4. Program DBSR_PREP

4.1. Outline of the DBSR_PREP calculations

The main goal of the DBSR_PREP program is to analyze the one-electron orbitals in the input target wavefunctions and assign consistent set-indexes if the orbitals are not orthogonal. Since the target states may be generated in the independent calculations, it is possible that the same spectroscopic notation was given to the different orbitals. For example, we may use different term-dependent radial functions for the same *nl*-orbital, or we may use the same spectroscopic notation for the correlated functions in different states. To distinguish such orbitals, we use an additional 'set number' or 'set index', e.g. nl_1, nl_2, …, nl_a, nl_b and so on. The DBSR_PREP program therefore analyses the input target files and, if necessary, assigns an individual set number to each orbital. It concerns both the *N*-electron target states and the (*N*+1)-electron configurations included in the close-coupling expansion for a more complete description of short-range correlations. In the bound-state calculations, these (*N*+1)-electron states are called as 'perturbers', because they are often used to describe the states that perturb the Rydberg series under consideration.

The list of input target states and perturbers are provided by the user in the file **target_jj**. DBSR_PREP sequentially reads all related *c*- and *bsw*-files and compares the one-electron radial functions. They are considered the same if their overlaps or first moments differ by less than a given tolerance:

$$\begin{aligned} &|< P_1 \,|\, P_2 > -1| \;\; \le \;\; \varepsilon, \\ &|< P_1 \,|\, r \,|\, P_1 > - < P_2 \,|\, r \,|\, P_2 >| \;\; \le \;\; \varepsilon, \\ &|< P_1 \,|\, 1/r \,|\, P_1 > - < P_2 \,|\, 1/r \,|\, P_2 >| \;\; \le \;\; \varepsilon. \end{aligned} \tag{4.1}$$

The radial functions are considered orthogonal if their overlap

$$| \;\; < P_1 \,|\, P_2 > \;\; | \;\; \le \;\; \varepsilon \;\; . \tag{4.2}$$

For a given subset of orthogonal orbitals, DBSR_PREP assigns the same set number. There are practically no restrictions on the number of different non-orthogonal orbitals.

Then DBSR_PREP rewrites the target *c*- and *bsw*-files with a new consistent spectroscopic notation. New target *c*-files receive the names **targ_001.c**, **targ_002.**c, and so on, and they are ordered according to the target energies. All target radial functions are placed in the single file **target.bsw**. The same procedure is then applied to the perturber files, and each perturber is now rewritten in the pair of files **pert_nnn.c** and **pert_nnn.bsw,** where **nnn** denotes the corresponding partial wave. All the above rewritings are recorded in the file **target_jj**, from which the user can see the relation between the input names and the new notation.

Another important task of DBSR_PREP is to make difference between physical and correlation orbitals, and to find one orthogonal set of orbitals which will mimics all physical orbitals in the target states. Such orbitals will be

called as substitution orbitals and are needed to imply the orthogonal constraints through the projection scheme. The physical orbitals are defined by their effective occupation number, and the list of these orbitals are created in the file **target_orb**. The DBSR_PREP also create the list of substitution orbitals, however, in the extensive RMPS calculations with many target states the user is advised to provide such orbitals through the file **target_sub.bsw.** The example how to create these files are given in section (???).

4.2. Data files

target_jj	File type: formatted sequential input. Description: list of target states and scattering channels. Prepared by user. Read and modified by program DBSR_PREP and DBSR_CONF; used in all following calculations by DBSR complex**.** Format: see section 4.3.
dbsr_par	File type: formatted sequential input. Description: optional input parameters for the given run. Written by user. Format: see section 3.2 and examples in section 14.
knot.dat	File type: formatted sequential input. Provided by user. Description: input parameters that define the *B*-spline grid; should be consistent with the calculation of target states; used in all following calculations by DBSR complex**.** Format: see section 12.2.
name.c	File type: formatted sequential input. Provided by user. Description: configuration expansion for one target state. Format: see section 12.5.
name.bsw	File type: unformatted sequential input. Description: contains *B*-spline representation of one-electron radial functions for one target state. These files are output of the DBSR_HF or DBSR_MCHF programs, or created by utilities r**w_bsw** (see section 13) if the target states were generated with GRASP. Format: see section 12.5
target_sub.bsw	File type: unformatted sequential input. Description: one-electron substitution orbitals used for orthogonality constrains by programs DBSR_CONF and DBSR_MAT. Provided by user (optional).
targ_nnn.c	File type: formatted sequential output. Created by program DBSR_PREP. Read by program DBSR_CONF.

