21. Program BSR_RECOUP (version 4)

21.1. Outline of the BSR_RECOUP calculations

The BSR_RECOUP program makes recoupling of the LS Hamiltonian/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.

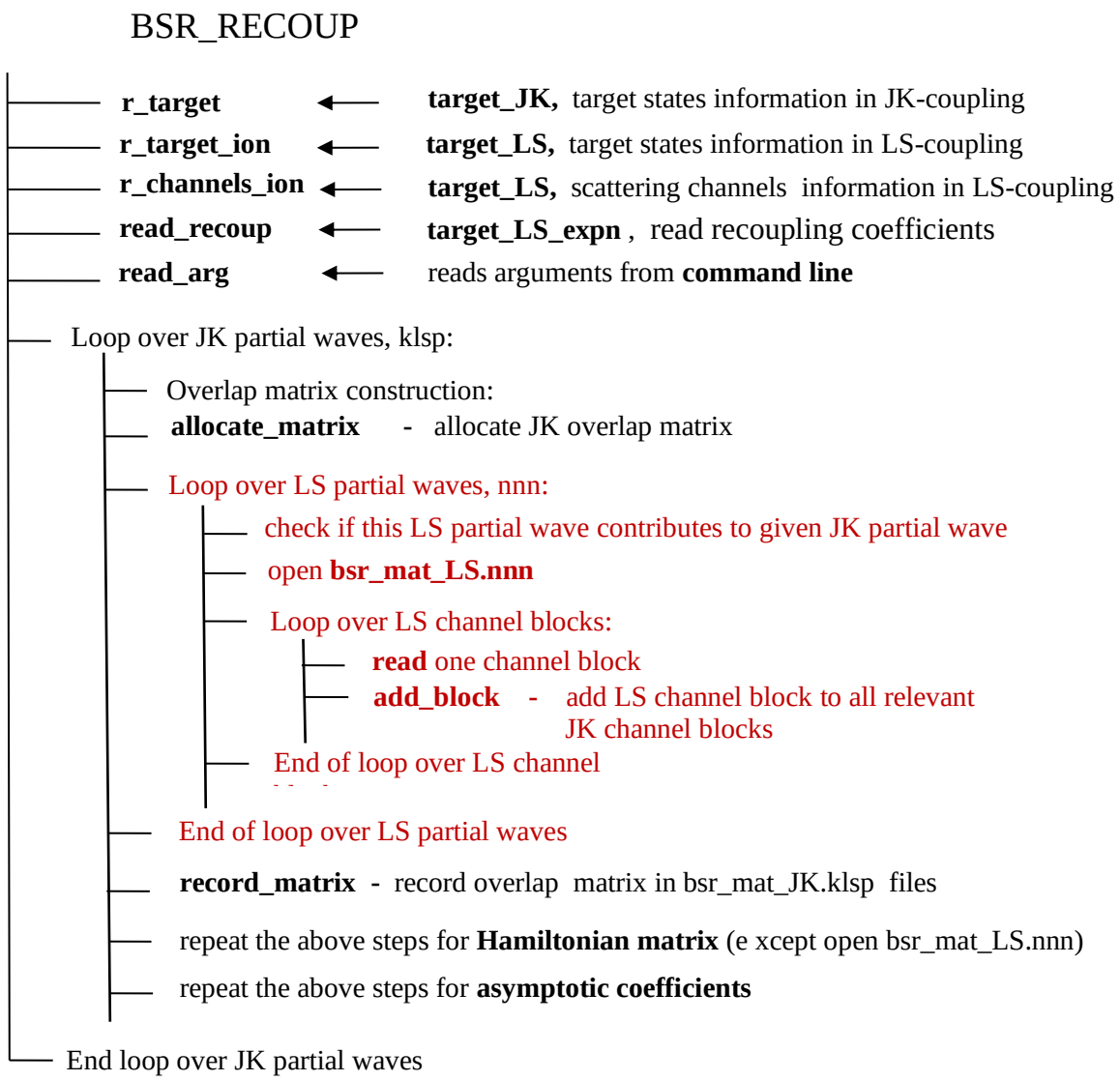

Fig. 21.1. Block diagram for the program BSR_RECOUP.

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:

$$T_{LS,jK} = < [(l_1 l_2)L, (s_1 s_2)S]J \mid (l_1 s_1) j_1, l_2]K, s_2, J >$$
$$= (-1)^{s_2+J-l_2-j_1} [L, S, j_1, K]^{1/2} \begin{Bmatrix} L & s_1 & K \\ s_2 & J & S \end{Bmatrix} \begin{Bmatrix} l_2 & l_1 & L \\ s_1 & K & j_1 \end{Bmatrix} \quad (21.1)$$

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 $3d^5$, $3d^4 4s$, $3d^3 4s^2$, $3d^4 4p$ and $3d^3 4s 4p$ 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

$$\Psi^{LS} = \sum_i c_i \psi_i^{LS} \ , \quad (21.2)$$

where the ψ_i^{LS} are the one-configuration wave function. The LSJ states we will represent as the expansions

$$\Psi^{LSJ} = \sum_i b_i \Psi_i^{LS}, \qquad (21.3)$$

where the expansion coefficients c_i in Ψ_i^{LS} are frozen from the LS CI calculations. The term-mixing coefficients b_i 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 $3d^4\,{}^1S$ 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(3d S)+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 (b_i 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 step is to run BSR_RECOUP to get the **bsr_mat_JK.nnn** with the Hamiltoniam 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 b_i 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=..
```