**Description of utility-programs for BSR complex (folder UTILS/BSR\_utils)**

In addition to the main BSR programs, a number of short utility-programs are available that assist in the processing and managing the data. This folder contains the utilities which directly working with B-splines or with files produced with the BSR programs.

**Quick-references to the utilities**

|  |  |
| --- | --- |
| **bound\_tab** | produces the total list of resulting bound states after BSR calculations |
| **bound\_bsw** | converts the close-coupling B-spline expansions to the c- and bsw-files for individual state |
| **w\_bsw** | converts the MCHF w-file to the BSR bsw-file |
| **bsw\_w** | converts the BSR bsw-file to the MCHF w-file |
| **bsw\_tab** | prepares the text files suitable for plotting the radial functions from bsw-file |
| **bsw123** | merging the set of bsw-files with user's choice of orbitals and with optional changing the spectroscopic notation |
| **bs\_hwf** | provides hydrogen-like bound and continuum pseudo-state orbitals'on the given B-spline basis |
| **print\_bs** | prints B-splines (in separate files) for given B-spline basis |
| **sum\_hh** | merges the set of **h.nnn** files to the final H.DAT |
| **h\_targb** | creates "**target**" file based on the "**H.DAT**" file |
| **h\_targn** | creates "**target**" file based on the set of **nnn/h.nnn** files |
| **target\_exp** | change **target** file to fit new experimental state energies, given in file **thresholds** |
| **target\_states** | provide information about target states including their labels |
| **zf\_bb\_bsr** | calculates f-values between solutions in set of **bound.nnn** |
| **zf\_cc\_bsr** | calculates f-values between set of {**name.c+name.bsw**} files |
| **bsr\_dd** | calculation of dipole matrix elements between R-matrix states saved in **rsol.nnn** files |
| **photo\_tab** | produces the tables for channel or total photoionization cross sections and asymmetry parameters |
| **photo\_collect** | collects data from **bsr\_phot.nnnn** files to final **bsr\_phot.nnn** file after MPI calculations if they not finished correctly |
|  |  |

**B O U N D \_ T A B**

|  |  |
| --- | --- |
| Description: | produces the total list of resulting bound states |
| Input files: | **bound.nnn** |
| Output files: | **bound.tab** |
| Call: | **bound\_tab** [**klsp =…**] |

This program sorts the energies of states recorded in different **bound.nnn** files and prints them in atomic units, eV or cm-1, relative to the lowest state. The user can define the range of partial waves and the energy range to restrict the output. The end of the file contains the parameters used by program. The range of partial waves is defined by **klsp1**, **klsp2**, and **klsp3**, as the initial, final and step for partial wave. **Emin**, **Emax** restrict the energy region under consideration (zero values mean no restrictions). Nuclear charge **Z** and **AWT** (if they are not zero) are used to define conversation factor from atomic units (Ry, au) to other units (eV, cm-1). **E0** defines the reference points to calculate excitation or bound energies. If reference point is not defined by user, the program chooses the energy of the first target state as the reference points. All above parameters can be redefined by corresponding command-line arguments (as parameter=value), or user can change these parameters directly in the **bound\_tab** file and re-run the program.

