Herman – Skillman Selfconsistent field code

Active participants:

Xaaaa Yaaaaa
Abaaa Baaaaaa
Caaaa Deeeee

All 3 participants worked on own unix computers

Mac OSX (2) Linux in virtual machine (1)

Common report collected and edited by L.K.

THIS IS A SHORTENED VERSION - for 2015 instructions

Task 1

Run the code with available input files inZ (in6, in18 .... in
Calculate several potentials (for several Z).
The name of the potentials and other output-files is taken from the first line of the input-line (the existing - from Z=2 to Z=28 are available)

Challenge: organizing the output data - you can quickly get too many ouput files. Efficient work depends on your organization. For example, copy the commands you have used, and allways delete all the files you do not need.It might be easier to re-compute (using your copied commends) than keeping all the output.

Optional Task 1a

example: construct in47 using the configurations given on the web description
The details of the input file are described in the links

hint: modify in28 to in47 adding the configurations as described in the above link.

```
Note: take care of the variables
 Z,   ncores,    nvales,     ion
 13       4          1         0          for Aluminium
```

Z=13, four filled orbitals, one partially filled orbital, and it is not ionized

Task 1 work 2014

We have combined the **herman3** and **hydrad3** results

Plots Using Matlab and Octave

Plots using SPREADSHEET
(OpenOffice Calc, Apple Mac Numbers, MS Excel)

Plots Using Matlab and Octave

BLUE **SELFCONSISTENT CASE**
RED **HYDROGEN LIKE CASES**

Prepared New INPUT files
in47.txt Silver and **in37.txt** Rubidium

Additional **in36.txt** Krypton

Input file in36   for Krypton

Input file in6 for Carbon

```
carb
    this is a normal carbon
 0,0.001,0.00001,441,1,40,0,0,0,0
 320
 1.00000 .99171 .98318 .97448 .96567 .95680 .94789 .93899 .93012 .92129
  .91254 .89528 .87840 .86196 .84597 .83042 .81531 .80061 .78631 .77239
  .75883 .73273 .70790 .68429 .66187 .64062 .62053 .60155 .58361 .56663
  .55051 .52049 .49296 .46751 .44388 .42191 .40148 .38252 .36492 .34861
  .33350 .30650 .28323 .26306 .24541 .22983 .21594 .20346 .19216 .18188
  .17252 .15627 .14302 .13249 .12426 .11780 .11262 .10829 .10448 .10104
  .09782 .09188 .08645 .08100 .07692 .07692 .07692 .07692 .07692 .07692
  .07692 .07692 .07692 .07692 .07692 .07692 .07692 .07692 .07692 .07692
  .07692 .07692 .07692 .07692 .07692 .07692 .07692 .07692 .07692 .07692
  .07692 .07692 .07692 .07692 .07692 .07692 .07692 .07692 .07692 .07692
  .07692 .07692 .07692 .07692 .07692 .07692 .07692 .07692 .07692 .07692
 6, 2, 1, 0
 100,   2,  -18.0
 200,   2,    -3.0
 210,   2,    -0.3
-1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
```

```
carb-pot.h-s

carb100.h-s
carb200.h-s
carb210.h-s

carbFILE.lst   carb_gnu.cmd
```

Terminal window example

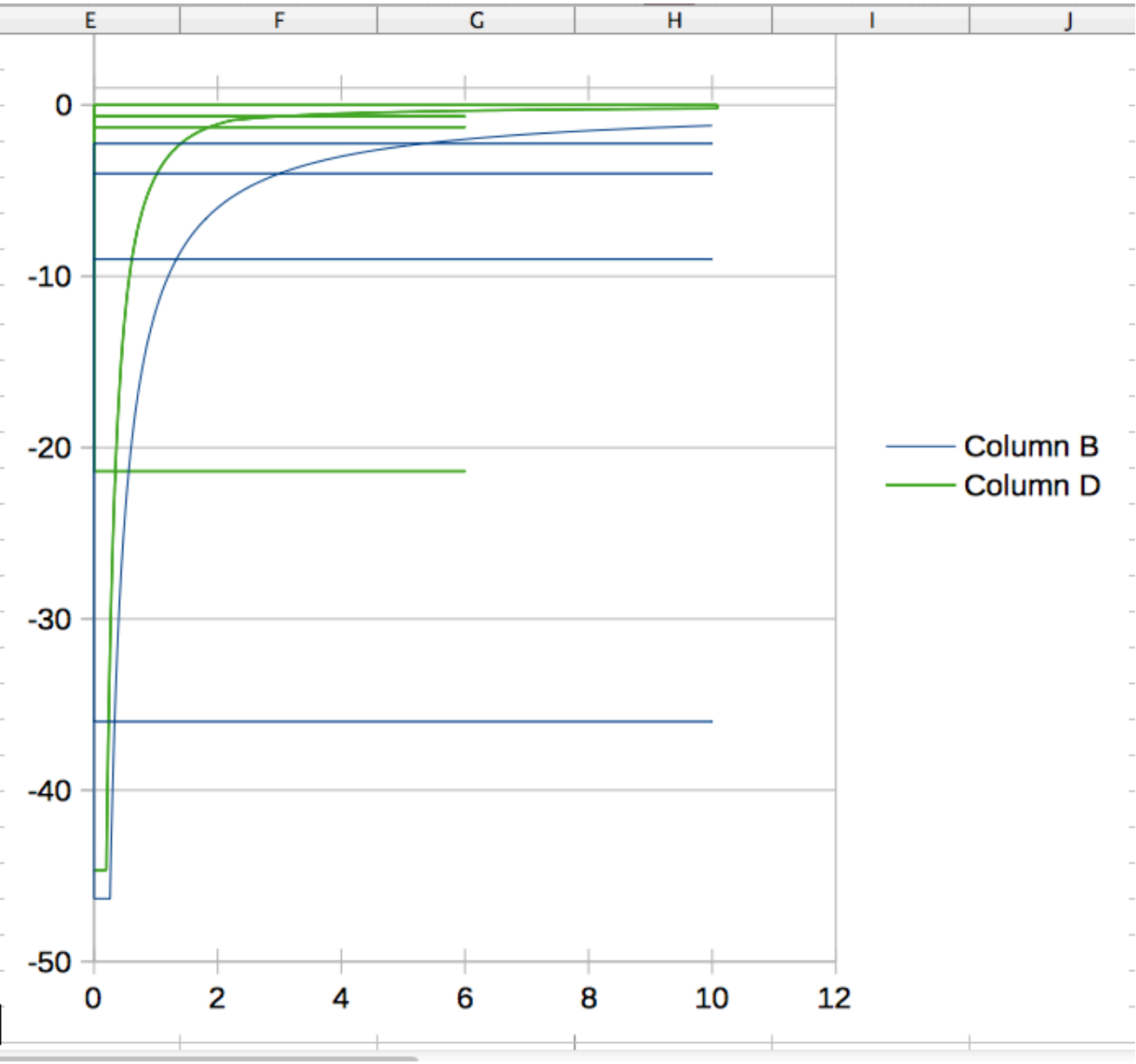
```
./herman3_MAC < in6
 ---------------------------------------
   Herman - Skilman Program - for MATLAB
 ---------------------------------------
     Iter    z              del      i(d)      x(d)    i   cut
      1      6.    2.5551960E+00    184     2.420    203     3.260
      2      6.    7.0718837E-01    268    10.620    238     6.060
      3      6.    2.4311793E-01    232     5.580    226     5.100
      4      6.    9.8627806E-02    225     5.020    222     4.780
      5      6.    2.3582503E-02    322    26.140    220     4.620
      6      6.    1.1793159E-02    322    26.140    220     4.620
      7      6.    1.3670921E-03    166     1.700    220     4.620
      8      6.    5.2976608E-04    166     1.700    220     4.620
  6.   2   1   0
     z  6   1
#  IDENT:  100 E =      -21.379372        0.000000        2.000000
#  IDENT:  200 E =       -1.289404        0.000000        2.000000
#  IDENT:  210 E =       -0.660353        1.000000        2.000000

Finished the loop
```

