**21. Program BSR\_RECOUP** (version 4)

*21.1. Outline of the BSR\_RECOUP calculations*

The BSR\_RECOUP program makes recoupling of the LS Hamiltionian/Overlap matrixes **bsr\_mat.nnn** to the JK coupling based on the target expansions over LS-states. It allows to switch from LS calculations to the semi-relativistic JK scheme. In general, the calculations of the Hamiltonian matrixes is more effective than the direct Breit-Pauli calculations.

BSR\_RECOUP

**read\_arg** reads arguments from **command line**

Loop over JK partial waves, klsp:

**target\_LS\_expn** , read recoupling coefficients

End loop over JK partial waves

Overlap matrix construction:

**read** one channel block

**r\_target**

**r\_target\_ion**

**target\_LS,** target states information in LS-coupling

**target\_JK,** target states information in JK-coupling

check if this LS partial wave contributes to given JK partial wave

**r\_channels\_ion**

**target\_LS,** scattering channels information in LS-coupling

**read\_recoup**

**allocate\_matrix -** allocate JK overlap matrix

Loop over LS partial waves, nnn:

Loop over LS channel blocks:

open **bsr\_mat\_LS.nnn**

**add\_block -** add LS channel block to all relevant

JK channel blocks

End of loop over LS channel blocks

End of loop over LS partial waves nnn:

**record\_matrix -** record overlap matrix in bsr\_mat\_JK.klsp files

repeat the above steps for **Hamiltonian matrix** (e xcept open bsr\_mat\_LS.nnn)

repeat the above steps for **asymptotic coefficients**

**F**ig. 21.1. Block diagram for the program BSR\_RECOUP.

*21.2. Data files*

The BSR\_BMAT uses all the files indicated in the description of the BSR\_BREIT and BSR\_MAT programs. The difference is in the final results files specified below.

|  |  |  |  |
| --- | --- | --- | --- |
| **target\_LS** | | File type: formatted sequential input.  Description: contains list of target states and scattering channels in LS-coupling. | |
| **target\_JK** | | File type: formatted sequential input.  Description: contains list of target states and scattering channels in JK-coupling. | |
| **target\_LS\_expn** | | | File type: unformatted sequential output.  Created by utility **make\_ target\_LS\_expn**  Description: contains mixing expansion coefficients other LS terms  for each JK target states. | |
| **target\_LS** | | File type: formatted sequential input.  Description: contains list of target states and scattering channels in LS-coupling.  Format: see sections 4.3 and 5.4. | |
| **bsr\_mat\_LS.nnn** | | File type: unformatted sequential **input**  Created by program BSR\_MAT.  Description: Overlap matrix, Hamiltonian matrix and asymptotic coefficients  in LS-coupling. | | | | |
| **bsr\_mat\_JK.nnn** | | | File type: unformatted sequential **output.**  Created by BSR\_RECORD.  Description: Overlap matrix, Hamiltonian matrix and asymptotic coefficients  in JK-coupling | |
| **bsr\_recoup.log** | | | File type: formatted sequential output.  Written by program BSR\_RECOUP.  Description: running and debug information. | |

*21.3 Input paramters*

Input parameter are limited and define the range of partial wave to be considered and the debug output level in the bsr\_recoup.log file.

|  |  |
| --- | --- |
| **klsp1** [1] | first partial wave under consideration. |
| **klsp2** [nlsp] | last partial wave under consideration. |
| **klsp** [1] | partial wave under consideration (overwrites **klps1** and **klsp2**) . |
| **mk** [7] | maximum multipole index in two-electron integrals. |
| **mb** [5000] | the size of one block in module **c\_data** used for accumulation of given type of integrals. |

*21.4 Data flow*

As seen from the block-scheme, Fig.21.1, the main operation is the reading of the channel block in LS-coupling and adding it to the corresponding JK-channel block, with preliminary multiplication on the LS-mixing coefficients and transformation coefficient. Transformation matrix from LS to JK coupling is defined by following expression:

 (21.1)

The main difficulty is that we need simultaneously several LS matrixes to construct one JK-matrix. In large-scale calculations it would be required too much RM memory. To avoid the memory problems, the program repeatedly read only one LS channel block and transfer it in different blocks of the JK matrix under consideration.

*21.4 MPI version*

MPI version, BSR\_RECOUP\_MPI, works along the same MPI distribution procedure as in the BSR\_MAT\_MPI. The JK Hamiltonian matrix is distributed over processors by channel blocks, and each processor calculated only the assigned blocks. Each processor repeatedly reads the needed **bsr\_mat\_LS.nnn** files with the LS results. It is a main drawback of the employed procedure, however, it allows consider very large-scaled cases. The master processor collect the results and records them to the **bsr\_mat\_JK.nnn** files.

*21.5 Example of using BSR\_RECOUP*

Example for using BSR\_RECOUP is given in the folder **Cr\_recoup**, which contains the simplified calculations of electron scattering on CrII (Tayal & Zatsarinny 2020).