**klsp sol label L S P E\_Ry E\_eV E\_cm E\_au**

**1 1 4s\_4s\_1S 0 1 1 -0.217888 -5.92898 -47820.4 -676.80847440**

**4 1 4s\_4p\_3P 1 3 -1 -0.147927 -4.02526 -32465.9 -676.73851340**

**3 1 4s\_4p\_1P 1 1 -1 -0.109965 -2.99226 -24134.2 -676.70055090**

**8 1 4s\_3d\_3D 2 3 1 -0.105841 -2.88004 -23229.1 -676.69642660**

**7 1 4s\_3d\_1D 2 1 1 -0.102908 -2.80023 -22585.4 -676.69349370**

**2 1 4s\_5s\_3S 0 3 1 -0.078572 -2.13803 -17244.4 -676.66915820**

**1 2 4s\_5s\_1S 0 1 1 -0.070551 -1.91976 -15483.9 -676.66113670**

**12 1 3d\_4p\_3F 3 3 -1 -0.059778 -1.62664 -13119.7 -676.65036440**

**4 2 4s\_5p\_3P 1 3 -1 -0.056834 -1.54651 -12473.5 -676.64741990**

**...............................................................................**

**5 9 3d\_kd\_1P 1 1 1 0.081296 2.21216 17842.3 -676.50928960**

**5 10 4p\_6p\_1P 1 1 1 0.083449 2.27072 18314.6 -676.50713740**

**\***

**Z = 20.000**

**AWT = 0.000**

**E0 = -676.59058592**

**Emax = 0.00000000**

**klsp1 = 1**

**klsp2 = 14**

**klsp3 = 1**

**au\_eV= 27.211055**

**au\_cm= 219471.99**

**nstate = 218**

**Figure** **1.** Example of the **bound\_tab** file.

**B O U N D \_ B S W**

|  |  |
| --- | --- |
| Description: | converts the close-coupling *B*-spline expansions to the *c*- and *bsw*-files |
| Input files: | **bound.nnn, bound\_bsw.inp, target, knot.dat, cfg.nnn, target.bsw** |
| Output files: | *c*- and *bsw*-files for given states, indicated in the input file |
| Call as: | **bound\_bsw** [**mode=…**](if given input file **bound\_bsw.inp**), or  **bound\_bsw klsp=... sol=... name=...** , where  **klsp** - partial wave index  **sol** - state index'  **name -** name for given state |

The results of the BSR bound-state calculations are recorded in the **bound.nnn** files in the form of the corresponding B-spline close-coupling expansions. The BOUND\_BSW utility collects the information for a given bound state indicated in the file **bound\_bsw.inp**, and records it as pair (**name.c** , **name.bsw**). These files can be used as input target files for the further BSR calculations or other applications.

Input file is usually created on the base of the **bound\_tab** file created by utility BOUND\_TAB and contains the list of states to be processed. Each line contains the information for one state as index of the partial wave, index of the state for given partial wave and assigned name. Asterisk denotes the end of the list. The names are usually assigned by user. In case of large-scale calculations with hundreds of states, it is more convenient to use additional optional argument **mode**. In this case, all names are assigned automatically as **mode\_nnn\_mmm**, where **nnn =<klsp>** – index of partial wave, **mmm=<sol>** index of the state. If needed to output a few individual states, the user can employ the command-argument option indicated above.

**B S W \_ W**

|  |  |
| --- | --- |
| Description: | converts the *bsw*-file to the *w*-file |
| Input files: | **name.bsw** |
| Output files: | **name.w** |
| Call: | **bsw\_w name.bsw** |

**W \_ B S W**

|  |  |
| --- | --- |
| Description: | converts the *w*-file to the *bsw*-file |
| Input files: | **name.w, knot.dat** |
| Output files: | **name.bsw** |
| Call: | **bsw\_w name.w** |

**B S W \_ T A B**

|  |  |
| --- | --- |
| Description: | prepares the text files suitable for plotting the radial functions from bsw-file |
| Input files: | **name.bsw** |
| Output files: | **name.tab** |
| Call as: | **bsw\_tab name.bsw** |

**B S W 1 2 3**

|  |  |
| --- | --- |
| Description: | merging the set of bsw-files with user's choice of orbitals and  with optional changing the spectroscopic notation |
| Input files: | set of bsw-files under consideration |
| Output files: | resulting **bsw-file** with chosen orbitals |
| Call as: | **bsw123** withinteractive input (knot.dat is not required) |

**B S \_H W F**

|  |  |
| --- | --- |
| Description: | provides hydrogen-like bound and continuum pseudo-state orbitals on the given B-spline basis |
| Input files: | **knot.dat** |
| Output files: | **nl\_nnn.bsw** and **nl\_nnn.c**  for each orbital 'nnn' |
| Call as: | **bs\_hwf l=... nsol=... ii=... jj=... emax=… eps\_tail=…** |
|  |  |
|  | **l**  - orbital momentum |
|  | **nsol** - number of solutions [1] |
|  | **ii** - zero B-splines in the beginning [*l*+1] ' |
|  | **jj** - zero B-splines in the end [1] ' |
|  | **emax** - maximum energy [100] ' |
|  | **eps\_tail** - tolerance for the last B-spline [1.d-7] |
|  | **(Z**-value is coming from **knot.dat)** |

