Test the RRKJ pseudization routine and check the results against ld1.x (carbon, LDA).

[1]

```
import numpy as np
import matplotlib.pyplot as plt

# add pstudio to the search path
import sys
sys.path.append('..')
```

[2]

```
from pstudio import AE, set_output
from pstudio.RRKJ import pseudize_RRKJ
from pstudio.pseudo import calculate_vpot
#set_output(sys.stdout)

ae = AE('C', xcname='LDA', relativity='SR')
ae.run()
```

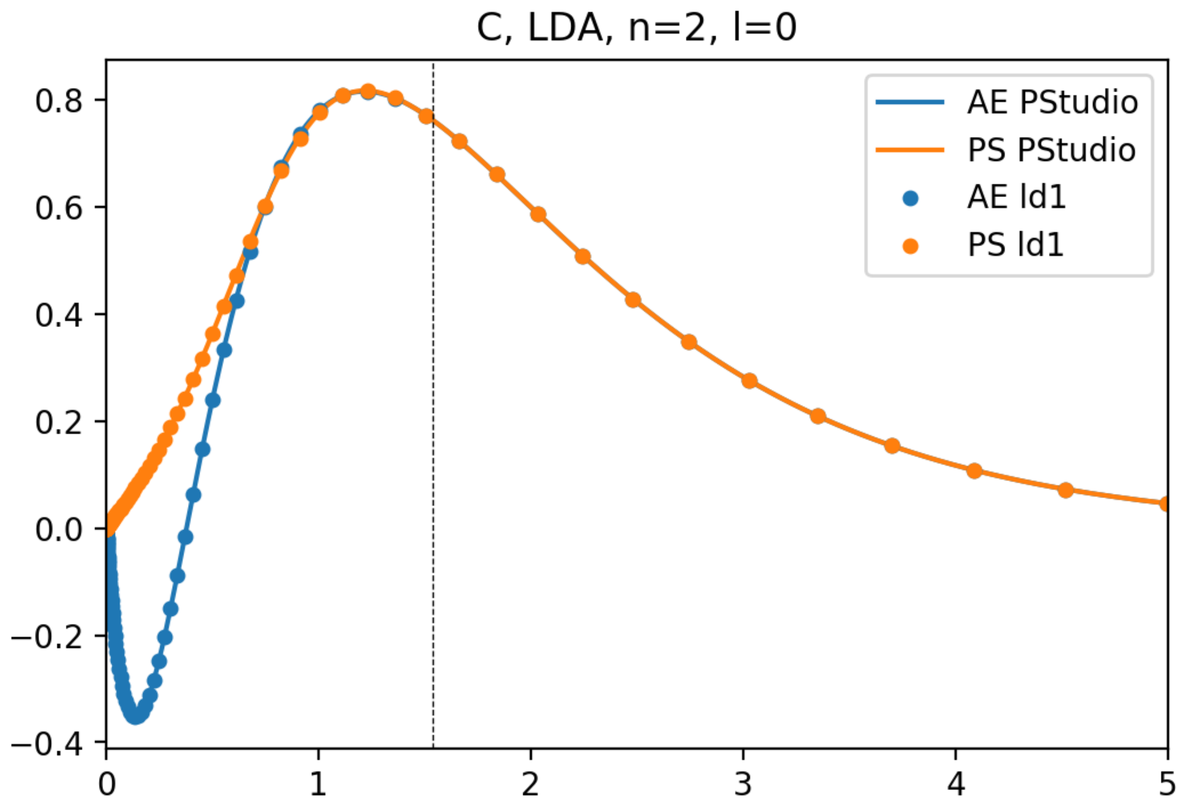
```
scalar relativistic atomic calculation for C (Carbon, Z=6)
configuration: 1s2 2s2 2p2, 6 electrons
exchange-correlation: lda_x+lda_c_pz
2001 radial gridpoints in [1e-05,100]

Converged in 63 iterations

Energy contributions:
------------------------------------------------------------------------
Kinetic:      +37.269733 Ha     +1014.161102 eV
Ionic:        -87.619337 Ha     -2384.243613 eV
Hartree:      +17.627276 Ha      +479.662609 eV
