QUANTY

How to calculate a many body energy level diagram ?

energy level diagram

In the part of the input file about the crystal field we replace the red text

```
-------------------------------------------------------------------------------
-- Define the crystal field term.
-------------------------------------------------------------------------------
if H_cf == 1 then
   -- PotentialExpandedOnClm('Oh', 2, {Eeg, Et2g})
   tenDq_3d = NewOperator('CF', NFermions, IndexUp_3d,
IndexDn_3d, PotentialExpandedOnClm('Oh', 2, {0.6, -0.4}))

   tenDq_3d_i = 2.5

   tenDq_3d_f = 2.5

   H_i = H_i + Chop(
       tenDq_3d_i * tenDq_3d)

   H_f = H_f + Chop(
       tenDq_3d_f * tenDq_3d)
end
```

energy level diagram

With the blue text

```
--------------------------------------------------------------------------------
-- Define the crystal field term.
--------------------------------------------------------------------------------
file = assert(io.open("Fe3p_EnergyLevelDiagram2", "w"))
   -- PotentialExpandedOnClm('Oh', 2, {Eeg, Et2g})
   tenDq_3d = NewOperator('CF', NFermions, IndexUp_3d,
IndexDn_3d, PotentialExpandedOnClm('Oh', 2, {0.6, -0.4}))
   for i=0, 600 do
  tenDq_3d_i = 0.01*i

   tenDq_3d_f = tenDq_3d_i

   H_i = H_i + Chop(
       tenDq_3d_i * tenDq_3d)

   H_f = H_f + Chop(
       tenDq_3d_f * tenDq_3d)
```

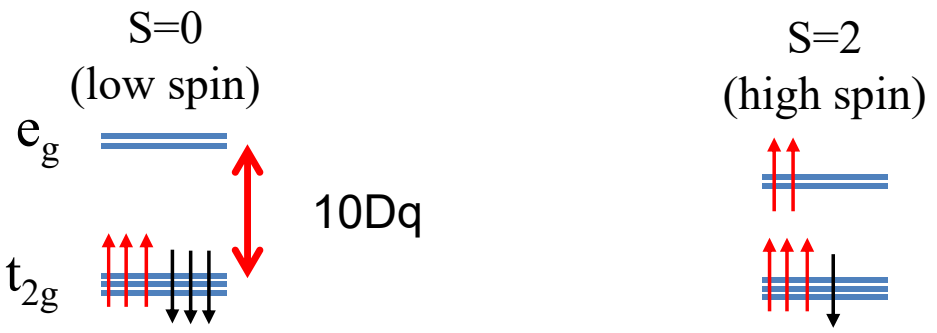
energy level diagram

*We add at the end of the input file the following lines where we tell the program to calculate the energy as Psis_i*H_i*Psis_i*

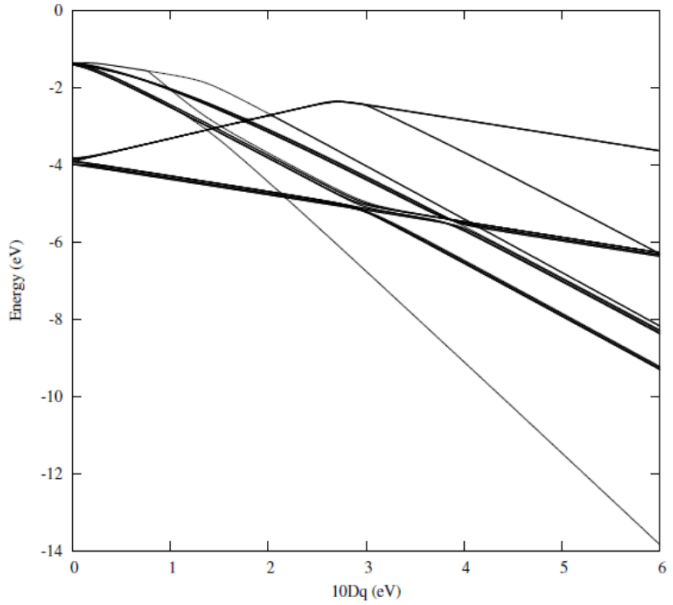
```
Eigensystem(H_i, Psis_i)
  for key,value in pairs(Psis_i) do
    energy = value * H_i * value
    file:write(string.format("%14.7E ",energy))
  end
  file:write("\n")
end
io.write("\n")
file:close()
```

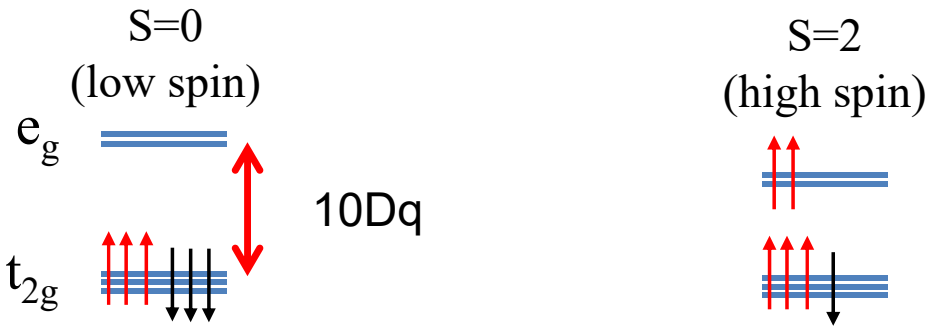
Co3+ 3d6

Different ground states are possible depending on 10Dq



Co3+ 3d6


Energy (eV)
10Dq (eV)
0
-2
-4
-6
-8
-10
-12
-14
0
1
2
3
4
5
6

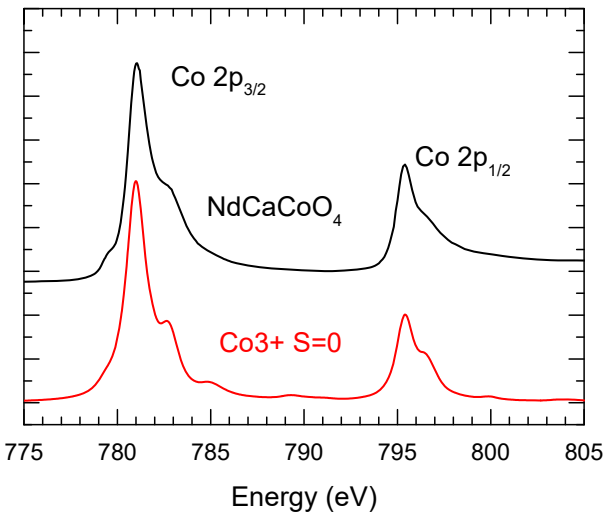

S=0
(low spin)
e_g
t_{2g}
10Dq
S=2
(high spin)

