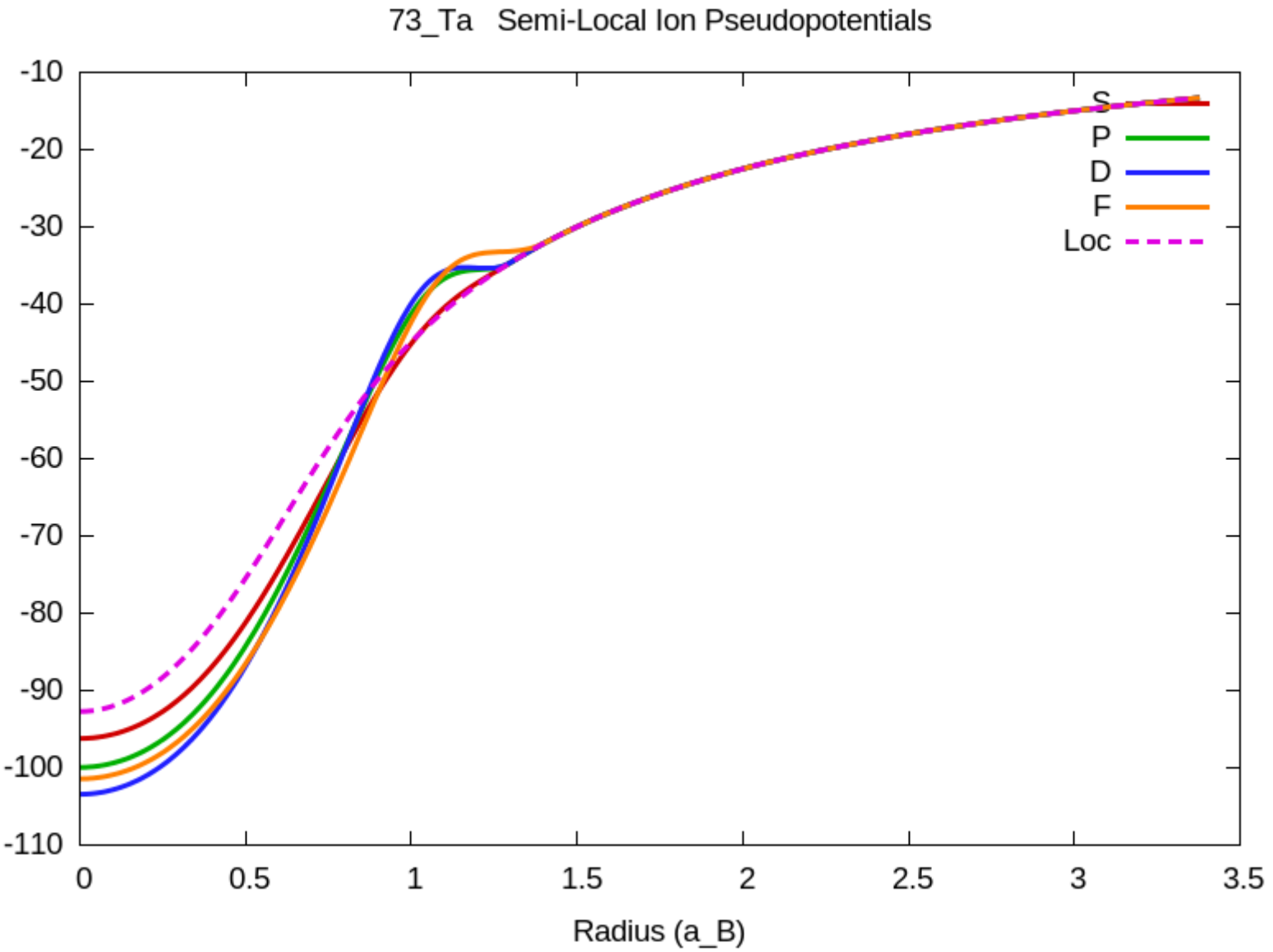
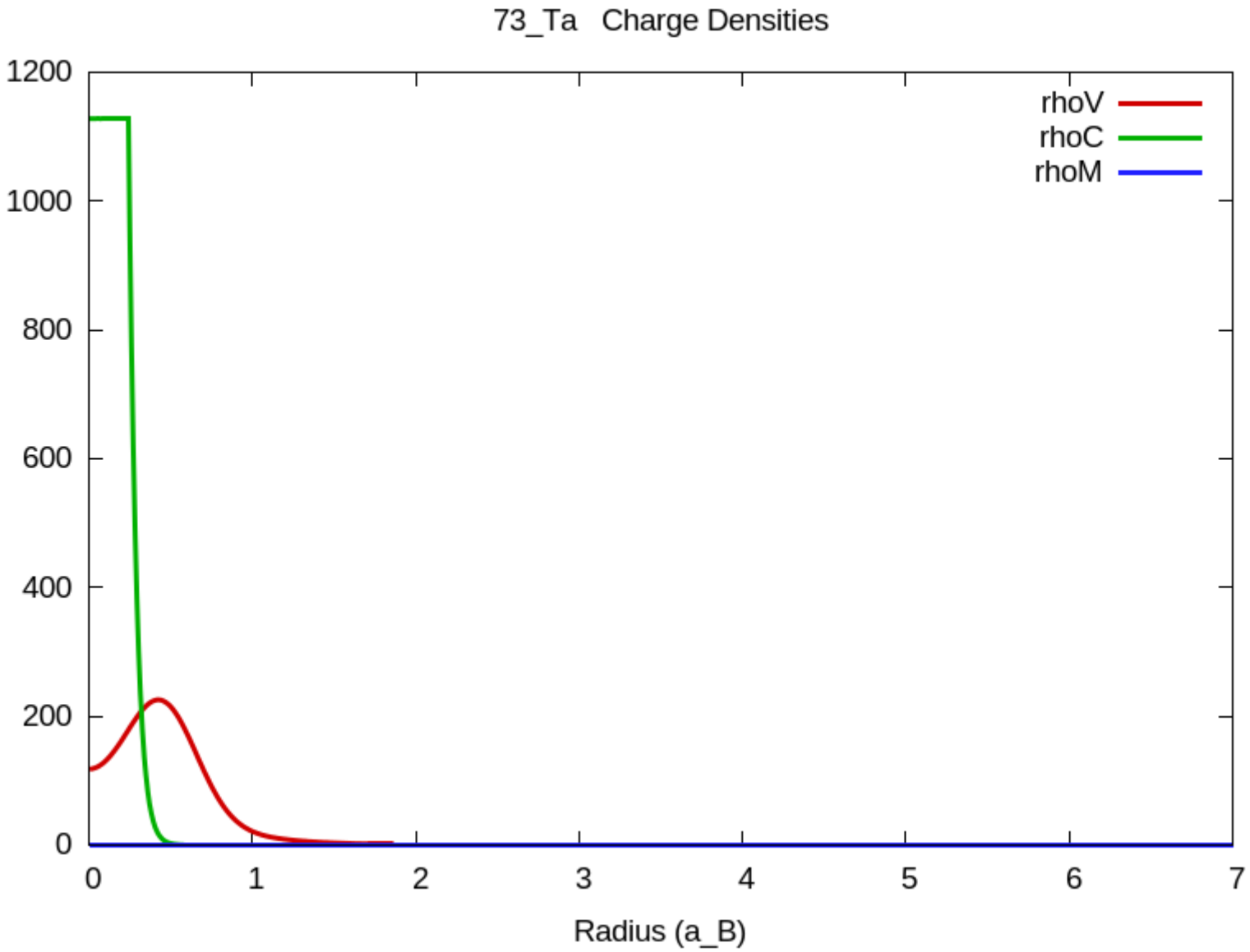
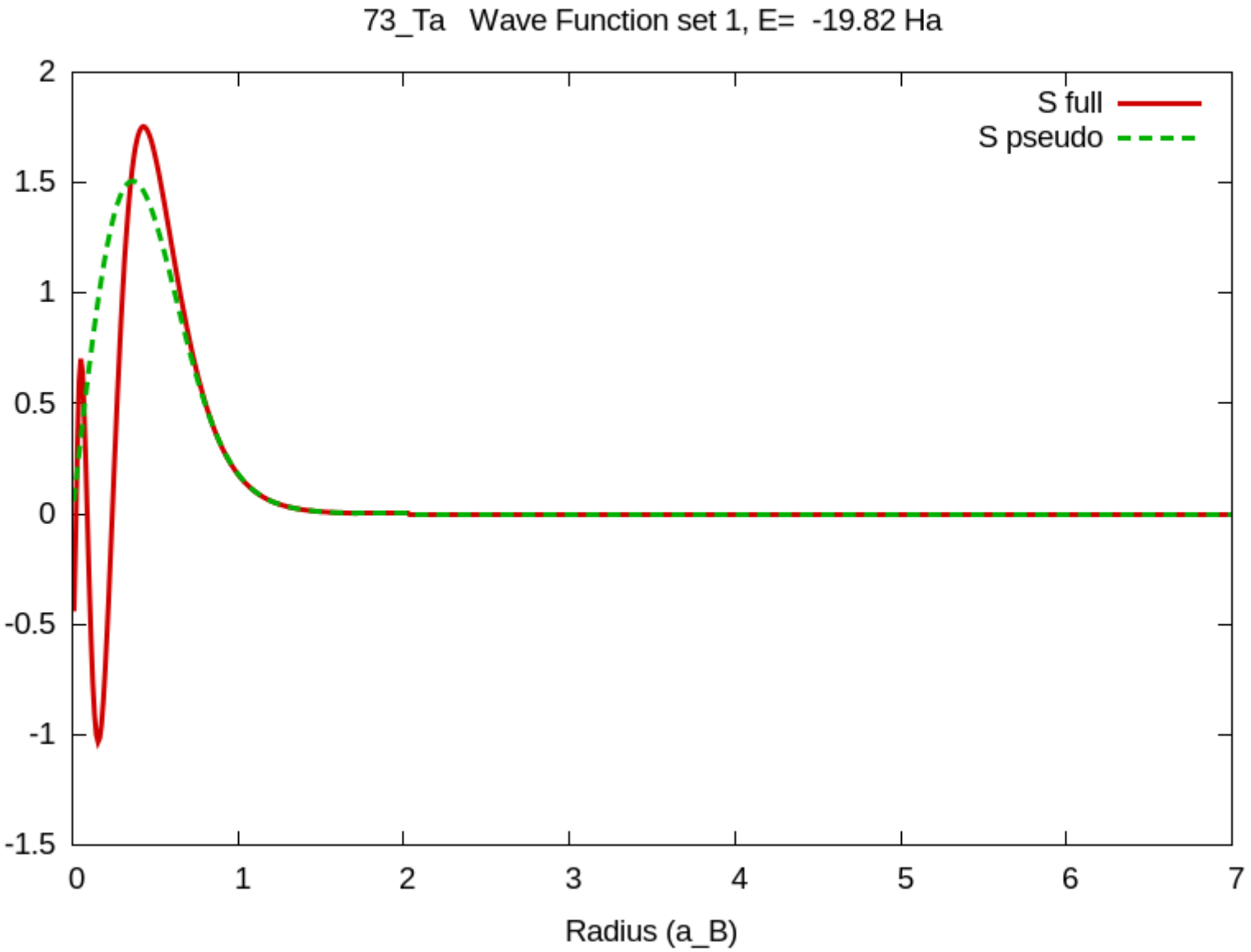
