4. Program BSR_PREP

4.1. Outline of the BSR_PREP calculations

This program provides initial preparations for BSR calculations. Since the input 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 can use different term-dependent radial functions for the same *nl*-orbital, or simply use the same spectroscopic notation for the correlated functions in different states. In order to distinguish between such orbitals, we use an additional 'set number' or 'set index', e.g. nl_1, nl_2, …, nl_a, nl_b and so on. It is difficult and very inconvenient for the user to keep track of all such cases by hand. The BSR_PREP program therefore analyses the input target files and, if necessary, assigns an individual set number to each orbital. The same concerns also the additional sets of (N+1)-electron configurations included in the close-coupling expansion (2.14) for a more complete description of short-range correlations. We will call these configurations 'perturbers', because they are often used in bound-state calculations to describe the states that perturb the Rydberg series under consideration. These additional (N+1)-electron configurations should be provided in separate files, and they should be distinguished from the configurations which are automatically generated for compensation of the orthogonality constraints imposed on the continuum orbitals (see the description of the BSR_CONF program).

The list of input target states and perturbers are provided by the user in the file **target**. BSR_PREP sequentially reads all *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, BSR_PREP assigns the same set number. There are practically no restrictions on the number of different non-orthogonal orbitals.

Then BSR_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 this information about target and perburbers states are recorded in the file **target**, from which the user can obtain the relation between the new standard and the input names.

4.2. Data files

target	File type: formatted sequential input. Written by user. Read and modified by program BSR_PREP and BSR_CONF**.** Description: list of target states and scattering channels. Format: see section 4.3.
bsr_par	File type: formatted sequential input. Written by user. Description: input parameters for given run. Format: see section 3.2 and examples in section 14.
knot.dat	File type: formatted sequential input. Prepared by user. Read and modified by routine **define_grid** from BSPLINE library. Description: input parameters that define the *B*-spline grid. Format: see section 12.2.
bsr_prep.log	File type: formatted sequential output. Written by program BSR_PREP**.** Read by user. Description: running information.
name.c	File type: formatted sequential input. Provided by user. Read by routine **r_confc** from ZCONF library. Description: configuration expansion for one target state. Format: see section 12.5.
name.bsw	File type: unformatted sequential input. Created by utilities **w_bsw** or **slater_bsw** (see section 13). Read by routine **read_bsw.** Description: contains *B*-spline representation of one-electron radial functions.
targ_nnn.c	File type: formatted sequential output. Created by program BSR_PREP. Read by program BSR_CONF. Description: contains configuration expansion for one target state **nnn,** with consistent spectroscopic notation for one-electron orbitals.
target.bsw	File type: unformatted sequential output. Created by program BSR_PREP. Read by program BSR_MAT Description: contains all one-electron target orbitals in the *B*-spline basis.
pert_nnn.c	File type: formatted sequential output. Created by program BSR_PREP.

	Read by program BSR_CONF. Description: contains configuration expansion for perturber **nnn,** with consistent spectroscopic notation for one-electron orbitals.
pert_nnn.bsw	File type: unformatted sequential output. Created by program BSR_PREP**.** Read by programs BSR_MAT. Description: contains one-electron orbitals in *B*-spline basis for pertuber **nnn**.
target_orb	File type: formatted sequential output. Created by program BSR_PREP. Read by program BSR_MAT. Description: contains list of one-electron physical orbitals, with their effective occupation numbers and the corresponding substitution orbitals.
target_sub.bsw	File type: unformatted sequential input/output. Created by program BSR_PREP or provided by user (optional). Read by programs BSR_CONF and BSR_MAT. Description: contains one-electron substitution orbitals used for orthogonality constraints.

4.3. Input parameters

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

eps_ovl [1.d-6]	tolerance for overlaps, see equation (4.1).
eps_phys [0.5]	minimum occupation number for orbital to be considered physical.
eps_sub [0.5]	tolerance for substitution orbitals.
eps_targ [2.d-8]	tolerance for target expansion coefficients.
ii_sub [0]	**ii_sub** = 1 prevents the automatic generation of substitution orbitals.
LT_min [0]	minimum *L*-value for the partial waves.
LT_max [25]	maximum *L*-value for the partial waves.
IS_min [-1]	minimum 2*S*+1-value for the partial waves.
IS_max [-1]	maximum 2*S*+1-value for the partial waves.
JJ_min [-1]	minimum 2*J*-value for the partial waves.
JJ_max [-1]	maximum 2*J*-value for the partial waves.