Terminal window

```
./hydrad3_MAC
# produces hydrogen radial functions
# Give the power of X**ifunc * hydrad(n,l,x)
      for Herman-Skillman Comparison power = 1
1
#  Hydrogenic functions  r** 1 * R(n,l,r) z,
# Give the  Z value of the nucleus
35.7
plot "w35.70hyd10.d" with lines
plot "w35.70hyd20.d" with lines
plot "w35.70hyd21.d" with lines
plot "w35.70hyd30.d" with lines
plot "w35.70hyd31.d" with lines
plot "w35.70hyd32.d" with lines
plot "w35.70hyd40.d" with lines
plot "w35.70hyd41.d" with lines
plot "w35.70hyd42.d" with lines
plot "w35.70hyd43.d" with lines
plot "p35.70pot.hyd" with lines
```

SPREADSHEET Plots Potentials/levels **Z=6 Carbon**

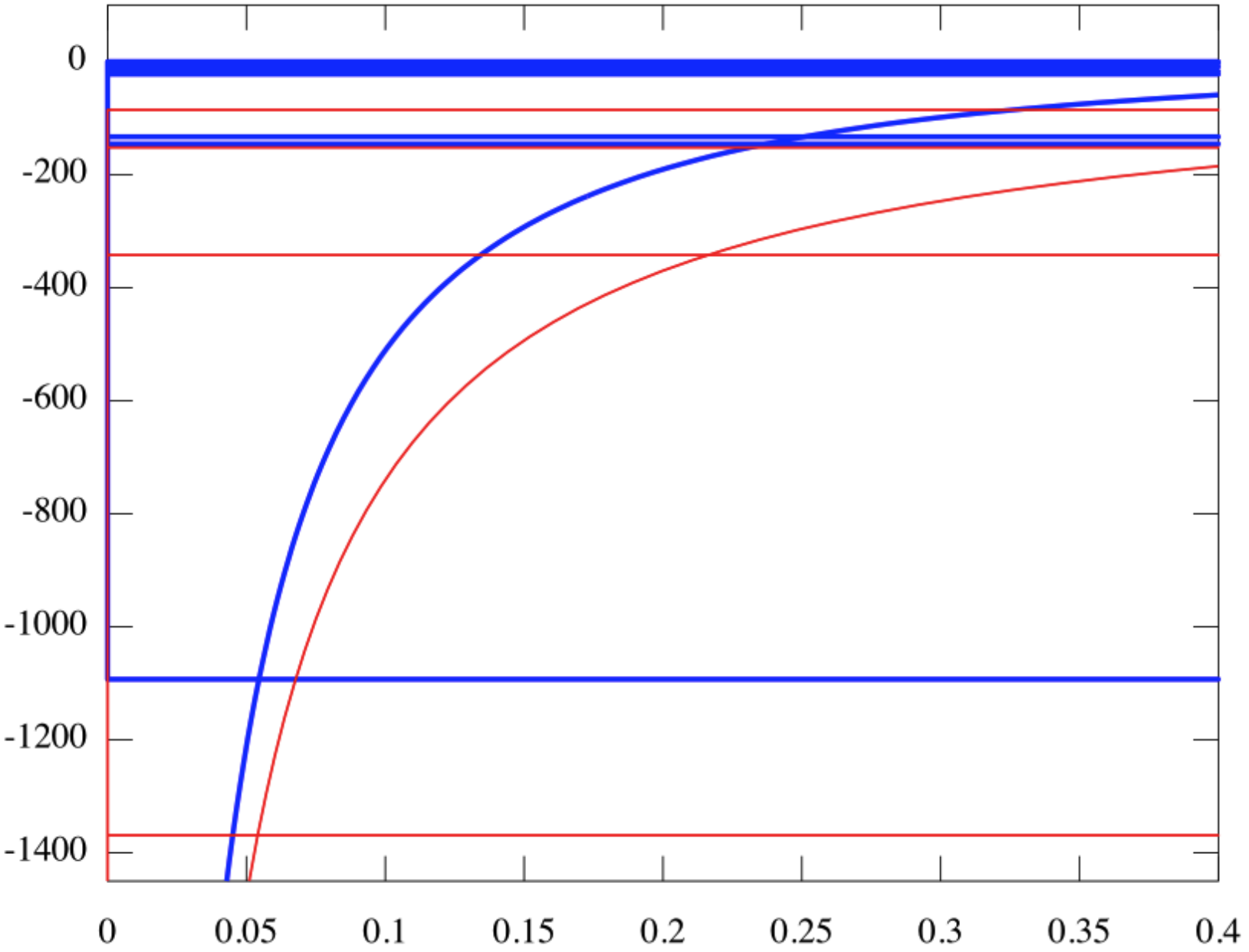
A	B	C	D
0.2993033	-40.09311	0.2777164	-28.965832
0.31032845	-38.668705	0.28258863	-28.288656
0.32175973	-37.29491	0.28746083	-27.635468
0.33361208	-35.96992	0.29233307	-27.00569
0.34590137	-34.69197	0.29720527	-26.398252
0.358643	-33.459457	0.3020775	-25.812168
0.37185398	-32.270733	0.3069497	-25.246315
0.385552	-31.124207	0.31182194	-24.699684
0.3997542	-30.018446	0.31669414	-24.170738
0.41447958	-28.95197	0.32156637	-23.659088
0.42974737	-27.923382	0.32643858	-23.163607
0.44557756	-26.931337	0.3313108	-22.683949
0.4619913	-25.974514	0.336183	-22.219412
0.47900927	-25.051706	0.3410552	-21.769339
0.49665406	-24.161688	0.35079965	-20.910383
0.5149493	-23.303265	0.3605441	-20.10229
0.533918	-22.47536	0.37028852	-19.34079
0.55358547	-21.67687	0.38003296	-18.622267
0.57397735	-20.906748	0.3897774	-17.943478
0.59512043	-20.163986	0.39952183	-17.301506
0.6170429	-19.447594	0.40926626	-16.69374
0.63977236	-18.756672	0.4190107	-16.117846
0.663339	-18.090298	0.42875513	-15.571714
0.6877745	-17.44758	0.43849957	-15.053406
0.7131094	-16.827713	0.448244	-14.5611515
0.7393775	-16.22987	0.45798844	-14.0933275
0.76661325	-15.653265	0.46773288	-13.648444
0.79485226	-15.097145	0.47747728	-13.225122



