Read transition density matrix

Initialize

```
> abbr,method:= "HCOOH", "B3LYPp2";
  fn:=cat(abbr,"_",method,"_rhot");
  #fn:="g09_opt_DFT_CB3LYP_tight_scrf-td";  convert2dos(cat(fn,".out"));
  fexists(cat(fn,".out"));
```

abbr, method := "HCOOH", "B3LYPp2"
fn := "HCOOH_B3LYPp2_rhot"
true

Load initial geometry

```
> Atoms:=ReadXYZ(cat(abbr,"_",method),printout):
 //5
```

Write input

```
> WriteInput(fn,"gau",Atoms,"TD(singlets,nstates=4)",'output'=["rwf"],
  'title'=cat(abbr," molecule: transition density matrix"),'method'=method,
  printout);
%rwf=HCOOH_B3LYPp2_rhot.rwf
# B3LYP 6-31g  TD(singlets,nstates=4)

HCOOH molecule: transition density matrix

0 1
C       0.00000000      0.43285900      0.00000000
O      -1.04628800     -0.45320100      0.00000000
O       1.18631800      0.12015500      0.00000000
H      -0.39242800      1.45121600      0.00000000
H      -0.72780500     -1.38400400      0.00000000
```

```
> SubmitJob(cat(fn,".gau"));
```

"953765.nano.lanl.gov"

```
> DownloadJob(cat(fn,".gau"),["s1e","evl","evc","rho","rhoa","rhob",633],
  'keepinp',printout);
Done HCOOH_B3LYPp2_rhot.s1e
Done HCOOH_B3LYPp2_rhot.evl
Done HCOOH_B3LYPp2_rhot.evc
Done HCOOH_B3LYPp2_rhot.rho
Done HCOOH_B3LYPp2_rhot.rhoa
Done HCOOH_B3LYPp2_rhot.rhob
Done HCOOH_B3LYPp2_rhot.633
Ready, HCOOH_B3LYPp2_rhot
```

true

Read number of electrons and orbitals, overlap and density matrices

```
> Na,Nb,N:=seq(ReadNumber(cat(fn,".out"),s),s=["Na","Nb","N"]);
  s1e:=ReadBIN(cat(fn,".s1e")):
  rho:=ReadBIN(cat(fn,".rho")):
  rhoa:=ReadBIN(cat(fn,".rhoa")):
  rhob:=ReadBIN(cat(fn,".rhob")):
```

Na, Nb, N := 12, 12, 31

Test

```
> Trace(rho.s1e)-Na-Nb;
  Norm(rho.s1e.rho/4-rho/2,Frobenius);
  Norm(rho-rhoa,Frobenius);
```

$-3.552714\,10^{-15}$

$1.070766\,10^{-14}$

0.000000

Read number of states and first few records

```
> ns:=op(FileTools[Binary][Read](cat(fn,".633"),integer[4],1,'byteorder'=
  'native'));
  FileTools[Binary][Read](cat(fn,".633"),integer[4],1+2*ns,'byteorder'=
  'native');
  FileTools[Binary][Read](cat(fn,".633"),float[8],10,'byteorder'='native');
  fclose(cat(fn,".633")):
```

ns := 4

[7, 0, 0, 0, 0, 0, 0, 0, 0]

[1.029187, −0.054659, 0.199518, −0.002889, 0.015802, 0.218704, −0.007388, 0.007526, −0.027191, 0.217524]

Read excited state and transition density matrices

```
> rhoe,rhot:=table(),table():
  for s from 1 to ns do
   rhoe[s]:=ReadBIN(cat(fn,".633"),'nodescription','code'=[2,8,31,1],
  'dimensions'=[N],'datapos'=8*(ns+1+(s-1)*N*(N+1)/2));
   Ma:=ReadBIN(cat(fn,".633"),'nodescription','code'=[2,8,22,1],'dimensions'=
  [N,N],'datapos'=8*(ns+1+ns*N*(N+1)/2+(2*s-2)*N^2));
   Mb:=ReadBIN(cat(fn,".633"),'nodescription','code'=[2,8,22,1],'dimensions'=
  [N,N],'datapos'=8*(ns+1+ns*N*(N+1)/2+(2*s-1)*N^2));
   if (Norm(Ma-Mb,Frobenius)>1e-8) then WARNING("Unpaired orbitals") end;
   rhot[s]:=Ma end:
```

Test

```
> for s from 1 to ns do printf("%2d%9.0g%9.0g%9.4f%9.4f\n",s,Trace(rhoe[s].
  s1e)-Na,Trace(rhot[s].s1e),Trace(rhoe[s].s1e.Transpose(rhoe[s]).s1e)-Na,
  Trace(rhot[s].s1e.Transpose(rhot[s]).s1e)) end;
```

```
 1        0   3e-031  -0.5009   1.0020
 2   4e-015  -2e-015  -0.7583   1.0113
 3   7e-015  -9e-030  -0.5130   1.0019
 4   4e-015  -3e-015  -0.7617   1.0250
```

NO and NTO weights

```
> R:=Matrix(MatrixFunction2(s1e,x->x^(1/2)),shape=symmetric):
  for s from 1 to ns do s,select(v->min(v,2-v)>.01,convert(2*SingularValues
  (R.rhoe[s].R),list)) end;
  Norm(R^2-s1e,Frobenius);
  for s from 1 to ns do s,select(`>`,convert(map(x->x^2,SingularValues(R.rhot
  [s].R)),list),.01) end;
```

1, [1.001169, 0.998881]

2, [1.535125, 1.461409, 0.538836, 0.464179]

3, [1.987550, 1.011294, 0.988933, 0.012250]

4, [1.987373, 1.603935, 1.390821, 0.606542, 0.396340, 0.013090]

$3.463684\,10^{-14}$

1, [1.000498]

2, [0.535691, 0.463670]

3, [0.988348, 0.012211]

4, [0.606168, 0.389469, 0.011535]

For symmetric matrices eigenvalues=singularvalues

```
> Norm(sort(SingularValues(R.rhoe[1].R))-sort(Eigenvalues(Matrix(R.rhoe[1].R,
  shape=symmetric))),2);
```

$1.874594\,10^{-15}$

```
> printf("%10.6f\n\n",rhoe[1][..5,..5]);
  printf("%10.6f\n",rhot[1][..5,..5]);
  1.029187  -0.054659  -0.002889  -0.007388  -0.000000
 -0.054659   0.199518   0.015802   0.007526  -0.000000
 -0.002889   0.015802   0.218704  -0.027191   0.000000
 -0.007388   0.007526  -0.027191   0.217524  -0.000000
 -0.000000  -0.000000   0.000000  -0.000000   0.318676

  0.000000  -0.000000  -0.000000   0.000000  -0.001785
 -0.000000   0.000000   0.000000   0.000000   0.002318
  0.000000  -0.000000  -0.000000   0.000000  -0.001768
 -0.000000   0.000000  -0.000000   0.000000  -0.001324
  0.005816  -0.006750   0.016201  -0.024713   0.000000
```

Dipole in an excited state

Generating cube file