4.4. Input data in file **target**

This file is created by the user and contains the description of the physical scattering model under consideration. The example of input **target** 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 a title for the given run. Then after a line-delimiter, the user provides some basic data such as the type of coupling (*LS* or semi-relativistic *JK*, *JJ*), the number of electrons, and the atomic number. The format for all quantities is the same as for the parameters in the file **bsr_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 provides the list of partial wave, placed after number of partial waves, `nlsp`. The description of each partial wave contains the total term (L,$2S$+1,π) in *LS* coupling or ($2J$,0,π) in semi-relativistic calculations. The perturber for a given partial wave, if any, is given by the name of the corresponding *c*-file in the corresponding line after position 18. Note that list of the partial waves can be generated by the program based on the additional arguments `LT_min, LT_max, IS_min, IS_max`, or `JJ_min`, `JJ_max`, which restrict the values of the total angular momentums. This requires additional preliminary run BSR_PREP with **nlsp**=0 in the target file.

BSR_PREP adds some additional information to the **target** file. An example of **target** after a run of BSR_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.c**, the term (L,$2S$+1,π), 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.c**, 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`, and the list of orbitals with new spectroscopic notation, including the set numbers. In the example shown, we used two different sets of orthogonal orbitals, for even-parity and odd-parity states, respectively. These sets differ by their indexes 1 and 2. Note that the 1s orbital represents the closed shell $1s^2$, and it is common for all configurations. These core orbitals should be orthogonal to all orbitals, and hence they do not need any additional set index.

New important feature of BSR_PREP3 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 physical orbitals for the given target state or

perturber are also recorded in the end of the corresponding **targ_nnn.c** or **pert_nnn.c** files. The BSR_PREP3 will also try to create the list of substitution orbitals itself, 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 (???).

Another new feature of BSR_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 + C
-------------------------------------------------------------------------
coupling = LS     !   non-relativistic calculations
nz =  6           !   nuclear charge
nelc = 6          !   number of electrons
-------------------------------------------------------------------------
ntarg = 36        !   number of target states
-------------------------------------------------------------------------
2p2_1S
2p2_1D
2p2_3P
2p3_3Do
2p3_5S
2p3s_3Po
2p3s_1Po
2p3p_1P
..........
3Po_ps4
3Do_ps3
-------------------------------------------------------------------------
nlsp = 64         !   number of partial waves
-------------------------------------------------------------------------
001    0    2    1   p_2Se
002    0    4    1
003    0    2   -1
004    0    4   -1   p_4So
005    1    2    1   p_2Pe
006    1    4    1   p_4Pe
007    1    2   -1   p_2Po
008    1    4   -1
009    2    2    1   p_2De
010    2    4    1
011    2    2   -1   p_2Do
012    2    4   -1
013    3    2    1
.........................
063   15    2   -1
064   15    4   -1
```

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

```
    e + C
--------------------------------------------------------------------------
coupling = LS     !   LS coupling
nz =  6           !   nuclear charge
nelc = 6          !   number of electrons
--------------------------------------------------------------------------
ntarg = 36        !   number of target states
--------------------------------------------------------------------------
2p2_3P.c              targ_001.c   1   3   1      -37.77853957    258  10
2p2_1D.c              targ_002.c   2   1   1      -37.72880614    263   0
2p2_1S.c              targ_003.c   0   1   1      -37.67441594    132   0
2p3_5S.c              targ_004.c   0   5  -1      -37.62901126     30  10
2p3s_3Po.c            targ_005.c   1   3  -1      -37.50336422    318   0
2p3s_1Po.c            targ_006.c   1   1  -1      -37.49458261    261   0
2p3_3Do.c             targ_007.c   2   3  -1      -37.48150929    233   0
2p3p_1P.c             targ_008.c   1   1   1      -37.46513100    169   0
.........................................................................
3Po_ps4.c             targ_035.c   1   3  -1      -36.72115047    318   0
3Do_ps3.c             targ_036.c   2   3  -1      -36.69897493    233   0
--------------------------------------------------------------------------
nct =  8091
nwt =    20
  1s 2s1 2p1 3p1 3d1 3s1 9s1 9p1 9d1 9f1 2s2 2p2 3d2 3p2 3s2 4s2 9s2 9p2
 9d2 9f2
--------------------------------------------------------------------------
nlsp =   64       !   number of partial waves
--------------------------------------------------------------------------
001    0    2    1   p_2Se.c               pert_001.c      31    6
002    0    4    1
003    0    2   -1
004    0    4   -1   p_4So.c               pert_004.c      28    9
005    1    2    1   p_2Pe.c               pert_005.c      63    6
006    1    4    1   p_4Pe.c               pert_006.c      40    6
007    1    2   -1   p_2Po.c               pert_007.c      84    6
008    1    4   -1
009    2    2    1   p_2De.c               pert_009.c      55    6
010    2    4    1
011    2    2   -1   p_2Do.c               pert_011.c     141   10
012    2    4   -1
013    3    2    1
.........................................................................
063   15    2   -1
064   15    4   -1
--------------------------------------------------------------------------
```

Fig.4.2. Example of the file **target** after a run of the BSR_PREP program.