Plots Octave Potentials/levels Z=36 Krypton

BLUE SELFCONSISTENT CASE

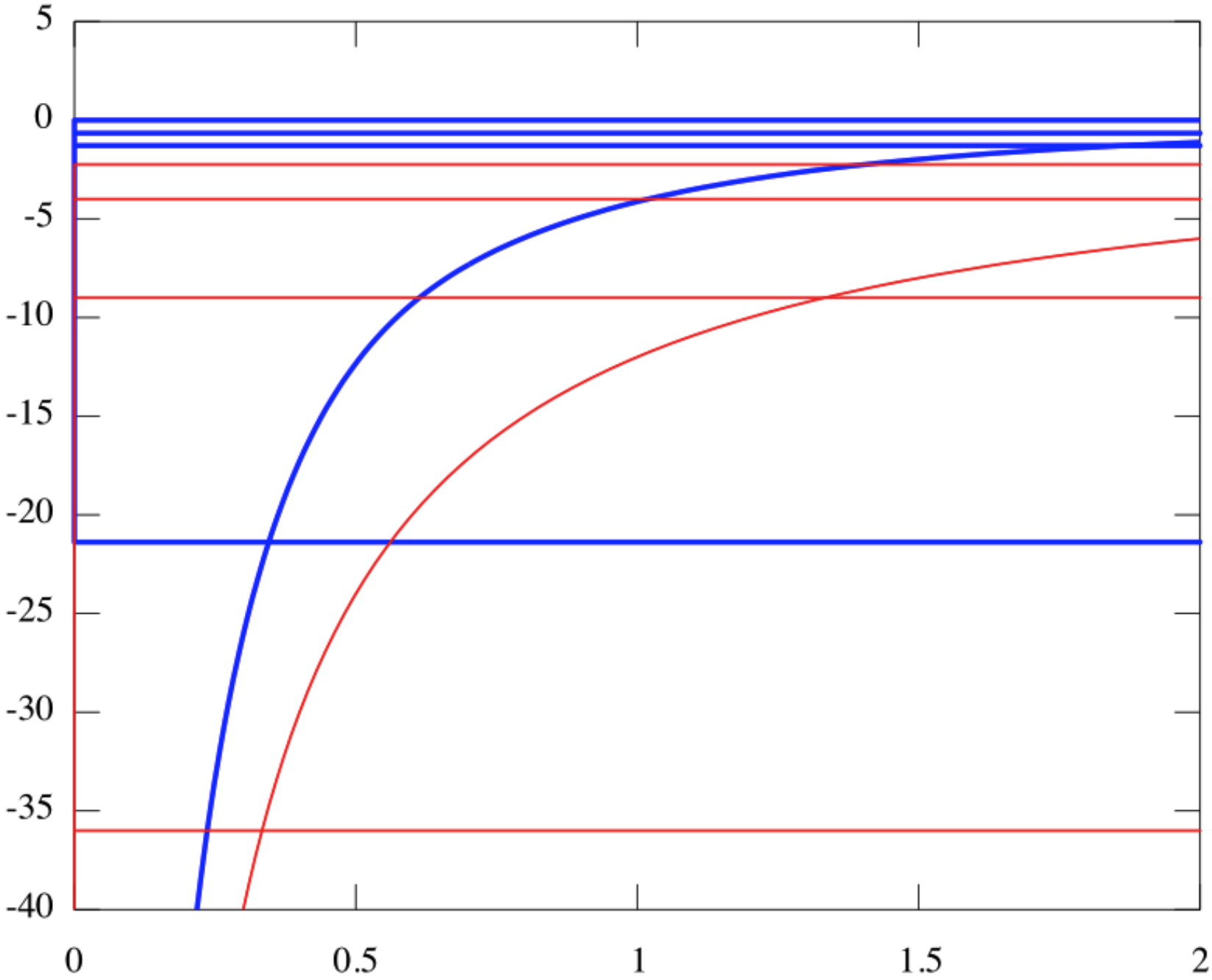
RED HYDROGEN LIKE CASES



Plots Octave Potentials/levels Z=6 Carbon

BLUE SELFCONSISTENT CASE

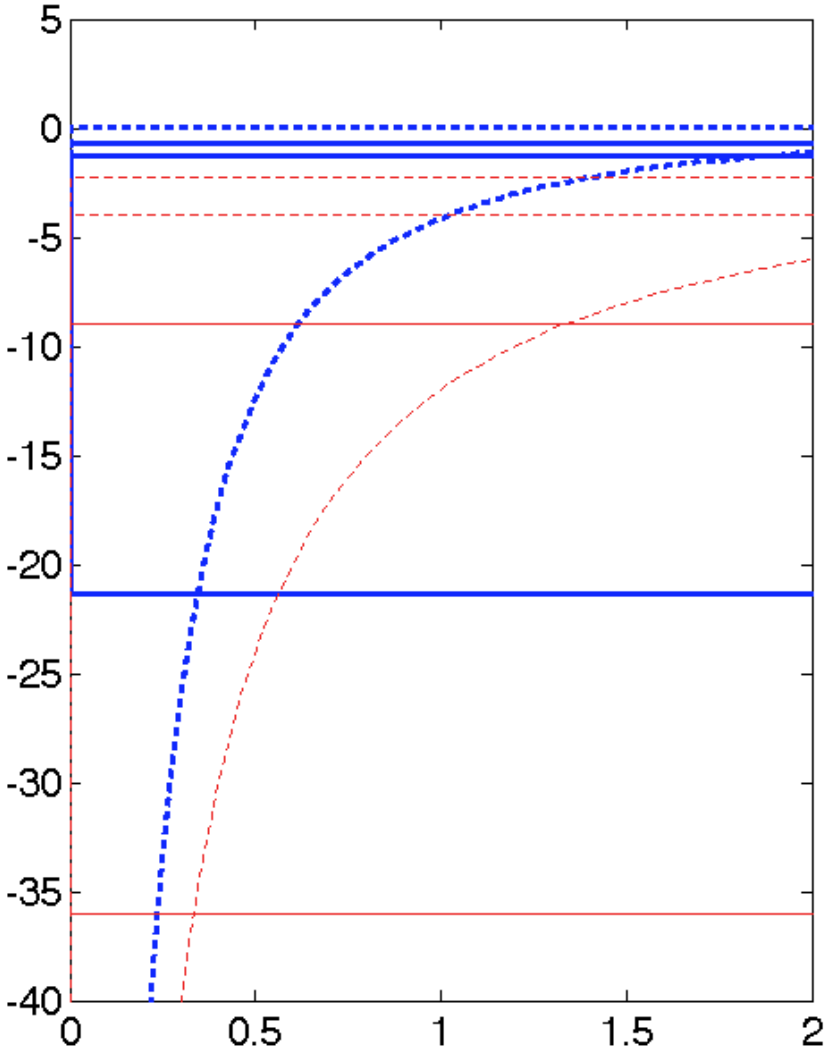
RED HYDROGEN LIKE CASES

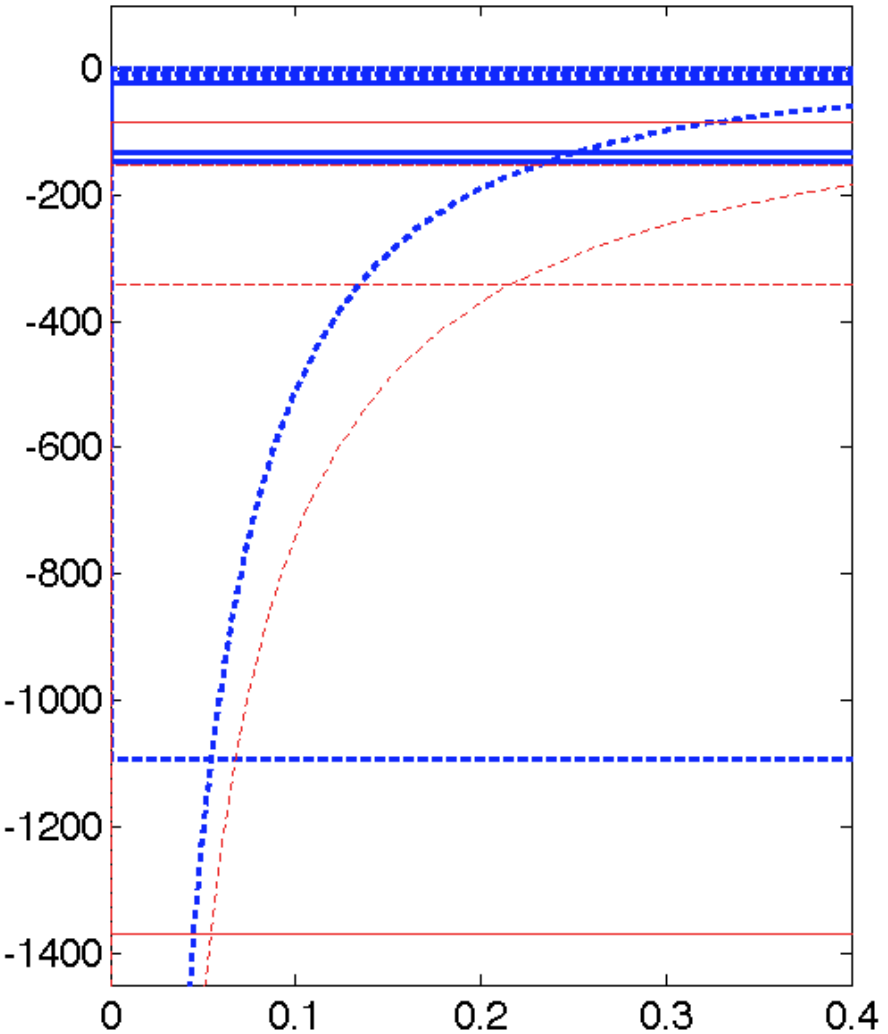


Plots Octave Potentials/levels
Z=6 Carbon and Z=36 Krypton

BLUE SELFCONSISTENT CASE

RED HYDROGEN LIKE CASES





Task 2
Find the alpha range parameter for different Z by studying the potentials output
example: `Alum-pot.h-s`

Method: for example EXCEL, OpenOffice-CALC or MATLAB

Plotting the potential is not too interesting. Instead, we start by
producing `-r*V(r)` - it should go from `Z` for small r to `1` for large r

Try to fit this by `Z_eff(r) = (Z-1)*exp(-r/potrange) + 1`

How would you do this efficiently?
Describe your method in the report ....

