Quick-Summary

edrix_run.py

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Starting

```
hahn@mccec0468 ~/Doc/Doc/PyC/RIX/python_rixs git AllSymmetries !?2 py edrixs_run.py -i RIXS_real.input -h
usage: edrixs_run.py [-h] -i FNAME [-p] [-s] [-t] [-w] [-f FNAME]

Reading the input-file for edrixs-run

optional arguments:
  -h, --help            show this help message and exit
  -i FNAME, --inflile FNAME
                        The name of the inputfile
  -p, --plot            Deactivating the plot-mode
  -s, --show            Deactivating the plot-showing-mode
  -t, --txt             Deactivating the txt-file-saving
  -w, --wavefunction    Activating the wave-function-printing
  -f FNAME, --fname FNAME
                        Filename of the outputs (default: output)
```

- Python 3.x is required plus:
  - Numpy, Sympy, matplotlib

Input-Example

- :electrons 6
- :symmetry ('Oh',-.35) ('Oh',-.35)
- :F2_dd 11.7794822567*0.8 11.7794822567*0.8
- F2_dd 13.006 13.006
- :F4_dd 7.32769083304*0.8 7.32769083304*0.8
- F4_dd 8.0844 8.0844
- :F2_dp 6.79309388088
- :G3_dp 2.84354556992
- :G1_dp 5.00094944056
- :SOC_d 0.052 0.052
- :SOC_p 8.4
- :B 0 0 0

Support of math-expressions

- :K 2
- :ABS -30 30 500 930
- :EMS -30 30 500 0
- :FHMW 0.85 0.20
- :Alpha 45
- :Phi 45
- :XES true
- :XAS true
- :RIXS true

: Activate the function

- XES true ('right',90) ('linear',-90)
- XAS true ('right',90) ('right',-40) ('left',-45) ('left',45)
- RIXS true ('left',90,'right',90) ('right',90,'right',90)

Crystal-Field-Models

Start-/Final-State

- :symmetry('Sp')('Td')

- :symmetry ('Td',+.35) ('Td',+.35)

- :symmetry ('Oh',-.35) ('Oh',-.35)

dq dt ds

- :symmetry ('D4h',1.4,0.13,-0.13) ('D4h',1.48,0.13,-0.13)

d_{xy} d_{xz} d_{yz} d_{x2y2} d_{z2}

- :symmetry ('real',0.0,0.0,0.0,0.13,0.13) ('real', 0.0,0.0,0.0,0.13,0.13)

L^2,S^2,J^2-Printing *for* d^9

edrixs >>> Ground-State Wavefunction ...

Energy(eV)	Energy(eV)	3d-alpha	3d-beta	2p-alpha	2p-beta	< S_x >	< S_y >	< S_z >	< S2 >	< L_x >	< L_y >	< L_z >	< L2 >	< LS >	< J2 >
-0.05200	0.00000	1 1 0 1 1	1 1 1 1 1	1 1 1	1 1 1	0.00000	0.00000	-0.10000	0.75000	0.00000	0.00000	-0.40000	6.00000	1.00000	8.75000
-0.05200	0.00000	1 1 1 1 1	0 1 1 1 1	1 1 1	1 1 1	0.00000	0.00000	0.10000	0.75000	0.00000	0.00000	0.40000	6.00000	1.00000	8.75000
-0.05200	0.00000	1 1 1 1 1	1 1 1 0 1	1 1 1	1 1 1	0.00000	0.00000	-0.30000	0.75000	0.00000	0.00000	-1.20000	6.00000	1.00000	8.75000
-0.05200	0.00000	0 1 1 1 1	1 1 1 1 1	1 1 1	1 1 1	0.00000	0.00000	0.50000	0.75000	0.00000	0.00000	2.00000	6.00000	1.00000	8.75000
-0.05200	0.00000	1 1 1 1 1	1 0 1 1 1	1 1 1	1 1 1	0.00000	0.00000	0.29957	0.75000	0.00000	0.00000	1.19829	6.00000	1.00000	8.75000
-0.05200	0.00000	1 0 1 1 1	1 1 1 1 1	1 1 1	1 1 1	0.00000	0.00000	-0.50000	0.75000	0.00000	0.00000	-2.00000	6.00000	1.00000	8.75000
0.07800	0.13000	1 1 1 0 1	1 1 1 1 1	1 1 1	1 1 1	0.00000	0.00000	0.10000	0.75000	0.00000	0.00000	-0.60000	6.00000	-1.50000	3.75000
0.07800	0.13000	1 1 1 1 0	1 1 1 1 1	1 1 1	1 1 1	0.00000	0.00000	-0.10000	0.75000	0.00000	0.00000	0.60000	6.00000	-1.50000	3.75000
0.07800	0.13000	1 1 1 1 1	1 1 1 1 1 0	1 1 1	1 1 1	0.00000	0.00000	0.30000	0.75000	0.00000	0.00000	-1.80000	6.00000	-1.50000	3.75000
0.07800	0.13000	1 1 1 1 1	1 1 0 1 1	1 1 1	1 1 1	0.00000	0.00000	-0.29925	0.75000	0.00000	0.00000	1.79552	6.00000	-1.50000	3.75000

