsilon_{n_k} \equiv \varepsilon_{n_k}^{(k)} (x_{k-1}...x_1) \) are solutions of the auxiliary parametric eigenvalue problems

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

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

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

\( \langle n'_k+1 | n_k \rangle = \int dx_N ... dx_{k+1} \psi_{n_k+1}^\dagger \psi_{n_k} \).

1. Eq(N) := \{ \langle H_N | n_N \rangle - \varepsilon_{n_N} | n_N \rangle = 0, \quad \langle \psi_{n_N}^{(N)} | \psi_{n_N}^{(N)} \rangle = \delta_{n_N n_N} \}

2. Eq(N) \rightarrow \{ n_N, \varepsilon_{n_N} \}

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

4. Eq(k) := \{ (\varepsilon_{n_k+1}^{(k+1)} - \varepsilon_{n_k}^{(k)} + H_k) \langle n_{k+1} | n_k \rangle \\
                                 + \sum_{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| := \sum_{n_{k+1}} \langle n_{k+1} | n_k \rangle

7. end for

8. \( \Psi = |n_1\rangle, \quad E_{n_1} = \varepsilon_{n_1}^{(1)} \)

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**References:**