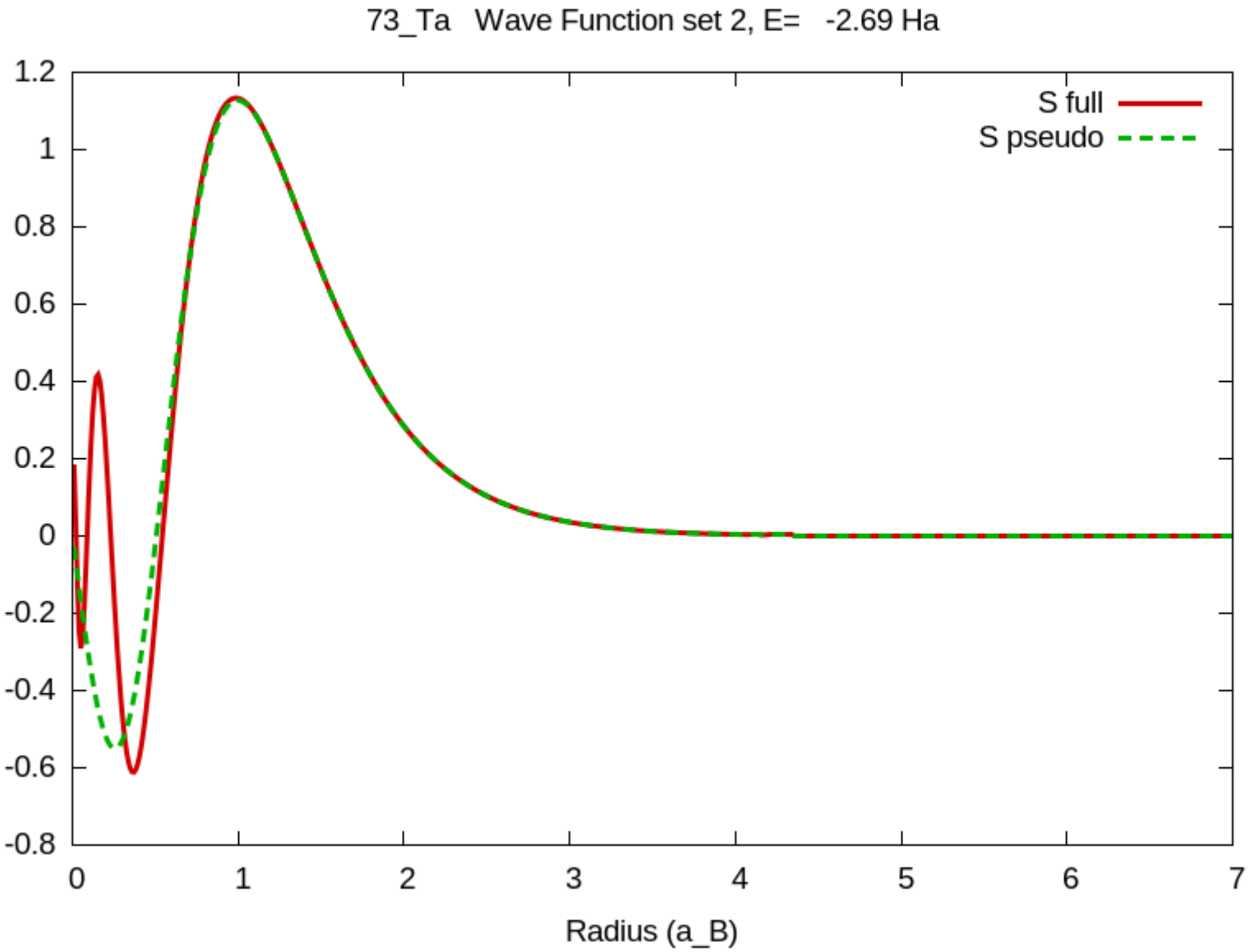
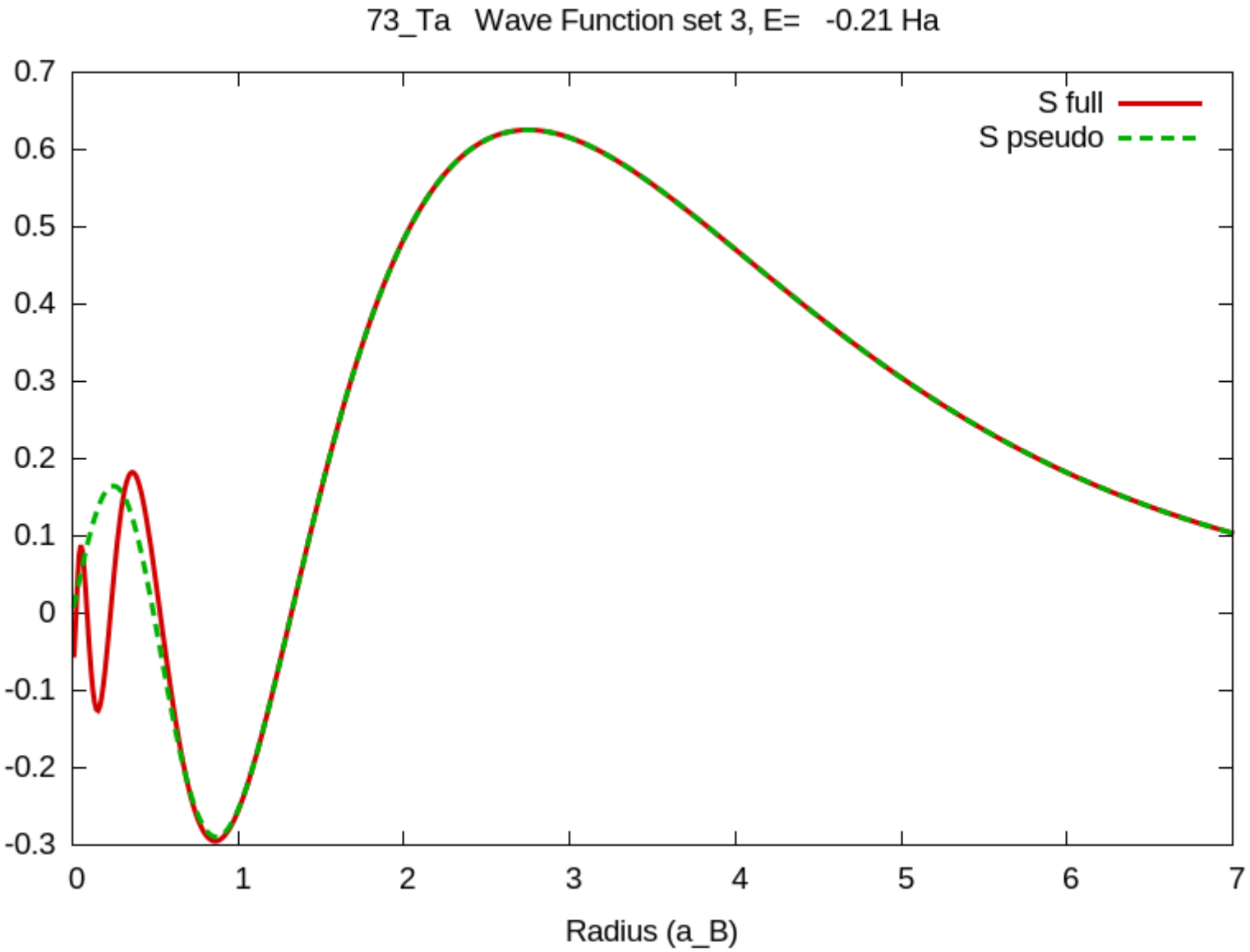
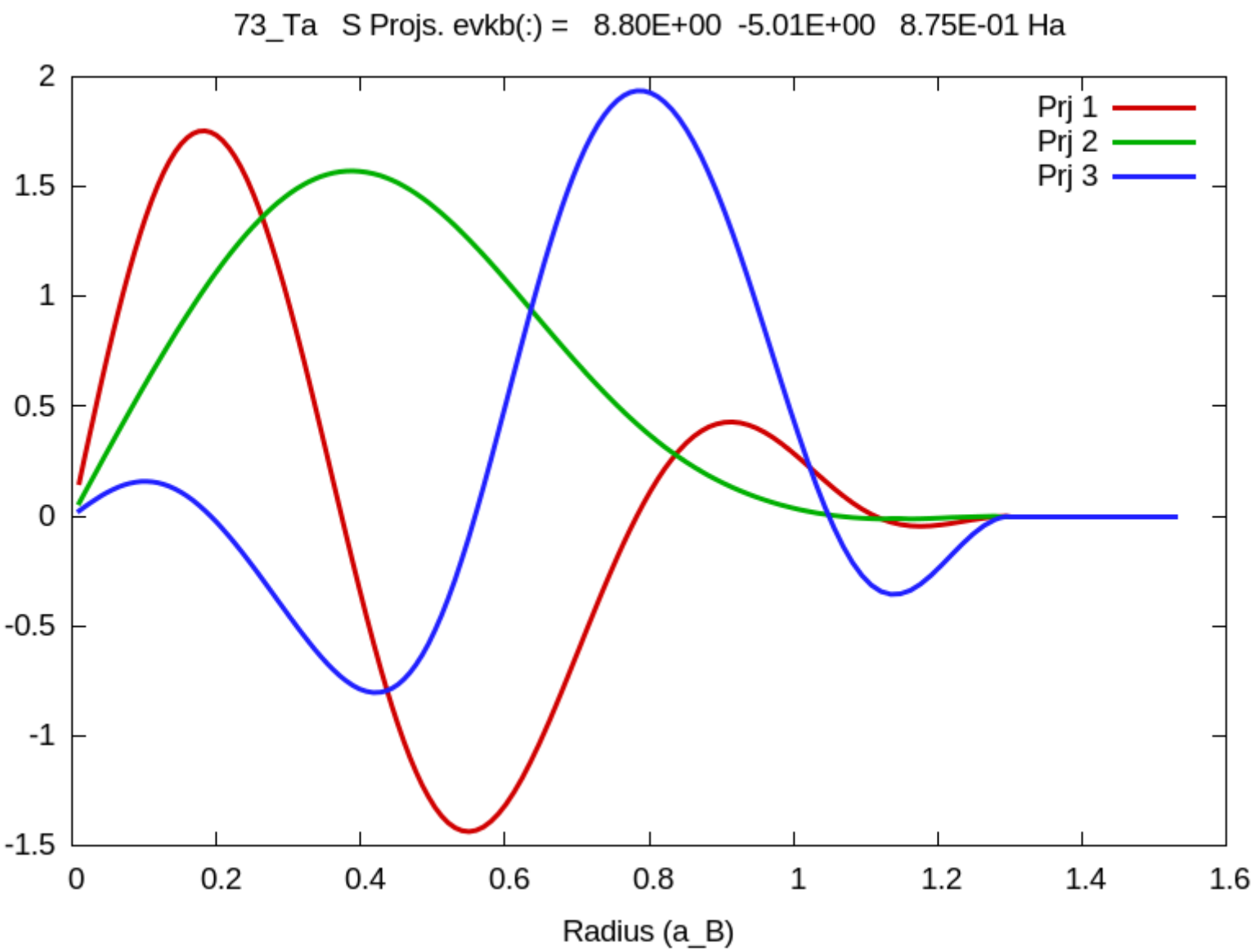