edrixs >>> Ground-State Wavefunction Done!

edrixs >>> Excited-State Wavefunction without 2p-coupling ...

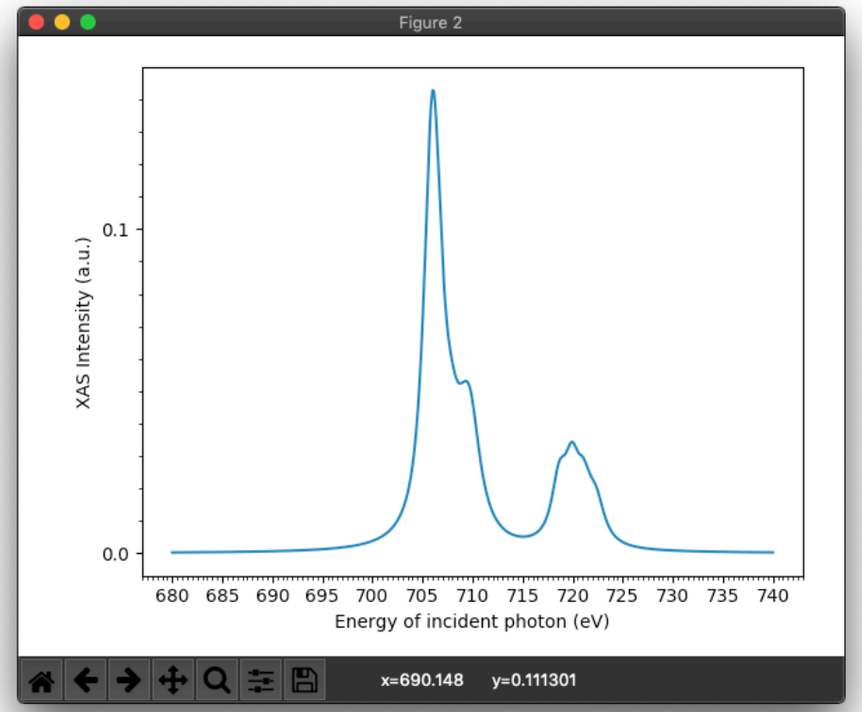
Energy(eV)	Energy(eV)	3d-alpha	3d-beta	2p-alpha	2p-beta	< S_x >	< S_y >	< S_z >	< S2 >	< L_x >	< L_y >	< L_z >	< L2 >	< LS >	< J2 >
-4.20000	0.00000	1 1 1 1 1	1 1 1 1 1	1 1 1	1 0 1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.20000	0.00000	1 1 1 1 1	1 1 1 1 1	1 1 1	0 1 1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.20000	0.00000	1 1 1 1 1	1 1 1 1 1	1 0 1	1 1 1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
-4.20000	0.00000	1 1 1 1 1	1 1 1 1 1	0 1 1	1 1 1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8.40000	12.60000	1 1 1 1 1	1 1 1 1 1	1 1 1	1 1 0	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
8.40000	12.60000	1 1 1 1 1	1 1 1 1 1	1 1 0	1 1 1	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

