Analyzing quantum impurity configuration

Weights of many-body states of the quantum impurity are stored in the ***hstate_weight_1.dat*** file if *solver=ct-qmc-w* and *measure_hstate_weight = yes* in the ***impurity_1.ini*** file. The example of the ***hstate_weight_1.dat*** file for the five-degenerate case, *nlm=5*, is presented below. In this case, the may-body state consists of five digits (columns) for one spin direction and the next five digits for the opposite (second quantization notations). The last column is a weight of the given configuration. The order of orbitals corresponds to the *cubic_harmonic_order* or *rhtm* token. Therefore, the probability to find three electrons siting in $d^{\uparrow}_{xy}$, $d^{\uparrow}_{xz}$ and $d^{\downarrow}_{x^2-y^2}$ is 0.0001989.

```
...
1 0 0 1 0 0 0 0 0 1     0.0001989
0 1 0 1 1 0 0 0 0 0     0.0002422
0 0 1 1 1 0 0 0 0 0     0.0132168
1 1 0 0 0 1 0 0 0 0     0.0000001
1 0 1 0 0 1 0 0 0 0     0.0000029
...
```

sector_statistics routine allows one to analyze the many-body configuration stored in this file. It requires the ***sector_statistics.ini*** file shown below.

```
10          !  spin-orbital degeneracy
2           !  number of sub-shells to analyze
t2g         !  sub-shell name
3           !  number of orbitals in sub-shell
1 2 4       !  orbitals positions
eg          !  sub-shell name
2           !  number of orbitals in sub-shell
3 5         !  orbitals positions
```

The first line contains spin-orbital degeneracy (2×*nlm*). The second line sets a number of sub-shells to analyze. Then for each sub-shell one needs to provide name, the orbital degeneracy and positions. One should note here that the doubled sum of the sub-shell degeneracies (fourth and seventh lines) must be equal to the spin-orbital degeneracy (first line). In the above example, one has two sub-shells to analyze. The first sub-shell is named **t2g** with the degeneracy equal to **3** and positions **1 2 4**. This order corresponds to the *rhtm=VASP* token. The second sub-shell is **eg** with the degeneracy equal to **2** and positions **3 5**.

The ***sector_statistics*** routine reads from standard input and writes to standard output and it has to be executed as:

```
[user]> sector_statistics < hstate_weight_1.dat > sector_statistics.out
```

One should note here that ***hstate_weight_1.dat*** file must be used as standard input. Below is a part of ***sector_statistics.out*** file.

```
          Sector statistics
 Ntot    Weight     Sz(i)      0           1           2           3           4           5
  0     0.0000000    |        ----        ----        ----        ----        ----        ----
  1     0.0000000    |        ----        ----        ----        ----        ----        ----
  2     0.0000000    |        ----        ----        ----        ----        ----        ----
  3     0.0000000    |        ----        ----        ----        ----        ----        ----
  4     0.0000000    |        ----        ----        ----        ----        ----        ----
  5     0.0000180    |        ----   0.0000051        ----   0.0000109        ----   0.0000020
  6     0.0090957    |   0.0000167        ----   0.0046116        ----   0.0044674        ----
  7     0.8118625    |        ----   0.0043162        ----   0.8075463        ----        ----
  8     0.1724999    |   0.0005869        ----   0.1719130        ----        ----        ----
  9     0.0064779    |        ----   0.0064779        ----        ----        ----        ----
 10     0.0000455    |   0.0000455        ----        ----        ----        ----        ----

SUM(Sz(i))      0           1           2           3           4           5
            0.000649    0.010799    0.176525    0.807557    0.004467    0.000002

          Orbital configurations
...
 Ntot    Weight
  7      0.8118625
Sz |  t2g  eg    Weight
  3|     3     4       0.0001444
  3|     4     3       0.0106125
  3|     5     2       0.7967894
  1|     3     4       0.0000066
  1|     4     3       0.0008948
  1|     5     2       0.0031132
  1|     6     1       0.0003016

 Ntot    Weight
  8      0.1724999
Sz |  t2g  eg    Weight
  2|     4     4       0.0009147
  2|     5     3       0.1396354
  2|     6     2       0.0313629
  0|     4     4       0.0000598
  0|     5     3       0.0004411
  0|     6     2       0.0000860
...
```

The beginning of the output file repeats the information that can be found in the ***amulet.out*** file. It reports the weights of different ionic and spin state configurations. In the above example, the effective quantum impurity under consideration is in d^7 and d^8 high spin states with probabilities 0.812 and 0.172, respectively.

Next blocks of the output file contain a similar information collected for sub-shells requested in the input file. One can see that for d^7 ionic state (block) the most probable configuration is $t_{2g}^5 e_g^2$ with S_z=3, while for d^8 block it is $t_{2g}^5 e_g^3$ with S_z=2.