73_Ta Semi-Local Ion Pseudopotentials
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
0
0.5
1
1.5
2
2.5
3
3.5
Radius (a_B)
S
P
D
F
Loc

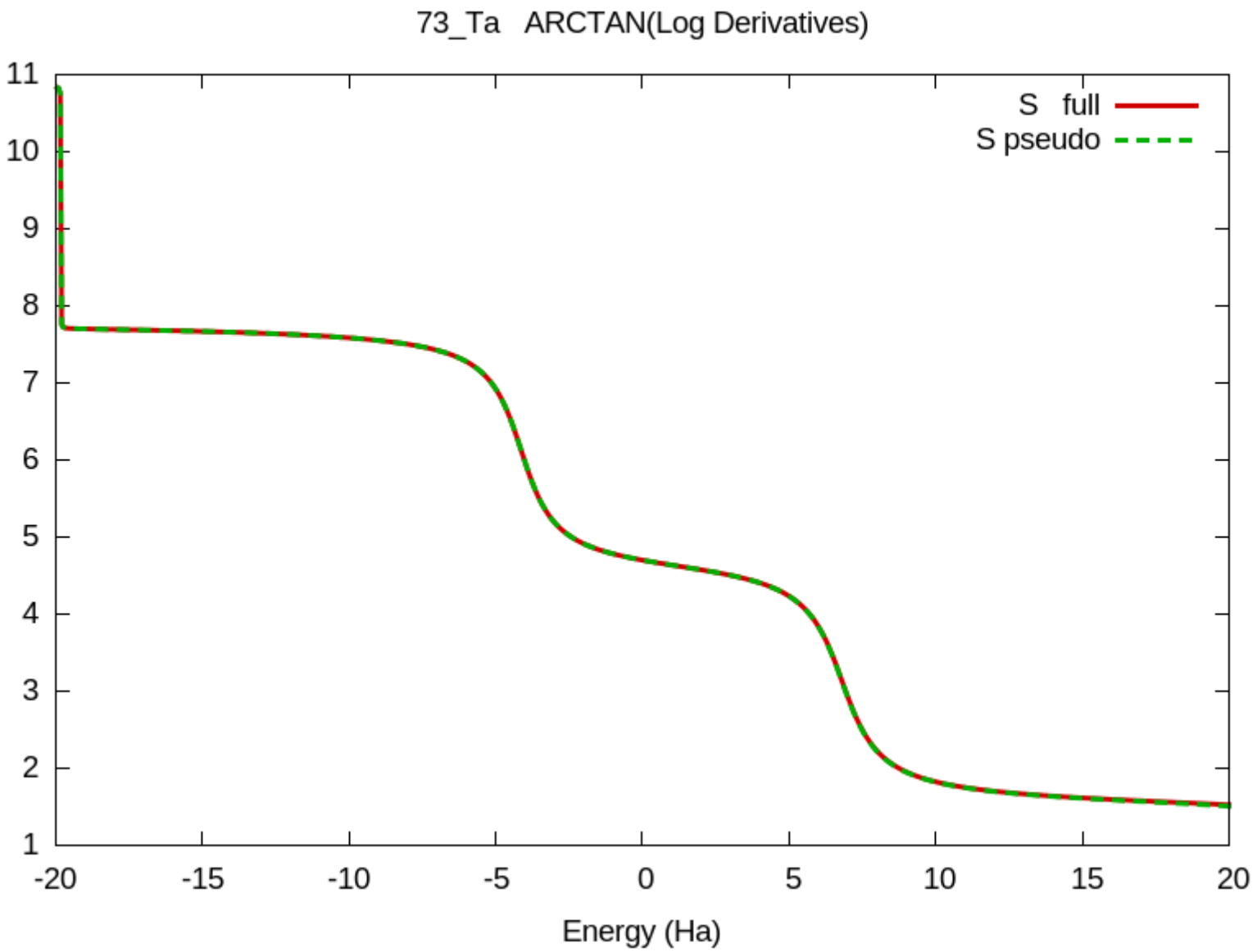

73_Ta Charge Densities
rhoV
rhoC
rhoM
1200
1000
800
600
400
200
0
0
1
2
3
4
5
6
7
Radius (a_B)

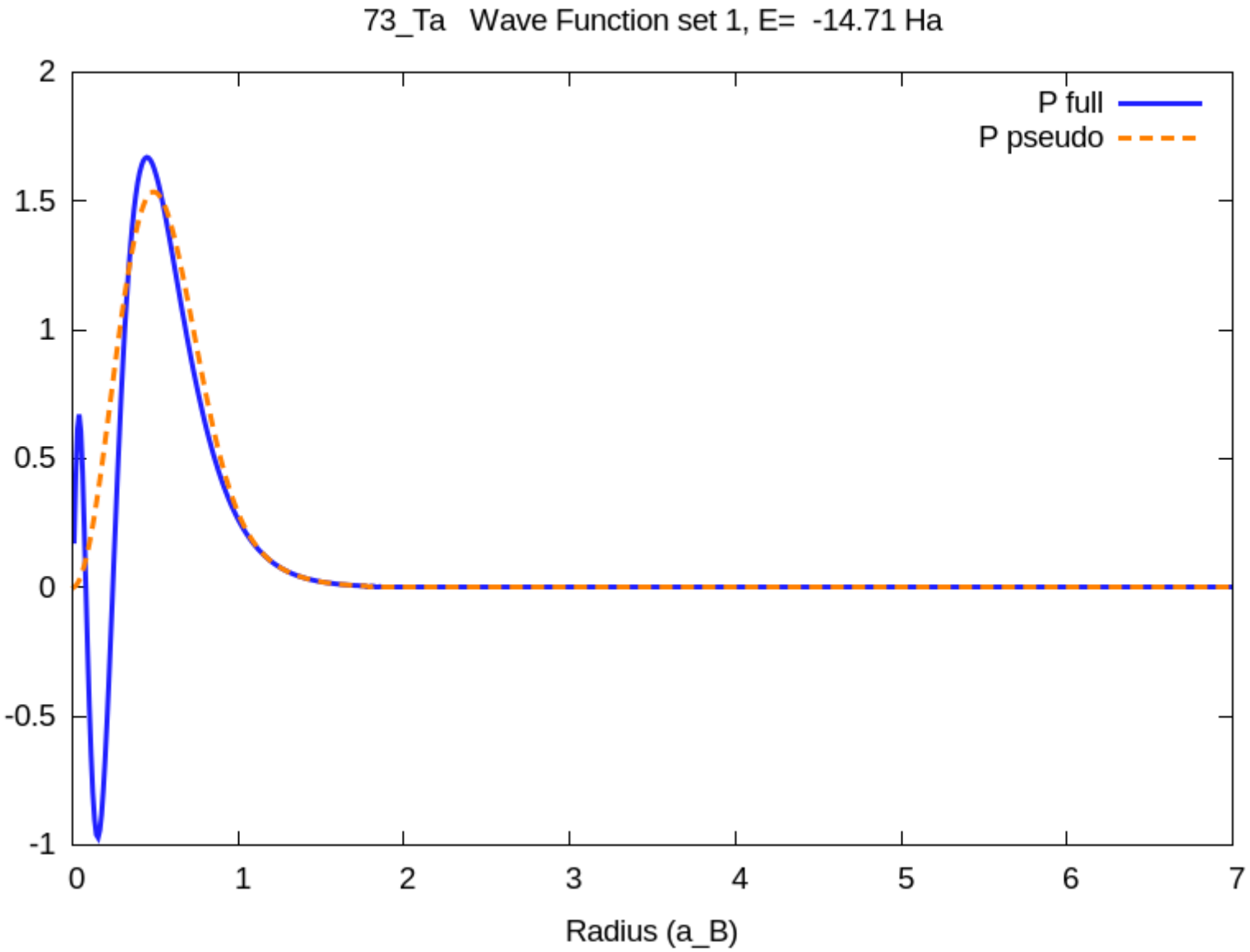

73_Ta Wave Function set 1, E= -19.82 Ha
S full
S pseudo
2
1.5
1
0.5
0
-0.5
-1
-1.5
0
1
2
3
4
5
6
7
Radius (a_B)

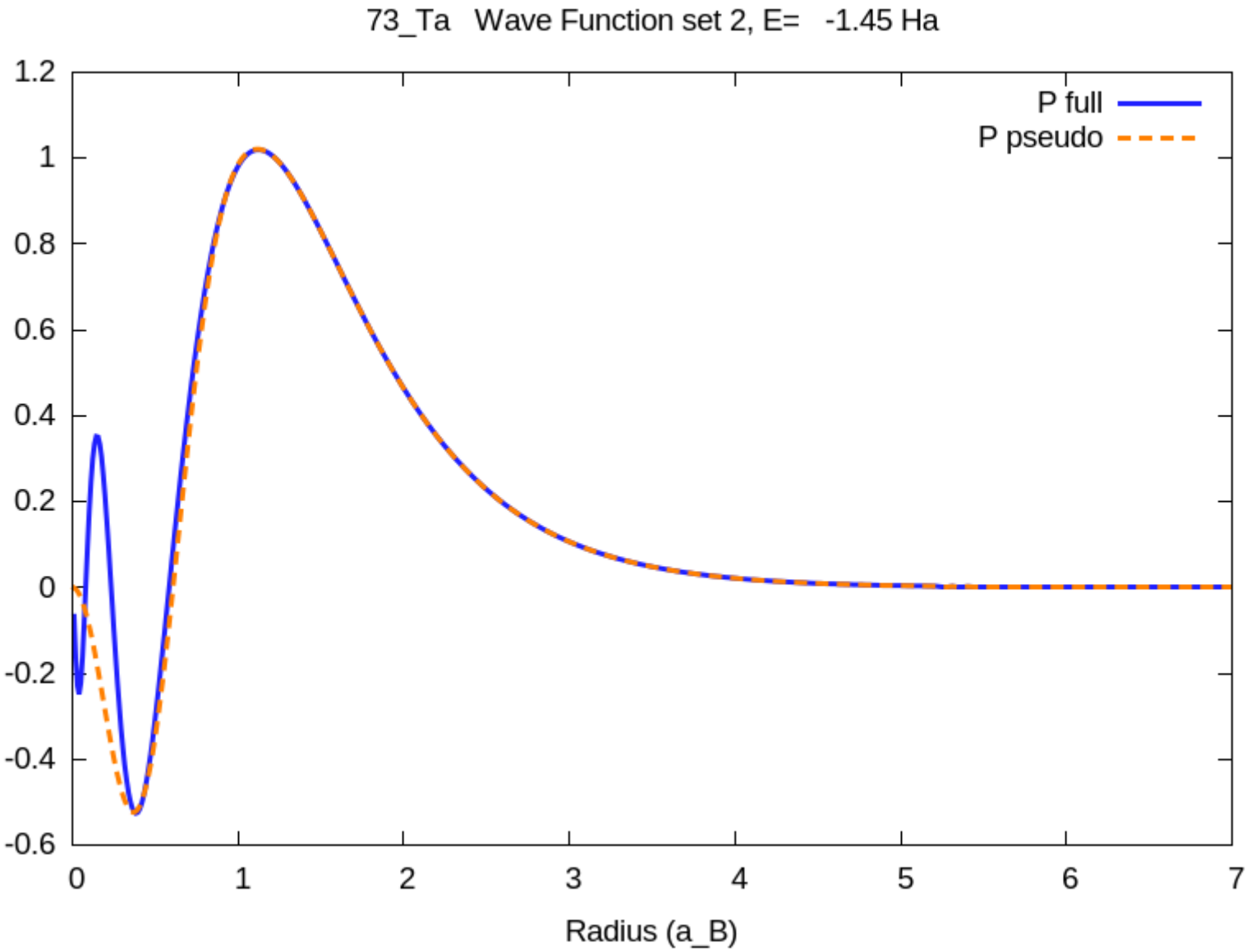

73_Ta Wave Function set 2, E= -2.69 Ha
S full
S pseudo
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
0
1
2
3
4
5
6
7
Radius (a_B)