```
      e + N+     bound-states calculations
-------------------------------------------------------------------------------
coupling = LS    !   non-relativistic calculations
nz =   7         !   nuclear charge
nelc =  6        !   number of electrons
-------------------------------------------------------------------------------
ntarg =  9       !   number of target states
-------------------------------------------------------------------------------
2p2_3P
2p2_1D
2p2_1S
2s_2p3_5S
2s_2p3_3D
2s_2p3_3P
2s_2p3_1D
2s_2p3_3S
2s_2p3_1P
-------------------------------------------------------------------------------
nlsp = 20        !  number of partial waves
-------------------------------------------------------------------------------
001    0    2    1
002    0    4    1
003    0    2   -1
004    0    4   -1
005    1    2    1
006    1    4    1
007    1    2   -1
008    1    4   -1
009    2    2    1
010    2    4    1
011    2    2   -1
012    2    4   -1
013    3    2    1
014    3    4    1
015    3    2   -1
016    3    4   -1
017    4    2    1
018    4    4    1
019    4    2   -1
020    4    4   -1
-------------------------------------------------------------------------------
kpert =  7        !  number of pertubers
-------------------------------------------------------------------------------
   1     2s_2p4_2S
   4     2p3_4S
   5     2s_2p4_2P
   6     2s_2p4_4P
   7     2p3_2P
   9     2s_2p4_2D
  11     2p3_2D
-------------------------------------------------------------------------------
```

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

```
        e + N+     bound-states calculations
-------------------------------------------------------------------------
coupling = LS     !   coupling scheme
nz       =    7    !   nuclear charge
nelc     =    6    !   number of electrons
-------------------------------------------------------------------------
ntarg    =    9    !   number of target states
-------------------------------------------------------------------------
2p2_3P               targ_001      1   3   1      -53.97574931   17    5
2p2_1D               targ_002      2   1   1      -53.90955467   24    3
2p2_1S               targ_003      0   1   1      -53.82661750   15    0
2s_2p3_5S            targ_004      0   5  -1      -53.77862021    9    7
2s_2p3_3D            targ_005      2   3  -1      -53.55181815   16    1
2s_2p3_3P            targ_006      1   3  -1      -53.46737181   18    1
2s_2p3_1D            targ_007      2   1  -1      -53.29836607   12    0
2s_2p3_3S            targ_008      0   3  -1      -53.26363494   14    0
2s_2p3_1P            targ_009      1   1  -1      -53.21478218   20    0
-------------------------------------------------------------------------
nct      =  145    !   total number of target configurations
nwt      =   18    !   total number of target orbitals
nsub     =    3    !   number of substitution orbitals
-------------------------------------------------------------------------
nlsp     =   20    !   number of partial waves
-------------------------------------------------------------------------
001    0    2    1   no                  pert_001     72    9
002    0    4    1
003    0    2   -1
004    0    4   -1   no                  pert_004     21    8
005    1    2    1   no                  pert_005     42    9
006    1    4    1   no                  pert_006     42    9
007    1    2   -1   no                  pert_007     67    8
008    1    4   -1
009    2    2    1   no                  pert_009     65    9
010    2    4    1
011    2    2   -1   no                  pert_011     53    9
012    2    4   -1
013    3    2    1
014    3    4    1
015    3    2   -1
016    3    4   -1
017    4    2    1
018    4    4    1
019    4    2   -1
020    4    4   -1
-------------------------------------------------------------------------
kpert    =    7    !   number of additional perturbers
-------------------------------------------------------------------------
  1   2s_2p4_2S
  4   2p3_4S
  5   2s_2p4_2P
  6   2s_2p4_4P
  7   2p3_2P
  9   2s_2p4_2D
 11   2p3_2D
-------------------------------------------------------------------------
```

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

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