XC:            -4.732032 Ha      -128.765157 eV
------------------------------------------------------------------------
Total:        -37.454308 Ha     -1019.183627 eV

state      eigenvalue      eigenvalue        rmax
------------------------------------------------------------------------
1s2         -9.961701 Ha  -271.071678 eV    0.175
2s2         -0.501784 Ha   -13.654238 eV    1.218
2p2         -0.199279 Ha    -5.422666 eV    1.189
```

```
[8]   # load LD1 results
      ld1ae = np.loadtxt('LD1_C-LDA-RRKJ/c.wfc')
      ld1ps = np.loadtxt('LD1_C-LDA-RRKJ/cps.wfc')
```

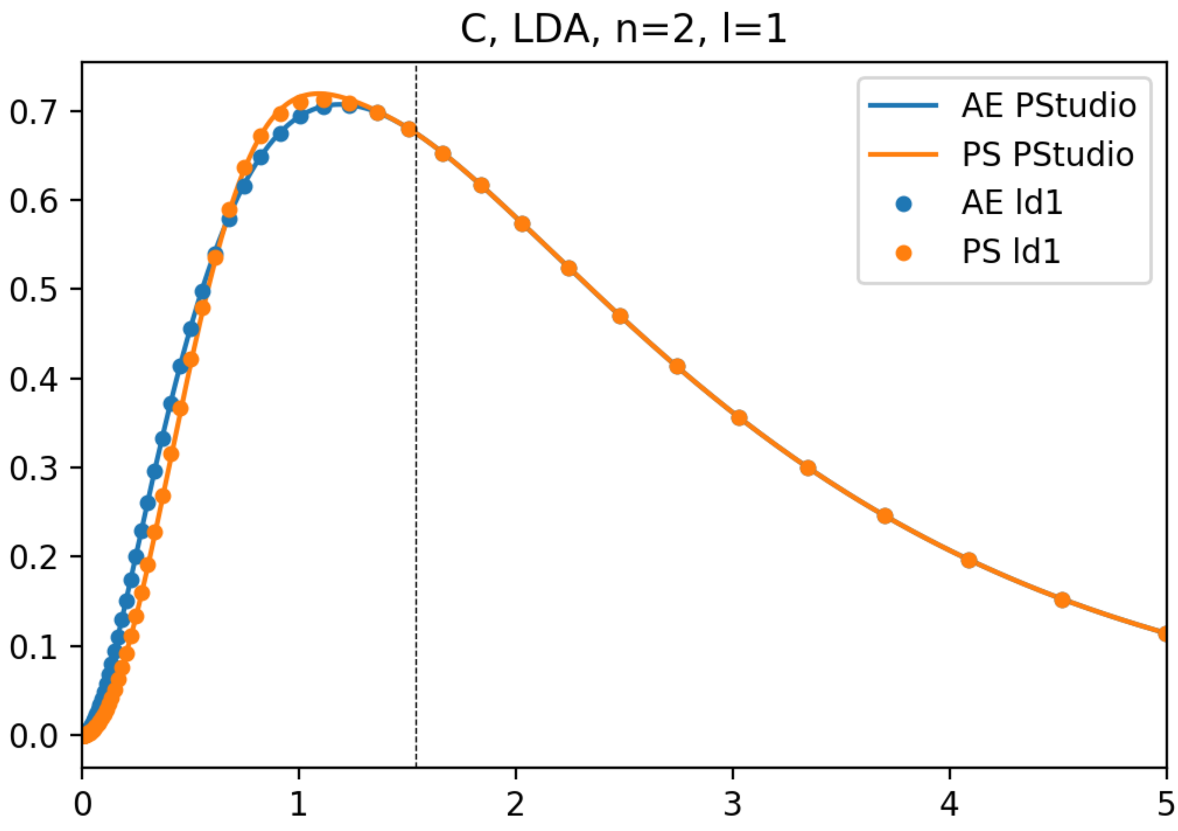
```
[9]   # loop over the valence orbitals
      r = ae.rgd.r
      ps = []
      ppot = []
      for orb in ae.orbitals[1:]:
          n = orb.n
          l = orb.l
          aeorb = orb.ur
          rc = 1.54

          print('Pseudizing n={0}, l={1}'.format(n,l))