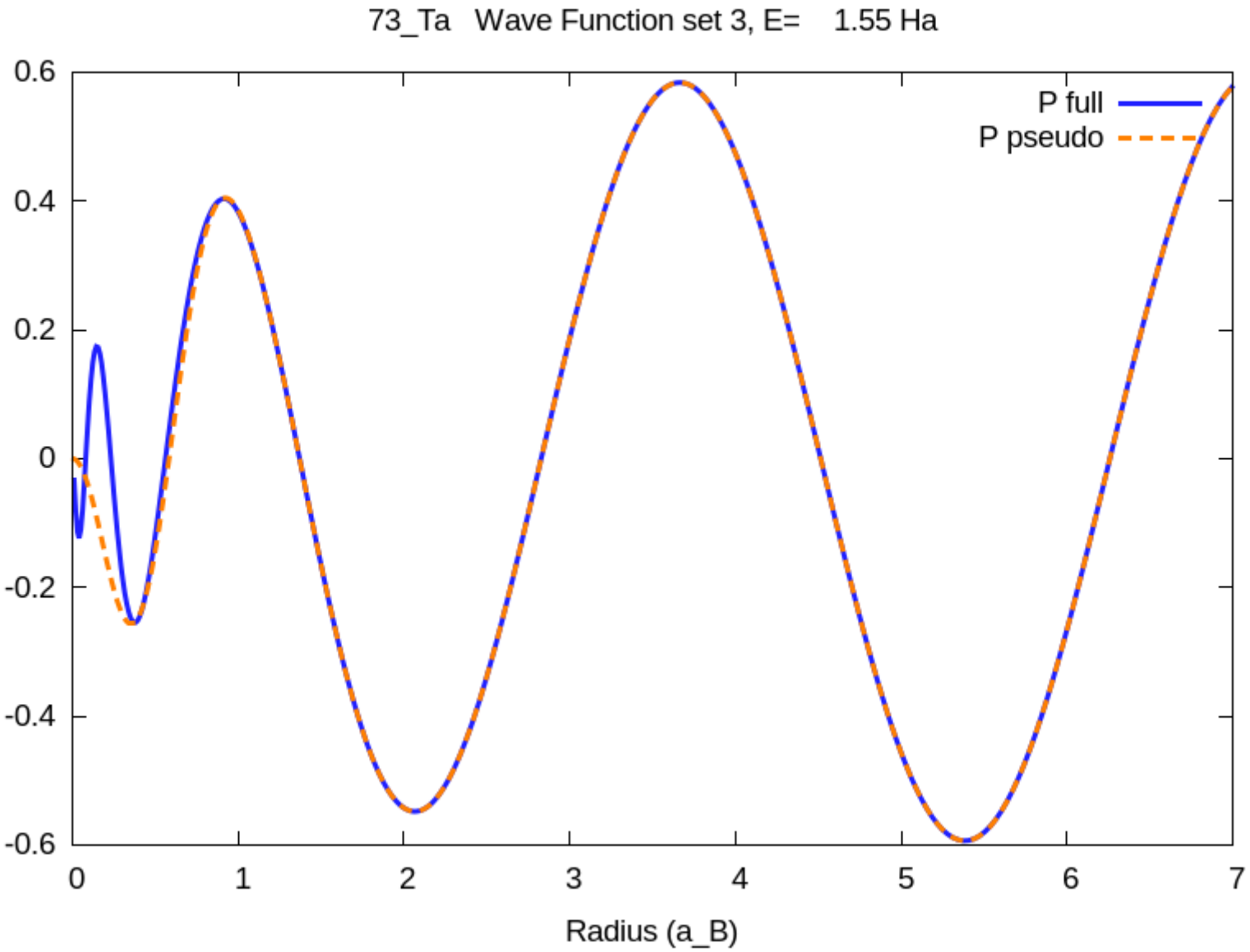

73_Ta Wave Function set 3, E= -0.21 Ha
S full
S pseudo
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-0.3
0
1
2
3
4
5
6
7
Radius (a_B)

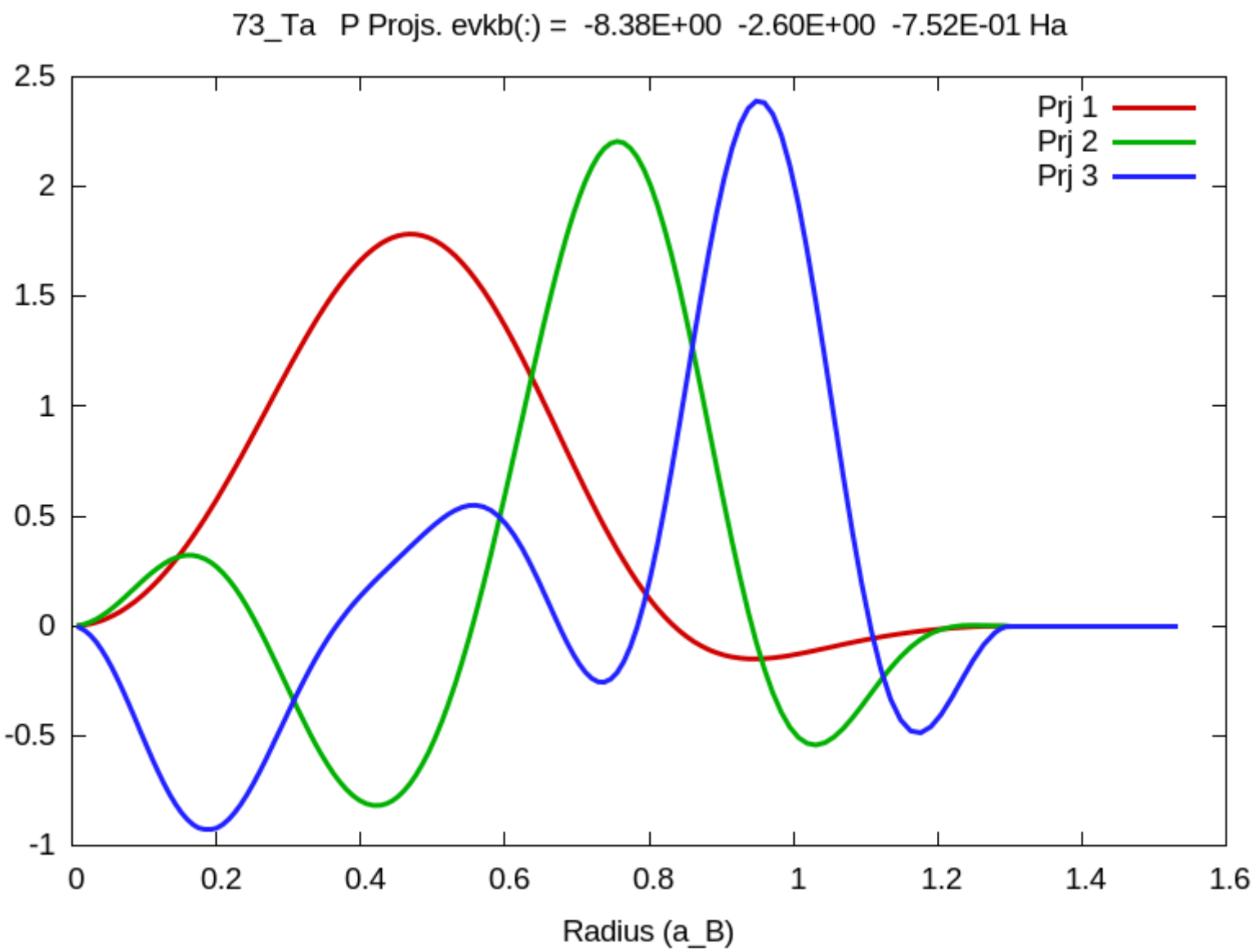

73_Ta S Projs. evkb(:) = 8.80E+00 -5.01E+00 8.75E-01 Ha
Prj 1
Prj 2
Prj 3
2
1.5
1
0.5
0
-0.5
-1
-1.5
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
Radius (a_B)

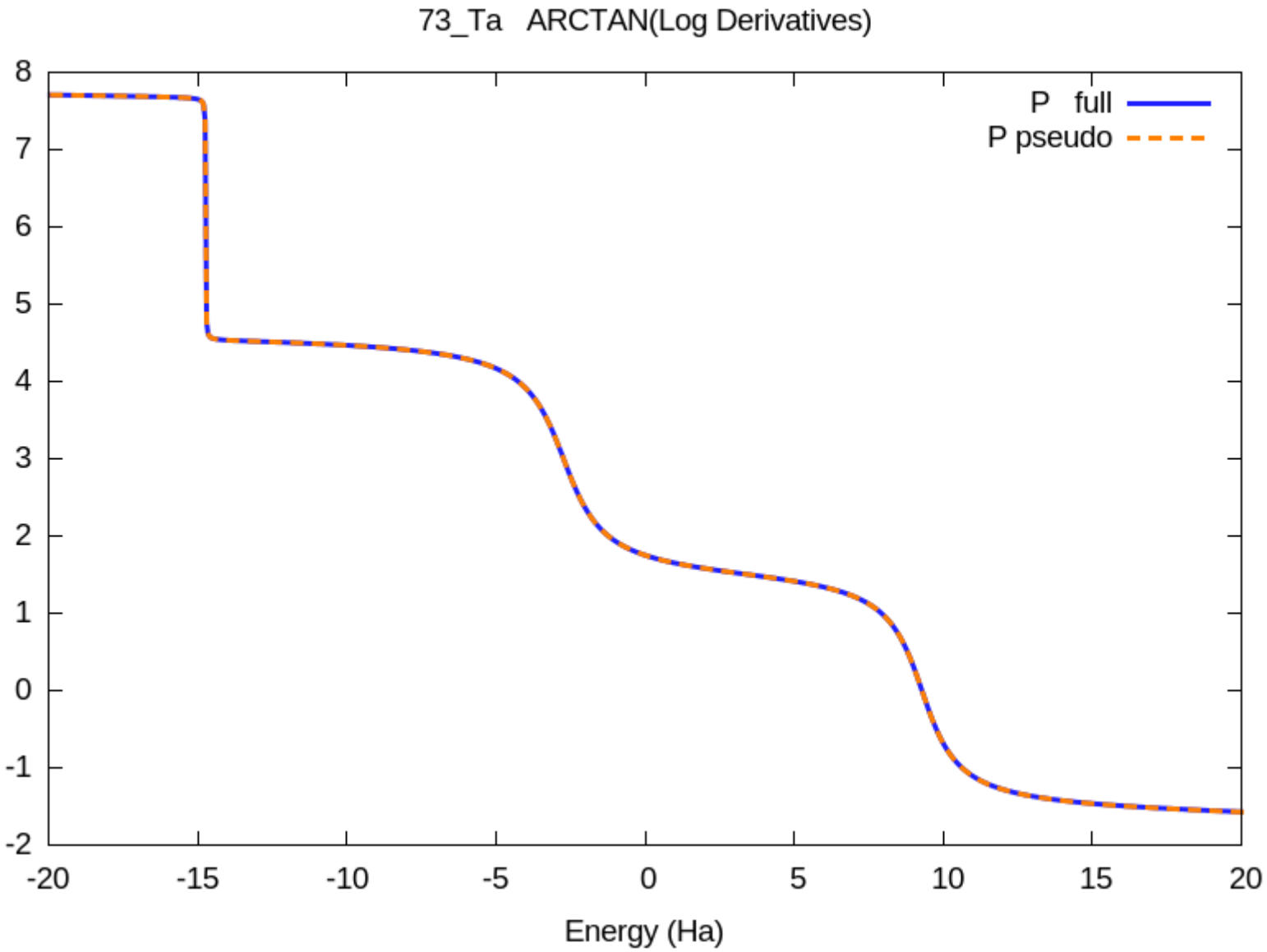

73_Ta ARCTAN(Log Derivatives)
S full
S pseudo
11
10
9
8
7
6
5
4
3
2
1
-20
-15
-10
-5
0
5
10
15
20
Energy (Ha)