Compare the `potrange` values for the different Z

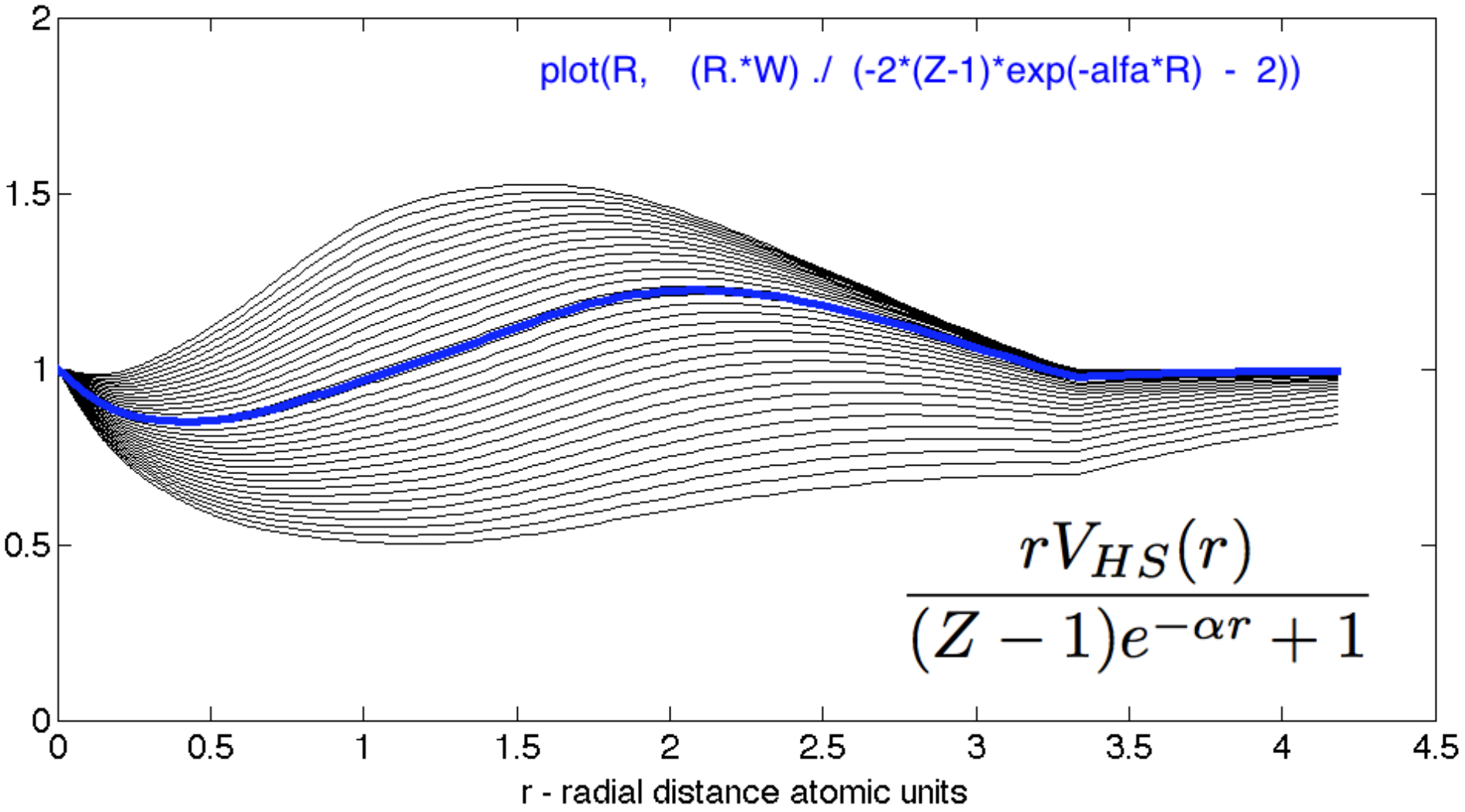
Task 2a
Model for Z-dependence of `potrange`
(`or` alpha in our lecture notes)

```
load pot1.txt
r=pot1(:,1); V=pot1(:,2);
plot(r,r.*V)
Z=13;  alfa=2;

plot(r,r.*V,'-k',r,-2*(Z-1)*exp(-alfa*r)-2,'b-');
set(gca,'xlim',[0 10])
r(100)  ,  r(300)      %%%  Testing r-values
R=r(1:270);  W=V(1:270);
plot(R,(R.*W)./(-2*(Z-1)*exp(-alfa*R)-2),'k-')

for alfa=1.0:0.005:3.3;
      alfa,
      plot(R,(R.*W)./(-2*(Z-1)*exp(-alfa*R)-2),'k-');
      set(gca,'ylim',[0 2]);
      pause;
end
```

$$V_{HS}(r) \longrightarrow \frac{(Z-1)}{r}e^{-\alpha r} + \frac{1}{r}$$

Because Rydberg energy unit FACTOR 2
(-2*(Z-1)*exp(-alfa*R)-2)

```
for alfa=1.0:0.05:3.3;alfa,
plot(R,(R.*W)./(-2*(Z-1)*exp(-alfa*R)-2),'k-');
hold on;set(gca,'ylim',[0 2]);pause;end
alfa=1.875000
plot(R,(R.*W)./(-2*(Z-1)*exp(-alfa*R)-2),'b-','linewidth',4)
set(gcf,'color','white');   set(gca,'fontsize',18)
```



```
load pot1.txt
r=pot1(:,1); V=pot1(:,2);
plot(r,r.*V)
Z=13;  alfa=2;
R=r(1:270);  W=V(1:270);

comp=(R.*W)./(-2*(Z-1)*exp(-alfa*R)-2);   %%  compares data / model
oness=comp*0+1;

sum(comp)                                 %%  just test
sum(oness)                                %%  gives the length
VAL=sum((comp-oness).^2)/sum(oness)    %%  average value

%%%   For manual detection of the minimum
for alfa=1.0:0.005:3.3;
     comp=(R.*W)./(-2*(Z-1)*exp(-alfa*R)-2);
     VAL=sum((comp-oness).^2)/sum(oness);
     fprintf(' %f    %f  \n',alfa,VAL);
end

%%%   For automatic detection   of the minimum
alfav=1.0:0.005:3.3;   VALv=alfav*0+1; NN=sum(VALv);
for N=1:NN;
    comp=(R.*W)./(-2*(Z-1)*exp(-alfav(N)*R)-2);
    VALv(N)=sum((comp-oness).^2)/sum(oness);
end
```

Task 3

Using the provided files
`in193d` and `in194s`
(i.e. in19 for the 19th electron in 3d or in 4s)
convince yourself from the output energies that
indeed, the 4s has lower energy

Copy the output of the two runs into your report and discuss the results

Optional: Show the same situation for the next alcalic metal, including the filling
of 5s before filling 4d.
For this you must study the Periodic table with configurations
and extend the input files considerably (as in the **optional task 1a** above)