	Description: contains configuration expansion for one target state **nnn,** with consistent spectroscopic notation for one-electron orbitals.
target.bsw	File type: unformatted sequential input. Created by program DBSR_PREP. Read by program DBSR_MAT. Description: contains all one-electron target orbitals in the *B*-spline basis.
target_orb	File type: formatted sequential input. Created by program DBSR_PREP. Read by program DBSR_CONF DBSR_MAT. Description: contains list of one-electron physical orbitals, with their effective occupation numbers and the corresponding substitution orbitals.
pert_nnn.c	File type: formatted sequential output. Created by program DBSR_PREP. Read by program DBSR_CONF. Description: contains configuration expansion for the perturber **nnn,** with consistent spectroscopic notation for one-electron orbitals.
pert_nnn.bsw	File type: unformatted sequential output. Created by program DBSR_PREP**.** Read by programs DBSR_MAT. Description: contains one-electron orbitals in *B*-spline basis for pertuber **nnn**.
dbsr_prep.log	File type: formatted sequential output. Written by program DBSR_PREP**.** Description: running information.

4.3. Input parameters

Input parameters can be provided in the command line or in the input file **dbsr_par** (data from the command line overwrite data from the input file). Below we describe the data from **dbsr_par** that are read by program DBSR_PREP. The default values for all data are indicated in the brackets.

eps_ovl [1.d-6]	tolerance for overlaps, see equation (4.1).
eps_core [1.d-5]	tolerance for orthogonality to the core orbitals.
eps_phys [0.25]	minimum occupation number for orbital to be considered as physical.
eps_sub [0.5]	tolerance for substitution orbitals.
JJ_min [1]	minimum 2*J*-value for the partial waves.
JJ_max [1]	maximum 2*J*-value for the partial waves.

All parameters are optional. The parameters **JJ_min** and **JJ_max** are used only when file target does not contains explicit description of the partial waves included into considerations (parameter **`nlsp`** = 0).

4.4. Input data in file **target_jj**

This file is created by the user and contains the description of the physical scattering model under consideration. If **target_jj** is absent, the program creates an example and suggests to user to fill in. The example of **target_jj** is given in Fig. 4.1. In addition to the data, the file also contains the dashed lines and comments placed behind the '!' character. The comments are optional, whereas the dashed lines are used to delimit different types of data and are part of the format. The first line is just a title for the given run. Then, after a line-delimiter, the user provides some basic data such the number of electrons, and the atomic number. The format for all quantities is the same as for the parameters in the file **dbsr_par:** `name = value`, where `name` should be placed at the beginning of the line. The next block of data is the list of target *c*-files, which should be placed after the number of target states, `ntarg`. Then user may provide the list of partial wave, placed after number of partial waves, `nlsp`. The description of each partial wave contains their index, total momentum as 2*J*-value and parity. The perturber for a given partial wave, if any, is given by the corresponding name, placed in the same line after position 13. Alternatively, user can indicate the `nlsp=0` and indicate the range of partial wave through the input parameters **JJ_min** and **JJ_max**.

DBSR_PREP adds some additional information to the **target** file. An example of **target** after a run of DBSR_PREP is given in Fig. 4.2. Now the target states are ordered by energy, and for each target state the program provides a new name **targ_nnn**, the term ($2J,\pi$), the energy, the number of configurations, and the number of new one-electron radial orbitals used in the description of a given target state. All this information was extracted from the corresponding target *c*-files. Similar information is also provided for the perturbers: new standard name **pert_nnn**, the number of configurations and the number of new one-electron radial orbitals used in the description of a given pertuber. Also provided are the total number of target configurations, `nct`, the total number of one-electron orbitals, `nwt`.