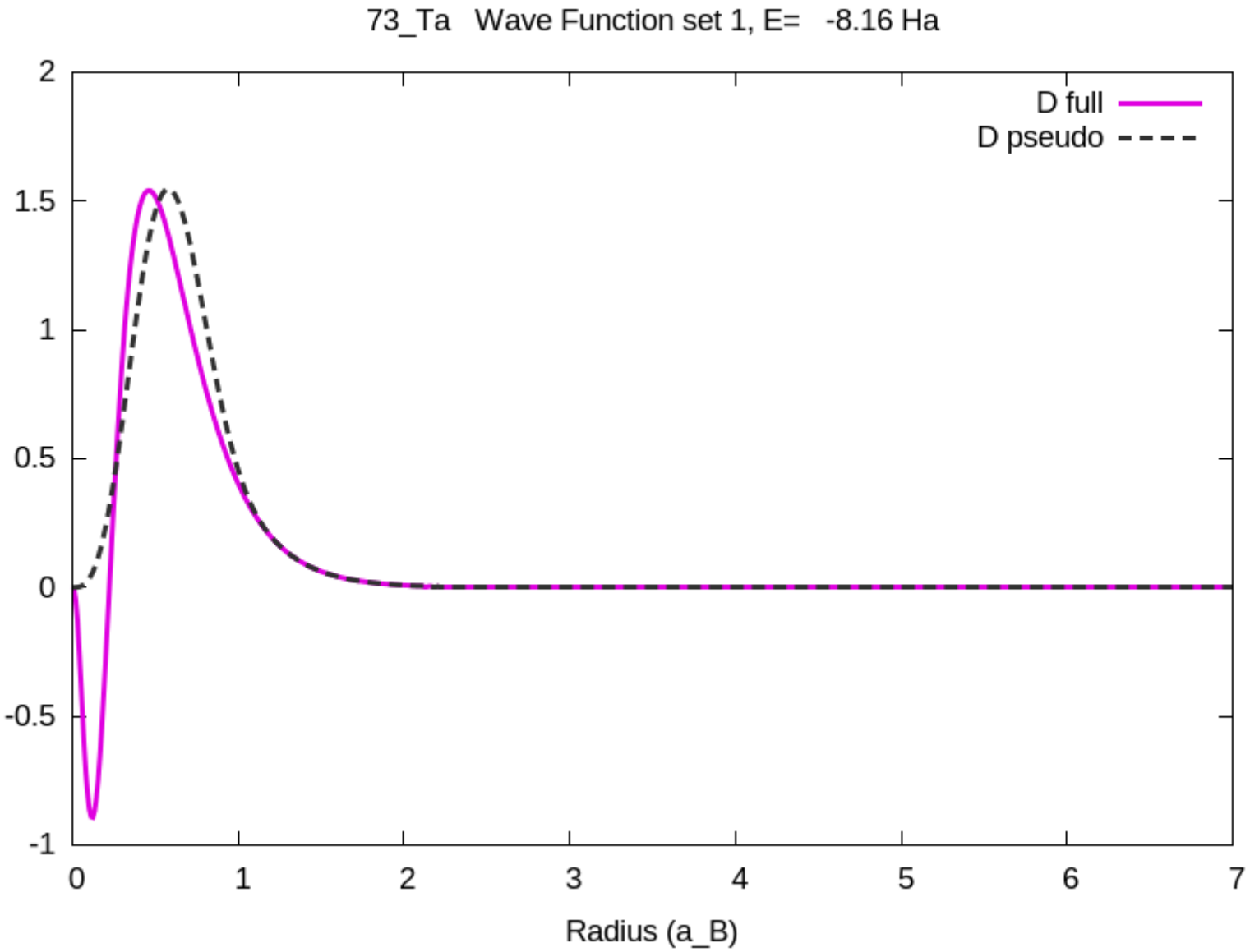

73_Ta Wave Function set 1, E= -14.71 Ha
P full
P pseudo
2
1.5
1
0.5
0
-0.5
-1
0
1
2
3
4
5
6
7
Radius (a_B)

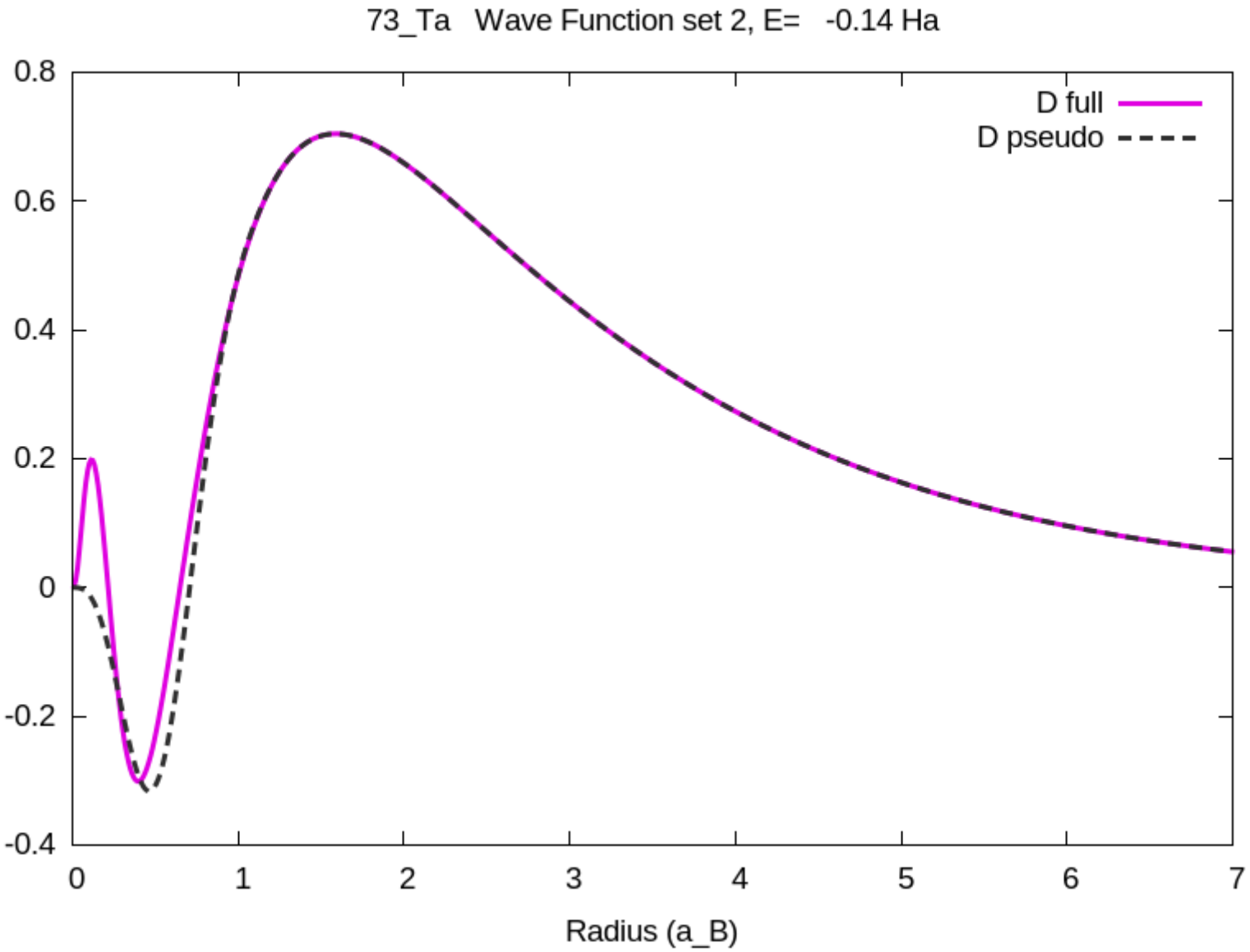

73_Ta Wave Function set 2, E= -1.45 Ha
P full
P pseudo
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
0
1
2
3
4
5
6
7
Radius (a_B)

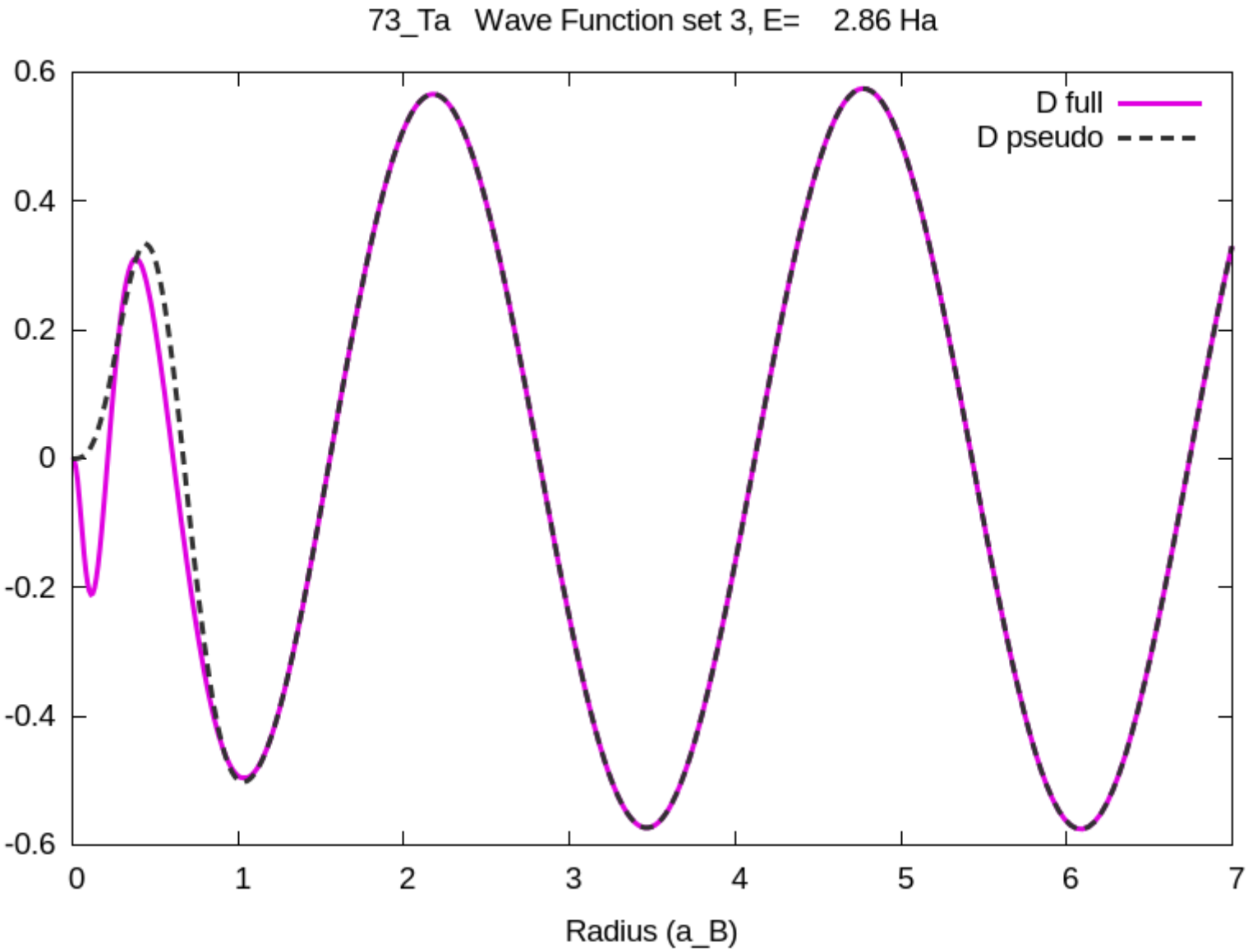

73_Ta Wave Function set 3, E= 1.55 Ha
P full
P pseudo
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
0
1
2
3
4
5
6
7
Radius (a_B)

