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Quasi-Relativistic Hartree-Fock Program

User's Guide

ver. 1.0

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1 Description of input data

qrhf program accepts input data that consist of separate lines which contain

- a label
- a label followed by a string of characters, integer(s) and/or real number(s)
- a string of characters, integer(s) and/or real number(s)

Real numbers can be written in a fixed-point or scientific notation. Note that

- labels and strings can be in upper or lower case,
- the compulsory labels must follow the order given below; the optional ones can be inserted anywhere before **stop** label,
- optional parameters are enclosed in square brackets,
- an exclamation mark or a hash placed anywhere in an input line starts a comment and what follows “!” or “#” is ignored.

1.1 Mandatory labels

The following labels must be specified in the specified order:

ATOM

Format: `ATOM atom term z nwf [nit [ncfg [nf [ng [nr [nl]]]]]`

`atom` – an eight character label describing the atom

`term` – an eight character label describing a term of the atom

`z` – a real equal to the atomic number

`nwf` – a number (integer) of wave functions (HF orbitals)

`nit` – a number of orbitals to undergo scf process (the default value is equal to nwf)

`ncfg` – a number of configurations (defaults to 1, the only allowed value in this version of the program)

`nf,ng,nr,nl` – number of F, G, R and L integrals to be read in (default values are zero). If any of these numbers is non-zero Fk, Gk, etc cards are read in (see below)

The ATOM card is followed by nwf electron (orbital) cards of the form

Format: ellab [occ [n l s meth acc ind]]

ellab – electron label (1s, 2s 2p, etc)

occ – occupation number (if not given it is set to the maximum value allowed for a given symmetry)

n,l – principal and orbital quantum numbers (if not given they are deduced from the electron label)

s – screening factor

meth – method of solution (default 0)

acc – acceleration factor (default 0)

inf – source of initial orbitals:

-1 – a file containing orbitals generated in a previous run

0 – screened hydrogenic approximation (default)

1 – unchanged

If iuf is zero and inf is omitted it defaults to 0.

SCF

Format: SCF nscftol [nscf [omit]]

nscftol – an integer specifying the initial level of convergence of the SCF procedure, i.e. scftol= 10^{nscftol} (default 10^{-20})

nscf – a maximum number of SCF iteration

omit – if this logical variable is equal f (or F) then orthogonalization between orbitals is enforced during a SCF iteration (default omit=.false.)

GRID

Format: GRID no [rhonew [rmax]]

no – a number of grid points in r (ρ) variable

rhonew – a new value of ρ_0 which defines the location of the first grid point for which $r \neq 0$ (if omitted or set to zero the ρ_0 is set to -6.0)

rmax – if rmax is set then the step size is calculated so that the given number of points cover the range specified; if rmax equals zero its value is calculated according to no, ρ_0 (or rhonew if given) and the default step size in ρ variable (see setgrid)

STOP

Format: STOP

This label denotes the end of input data (any subsequent cards are ignored)

1.2 Optional labels

The following additional labels can be specified in any order:

ALPHA

Format: ALPHA alpha

Change the α parameter used to scale local exchange values ($\alpha = 2/3$ by default)

CONT

Format: CONT new|scaled|rel

Use this label to continue calculations with some of the input parameters modified:

new – another case with new initial functions

scaled – a new case with scaled orbitals as a source of initial functions (scale results for another member of the isoelectronic sequence)

rel – a previous case with (some of) relativistic parameters changed.

Note that only **STOP** can follow this card.

DEBUG

Format: DEBUG i1 [i2 [.. [...] ...] i100]]

Up to 100 integers (ranging from 1 to 100) can be used to request additional printouts (of debugging character). To make use of this feature insert in a place of interest the following instruction:

```
if (idbg(i).ne.0) then
...
endif
```

FERMI

Format: FERMI [atweight]

Use a finite nucleus model with the Fermi charge distribution. If atomic mass is not specified it is taken from *The 1983 Atomic Mass Evaluation* by Wapstra and Audi (see blk-data).

GAUSS

Format: GAUSS [atweight]

Use a finite nucleus model with the Gaussian charge distribution. If atomic mass is not specified it is taken from *The 1983 Atomic Mass Evaluation* by Wapstra and Audi (see blk-data).

INOUT

Format: INOUT iuf ouf [oud [ouh]]

iuf – a unit number (integer) for reading functions from a previous run

ouf – a unit number (integer) for writing functions from the current run

oud, ouh – additional (optional) unit numbers can be specified to obtain F and G integrals (oud) and energy matrix (ouh) (by default oud=ouh=0)

If inf/ouf are set to zero no orbitals are read/written.