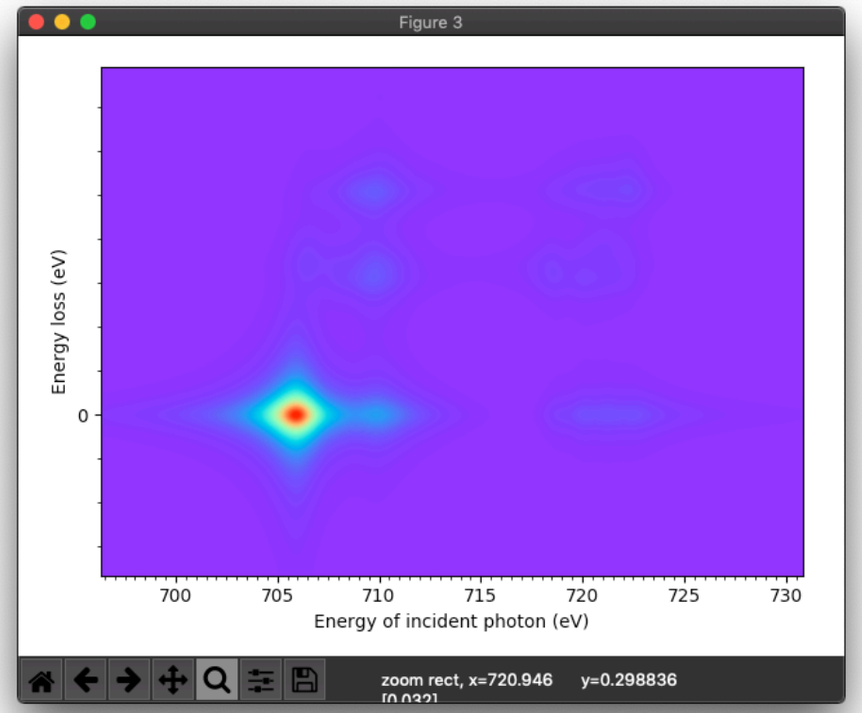
edrixs >>> Excited-State Wavefunction without 2p-coupling Done!

edrixs >>> Excited-State Wavefunction with 2p-coupling ...

Energy(eV)	Energy(eV)	3d-alpha	3d-beta	2p-alpha	2p-beta	< S_x >	< S_y >	< S_z >	< S2 >	< L_x >	< L_y >	< L_z >	< L2 >	< LS >	< J2 >
-4.20000	0.00000	1 1 1 1 1	1 1 1 1 1	1 1 1	1 0 1	0.00000	0.00000	-0.16667	0.75000	0.00000	0.00000	-0.33333	2.00000	0.50000	3.75000
-4.20000	0.00000	1 1 1 1 1	1 1 1 1 1	1 1 1	0 1 1	0.00000	0.00000	0.16667	0.75000	0.00000	0.00000	0.33333	2.00000	0.50000	3.75000
-4.20000	0.00000	1 1 1 1 1	1 1 1 1 1	1 0 1	1 1 1	0.00000	0.00000	-0.50000	0.75000	0.00000	0.00000	-1.00000	2.00000	0.50000	3.75000
-4.20000	0.00000	1 1 1 1 1	1 1 1 1 1	0 1 1	1 1 1	0.00000	0.00000	0.50000	0.75000	0.00000	0.00000	1.00000	2.00000	0.50000	3.75000
8.40000	12.60000	1 1 1 1 1	1 1 1 1 1	1 1 1	1 1 0	0.00000	0.00000	0.16667	0.75000	0.00000	0.00000	-0.66667	2.00000	-1.00000	0.75000
8.40000	12.60000	1 1 1 1 1	1 1 1 1 1	1 1 0	1 1 1	0.00000	0.00000	-0.16667	0.75000	0.00000	0.00000	0.66667	2.00000	-1.00000	0.75000

D5-Sp-*Example*





- :electrons 5
- :symmetry ('Sp') ('Sp')
- :F2_dd
  11.7794822567*0.34
  11.7794822567*0.34
- :F4_dd
  7.32769083304*0.34
  7.32769083304*0.34
- :F2_dp 6.79309388088
- :G3_dp 2.84354556992
- :G1_dp 5.00094944056
- :SOC_d 0.052 0.052
- :SOC_p 8.4
- :B 0 0 0
- :K 2
- :ABS -30 30 2500 710
- :EMS -5 25 2500 0
- :FHMW 0.85 0.20
- :Alpha 45
- :Phi 45
- :XES true
- :XAS true
- :RIXS true

Slater-Condon-Database

```
hahn@mccec0468 ~/Doc/Doc/PyC/RIX/python_rixs git AllSymmetries 2 py database.py
Element?
        Fe
Oxidation-State?
        2+
Edge?
        L3
Groundstate-Parameters
('F2(3d,3d)', 10.9664479746)
('F4(3d,3d)', 6.81536070296)
('SOC(3d)', 0.051979504)
Excitedstate-Paramters
('F2(2p,2p)', 50.8607812484)
('F2(3d,3d)', 11.7794822567)
('F4(3d,3d)', 7.32769083304)
('F2(2p,3d)', 6.79309388088)
('G3(2p,3d)', 2.84354556992)
('G1(2p,3d)', 5.00094944056)
('SOC(2p)', 8.200923368)
('SOC(3d)', 0.066539208)
```