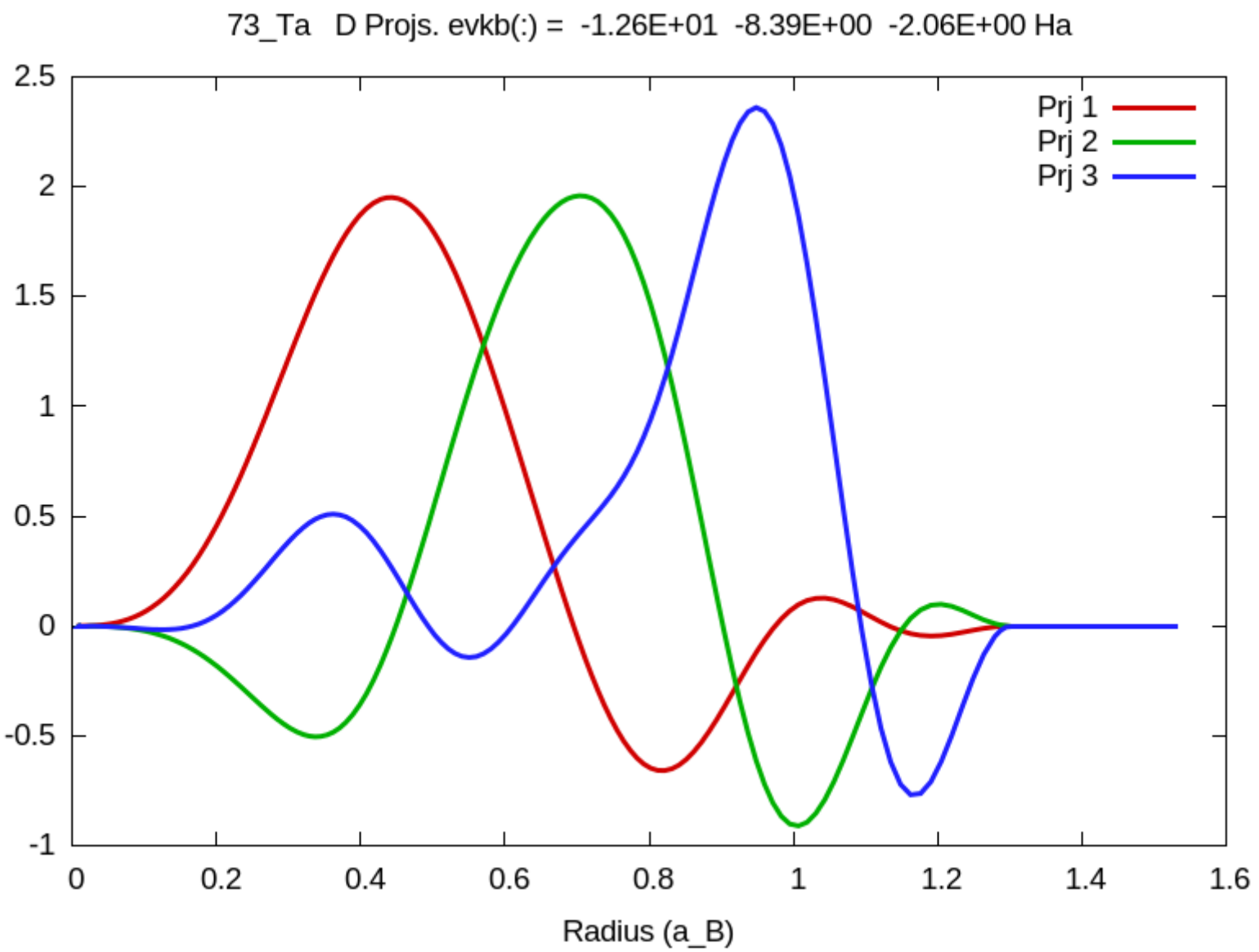

73_Ta P Projs. evkb(:) = -8.38E+00 -2.60E+00 -7.52E-01 Ha
Prj 1
Prj 2
Prj 3
2.5
2
1.5
1
0.5
0
-0.5
-1
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
Radius (a_B)

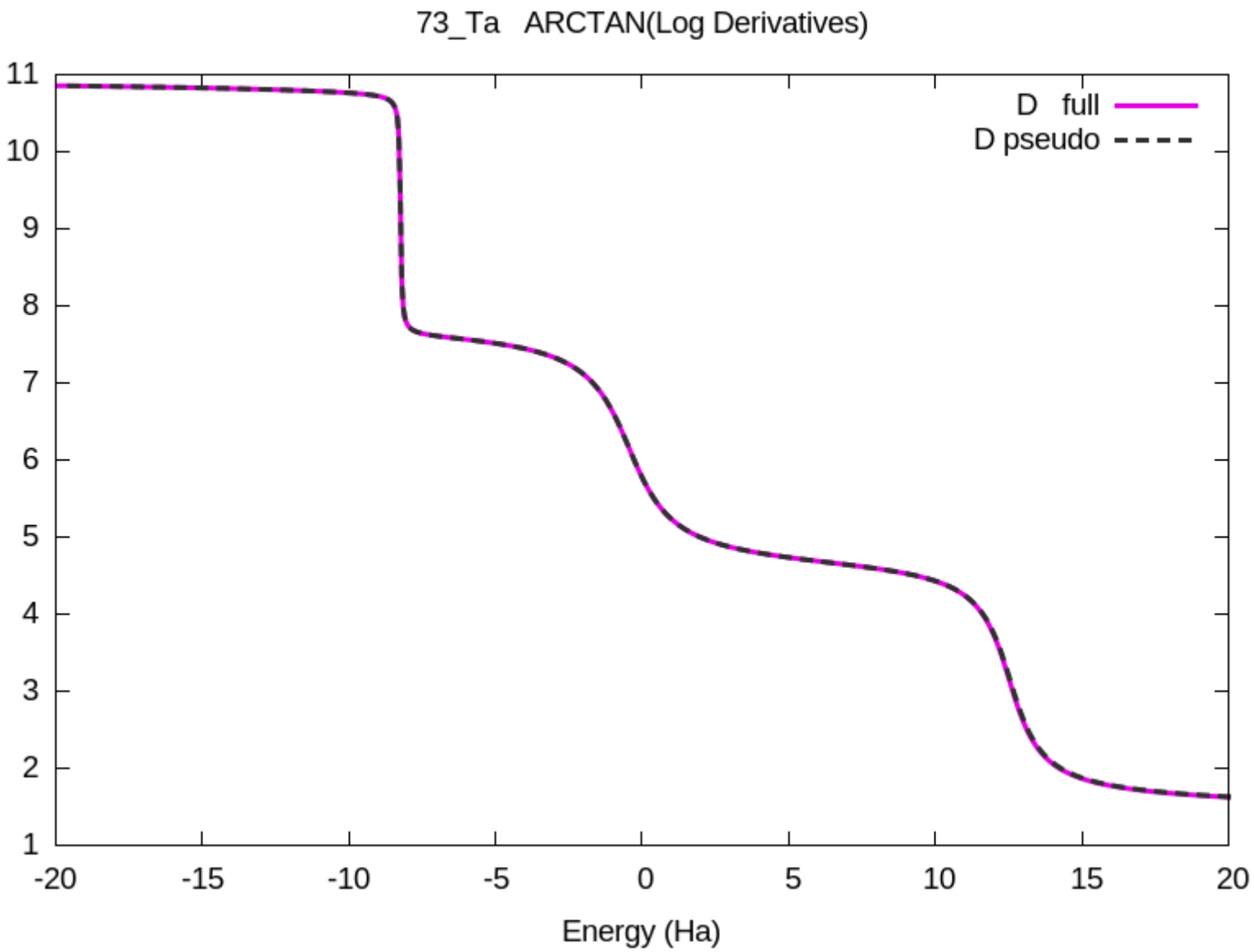

73_Ta ARCTAN(Log Derivatives)
P full
P pseudo
8
7
6
5
4
3
2
1
0
-1
-2
-20
-15
-10
-5
0
5
10
15
20
Energy (Ha)