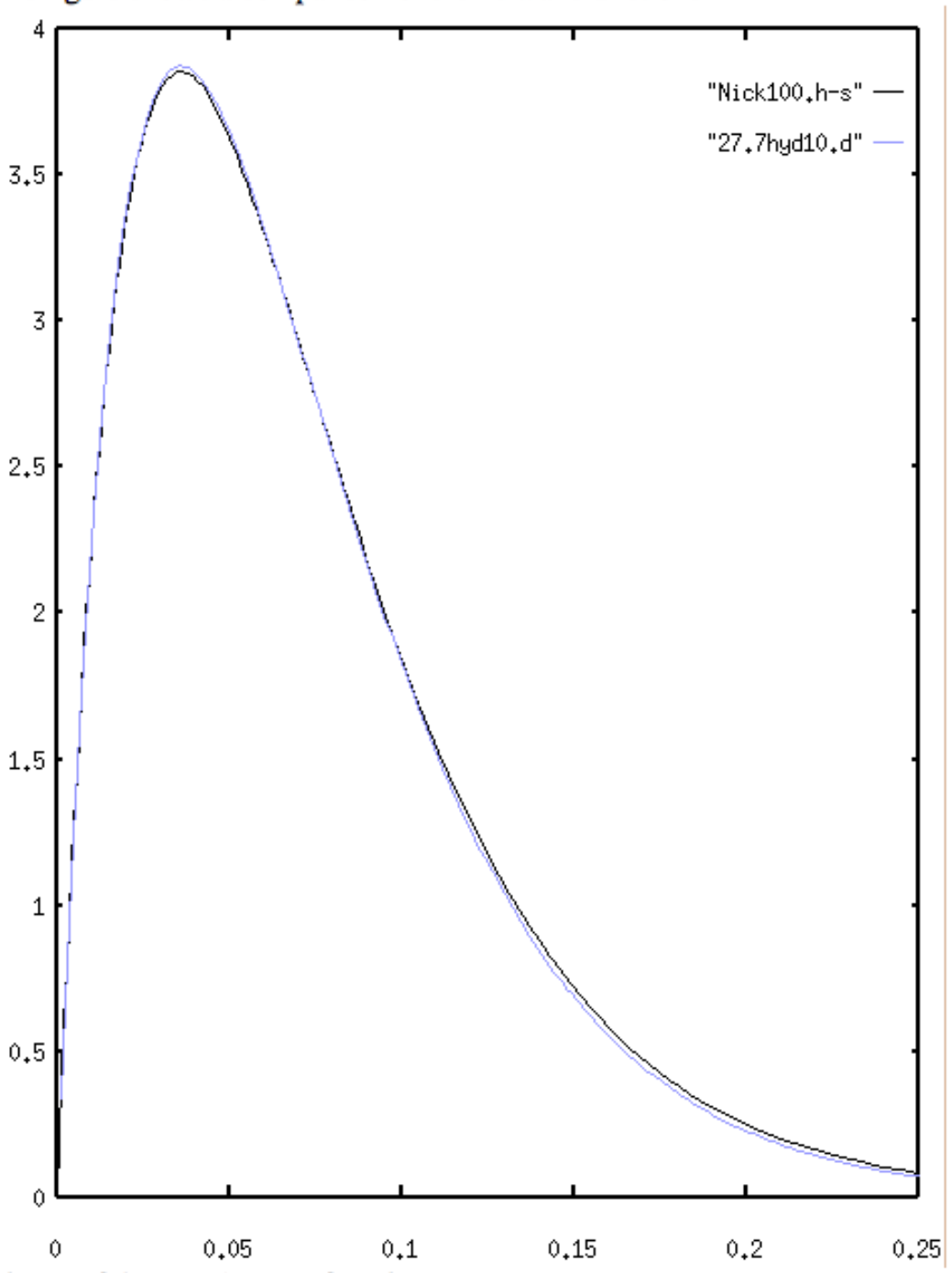
Optional Task 4
Follow the instructions at http://web.ift.uib.no/AMOS/Hartree/
and perform a study of radial wavefunctions,
comparing the hydrogen-like with the output in files of the type.

This is best done in MATLAB or OCTAVE, but it can also be done using a spreadsheet program, like in the tasks above.

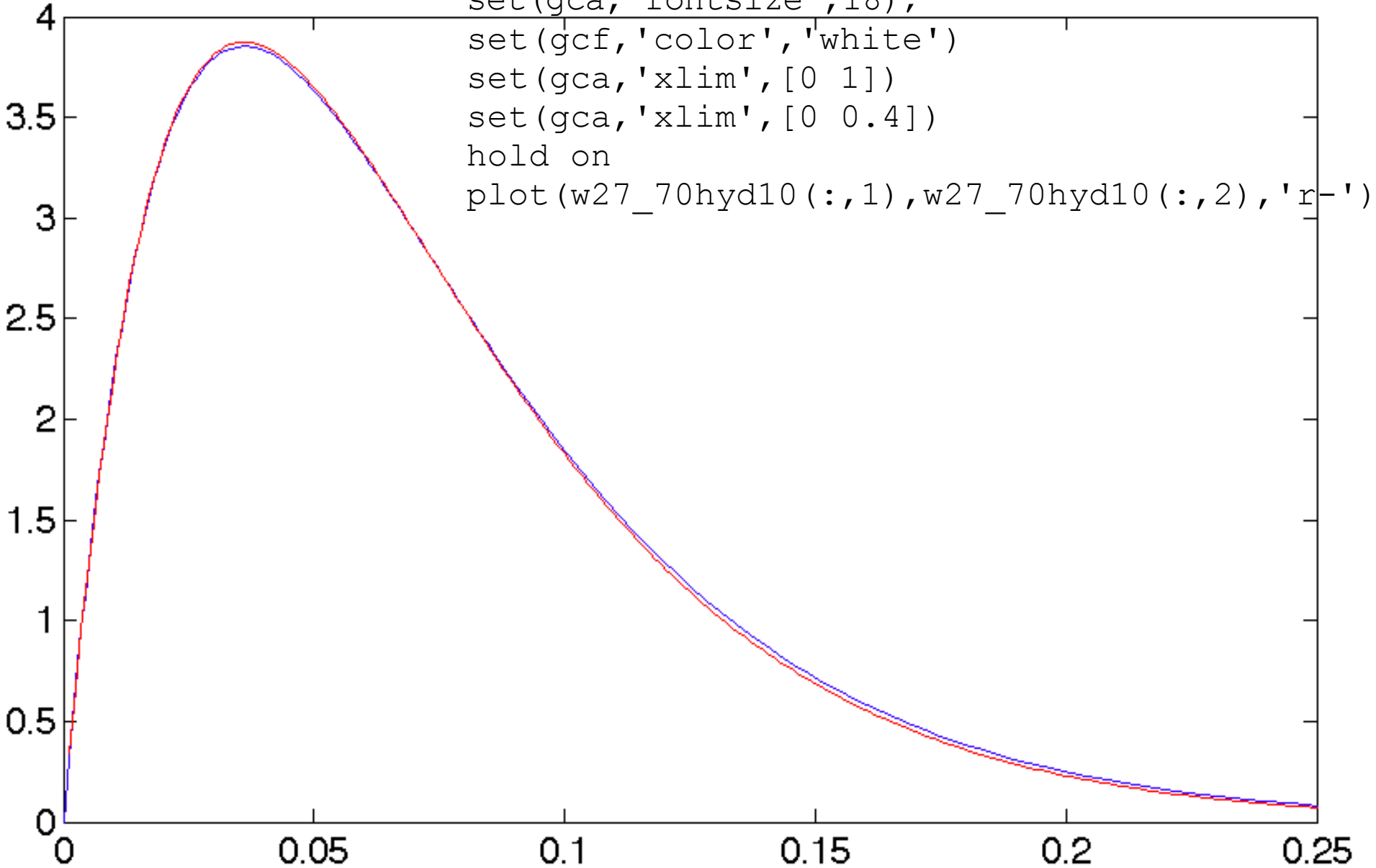
This requires also to run the other program for hydrogenic functions, radhyd3.exe
This asks for parameter 1 (enter 1) and then parameter Z
It produces many data files (listed in the commands)