Program also create the file **target.bsw** which contains all one-electron orbitals, used for the description of target states, with consistent set indexes. The output file **target_orb** contains the list of physical orbitals with indication of corresponding substitution orbitals used for orthogonality constraints.

Another new feature of DBSR_PREP3 is the possibility to add perturbers through `kpert` list (see example in Fig.4.3 and Fig.4.4). This list consists from the partial wave index and the name of the perturber. These perturbers can be generated in the separate MCHF calculations and their configuration expansions will be kept the same during the calculations. Any number of additional perturbers are allowed.

```
  e + Xe+
------------------------------------------------------------------------
nz    =   54      !   nuclear charge
nelc  =   53      !   number of electrons
------------------------------------------------------------------------
ntarg =    3      !   number of target states
------------------------------------------------------------------------
5p5_j3
5p5_j1
5s5p6_j1
------------------------------------------------------------------------
nlsp  =   11      !   number of partial waves
------------------------------------------------------------------------
  1.    0   1      5p6_j0
  2.    0  -1
  3.    2   1
  4.    2  -1
  5.    4   1
  6.    4  -1
  7.    6   1
  8.    6  -1
  9.    8   1
 10.    8  -1
 11.   10   1
------------------------------------------------------------------------
```

Fig.4.1. Example of input file **target_jj** prepared by the user.

```
  e + Xe+
------------------------------------------------------------------------
nz    =   54      !   nuclear charge
nelc  =   53      !   number of electrons
------------------------------------------------------------------------
ntarg =    3      !   number of target states
------------------------------------------------------------------------
5p5_j3                targ_001       3  -1    -7446.56423993    1    0
5p5_j1                targ_002       1  -1    -7446.51524601    1    0
5s5p6_j1              targ_003       1   1    -7446.00375949    1    3
------------------------------------------------------------------------
nct =      3
nwt =     20
------------------------------------------------------------------------
nlsp  =   11      !   number of partial waves
------------------------------------------------------------------------
  1.    0   1      5p6_j0                         pert_001      1    3
  2.    0  -1
  3.    2   1
  4.    2  -1
  5.    4   1
  6.    4  -1
  7.    6   1
  8.    6  -1
  9.    8   1
 10.    8  -1
 11.   10   1
------------------------------------------------------------------------
```

Fig.4.2. Example of the file **target_jj** after a run of the DBSR_PREP program.

```
    e + Xe+     bound states
-------------------------------------------------------------------
nz    =   54      !   nuclear charge
nelc  =   53      !   number of electrons
-------------------------------------------------------------------
ntarg =    3      !   number of target states
-------------------------------------------------------------------
5p5_j3
5p5_j1
5s5p6_j1
-------------------------------------------------------------------
nlsp  =   11      !   number of partial waves
-------------------------------------------------------------------
  1.   0   1
  2.   0  -1
  3.   2   1
  4.   2  -1
 ...........
 11.  10   1
-------------------------------------------------------------------
kpert =    1      !   number of additional perturbers
-------------------------------------------------------------------
  1     5p6_j0
-------------------------------------------------------------------
```

Fig.4.3. Example of input file **target_jj** (prepared by the user) which illustrate new option for the introduction of perturbers through the **kpert** parameter.

```
  e + Xe+     bound states
-------------------------------------------------------------------------
nz    =   54      !   nuclear charge
nelc  =   53      !   number of electrons
-------------------------------------------------------------------------
ntarg =    3      !   number of target states
-------------------------------------------------------------------------
5p5_j3               targ_001       3  -1    -7446.48480535    1    3
5p5_j1               targ_002       1  -1    -7446.43571440    1    0
5s5p6_j1             targ_003       1   1    -7445.92429625    1    3
-------------------------------------------------------------------------
nct =      3
nwt =     20
-------------------------------------------------------------------------
nlsp  =   11      !   number of partial waves
-------------------------------------------------------------------------
  1.   0   1      no                                pert_001      1    3
  2.   0  -1
  3.   2   1
  4.   2  -1
 ...........
 11.  10   1
-------------------------------------------------------------------------
kpert =    1      !   number of additional perturbers
-------------------------------------------------------------------------
  1     5p6_j0
-------------------------------------------------------------------------
```

Fig.4.4. Example of the file **target_jj** after a run of the DBSR_PREP program (compare with Fig.4.3).