          psorb, d2psorb = pseudize_RRKJ(aeorb, l, rc, ae.rgd,
      verbose=True)
          vpot = calculate_vpot(ae.vtot, ae.rgd, rc, l, orb.e, psorb,
      d2psorb)

          ps.append(psorb)
          ppot.append(vpot)
          print()

          plt.figure(figsize=(6,4), dpi=200)
          plt.plot(r, aeorb, color='C0', label='AE PStudio')
          plt.plot(r, psorb, color='C1', label='PS PStudio')
          if l == 0:
              plt.plot(ld1ae[::20,0], -ld1ae[::20,2], linestyle='none',
      marker='o', markersize=4, color='C0', label='AE ld1')
              plt.plot(ld1ps[::20,0], ld1ps[::20,1], linestyle='none',
      marker='o', markersize=4, color='C1', label='PS ld1')
          else:
              plt.plot(ld1ae[::20,0], ld1ae[::20,1], linestyle='none',
      marker='o', markersize=4, color='C0', label='AE ld1')
              plt.plot(ld1ps[::20,0], ld1ps[::20,2], linestyle='none',
      marker='o', markersize=4, color='C1', label='PS ld1')

          plt.axvline(rc, linestyle='dashed', color='black',
      linewidth=0.5)
          plt.xlim(0,5)
          plt.title('C, LDA, n={0}, l={1}'.format(n,l))
          plt.legend()
          plt.show()

          print()
```

```
Pseudizing n=2, l=0
RRKJ3 pseudization: l=0 rc=1.5382
AE norm within rc        : +0.542046
```

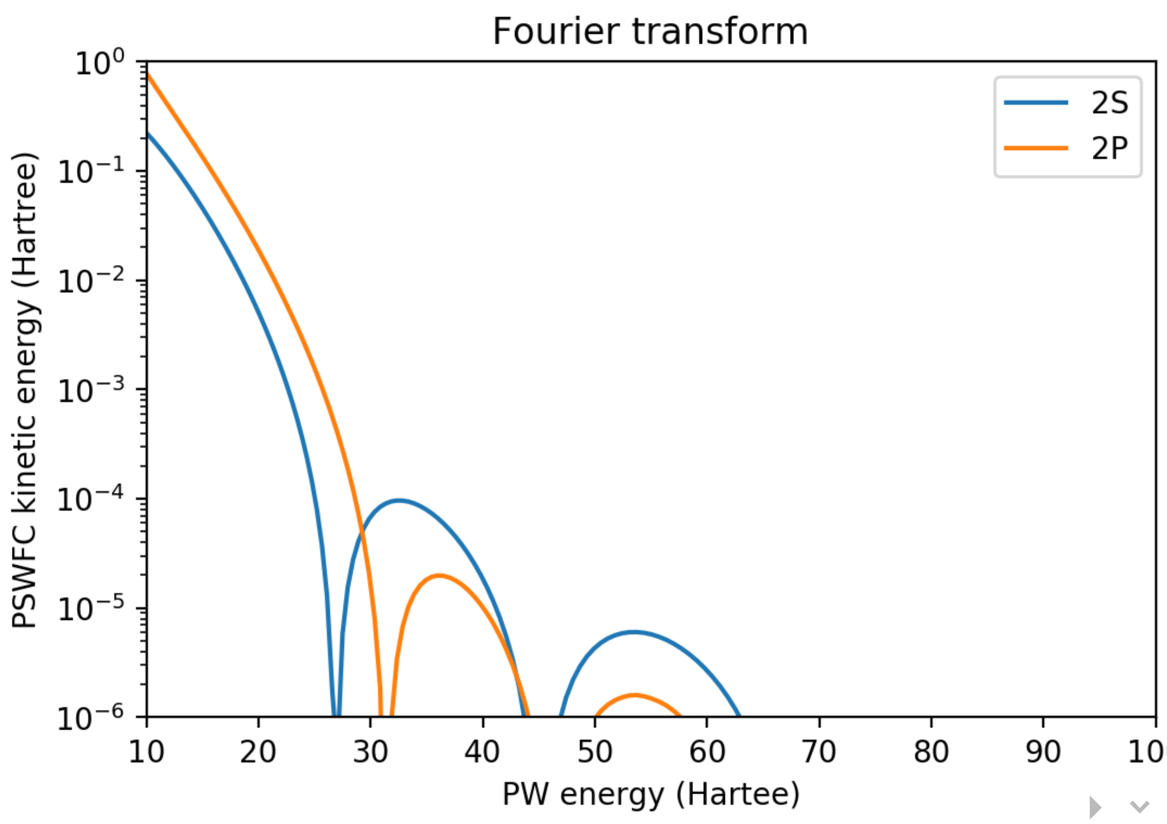
```
0-th AE derivative at rc: +0.762039
1-th AE derivative at rc: -0.286792
2-th AE derivative at rc: -0.507802
qi                 :  [1.21630917 3.14118716 5.15350006]
estimated cutoff : 13.2793 Ha
RRKJ coefficients: [0.9513780164843818, -0.18781477552128958,
-0.23024792136890476]
norm error         : 1.1102230246251565e-16
```



```
Pseudizing n=2, l=1
RRKJ3 pseudization: l=1 rc=1.5382
AE norm within rc        : +0.475565
0-th AE derivative at rc: +0.675043
1-th AE derivative at rc: -0.161338
2-th AE derivative at rc: -0.287611