OUT2DFH

Format: OUT2DFH out2dhf

out2dhf – an optional unit number (integer) for writing configuration information and orbitals in a (text) format suitable for the x2dhf program

PRINT

Format: PRINT

If present additional printout is produced

PRINT

Format: print [i_1 [$i_2 \dots$] i_{40}]

Up to 40 different printing flags can be set at a time. If the integer i_k is encountered the printing flag i_k is set, i.e. $\text{iprint}(i_k) = 1$ ($1 \leq i_k < 999$). These are used to generate additional printouts by adding the lines of the form

```
      if (iprint(ik).eq.1) then
        print *, 'printing something ...'
      ...
    endif
```

QPOT

Format: QPOT [qpot [state [reldamp]]]

qpot – an optional integer for selecting one of the following one-particle quasirelativistic potentials:

0 – no relativistic correction

- 1 – Cowan and Griffin (see qpotcg)
- 2 – Wood and Boring (default, see qpotwb)
- 3 – Barthelat, Pelissier and Durand (see qpotbpd)
- 4 – Karwowski and Klobukowski (see qpotkk)

If omitted the Wood and Boring relativistic correction is used.

state – ± 1 if $j = l \pm 1/2$ ($\kappa = j + 1/2$ or $-j - 1/2$)

It is assumed that the atomic configuration consists of (i) only closed shells, (ii) closed shell plus a single electron in a valence shell or (iii) closed shell plus an open shell having a single hole. In the first case the total angular momentum is zero and in the latter two cases is equal to $j = l \pm 1/2$ where l is the orbital quantum number of the open shell.

REL

Format: REL [reldamp [reldampsf]]

reldamp – an optional real number used to scale the velocity of light in order to switch relativistic effects gradually and avoid SCF instabilities (default 1.0). In subsequent cases (as determined by CONT label) this value is decreased by reldampsf (2.0 by default)

reldampsf – if reldamp is greater than 1 than additional runs of the program are needed to reduce this value eventually to 1.0 (this can be achieved by using CONT card). reldampsf (2.0 by default) determines the factor by which reldamp is decreased in each run

XPOT

Format: XPOT lda|cowan1|cowan2

Set a type of the local exchange potential to be used in a quasirelativistic potential (cowan1, i.e. is used by default)

2 Examples of input data

2.1 Ar

Quasirelativistic Hartree-Fock ground state of the Ar atom with the default (Wood and Boring) potential.

```
inout 0 0
atom  Ar S 18.0 5 5
      1s
      2s
      2p
      3s
      3p
scf    -12 80
grid  1500 -12 15000
!rel 10
qpot 2
!cont rel
stop
```


2.2 At

(QR)HF ground state of the At atom

1. HF calculations on the default grid.

```
inout 0 10
atom At 2P 85.0 15 15
1s
2s
2p
3s
3p
3d
4s
4p
4d
4f
5s
5p
5d
6s
6p 5
scf -10 80
!grid 3500 -10 1500
stop
```

2. HF calculations on a refined grid. Converged orbitals are written to the fort.10 file.

```
inout 0 10
atom At 2P 85.0 15 15
1s
2s
2p
3s
3p
3d
4s
4p
4d
4f
```

```

5s
5p
5d
6s
6p 5
scf -10 80
grid 3500 -10 1500
stop

```

3. QRHF calculations employing HF orbitals and the default QR potential.
Initial orbitals are taken from the previous HF calculations.

```

inout 10 12
atom At 2P 85.0 15 15
1s
2s
2p
3s
3p
3d
4s
4p
4d
4f
5s
5p
5d
6s
6p 5
scf -10 80
grid 3500 -10 1500
!xpot lda
rel 10 1.1
qpot 2 +1
cont rel
stop

```

2.3 Au

(QR)HF ground state of the Au atom.

1. Hartree-Fock calculations on a refined grid.

```
inout 0 10
atom Au 2D 79.0 14 14
1s
2s
2p
3s
3p
3d
4s
4p
4d
4f
5s
5p
5d 9
6s
scf -12 120
grid 2500 -8 15000
stop
```

2. QRHF calculations employing HF orbitals and the default QR.

```
inout 10 12
atom Au 2D 79.0 14 14
1s
2s
2p
3s
3p
3d
4s
4p
4d
4f
5s
5p
5d 9
```

```
6s
scf -12 120
grid 2500 -8 15000
!alpha 0.7
xpot cowan1
rel 20
!rel 20 1.2
qpot 2
cont rel
stop
```