Figure of the two 1s wavefunctions for Ni

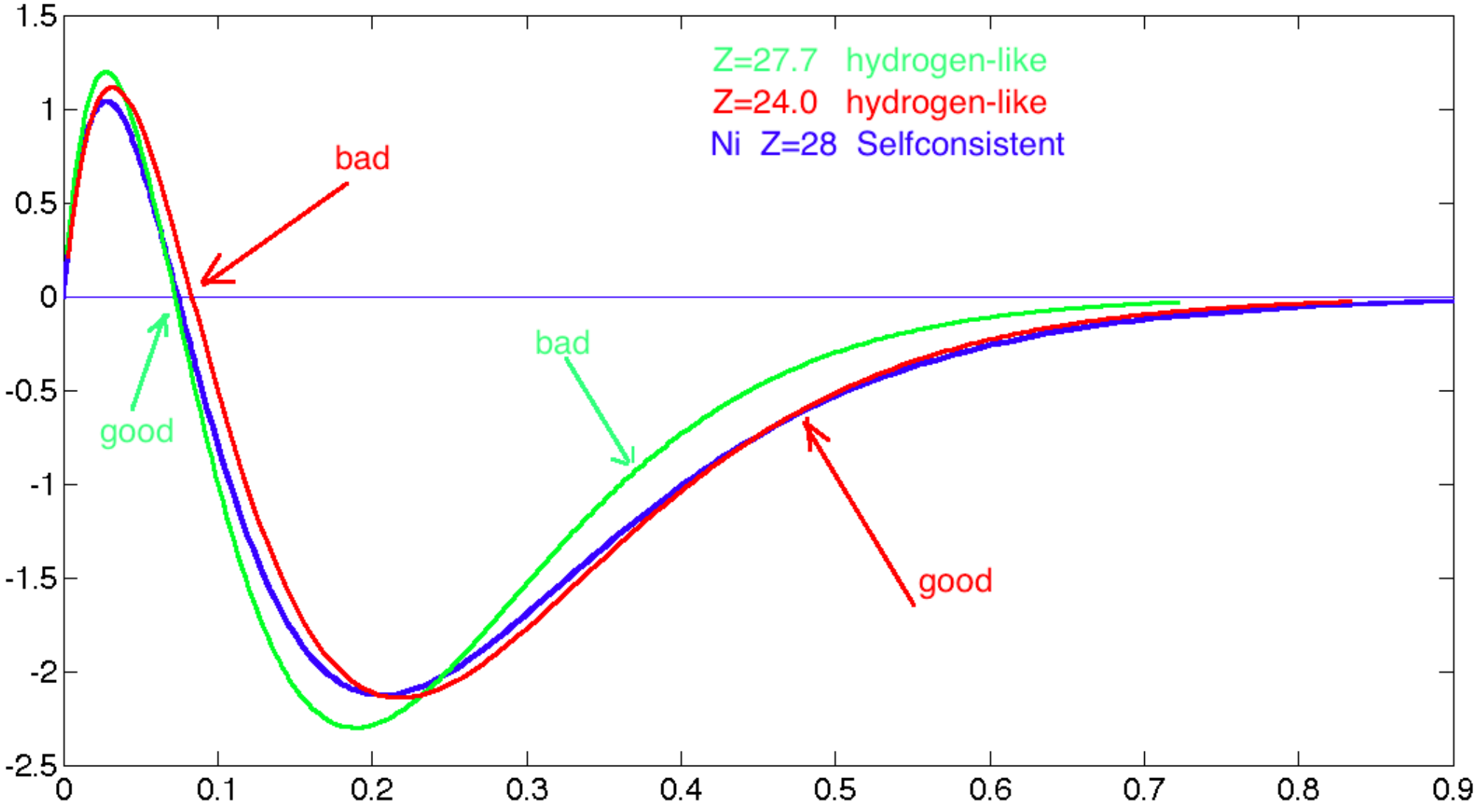
The figure shows a comparison of the 1s wavefunctions