qi                 :  [1.89253659 4.01747702 6.08313779]
estimated cutoff : 18.5023 Ha
RRKJ coefficients: [1.5167470916476324, 0.7727604193095149,
0.16001840742104906]
norm error         : -1.2323475573339238e-14
```

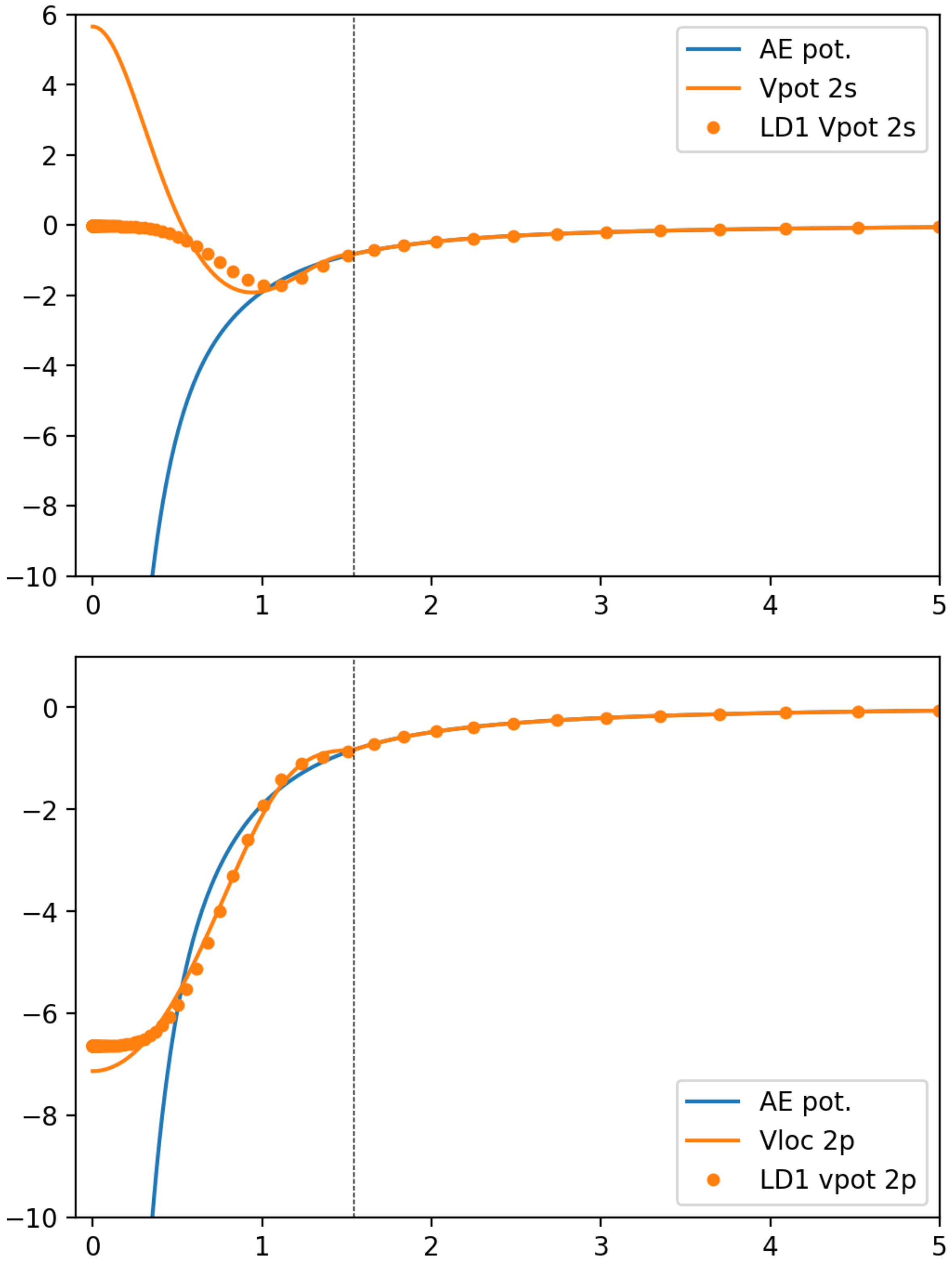


```
[5]     plt.figure(figsize=(6,4), dpi=200)

        q, fq = ae.rgd.fft(ps[0], l=0)
        plt.plot(0.5*q*q, 0.5*fq*fq*q*q, label='2S')
        q, fq = ae.rgd.fft(ps[1], l=1)
        plt.plot(0.5*q*q, 0.5*fq*fq*q*q, label='2P')

        plt.xlim(10,100)
        plt.xlabel('PW energy (Hartee)')

        plt.ylim(1e-6, 1)
        plt.yscale('log')
        plt.ylabel('PSWFC kinetic energy (Hartree)')

        plt.title('Fourier transform')
        plt.legend()
        plt.show()
```



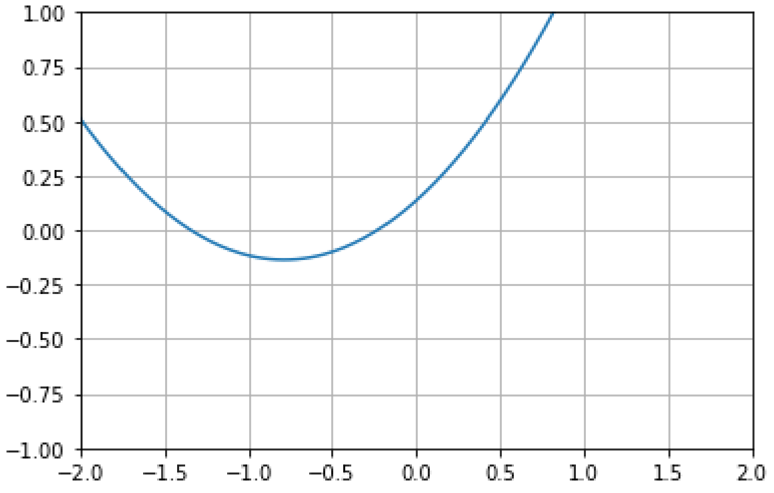
In ld1.x the screened pseudopotential is always calculated using the TM method, hence we cannot compare!