2.4 C

Hartree-Fock ^3P state of the C atom.

```
! carbon 3P term HF
inout 0 0 0 1
atom C 3P 6.0 3 3 1 1
      1s 2 1 0 5.0 0 0 0
      2s 2 2 0 2.0 0 0 0
      2p 2 2 1 1.0 0 0 0
      -0.12 F 2 3 1 3 1
scf -12 120
grid 3000 -10 2000
rel 50
qpot 2
cont rel
stop
```

2.5 Ca

Hartree-Fock ground state of the Ca atom.

```
inout 0 0 0
atom  Ca S 20.0 6 6
      1s
      2s
      2p
      3s
      3p
      4s
scf    -12 180
grid  2500 -10 15000
rel 20
qpot 2
cont rel
stop
```

2.6 H

Ground state of the H atom.

```
inout 0 0
atom  H S 1.0 1 1
      1s 1
scf    -10 20
grid 5000 -6 10000
!gauss
!xpot lda
!qpot 2 1
stop
```

point nucleus

DHF = -0.5000066565975E+00

```
RHF (WB) = -0.50000665659750E+00 grid 2500 -10 1000
          -0.50000665659655E+00 grid 2500  -8 1000
          -0.50000665655720E+00 grid 2500  -6 1000
          -0.50000654104435E+00 grid   500  -4 1000
          -0.50000654353068E+00 grid 1000  -4 1000
          -0.50000654407969E+00 grid 1000  -4  100
```

2.7 Ne

(QR)HF ground state of the Ne atom.

1. HF calculation on a refined grid.

```
inout 0 0 6
!out2dhf 10
atom Ne S 10.0 3 3 1
      1s 2
      2s 2
      2p 6
scf -12 80
grid 2500 -12 12000
stop
```

2. QRHF calculations on the same grid.

```
inout 0 0 6
!out2dhf 10
atom Ne S 10.0 3 3 1
      1s 2
      2s 2
      2p 6
scf -12 80
grid 2500 -12 12000
rel 10
qpot 2
cont rel
stop
```


2.8 Rb

(QR)HF ground state of the Rb atom.

1. HF calculation on the default grid.

```
inout 0 0 0
atom Rb S 37.0 9 9
    1s  2  1  0    0.07  0 0 0
    2s  2  2  0    3.98  0 0 0
    2p  6  2  1    5.15  0 0 0
    3s  2  3  0   10.9   0 0 0
    3p  6  3  1   13.0   0 0 0
    3d 10  3  2   16.86  0 0 0
    4s  2  4  0   21.00  0 0 0
    4p  6  4  1   23.74  0 0 0
    5s  1  5  0   30.34  0 0 0
scf -12 100
!grid 1500 -10 10000
stop
```

2. HF calculation on a refined grid.

```
inout 0 0 0
atom Rb S 37.0 9 9
    1s  2  1  0    0.07  0 0 0
    2s  2  2  0    3.98  0 0 0
    2p  6  2  1    5.15  0 0 0
    3s  2  3  0   10.9   0 0 0
    3p  6  3  1   13.0   0 0 0
    3d 10  3  2   16.86  0 0 0
    4s  2  4  0   21.00  0 0 0
    4p  6  4  1   23.74  0 0 0
    5s  1  5  0   30.34  0 0 0
scf -12 100
grid 1500 -10 10000
stop
```

2.9 Rn

Hartree-Fock ground state of the Rn atom.

```
inout 0 10
atom Rn S 86.0 15 15
 1s
 2s
 2p
 3s
 3p
 3d
 4s
 4p
 4d
 4f
 5s
 5p
 5d
 6s
 6p
scf -10 80
grid 2500 -10 1500
!xpot cowan1
!rel 20
!qpot 2
!cont rel
stop
```

2.10 Th⁺⁸⁹

1. ²S ground state of the Th⁺⁸⁹ one-electron system (point nucleus model).

```
inout 0 0
atom  U S 90.0 1 1
      1s 1
scf    -10 120
grid 2500 -10 1000
rel 20 2
qpot 2 1
cont rel
stop
```

point nucleus

DHF = -4.6177576543E+03

RHF (WB) = -4.6177576541103E+03 rho=-10
-4.6177576539497E+03 rho=-8
-4.6177576550871E+03 rho=-6
-4.6177371783313E+03 rho=-4 non-converged

2. ²S ground state of the Th⁺⁸⁹ one-electron system (finite nucleus model).

```
inout 0 0
atom  U S 90.0 1 1
      1s 1
scf    -10 120
grid 2500 -10 1000
gauss
rel 20 2
qpot 2 1
cont rel
stop
```

finite nucleus: gauss, 232.0380508

DHF = -4.6120559360E+03

RHF (WB) = -4.6120562084455E+03 rho=-8
-4.6120559366543E+03 rho=-10

