**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, …, *nla*, *nlb* 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:

 (4.1)

The radial functions are considered orthogonal if their overlap

. (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.

* 1. *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*,2*S*+1,*π*) in *LS* coupling or (2*J*,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*,2*S*+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 1s2, 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.