```
[6]    # load the screeend potentials from ld1.x
       ld1_vloc2s = np.loadtxt('LD1_C-LDA-RRKJ/c.screen-vloc0')
       ld1_vloc2p = np.loadtxt('LD1_C-LDA-RRKJ/c.screen-vloc1')

       fig = plt.figure(figsize=(6,4), dpi=200)
       plt.plot(r, ae.vtot, color='C0', label='AE pot.')
       plt.plot(r, ppot[0], color='C1', label='Vpot 2s')
       plt.plot(ld1_vloc2s[::20,1], ld1_vloc2s[::20,2]/2, color='C1',
       linestyle='none', marker='o', markersize=4, label='LD1 Vpot 2s')

       plt.axvline(rc, linestyle='dashed', color='black', linewidth=0.5)
       plt.xlim(-0.10,5)
       plt.ylim(-10,6)
       plt.legend()
       plt.show()


       fig = plt.figure(figsize=(6,4), dpi=200)
       plt.plot(r, ae.vtot, color='C0', label='AE pot.')
       plt.plot(r, ppot[1], color='C1', label='Vloc 2p')
       plt.plot(ld1_vloc2p[::20,1], ld1_vloc2p[::20,2]/2, color='C1',
       linestyle='none', marker='o', markersize=4, label='LD1 vpot 2p')

       plt.axvline(rc, linestyle='dashed', color='black', linewidth=0.5)
       plt.xlim(-0.10,5)
       plt.ylim(-10,1)
       plt.legend()
       plt.show()
```

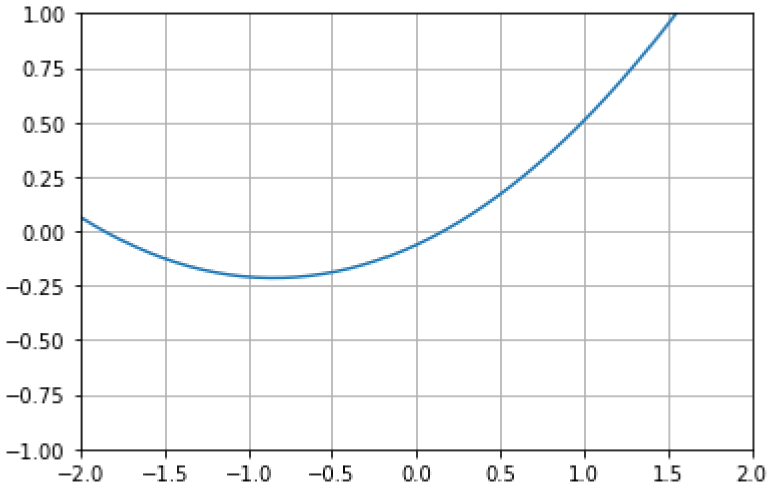


```
[7]   for orb in ae.orbitals[1:]:
          n = orb.n
          l = orb.l
          aeorb = orb.ur
          print('Pseudizing n={0}, l={1}'.format(n,l))
          psorb = pseudize_RRKJ(aeorb, l, 1.54, ae.rgd, verbose=False,
      plot_c2=True)
          plt.xlim(-2,2)
          plt.ylim(-1,1)
          plt.show()
          print()
```

```
Pseudizing n=2, l=0
```



```
Pseudizing n=2, l=1
```


1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0