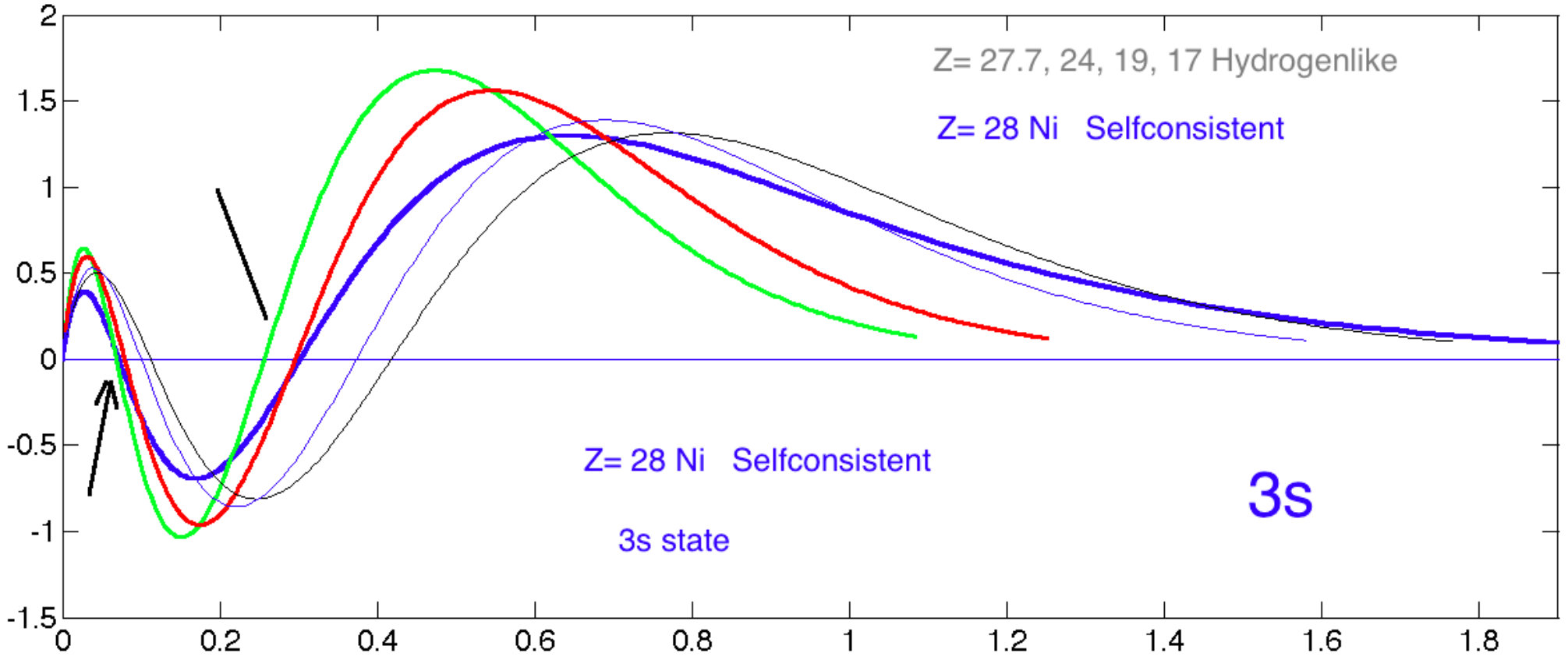


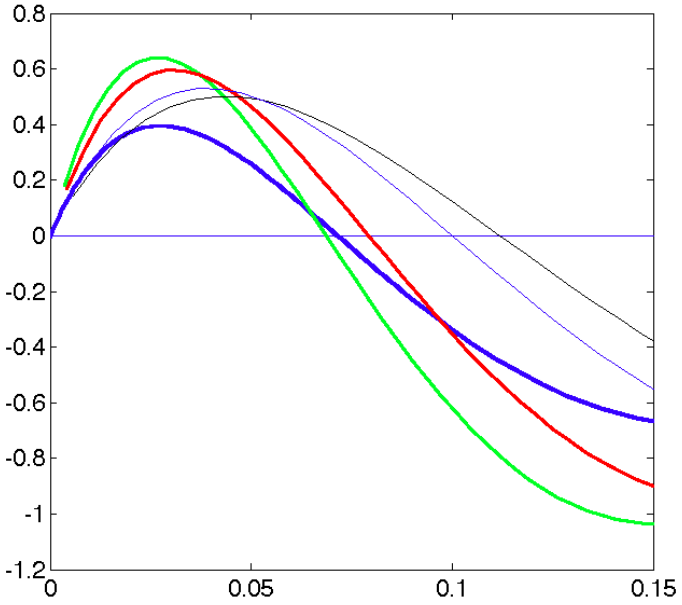
```
load 'z28n100.h-s'
load 'w27.70hyd10.d'
plot(z28n100(:,1),z28n100(:,2))
set(gca,'fontsize',18);
set(gcf,'color','white')
set(gca,'xlim',[0 1])
set(gca,'xlim',[0 0.4])
hold on
plot(w27_70hyd10(:,1),w27_70hyd10(:,2),'r-')
```

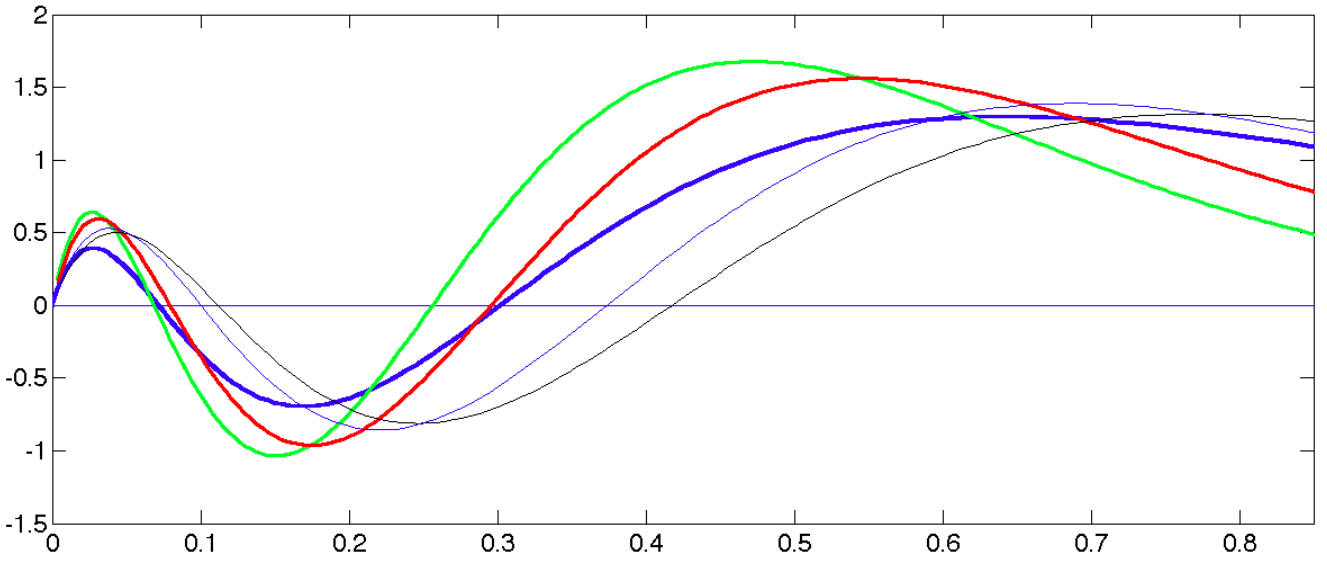


```
load 'z28n210.h-s';     load 'w27.70hyd20.d';  load 'w24.00hyd20.d';
figure(2)
set(gca,'fontsize',18);   set(gcf,'color','white')
plot(z28n200(:,1),z28n200(:,2),'b-','linewidth',3)
set(gca,'xlim',[0 0.9])
hold on
plot([0 5],[0 0])     %   Draw x-axis at 0
plot(w27_70hyd20(:,1),w27_70hyd20(:,2),'g-','linewidth',2)
plot(w24_00hyd20(:,1),w24_00hyd20(:,2),'r-','linewidth',2)
```




Z= 27.7, 24, 19, 17 Hydrogenlike
Z= 28 Ni Selfconsistent
Z= 28 Ni Selfconsistent
3s state
3s





MATLAB COMMANDS STORAGE – for 2015

```
figure(1)
load 'z28n100.h-s';    load 'w27.70hyd10.d'
plot(z28n100(:,1),z28n100(:,2))
set(gca,'fontsize',18);   set(gcf,'color','white')
set(gca,'xlim',[0 1])
set(gca,'xlim',[0 0.4])
hold on
plot(w27_70hyd10(:,1),w27_70hyd10(:,2),'r-')


load 'z28n210.h-s';    load 'w27.70hyd20.d';  load
'w24.00hyd20.d';
figure(2)
set(gca,'fontsize',18);   set(gcf,'color','white')
plot(z28n200(:,1),z28n200(:,2),'b-','linewidth',3)
set(gca,'xlim',[0 0.9])
hold on
plot([0 5],[0 0])    %   Draw x-axis at 0
plot(w27_70hyd20(:,1),w27_70hyd20(:,2),'g-','linewidth',2)
plot(w24_00hyd20(:,1),w24_00hyd20(:,2),'r-','linewidth',2)
```