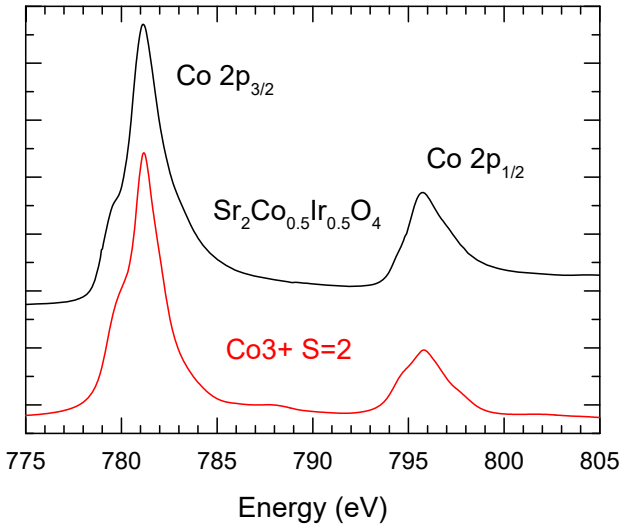
Crystal field multiplet theory

Co^{3+} 2p XAS

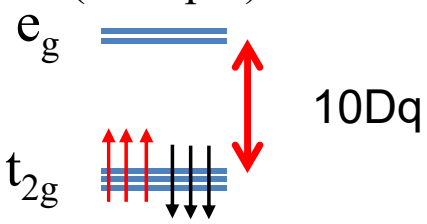
Dipole transition

$3d^6 \rightarrow 2p^5 3d^7$

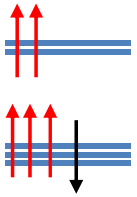




S=0
(low spin)



S=2
(high spin)



Eigenvalues

How to check what are these states? Calculate the quantum numbers!

Eigenvalues

I add the definition of the Tz operators (intra-atomic dipole moment)

```
Jx_3d = NewOperator('Jx', NFermions, IndexUp_3d,
IndexDn_3d)
Jy_3d = NewOperator('Jy', NFermions, IndexUp_3d,
IndexDn_3d)
Jz_3d = NewOperator('Jz', NFermions, IndexUp_3d, IndexDn_3d)
Jsqr_3d = NewOperator('Jsqr', NFermions, IndexUp_3d,
IndexDn_3d)
Jplus_3d = NewOperator('Jplus', NFermions, IndexUp_3d,
IndexDn_3d)
Jmin_3d = NewOperator('Jmin', NFermions, IndexUp_3d,
IndexDn_3d)

OppTx   =NewOperator("Tx"
,NFermions,IndexUp_3d,IndexDn_3d)
OppTy   =NewOperator("Ty"
,NFermions,IndexUp_3d,IndexDn_3d)
OppTz   =NewOperator("Tz"
,NFermions,IndexUp_3d,IndexDn_3d)
```

Eigenvalues

I add Tz in the list of operators

```
if H_3d_Ld_hybridization == 1 then
   Operators = {H_i, Ssqr, Lsqr, Jsqr, Sz, Lz, Jz, OppTz, N_2p, N_3d,
N_Ld, 'dZ'}
   header = 'Analysis of the initial Hamiltonian:\n'
   header = header ..
'================================================
================================================
===============\n'
   header = header .. 'State       <E>    <S^2>    <L^2>    <J^2>
<Sz>    <Lz>    <Jz>   <Tz>  <N_2p>   <N_3d>   <N_Ld>
dZ\n'
   header = header ..
'================================================
================================================
===============\n'
   footer =
'================================================
================================================
```

Eigenvalues

I add the following blue lines to tell the program to save the calculated eigenvalues in an obj file with the same name as the input file

```
outputname = debug.getinfo(1,"S")
outputname = string.gsub(outputname.source,"@","")
outputname = string.gsub(outputname,".lua","")
tempfile = io.open(outputname.."_.obj","w")
io.output(tempfile)

io.write(header)
for i, Psi in ipairs(Psis_i) do
   io.write(string.format('%5d', i))
   for j, Operator in ipairs(Operators) do
      if j == 1 then
         io.write(string.format('%12.6f', Complex.Re(Psi * Operator * Psi)))
      elseif Operator == 'dZ' then
         io.write(string.format('%12.2E', dZ[i]))
      else
         io.write(string.format('%10.4f', Complex.Re(Psi * Operator * Psi)))
      end
   end
   io.write("\n")
end
io.write(footer)
```

Eigenvalues

*The black lines are telling the program to calculate the eigenvalue Psi*Operator*Psi of the list Operators for the i state*

```
outputname = debug.getinfo(1,"S")
outputname = string.gsub(outputname.source,"@","")
outputname = string.gsub(outputname,".lua","")
tempfile = io.open(outputname.."_.obj","w")
io.output(tempfile)

io.write(header)
for i, Psi in ipairs(Psis_i) do
   io.write(string.format('%5d', i))
   for j, Operator in ipairs(Operators) do
      if j == 1 then
         io.write(string.format('%12.6f', Complex.Re(Psi * Operator * Psi)))
      elseif Operator == 'dZ' then
         io.write(string.format('%12.2E', dZ[i]))
      else
         io.write(string.format('%10.4f', Complex.Re(Psi * Operator * Psi)))
      end
   end
   io.write("\n")
end
io.write(footer)
```