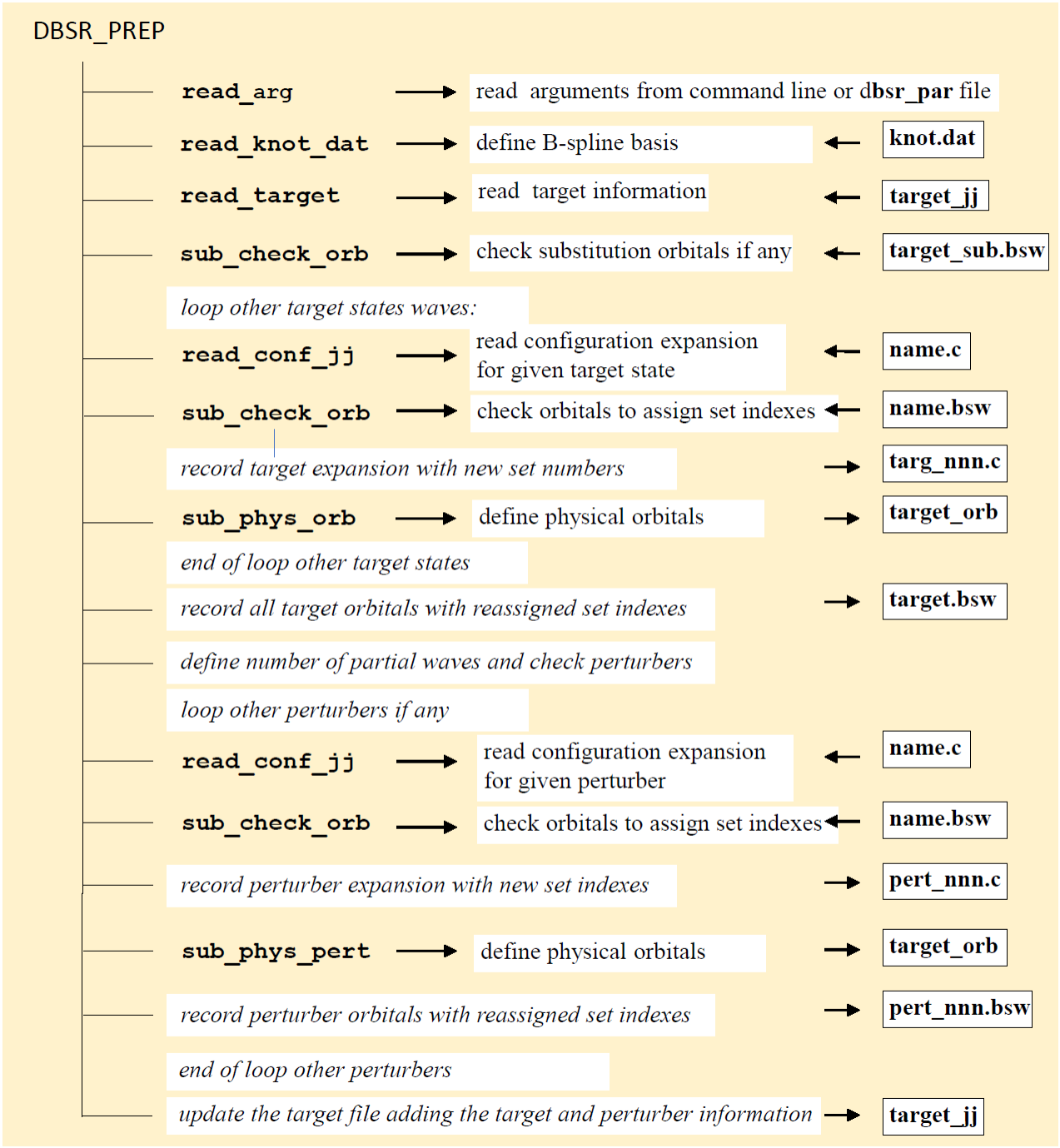

Fig.4.5. Block-scheme for the DBSR_PREP program.