Supposed we have done the standard LS calculations for e-CrII problem. The LS target calculations is given in sub-folder **hf\_target\_LS**, where we obtained HF target state for all LS terms of the 3d5, 3d44s, 3d34s2, 3d44p and 3d34s4p configurations. Overall it adds up to 192 LS states which all have been used in the original calculations. For example, we restrict the LS scattering calculations with first 20 target states of CrII. These calculations are given in sub-folder **sct\_LS**.

We want now to switch to JK calculations using, in part the existing, LS calculations. First we should obtain the corresponding fine-structure LSJ states through the spin-orbit term mixing of the LS wave functions. Each LS state is presented by the configuration expansion

 , (21.2)

where the are the one-configuration wave function. The LSJ states we will represent as the expansions

, (21.3)

where the expansion coefficients *ci* in  are frozen from the LS CI calculations. The term-mixing coefficients *bi* can be obtained using the BSR bound calculations where each LS states is represented by perturber in the **kpert** option. The used may proceed as following. Create new sub-folder, **bsr\_target\_LSJ**, and copy there all LS target *c*- and *bsw*- files, together with the knot.dat file, which should kept the same in all following calculations.

To create the target file where each LS state is represented as perturber, the user can use the utility **target\_kpert**, preliminary rename the target file for LS-calculations in target\_LS (more detailed see in the description of utility-programs, chapter BSR\_UTILS). If to look in the new target file we found that there is 14 different J-values for LSJ states. We also see that all LS states are recoded as pertubers but BSR target file should contains at least one scattering channel. We choose the 3d4 1S states of CrIII ion as target states here to be able run the programs (any CrIII state can be chosen, it will have no influence on the results). Now we ready to make standard BSR bound calculations with inclusion spin-orbit interaction in the usual bound-states mode.

**bsr\_prep3**

**bsr\_conf3**

**bsr\_breit4 klsp1=1 klsp2=14 oper=1111000**

**bsr\_mat4 klsp1=1 klsp2=14 ipert\_ch=0 mso=1**

**bsr\_hd4 klsp1=1 klsp2=14 itype=-1**

**bound\_tab EM=-1040**

Note that we include spin-orbit interaction in the BSR\_BREIT run (**oper=1111000**). **mso=1** for BSR\_MAT also includes to inclusion of spin-orbit interaction for construction of the Hamiltonian matrix. Additional parameter **ipert\_ch=0** guarantees that the interaction between perturbers and scattering channels is switched off, and the scattering channels have no influence on the mixing of perturbers.

The resulting **bound\_tab** file contains the list of obtained LSJ states (67 fine-structure levels in our example, after disregarding all fake bound states from channel part, CrIII(3dS)+nl ). Now we copy the bound\_tab in **bound\_bsw.inp** file and choose the LSJ states which we are want in the JK scattering calculations Rinning

**bound\_bsw mode=sol**

we obtain all LSJ target states as pares of the **sol\_nnn\_mmm.c**  and **sol\_nnn\_mmm.bsw**  files, where **nnn** - index of partial wave (with specific Jπ-value) and **mmm** – index of the solution.

**IMPORTANT NOTE:** at this stage, there is option of the **fine-tuning** of the energies of the LS terms, in order to improve the energies of the corresponding LSJ states and thereby to get more accurate spin-orbit mixing. The **target\_kpert** utility also creates the **thresholds\_kpert** file with the list of the all LS states and their energies. The third column contain possible corrections to the LS term (originally recorded as zeros) which can be estimated from the comparison of theoretical and experimental energies. When correction have been chosen, the user should repeat the BSR\_HD run to get bound.nnn files with corrected energies and spin-orbit mixing coefficients (*bi* in Eq. 21.3):

**bsr\_hd4 klsp1=1 klsp2=14 itype=-1 iexp\_pert=1**

where **iexp\_pert** parameter indicates that the program should include the LS term corrections from the **threshold\_kpert** file. Sometimes it may require a sequence of runs for better adjusting the LSJ energies.

Now we ready to begin JK scattering calculation. To do that let's first create the sub-folder **sct\_JK** and copy there all LSJ target states (sol\_nnn\_mmm in the example). Then we move all LS **bsr\_mat.nnn** files from the **sct\_LS** folder and rename them as **bsr\_mat\_LS.nnn**.Next stepis to run BSR\_RECOUP to get the **bsr\_mat\_JK.nnn** with theHamiltoniam matrix in the JK-coupling.Preliminary we need to run the utility program **make\_targt\_LS\_expn** to get the **targ\_LS\_expn** file with all term-mixing coefficients *bi* needed for the BSR\_RECOUP run. (developer: can we put this stage directly in BSR\_RECOUP ?):

**targ\_LS\_expn**

**bsr\_recoup4 klsp1=.. klsp2=..**

As results, we get **bsr\_mat\_JK.nnn** files with all spin-orbit interaction except the spin-orbit corrections for the scattering electron. If needed (usually it is small) it can be added by run

**bsr\_breit4 klsp1=.. klsp2=.. oper=0001000**

**bsr\_mat4 klsp1=.. klsp2=.. mode=7**

Finally, we run BSR\_HD4 to get **h.nnn** files in the JK-coupling:

**bsr\_hd4 klsp1=.. klsp2=..**