Eigenvalues for 10Dq=2.5 eV Co3+

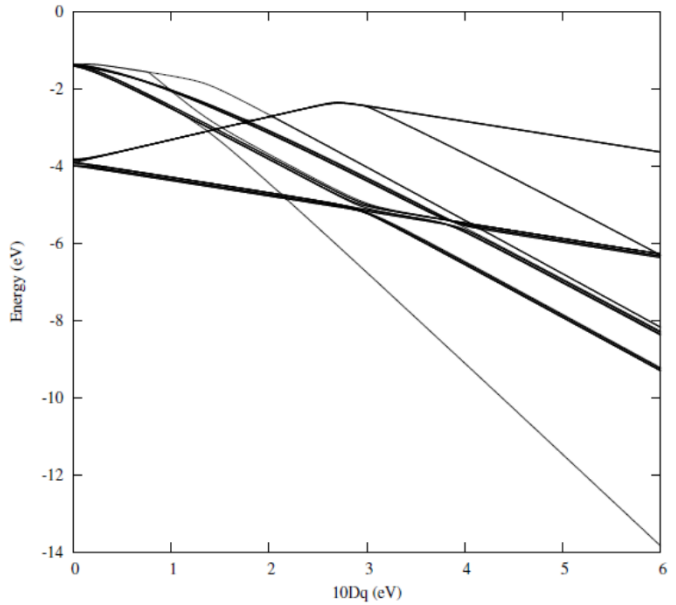
Analysis of the initial Hamiltonian:

State	<E>	<S^2>	<L^2>	<J^2>	<Sz>	<Lz>	<Jz>	<Tz>	<N_2p>	<N_3d>	dZ
1	-5.601363	0.0452	25.9689	25.9723	-0.0000	0.0000	0.0000	0.0000	6.0000	6.0000	1.00E+00
2	-4.981989	5.9845	6.0353	18.1117	-1.4907	-0.5302	-2.0209	0.0226	6.0000	6.0000	7.07E-313
3	-4.981989	5.9845	6.0353	18.1117	0.1639	0.0583	0.2222	-0.0025	6.0000	6.0000	7.07E-313
4	-4.981989	5.9845	6.0353	18.1117	1.3268	0.4719	1.7987	-0.0201	6.0000	6.0000	7.07E-313
5	-4.955096	5.9050	6.2265	14.5305	0.0000	-0.0000	0.0000	0.0000	6.0000	6.0000	0.00E+00
6	-4.955096	5.9050	6.2265	14.5305	-0.0000	0.0000	-0.0000	0.0000	6.0000	6.0000	0.00E+00
7	-4.949304	5.9390	6.1471	14.1361	0.2915	-0.1737	0.1179	0.0707	6.0000	6.0000	0.00E+00
8	-4.949304	5.9390	6.1471	14.1361	-0.5174	0.3082	-0.2092	-0.1254	6.0000	6.0000	0.00E+00
9	-4.949304	5.9390	6.1471	14.1361	0.2258	-0.1345	0.0913	0.0547	6.0000	6.0000	0.00E+00
10	-4.915902	5.7924	6.5142	9.1372	-0.0000	0.0000	-0.0000	0.0000	6.0000	6.0000	0.00E+00
11	-4.906102	5.8589	6.3366	8.8114	0.0000	-0.0002	-0.0001	0.0000	6.0000	6.0000	0.00E+00
12	-4.906102	5.8589	6.3366	8.8114	0.0938	-0.3599	-0.2661	0.0592	6.0000	6.0000	0.00E+00
13	-4.906102	5.8589	6.3366	8.8114	-0.0938	0.3601	0.2662	-0.0593	6.0000	6.0000	0.00E+00
14	-4.900441	5.8570	6.3375	8.4548	-0.1419	0.0712	-0.0708	-0.0095	6.0000	6.0000	0.00E+00
15	-4.900441	5.8570	6.3375	8.4548	-0.8213	0.4119	-0.4094	-0.0550	6.0000	6.0000	0.00E+00
16	-4.900441	5.8570	6.3375	8.4548	0.9632	-0.4830	0.4802	0.0645	6.0000	6.0000	0.00E+00
17	-4.499276	2.0812	17.4623	21.3952	0.0000	0.0000	0.0000	-0.0000	6.0000	6.0000	0.00E+00
18	-4.499276	2.0812	17.4623	21.3952	0.0000	0.0000	0.0000	-0.0000	6.0000	6.0000	0.00E+00
19	-4.489580	2.1468	17.2905	20.7733	0.5136	0.2529	0.7665	0.2768	6.0000	6.0000	0.00E+00
20	-4.489580	2.1468	17.2905	20.7733	-0.5096	-0.2509	-0.7606	-0.2746	6.0000	6.0000	0.00E+00
21	-4.489580	2.1468	17.2905	20.7733	-0.0040	-0.0020	-0.0059	-0.0021	6.0000	6.0000	0.00E+00
22	-4.424474	2.1855	17.6030	18.7588	-0.4593	-0.3182	-0.7775	-0.3529	6.0000	6.0000	0.00E+00
23	-4.424474	2.1855	17.6030	18.7588	-0.0383	-0.0266	-0.0649	-0.0294	6.0000	6.0000	0.00E+00
24	-4.424474	2.1855	17.6030	18.7588	0.4976	0.3448	0.8424	0.3824	6.0000	6.0000	0.00E+00
25	-4.374459	2.1578	18.0001	17.8772	0.0000	-0.0000	0.0000	-0.0000	6.0000	6.0000	0.00E+00
26	-3.766484	1.9493	20.3029	22.0513	-0.4818	-0.0628	-0.5446	0.2165	6.0000	6.0000	0.00E+00
27	-3.766484	1.9493	20.3029	22.0513	0.4665	0.0608	0.5273	-0.2096	6.0000	6.0000	0.00E+00
28	-3.766484	1.9493	20.3029	22.0513	0.0153	0.0020	0.0173	-0.0069	6.0000	6.0000	0.00E+00

Eigenvalues for 10Dq=2.5 eV Co3+

Analysis of the initial Hamiltonian:

State	<E>	<S^2>	<L^2>	<J^2>	<Sz>	<Lz>	<Jz>	<Tz>	<N_2p>	<N_3d>	dZ
1	-5.601363	0.0452	25.9689	25.9723	-0.0000	0.0000	0.0000	0.0000	6.0000	6.0000	1.00E+00
2	-4.981989	5.9845	6.0353	18.1117	-1.4907	-0.5302	-2.0209	0.0226	6.0000	6.0000	7.07E-313
3	-4.981989	5.9845	6.0353	18.1117	0.1639	0.0583	0.2222	-0.0025	6.0000	6.0000	7.07E-313
4	-4.981989	5.9845	6.0353	18.1117	1.3268	0.4719	1.7987	-0.0201	6.0000	6.0000	7.07E-313
5	-4.955096	5.9050	6.2265	14.5305	0.0000	-0.0000					
6	-4.955096	5.9050	6.2265	14.5305	-0.0000	0.0000					
7	-4.949304	5.9390	6.1471	14.1361	0.2915	-0.1737					
8	-4.949304	5.9390	6.1471	14.1361	-0.5174	0.3082					
9	-4.949304	5.9390	6.1471	14.1361	0.2258	-0.1345					
10	-4.915902	5.7924	6.5142	9.1372	-0.0000	0.0000					
11	-4.906102	5.8589	6.3366	8.8114	0.0000	-0.0002					
12	-4.906102	5.8589	6.3366	8.8114	0.0938	-0.3599					
13	-4.906102	5.8589	6.3366	8.8114	-0.0938	0.3601					
14	-4.900441	5.8570	6.3375	8.4548	-0.1419	0.0712					
15	-4.900441	5.8570	6.3375	8.4548	-0.8213	0.4119					
16	-4.900441	5.8570	6.3375	8.4548	0.9632	-0.4830					
17	-4.499276	2.0812	17.4623	21.3952	0.0000	0.0000					
18	-4.499276	2.0812	17.4623	21.3952	0.0000	0.0000					
19	-4.489580	2.1468	17.2905	20.7733	0.5136	0.2529					
20	-4.489580	2.1468	17.2905	20.7733	-0.5096	-0.2509					
21	-4.489580	2.1468	17.2905	20.7733	-0.0040	-0.0020					
22	-4.424474	2.1855	17.6030	18.7588	-0.4593	-0.3182					
23	-4.424474	2.1855	17.6030	18.7588	-0.0383	-0.0266					
24	-4.424474	2.1855	17.6030	18.7588	0.4976	0.3448					
25	-4.374459	2.1578	18.0001	17.8772	0.0000	-0.0000	0.0000	-0.0000	6.0000	6.0000	0.00E+00
26	-3.766484	1.9493	20.3029	22.0513	-0.4818	-0.0628	-0.5446	0.2165	6.0000	6.0000	0.00E+00
27	-3.766484	1.9493	20.3029	22.0513	0.4665	0.0608	0.5273	-0.2096	6.0000	6.0000	0.00E+00
28	-3.766484	1.9493	20.3029	22.0513	0.0153	0.0020	0.0173	-0.0069	6.0000	6.0000	0.00E+00



Eigenvalues for 10Dq=1.0 eV Co3+

Analysis of the initial Hamiltonian:

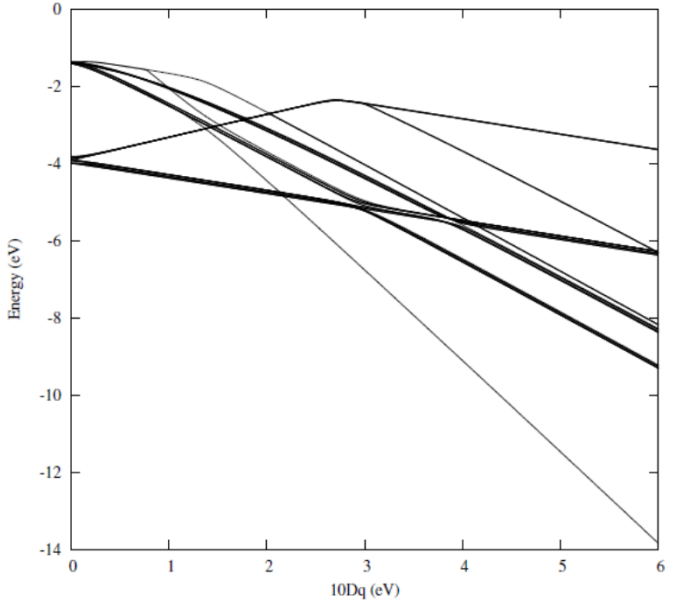
State	<E>	<S^2>	<L^2>	<J^2>	<Sz>	<Lz>	<Jz>	<Tz>	<N_2p>	<N_3d>	dZ
1	-4.382181	5.9935	6.0096	18.2569	0.0002	0.0001	0.0003	-0.0000	6.0000	6.0000	3.33E-01
2	-4.382181	5.9935	6.0096	18.2569	0.6056	0.2296	0.8352	-0.0120	6.0000	6.0000	3.33E-01
3	-4.382181	5.9935	6.0096	18.2569	-0.6058	-0.2297	-0.8355	0.0120	6.0000	6.0000	3.33E-01
4	-4.349380	5.9896	6.0116	14.8683	-0.0000	0.0000	-0.0000	0.0000	6.0000	6.0000	9.82E-18
5	-4.349380	5.9896	6.0116	14.8683	-0.0000	-0.0000	-0.0000	0.0000	6.0000	6.0000	9.82E-18
6	-4.346127	5.9923	6.0099	14.5032	0.7225	-0.2876	0.4348	0.1860	6.0000	6.0000	2.25E-19
7	-4.346127	5.9923	6.0099	14.5032	0.0036	-0.0014	0.0022	0.0009	6.0000	6.0000	2.25E-19
8	-4.346127	5.9923	6.0099	14.5032	-0.7261	0.2891	-0.4370	-0.1870	6.0000	6.0000	2.25E-19
9	-4.302170	5.9818	6.0131	9.8231	-0.0000	0.0000	-0.0000	0.0000	6.0000	6.0000	1.58E-41
10	-4.294778	5.9878	6.0073	8.8454	-0.0009	0.0014	0.0004	-0.0005	6.0000	6.0000	2.98E-45
11	-4.294778	5.9878	6.0073	8.8454	-0.1907	0.2759	0.0852	-0.0973	6.0000	6.0000	2.98E-45
12	-4.294778	5.9878	6.0073	8.8454	0.1916	-0.2773	-0.0857	0.0978	6.0000	6.0000	2.98E-45
13	-4.289829	5.9905	6.0041	8.1825	0.0981	-0.0533	0.0449	0.0120	6.0000	6.0000	9.54E-48
14	-4.289829	5.9905	6.0041	8.1825	-0.9937	0.5394	-0.4543	-0.1220	6.0000	6.0000	9.54E-48
15	-4.289829	5.9905	6.0041	8.1825	0.8956	-0.4862	0.4095	0.1100	6.0000	6.0000	9.54E-48
16	-3.324902	5.9924	6.0091	12.0012	-0.0000	-0.0000	-0.0000	-0.0000	6.0000	6.0000	0.00E+00
17	-3.324181	5.9899	6.0088	11.5691	0.0073	-0.0016	0.0058	-0.0020	6.0000	6.0000	0.00E+00
18	-3.324181	5.9899	6.0088	11.5691	0.2742	-0.0590	0.2152	-0.0749	6.0000	6.0000	0.00E+00
19	-3.324181	5.9899	6.0088	11.5691	-0.2816	0.0606	-0.2210	0.0769	6.0000	6.0000	0.00E+00
20	-3.323467	5.9874	6.0086	11.1406	0.0000	-0.0000	0.0000	-0.0000	6.0000	6.0000	0.00E+00
21	-3.323467	5.9874	6.0086	11.1406	-0.0000	-0.0000	-0.0000	-0.0000	6.0000	6.0000	0.00E+00
22	-3.322423	5.9858	6.0099	10.6648	-0.1232	-0.0101	-0.1333	-0.0352	6.0000	6.0000	0.00E+00
23	-3.322423	5.9858	6.0099	10.6648	-0.0413	-0.0034	-0.0447	-0.0118	6.0000	6.0000	0.00E+00
24	-3.322423	5.9858	6.0099	10.6648	0.1645	0.0135	0.1780	0.0470	6.0000	6.0000	0.00E+00
25	-3.321407	5.9841	6.0106	10.1912	0.0000	-0.0000	0.0000	-0.0000	6.0000	6.0000	0.00E+00
26	-2.516926	2.0002	19.1429	24.0481	-0.0000	-0.0000	-0.0000	0.0000	6.0000	6.0000	0.00E+00
27	-2.516926	2.0002	19.1429	24.0481	0.0000	-0.0000	-0.0000	-0.0000	6.0000	6.0000	0.00E+00
28	-2.510489	2.0045	19.1143	23.4426	0.0024	0.0020	0.0043	0.0010	6.0000	6.0000	0.00E+00
29	-2.510489	2.0045	19.1143	23.4426	-0.4971	-0.4142	-0.9113	-0.2071	6.0000	6.0000	0.00E+00
30	-2.510489	2.0045	19.1143	23.4426	0.4947	0.4123	0.9070	0.2062	6.0000	6.0000	0.00E+00
31	-2.496527	1.7044	21.1142	20.3534	0.0000	-0.0000	0.0000	-0.0000	6.0000	6.0000	0.00E+00
32	-2.447568	2.0093	20.0735	20.9250	0.4928	0.5393	1.0321	0.3462	6.0000	6.0000	0.00E+00
33	-2.447568	2.0093	20.0735	20.9250	-0.1882	-0.2060	-0.3943	-0.1322	6.0000	6.0000	0.00E+00
34	-2.447568	2.0093	20.0735	20.9250	-0.3046	-0.3333	-0.6379	-0.2139	6.0000	6.0000	0.00E+00

length : 14,884 lines : 126 Ln : 1 Col : 1 Sel : 0 | 0 Unix (LF) UTF-8 INS

Eigenvalues for 10Dq=1.0 eV Co3+

Analysis of the initial Hamiltonian:

State	<E>	<S^2>	<L^2>	<J^2>	<Sz>	<Lz>	<Jz>	<Tz>	<N_2p>	<N_3d>	dZ
1	-4.382181	5.9935	6.0096	18.2569	0.0002	0.0001	0.0003	-0.0000	6.0000	6.0000	3.33E-01
2	-4.382181	5.9935	6.0096	18.2569	0.6056	0.2296	0.8352	-0.0120	6.0000	6.0000	3.33E-01
3	-4.382181	5.9935	6.0096	18.2569	-0.6058	-0.2297	-0.8355	0.0120	6.0000	6.0000	3.33E-01
4	-4.349380	5.9896	6.0116	14.8683	-0.0000	0.0000	-0.0000	0.0000	6.0000	6.0000	9.82E-18
5	-4.349380	5.9896	6.0116	14.8683	-0.0000	-0.0000	-0.0000	0.0000	6.0000	6.0000	9.82E-18
6	-4.346127	5.9923	6.0099	14.5032	0.7225						5E-19
7	-4.346127	5.9923	6.0099	14.5032	0.0036						5E-19
8	-4.346127	5.9923	6.0099	14.5032	-0.7261						5E-19
9	-4.302170	5.9818	6.0131	9.8231	-0.0000						8E-41
10	-4.294778	5.9878	6.0073	8.8454	-0.0009						8E-45
11	-4.294778	5.9878	6.0073	8.8454	-0.1907						8E-45
12	-4.294778	5.9878	6.0073	8.8454	0.1916						8E-45
13	-4.289829	5.9905	6.0041	8.1825	0.0981						4E-48
14	-4.289829	5.9905	6.0041	8.1825	-0.9937						4E-48
15	-4.289829	5.9905	6.0041	8.1825	0.8956						4E-48
16	-3.324902	5.9924	6.0091	12.0012	-0.0000						0E+00
17	-3.324181	5.9899	6.0088	11.5691	0.0073						0E+00
18	-3.324181	5.9899	6.0088	11.5691	0.2742						0E+00
19	-3.324181	5.9899	6.0088	11.5691	-0.2816						0E+00
20	-3.323467	5.9874	6.0086	11.1406	0.0000						0E+00
21	-3.323467	5.9874	6.0086	11.1406	-0.0000						0E+00
22	-3.322423	5.9858	6.0099	10.6648	-0.1232						0E+00
23	-3.322423	5.9858	6.0099	10.6648	-0.0413						0E+00
24	-3.322423	5.9858	6.0099	10.6648	0.1645						0E+00
25	-3.321407	5.9841	6.0106	10.1912	0.0000						0E+00
26	-2.516926	2.0002	19.1429	24.0481	-0.0000						0E+00
27	-2.516926	2.0002	19.1429	24.0481	0.0000						0E+00
28	-2.510489	2.0045	19.1143	23.4426	0.0024	0.0020	0.0043	0.0010	6.0000	6.0000	0.00E+00
29	-2.510489	2.0045	19.1143	23.4426	-0.4971	-0.4142	-0.9113	-0.2071	6.0000	6.0000	0.00E+00
30	-2.510489	2.0045	19.1143	23.4426	0.4947	0.4123	0.9070	0.2062	6.0000	6.0000	0.00E+00
31	-2.496527	1.7044	21.1142	20.3534	0.0000	-0.0000	0.0000	-0.0000	6.0000	6.0000	0.00E+00
32	-2.447568	2.0093	20.0735	20.9250	0.4928	0.5393	1.0321	0.3462	6.0000	6.0000	0.00E+00
33	-2.447568	2.0093	20.0735	20.9250	-0.1882	-0.2060	-0.3943	-0.1322	6.0000	6.0000	0.00E+00
34	-2.447568	2.0093	20.0735	20.9250	-0.3046	-0.3333	-0.6379	-0.2139	6.0000	6.0000	0.00E+00



length : 14,884 lines : 126 Ln : 1 Col : 1 Sel : 0 | 0 Unix (LF) UTF-8 INS

Eigenvalues for Charge Transfer Calculations

- *One should calculate the eigenvalues of the total Lsqr, Ssqr and Jsqr, including the ligand contribution*

Eigenvalues for Charge Transfer Calculations

- *We add the operators acting on the Ligands*

```
-- operators acting on the ligand shell

LxL     = NewOperator("Lx",    NFermions,IndexUp_Ld,IndexDn_Ld)
LyL     = NewOperator("Ly",    NFermions,IndexUp_Ld,IndexDn_Ld)
LzL     = NewOperator("Lz",    NFermions,IndexUp_Ld,IndexDn_Ld)
LsqrL   = NewOperator("Lsqr",  NFermions,IndexUp_Ld,IndexDn_Ld)
SxL     = NewOperator("Sx",    NFermions,IndexUp_Ld,IndexDn_Ld)
SyL     = NewOperator("Sy",    NFermions,IndexUp_Ld,IndexDn_Ld)
SzL     = NewOperator("Sz",    NFermions,IndexUp_Ld,IndexDn_Ld)
SsqrL   = NewOperator("Ssqr",  NFermions,IndexUp_Ld,IndexDn_Ld)
JxL     = NewOperator("Jx",    NFermions,IndexUp_Ld,IndexDn_Ld)
JyL     = NewOperator("Jy",    NFermions,IndexUp_Ld,IndexDn_Ld)
JzL     = NewOperator("Jz",    NFermions,IndexUp_Ld,IndexDn_Ld)
JsqrL   = NewOperator("Jsqr",  NFermions,IndexUp_Ld,IndexDn_Ld)
TxL     = NewOperator("Tx",    NFermions,IndexUp_Ld,IndexDn_Ld)
TyL     = NewOperator("Ty",    NFermions,IndexUp_Ld,IndexDn_Ld)
TzL     = NewOperator("Tz",    NFermions,IndexUp_Ld,IndexDn_Ld)
```

Eigenvalues for Charge Transfer Calculations

- *We add the operators acting on the total cluster*

```
-- Operators acting on the total cluster

Lx = Lx_3d + LxL
Ly = Ly_3d + LyL
Lz = Lz_3d + LzL
Lsqr = Lx * Lx + Ly * Ly + Lz * Lz
Sx = Sx_3d + SxL
Sy = Sy_3d + SyL
Sz = Sz_3d + SzL
Ssqr = Sx * Sx + Sy * Sy + Sz * Sz
Jx = Jx_3d + JxL
Jy = Jy_3d + JyL
Jz = Jz_3d + JzL
Jsqr = Jx * Jx + Jy * Jy + Jz * Jz
Tx = Tx_3d + TxL
Ty = Ty_3d + TyL
Tz = Tz_3d + TzL
```

Eigenvalues for Charge Transfer Calculations

- *We update the list of the operators*

```
 Operators = {H_i, Ssqr_3d, Lsqr_3d, Jsqr_3d, Sz_3d, Lz_3d, Jz_3d, Tz_3d, Ssqr, Lsqr, Jsqr,
Sz, Lz, Jz, Tz, N_2p, N_3d, N_Ld, 'dZ'}
   header = 'Analysis of the initial Hamiltonian:\n'
   header = header ..
'================================================================================
============================================\n'
   header = header .. 'State      <E>    <S^2_d>   <L^2_d>   <J^2_d>   <Sz_d>   <Lz_d>
<Jz_d>    <Tz_d>    <S^2>    <L^2>    <J^2>    <Sz>    <Lz>    <Jz>    <Tz>   <N_2p>
<N_3d>   <N_Ld>       dZ\n'
   header = header ..
'================================================================================
============================================\n'
   footer =
'================================================================================
============================================\n'
```

Eigenvalues for charge transfer calculations of Co3+

Analysis of the initial Hamiltonian:

State	<E>	<S^2_d>	<L^2_d>	<J^2_d>	<Sz_d>	<Lz_d>	<Jz_d>	<Tz_d>	<S^2>	<L^2>	<J^2>	<Sz>	<Lz>	<Jz>	<Tz>	<N_2p>	<N_3d>	<N_Ld>
1	-7.464030	5.2694	7.1648	18.1919	-0.1177	-0.0479	-0.1656	0.0021	5.9911	6.6247	18.8847	-0.1281	-0.0482	-0.1763	0.0022	6.0000	6.3215	9.6785	3.34E-01
2	-7.464030	5.2694	7.1647	18.1918	0.0037	0.0015	0.0052	-0.0001	5.9911	6.6247	18.8848	0.0040	0.0015	0.0055	-0.0001	6.0000	6.3215	9.6785	3.34E-01
3	-7.464028	5.2695	7.1650	18.1920	0.1140	0.0464	0.1604	-0.0020	5.9911	6.6244	18.8843	0.1242	0.0467	0.1709	-0.0021	6.0000	6.3215	9.6785	3.33E-01
4	-7.431946	5.2593	7.1774	15.0218	-0.0000	-0.0000	-0.0000	-0.0000	5.9778	6.6411	15.3796	-0.0000	-0.0000	-0.0000	-0.0000	6.0000	6.3218	9.6782	2.26E-17
5	-7.431944	5.2595	7.1780	15.0228	0.0000	-0.0000	0.0000	-0.0000	5.9779	6.6409	15.3786	0.0000	-0.0000	0.0000	-0.0000	6.0000	6.3217	9.6783	2.25E-17
6	-7.428516	5.2652	7.1680	14.7195	0.0033	-0.0014	0.0019	0.0008	5.9850	6.6315	15.0553	0.0035	-0.0014	0.0021	0.0009	6.0000	6.3215	9.6785	4.22E-19
7	-7.428514	5.2650	7.1683	14.7192	0.0027	-0.0012	0.0015	0.0007	5.9850	6.6314	15.0552	0.0029	-0.0012	0.0017	0.0007	6.0000	6.3216	9.6784	4.21E-19
8	-7.428513	5.2649	7.1686	14.7191	-0.0060	0.0025	-0.0034	-0.0015	5.9850	6.6316	15.0555	-0.0065	0.0026	-0.0039	-0.0016	6.0000	6.3217	9.6783	4.20E-19
9	-7.385551	5.2430	7.1896	10.2547	-0.0000	0.0000	-0.0000	-0.0000	5.9560	6.6634	10.1427	-0.0000	0.0000	-0.0000	-0.0000	6.0000	6.3218	9.6782	9.37E-41
10	-7.378085	5.2554	7.1669	9.5034	0.0475	-0.0726	-0.0251	0.0230	5.9720	6.6366	9.3219	0.0516	-0.0742	-0.0226	0.0249	6.0000	6.3216	9.6784	1.62E-44
11	-7.378085	5.2554	7.1669	9.5034	-0.0475	0.0726	0.0251	-0.0230	5.9720	6.6366	9.3219	-0.0516	0.0742	0.0226	-0.0249	6.0000	6.3216	9.6784	1.62E-44
12	-7.378076	5.2552	7.1683	9.5042	0.0000	0.0000	0.0000	-0.0000	5.9720	6.6363	9.3210	0.0000	0.0000	0.0000	-0.0000	6.0000	6.3217	9.6783	1.60E-44
13	-7.373315	5.2598	7.1589	8.9959	-0.9121	0.5229	-0.3892	-0.1016	5.9778	6.6259	8.7587	-0.9917	0.5328	-0.4589	-0.1104	6.0000	6.3216	9.6784	6.38E-47
14	-7.373315	5.2597	7.1591	8.9959	0.9084	-0.5208	0.3876	0.1012	5.9778	6.6262	8.7589	0.9877	-0.5306	0.4571	0.1100	6.0000	6.3216	9.6784	6.38E-47
15	-7.373311	5.2596	7.1590	8.9960	0.0037	-0.0021	0.0016	0.0004	5.9778	6.6263	8.7591	0.0040	-0.0021	0.0018	0.0005	6.0000	6.3217	9.6783	6.36E-47
16	-6.446951	1.7470	18.5776	19.2331	-0.0000	0.0000	0.0000	-0.0000	1.4728	20.9261	20.8699	-0.0000	0.0000	0.0000	-0.0000	6.0000	6.4337	9.5663	0.00E+00
17	-6.444491	2.2857	16.3110	21.4314	-0.0000	-0.0000	-0.0000	0.0000	2.0121	18.4047	23.3263	-0.0000	-0.0000	-0.0000	0.0000	6.0000	6.4342	9.5658	0.00E+00
18	-6.444488	2.2857	16.3184	21.4394	-0.0000	0.0000	0.0000	-0.0000	2.0121	18.4143	23.3362	-0.0000	0.0000	0.0000	-0.0000	6.0000	6.4342	9.5658	0.00E+00
19	-6.436759	2.2909	16.2817	20.7287	0.0408	0.0297	0.0705	0.0159	2.0196	18.3666	22.5868	0.0413	0.0304	0.0717	0.0182	6.0000	6.4338	9.5662	0.00E+00
20	-6.436759	2.2909	16.2848	20.7333	0.4437	0.3230	0.7667	0.1729	2.0196	18.3705	22.5929	0.4495	0.3305	0.7800	0.1986	6.0000	6.4338	9.5662	0.00E+00
21	-6.436758	2.2908	16.2848	20.7328	-0.4844	-0.3530	-0.8374	-0.1888	2.0195	18.3703	22.5920	-0.4908	-0.3612	-0.8520	-0.2168	6.0000	6.4338	9.5662	0.00E+00
22	-6.374217	2.2954	16.7609	18.2360	0.4551	0.4252	0.8803	0.2839	2.0318	18.9427	20.2186	0.4607	0.4411	0.9018	0.3135	6.0000	6.4341	9.5659	0.00E+00
23	-6.374215	2.2951	16.7607	18.2360	0.0001	0.0001	0.0003	0.0001	2.0318	18.9420	20.2190	0.0002	0.0001	0.0003	0.0001	6.0000	6.4341	9.5659	0.00E+00
24	-6.374214	2.2950	16.7615	18.2381	-0.4551	-0.4255	-0.8806	-0.2840	2.0318	18.9424	20.2207	-0.4608	-0.4414	-0.9022	-0.3136	6.0000	6.4340	9.5660	0.00E+00
25	-6.308407	5.2772	7.5998	12.3657	-0.0000	0.0000	-0.0000	-0.0000	5.9511	6.7064	11.9500	-0.0000	0.0000	-0.0000	-0.0000	6.0000	6.3059	9.6941	0.00E+00
26	-6.308404	5.2769	7.6001	12.3663	-0.0001	-0.0000	-0.0001	-0.0000	5.9509	6.7067	11.9503	-0.0001	-0.0000	-0.0001	-0.0000	6.0000	6.3059	9.6941	0.00E+00
27	-6.308063	5.2881	7.5754	12.6366	0.0045	-0.0008	0.0037	-0.0010	5.9660	6.6714	12.2811	0.0048	-0.0008	0.0040	-0.0012	6.0000	6.3055	9.6945	0.00E+00
28	-6.308062	5.2881	7.5753	12.6365	-0.4345	0.0789	-0.3556	0.1052	5.9659	6.6717	12.2814	-0.4707	0.0834	-0.3873	0.1330	6.0000	6.3054	9.6946	0.00E+00
29	-6.308061	5.2880	7.5754	12.6366	0.4402	-0.0787	0.3614	-0.1042	5.9659	6.6718	12.2816	0.4767	-0.0832	0.3935	-0.1317	6.0000	6.3055	9.6945	0.00E+00
30	-6.307943	5.2972	7.5537	12.9330	-0.0000	-0.0000	-0.0000	-0.0000	5.9780	6.6412	12.6337	-0.0000	-0.0000	-0.0000	-0.0000	6.0000	6.3050	9.6950	0.00E+00
31	-6.307862	5.2771	7.5826	12.0264	0.0006	0.0000	0.0006	0.0001	5.9505	6.6872	11.5554	0.0006	0.0000	0.0006	0.0002	6.0000	6.3058	9.6942	0.00E+00
32	-6.307860	5.2769	7.5833	12.0265	-0.4528	-0.0374	-0.4902	-0.1038	5.9505	6.6874	11.5551	-0.4896	-0.0357	-0.5253	-0.1306	6.0000	6.3059	9.6941	0.00E+00
33	-6.307858	5.2767	7.5834	12.0269	0.4423	0.0380	0.4803	0.1037	5.9504	6.6874	11.5555	0.4783	0.0363	0.5146	0.1305	6.0000	6.3059	9.6941	0.00E+00
34	-6.307020	5.2777	7.5731	11.6727	-0.0000	0.0000	-0.0000	0.0000	5.9515	6.6764	11.1544	-0.0000	0.0000	-0.0000	0.0000	6.0000	6.3057	9.6943	0.00E+00
35	-6.113902	0.8839	22.4275	22.1669	-0.0000	0.0000	0.0000	0.0000	0.5701	25.2116	25.0477	-0.0000	0.0000	0.0000	0.0000	6.0000	6.4381	9.5619	0.00E+00
36	-6.036416	2.3082	18.1365	20.3726	-0.4244	-0.1145	-0.5389	0.1469	1.9953	20.5676	22.1195	-0.4258	-0.0944	-0.5202	0.1722	6.0000	6.4494	9.5506	0.00E+00
37	-6.036413	2.3089	18.1255	20.3832	-0.0163	-0.0045	-0.0208	0.0056	1.9955	20.5542	22.1317	-0.0163	-0.0037	-0.0201	0.0066	6.0000	6.4494	9.5506	0.00E+00
38	-6.036398	2.3094	18.1245	20.3799	0.4400	0.1245	0.5645	-0.1520	1.9960	20.5539	22.1290	0.4415	0.1043	0.5458	-0.1782	6.0000	6.4495	9.5505	0.00E+00
39	-6.025961	2.3399	17.9779	20.5385	0.0000	0.0000	0.0000	0.0000	2.0247	20.3885	22.3953	0.0000	0.0000	0.0000	0.0000	6.0000	6.4500	9.5500	0.00E+00
40	-6.025960	2.3400	17.9758	20.5403	0.0000	-0.0000	0.0000	-0.0000	2.0247	20.3863	22.3970	0.0000	-0.0000	0.0000	-0.0000	6.0000	6.4500	9.5500	0.00E+00