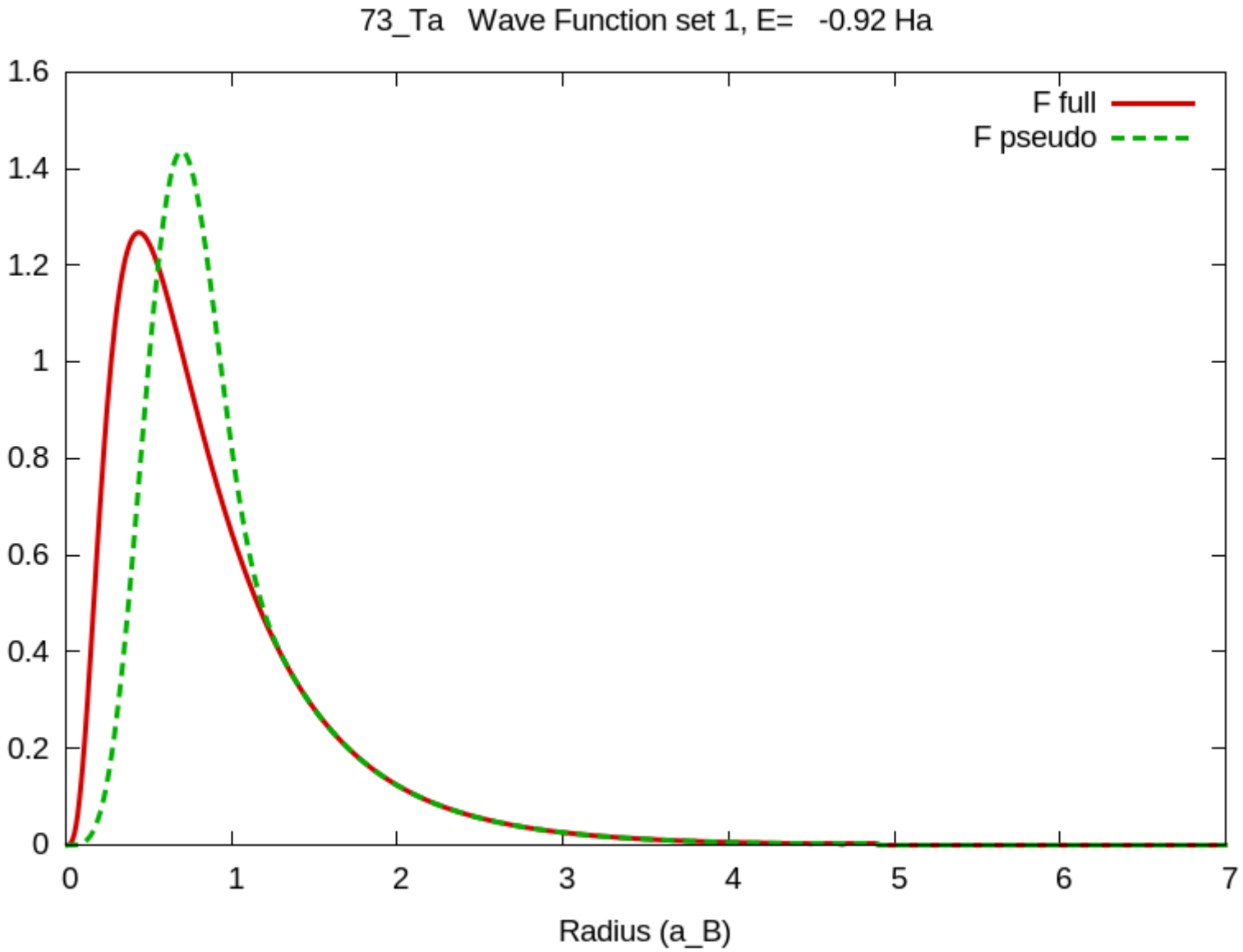

73_Ta Wave Function set 1, E= -8.16 Ha
D full
D pseudo
2
1.5
1
0.5
0
-0.5
-1
0
1
2
3
4
5
6
7
Radius (a_B)

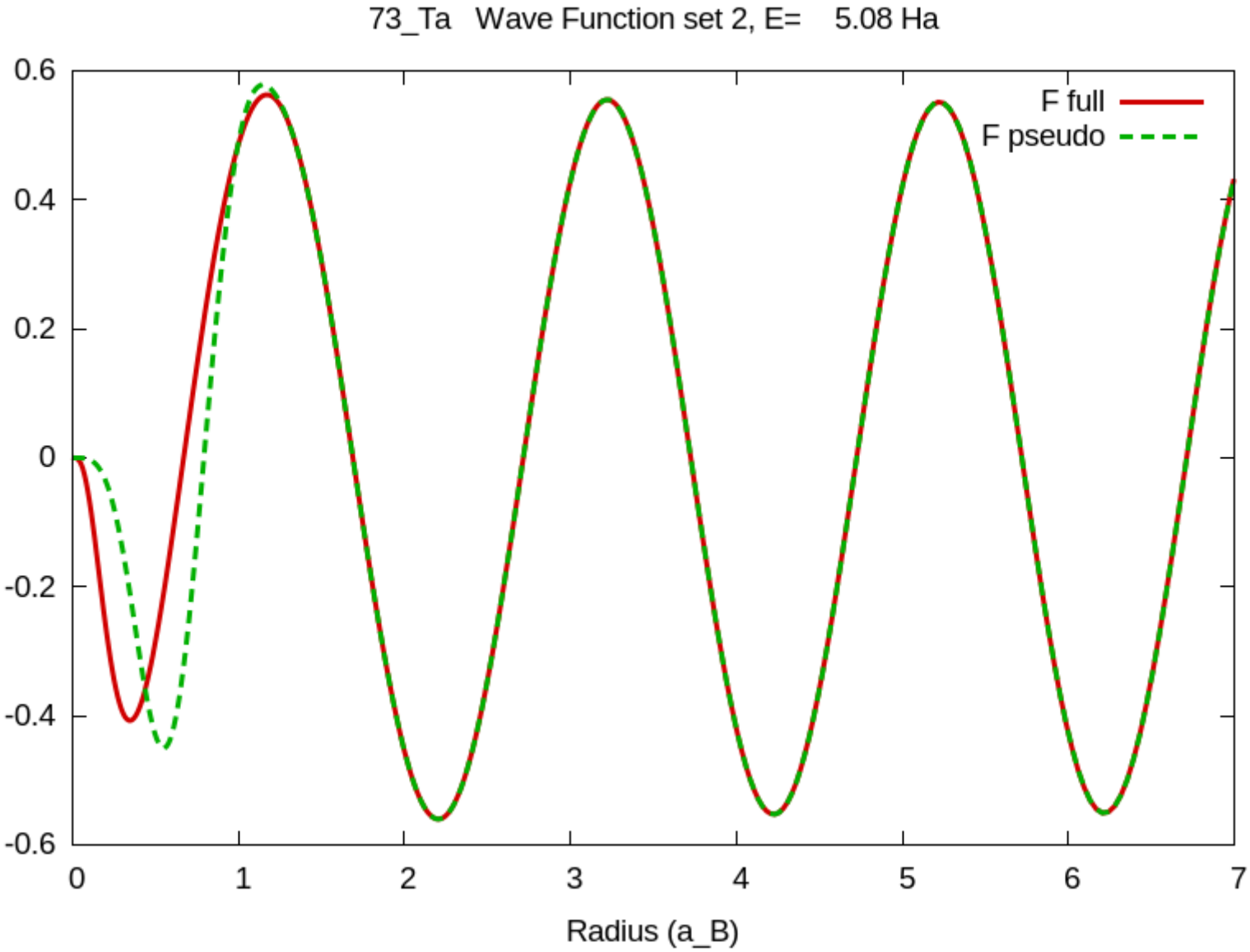

73_Ta Wave Function set 2, E= -0.14 Ha
D full
D pseudo
0.8
0.6
0.4
0.2
0
-0.2
-0.4
0
1
2
3
4
5
6
7
Radius (a_B)

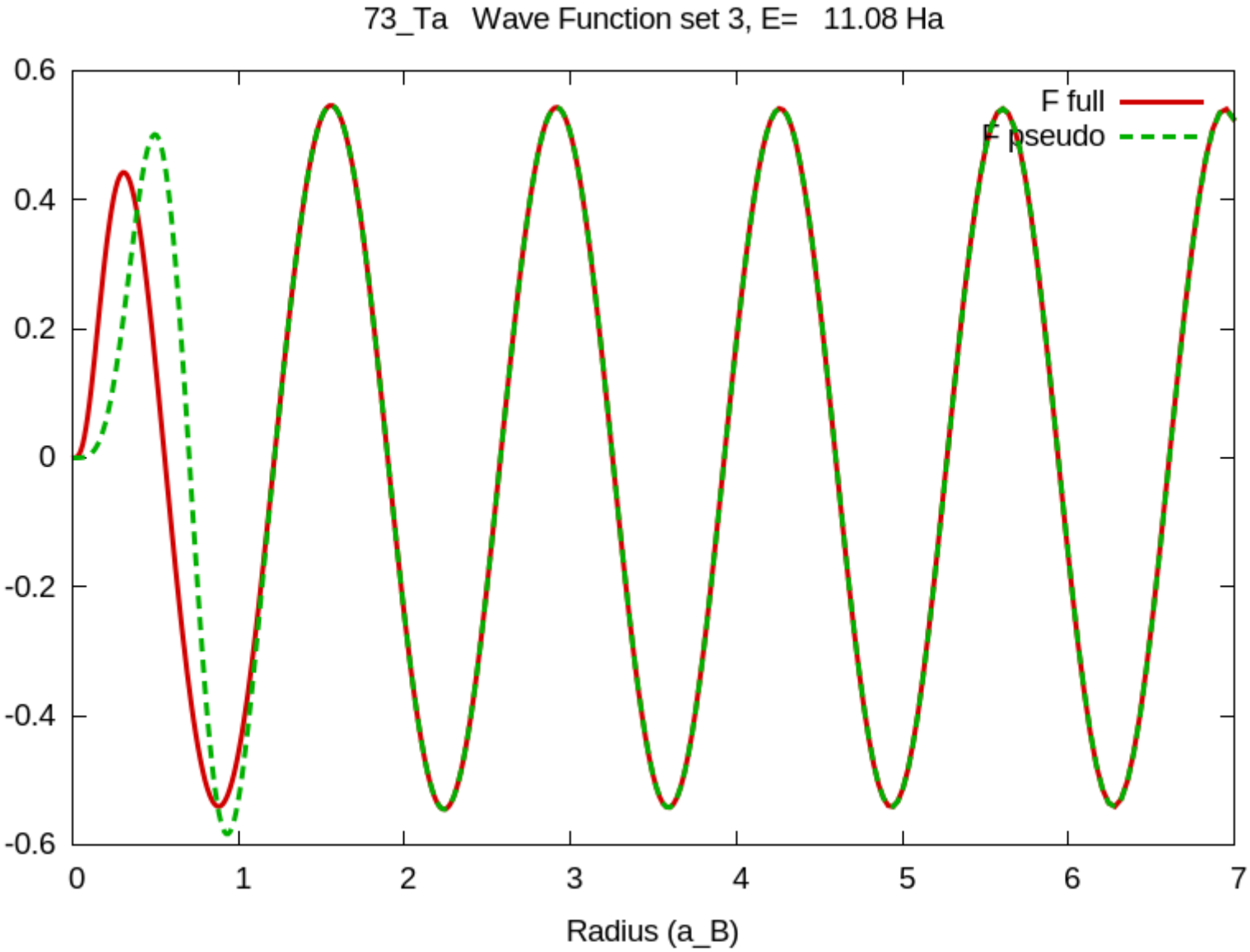

73_Ta Wave Function set 3, E= 2.86 Ha
D full
D pseudo
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
0
1
2
3
4
5
6
7
Radius (a_B)