**P R I N T \_ B S**

|  |  |
| --- | --- |
| Description: | prints B-splines (in separate files) for given B-spline basis |
| Input files: | **knot.dat** |
| Output files: | **bs\_nnn**  for each spline 'nnn' |
| Call as: | **print\_bs** |

**S U M \_ H H**

|  |  |
| --- | --- |
| Description: | merges the set of **h.nnn** files to the final **H.DAT** |
| Input files: | **h.nnn** |
| Output files: | **H.DAT** |
| Call as: | **sum\_hh**  [**ih1=… ih2=… folder=…**]  ih1 – initial nnn-index [1]  ih2 – final nnn-index [999]  folder – if > 0, we suppose paths: nnn/h.nnn |

**H \_ T A R G B**

|  |  |
| --- | --- |
| Description: | creates "**target**" file based on the "**H.DAT**" file |
| Input files: | **H.DAT** |
| Output files: | **target.h** |
| Call as: | **h\_targb** [**h=…**], where **h** can be used to redefine input name |

**H \_ T A R G N**

|  |  |
| --- | --- |
| Description: | creates "**target**" file based on the set of **nnn/h.nnn** files  (used in large-scaled calculations where each partial wave is considered in the separate folder) |
| Input files: | **nnn/h.nnn or nnn/H.DAT** |
| Output files: | **target.hhh** |
| Call as: | **h\_targn klsp=…**, where **klsp** defines number of **nnn** folders |

**T A R G E T \_ E X P**

|  |  |
| --- | --- |
| Description: | change **target** file to fit new experimental state energies, given in file **thresholds** (see also BSR\_HD, parameter iexp) |
| Input files: | **target.theory + thresholds** |
| Output files: | **target.exp** |
| Call as: | **target\_exp** [**targ1=... targ2=... thresholds=...**]  parameter are used to re-define the default names |

**T A R G E T \_ S T A T E S**

|  |  |
| --- | --- |
| Description: | provide information about target states including their labels |
| Input files: | **target + {name.c}** |
| Output files: | **target\_states** |
| Call as: | **target\_states** [**inp=... out=...**]  parameter are used to re-define the default names |

**B S R \_ D D**

|  |  |
| --- | --- |
| Description: | calculation of dipole matrix elements between R-matrix states saved in **rsol.nnn** files |
| Input files: | **{rsol.nnn}, cfg.nnn, target.bsw, knot.dat** |
| Output files: | **dd\_nnn\_mmm**  (nnn,mmm - indexes of partial waves) |
| Call as: | **bsr\_dd klsp=...**  klsp – number of partial waves  Program makes SYSTEM CALLS to MULT3 and BSR\_DMAT3 |

**Z F \_ B B \_ B S R**

|  |  |
| --- | --- |
| Description: | calculates f-values between solutions in set of **bound.nnn** |
| Input files: | **bound.nnn , cfg.nnn, target.bsw, knot.dat +** [**zf\_bb.inp**] |
| Output files: | **zf\_res** |
| Call as: | **zf\_bb\_bsr** [**klsp=… msol=… atype=… gf=…** ]  or provide input file **zf\_bb\_inp** with:  **atype** = E1 |E2|M1|… - multipole index  **gf** = f |g - output f- or gf-values'  **klsp**= ... - number of **bound.nnn** files to be considered  **msol** = … - maximum number of solutions in **bound.nnn**  followed by the list of ilsp(i), mstates(i), i=1,klsp for each partial wave in separate line, where ilsp -index of partial and mstates -number of states  Program makes SYSTEM CALLS to MULT3 and BSR\_DMAT3 |

**Z F \_ C C \_ B S R**

|  |  |
| --- | --- |
| Description: | calculates f-values between set of {**name.c+name.bsw**} files |
| Input files: | **{name.c+name.bsw}, knot.dat, zf\_cc.inp** |
| Output files: | **zf\_res** |
| Call as: | **zf\_cc\_bsr** [**inp**=…]  input file contains:  **atype** = E1 |E2|M1|... - multipole index  **gf** = f |g - output f- or gf-values  **param** =… - additional parameters for bsr\_dmat3  **nfiles**= ... - number of c-files  followed by list of c-files in separate lines  Program makes SYSTEM CALLS to MULT3 and BSR\_DMAT3 |