Eigenvalues - Temperature

One can use the calculated eigenvalues of Tz operator to extract the Sz value or the Lz/Sz ratio given by the sum rules applied to the XMCD spectrum.

Also it is good to compare the calculated Lz, Sz values with the Lz, Sz values given by the application of the sum rules.

However one should always consider the thermal population of the levels

Eigenvalues - Temperature

```
io.output(tempfile) T = 10 * EnergyUnits.Kelvin.value
Egrd = Psis_i[1] * H_i  * Psis_i[1]´
-- we will calculate the partition function Z
Z=0
-- the total magnetic moment M
M=0
-- the total spin moment MS
MS=0
-- the total angular moment ML
ML=0

-- and now we can make the sums
for j=1, 3 do
  Z  = Z  + exp(-(Psis_i[j] * H_i * Psis_i[j] - Egrd)/T)
  M  = M  + Psis_i[j] * (2 * OppSz + OppLz) * Psis_i[j] * exp(-(Psis_i[j] * H_i * Psis_i[j] - Egrd)/T)
  MS = MS + Psis_i[j] * (OppSz)           * Psis_i[j] * exp(-(Psis_i[j] * H_i * Psis_i[j] - Egrd)/T)
  ML = ML + Psis_i[j] * (OppLz)           * Psis_i[j] * exp(-(Psis_i[j] * H_i * Psis_i[j] - Egrd)/T)
end
-- In order to normalize we should device by the partition function Z
M  = M  / Z
MS = MS / Z
ML = ML / Z
```