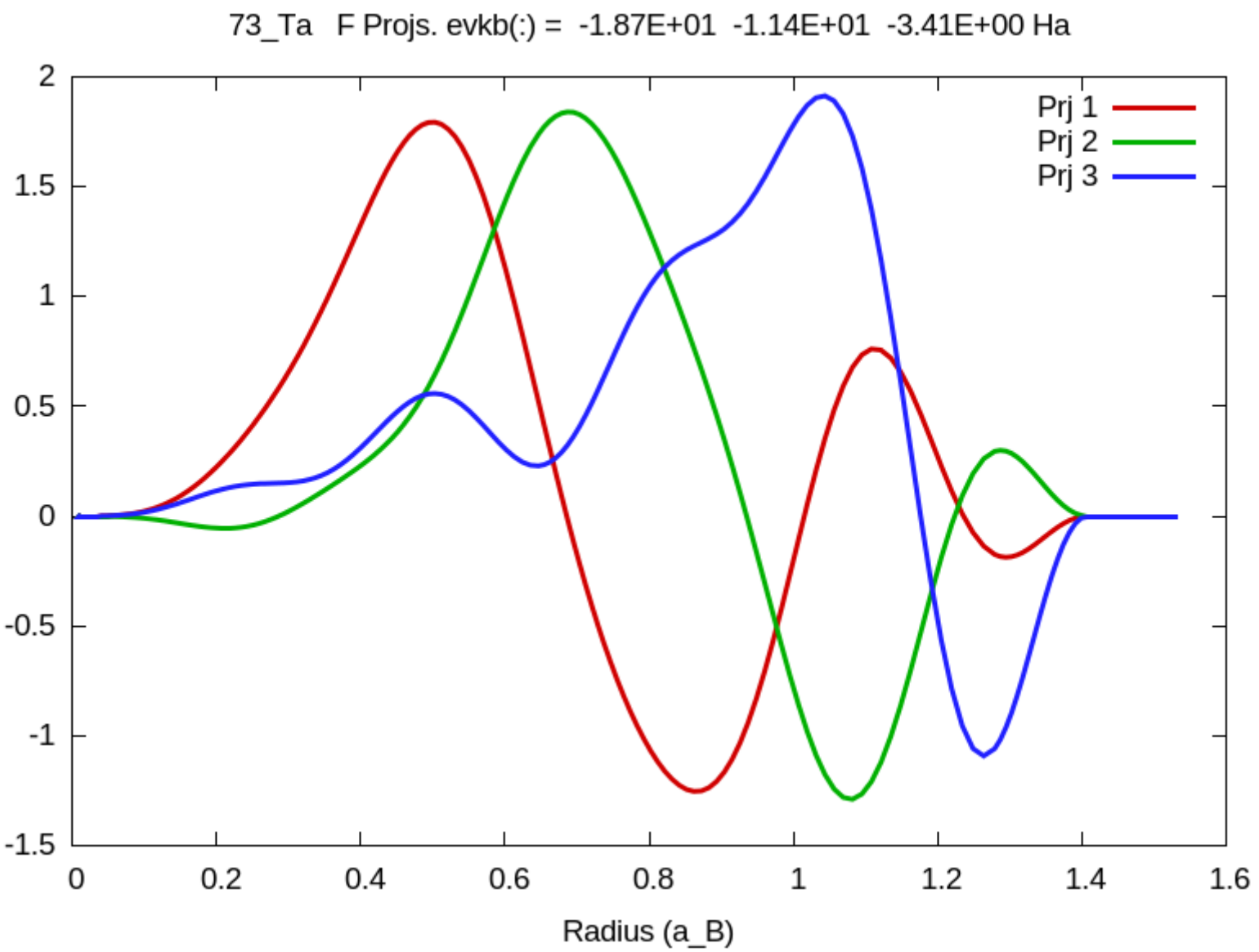

73_Ta D Projs. evkb(:) = -1.26E+01 -8.39E+00 -2.06E+00 Ha
Prj 1
Prj 2
Prj 3
2.5
2
1.5
1
0.5
0
-0.5
-1
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
Radius (a_B)

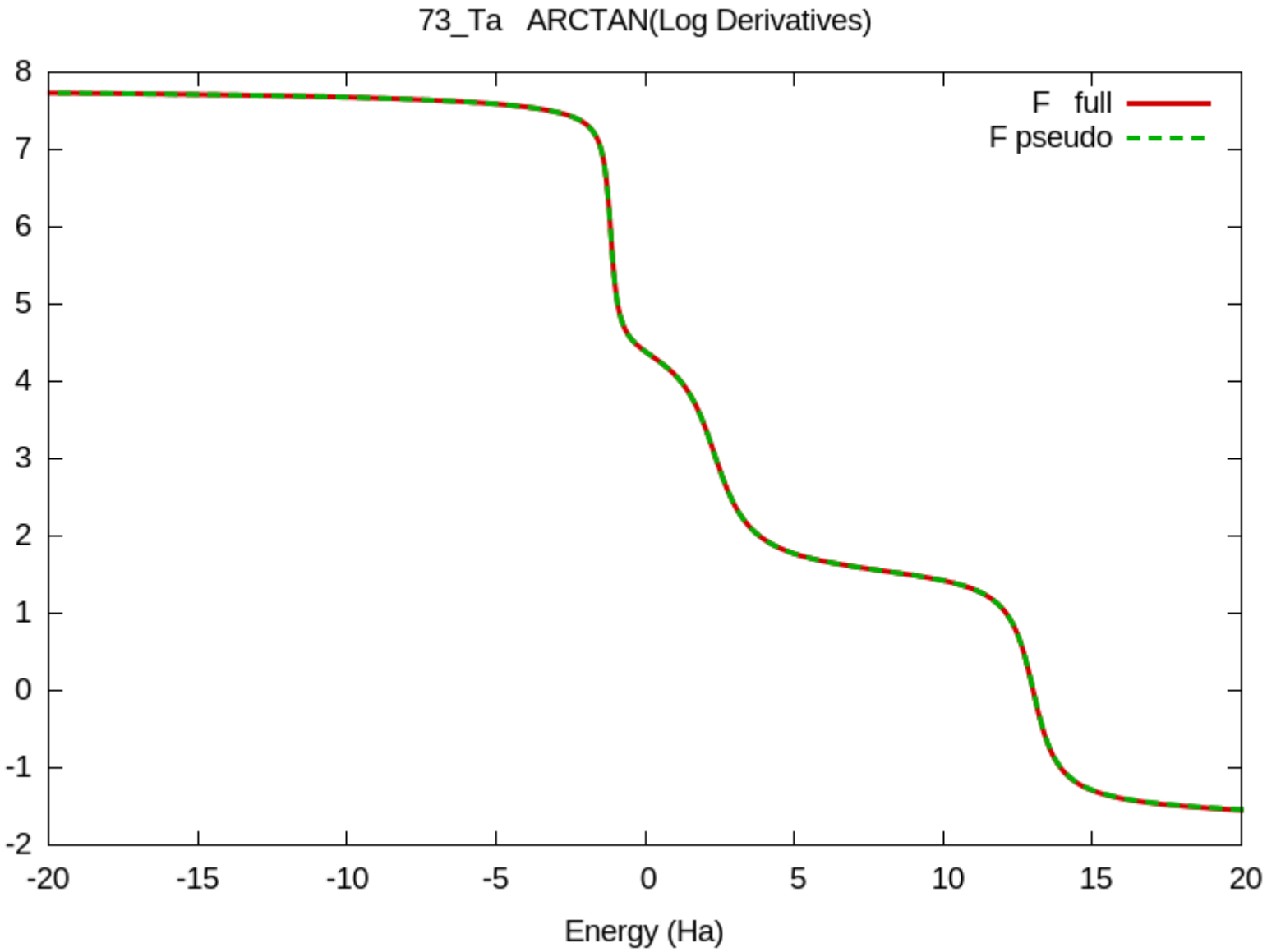

73_Ta ARCTAN(Log Derivatives)
D full
D pseudo
11
10
9
8
7
6
5
4
3
2
1
-20
-15
-10
-5
0
5
10
15
20
Energy (Ha)

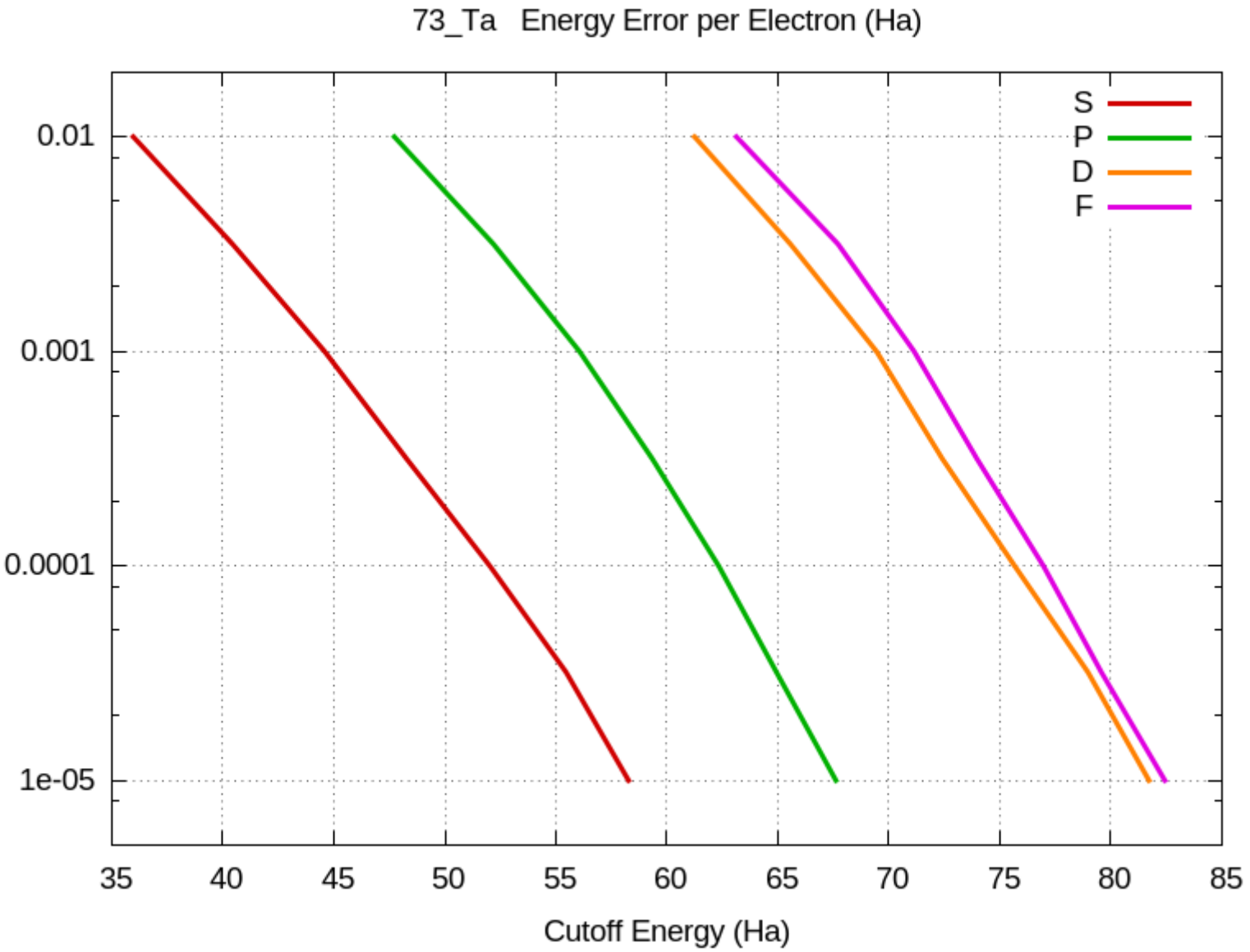

73_Ta Wave Function set 1, E= -0.92 Ha
F full
F pseudo
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
1
2
3
4
5
6
7
Radius (a_B)


73_Ta Wave Function set 2, E= 5.08 Ha
F full
F pseudo
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
0
1
2
3
4
5
6
7
Radius (a_B)


73_Ta Wave Function set 3, E= 11.08 Ha
F full
F pseudo
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
0
1
2
3
4
5
6
7
Radius (a_B)


73_Ta F Projs. evkb(:) = -1.87E+01 -1.14E+01 -3.41E+00 Ha
Prj 1
Prj 2
Prj 3
2
1.5
1
0.5
0
-0.5
-1
-1.5
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
Radius (a_B)


73_Ta ARCTAN(Log Derivatives)
F full
F pseudo
8
7
6
5
4
3
2
1
0
-1
-2
-20
-15
-10
-5
0
5
10
15
20
Energy (Ha)


73_Ta Energy Error per Electron (Ha)
0.01
0.001
0.0001
1e-05
35
40
45
50
55
60
65
70
75
80
85
Cutoff Energy (Ha)
S
P
D
F