**P H O T O \_ T A B**

|  |  |
| --- | --- |
| Description: | produces the tables for channel or total photoionization cross sections and asymmetry parameters |
| Input files: | **bsr\_phot.nnn, target** |
| Output files: | indicated by user |
| Call as: | **photo\_tab**  with interactive response from command line |

This utility serves for processing the data recorded during photoionization calculations with program BSR\_PHOT. The program BSR\_PHOT can be run for different energy intervals and different partial waves separately. The results are accumulated in files **bsr\_phot.nnn**. Then final tables for channel or total cross sections and asymmetry parameters may be generated with the utility **photo\_tab**. More detailed description of this utility and used formulas are given in the BSR\_PHOT write-up.

**P H O T O \_ C O L E C T**

|  |  |
| --- | --- |
| Description: | collects data from **bsr\_phot.nnnn** files to final **bsr\_phot.nnn** file after MPI calculations if they not finished correctly |
| Input files: | **bsr\_phot.nnnn** |
| Output files: | **bsr\_phot.nnn, photo.nnn** |
| Call as: | **photo\_collect klsp=… np=…**  **klsp** – index of partial wave under consideration  **np** – number of processors |

In MPI versions of BSR\_PHOT, each processor considers different set of photon energies and records results into separate **bsr\_phot.nnnn** files, where **nnnn** – index of the processor. In the end of calculations, the information collect into the **bsr\_phot.nnn** file, where the **nnn** – index of partial wave under consideration. If the calculations finished not correctly (time limits or problem for some energy), the **photo\_collect** utility may be used to collect the results for energies which were processed correctly.

**f \_ v a l u e s**

|  |  |
| --- | --- |
| Description: | calculation of f-values for transition between target states based on the asymptotic coefficients in the H.DAT file |
| Input files: | **H.DAT** or **h.nnn, target** |
| Output files: | **f\_values** or **f\_values.nnn** |
| Call as: | **f\_values**  [**h**=… **klsp**=…]  h [H.DAT] – alternative name for input file  klsp [1] - partial wave index to choose **h.nnn** file for the process |

**s \_ v a l u e s**

|  |  |
| --- | --- |
| Description: | calculation of s-values for transition between target states based on the asymptotic coefficients in the H.DAT file |
| Input files: | **H.DAT** or **h.nnn, target** |
| Output files: | **s\_values** or **s\_values.nnn** |
| Call as: | **s\_values** [**h**=.. **klsp1**=… **klsp2**=… **L1**=… **L2**=...]  h [H.DAT] - alternative name for H.DAT file  klsp1[0] - |

|  |  |
| --- | --- |
| h [H.DAT] | alternative name for H.DAT file |
| klsp1[0] | minimum index of partial wave to be considered |
| klsp2[0] | maximum index of partial wave to be considered |
| L1[-1] | minimum total orbital moment to be considered |
| L2[-1] | maximum total orbital moment to be considered |
|  |  |

**Asymptotic coefficients decomposition**

**LS coupling**

The long-range potential coefficients coupling two channels are

 (1)

In tensor notation

 (2)

where

 (3)

and

 . (4)

To evaluate expression (2), we may use the general expression (see, e.g., Cowan 1981, Eq.11.47) for matrix elements of a scalar product when angular momenta *j*1, *j*2 correspond to different subsystems

 (5)

Then coefficients (2) are reduced to

 (6)

This expression can be used for determination radiative matrix elements for transitions between target states from the asymptotic coefficients in *LS* coupling case.

**jj coupling**

 (7)

Here we can use the uncoupling formula when operator operates only within the first subspace (see Cowam 1981, Eq.11.38):

 (8)

Then

 (9)

**jK coupling**

 (10)

First we should uncoupled the *J*1 and *J*2 by transferring to *jj*-coupling (Cowan 1981, Eq.9.25):

 (11)

Then

 (12)

Now let reduce sum over *j*1, using the sum rule (Cowan 1981, Eq. 5.33):

 (13)

where S = *j*1 + *j*2 + *j*3 + *l*1 + *l*2 + *l*3 + *l'*1 + *l'*2 + *l'*3. Then

 (14)

Using the orthogonal relation (Cowan 1981, Eq.5.31)

 (15)

finally obtain

 (16)