APE_post_process

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```
In [19]: %matplotlib inline
         import numpy as np
         import scipy as sp
         import matplotlib.pyplot as plt
         import pandas as pd
         import pickle
         import sys
         import os

         from DFT_KIT.core import general_tool
         from DFT_KIT.core import calculator,job
         from DFT_KIT.calculator import APE
```

```
In [39]: #Bismuth
         os.chdir('/Users/shiangfang/Shiang DrobBox/Dropbox/Physics Research/Tim Kaxiras Group/

         dft_job=job.job(subdir=False,job_manager_mode=False,write_post_process=False)
         dft_calc=APE.calculator_APE(True,dft_job,None)
```

```
In [42]: biwfs1=dft_calc.post_process_read_ae('wf-6s0.5')
         biwfs2=dft_calc.post_process_read_pp('wf-6s0.5')

         plt.plot(biwfs1[:,0],biwfs1[:,1],biwfs2[:,0],biwfs2[:,1])
         plt.ylim([-1,1])
         plt.xlim([0,8])
         plt.title('Bismuth 6S J=1/2')
         plt.xlabel('radius (a.u.)')
```
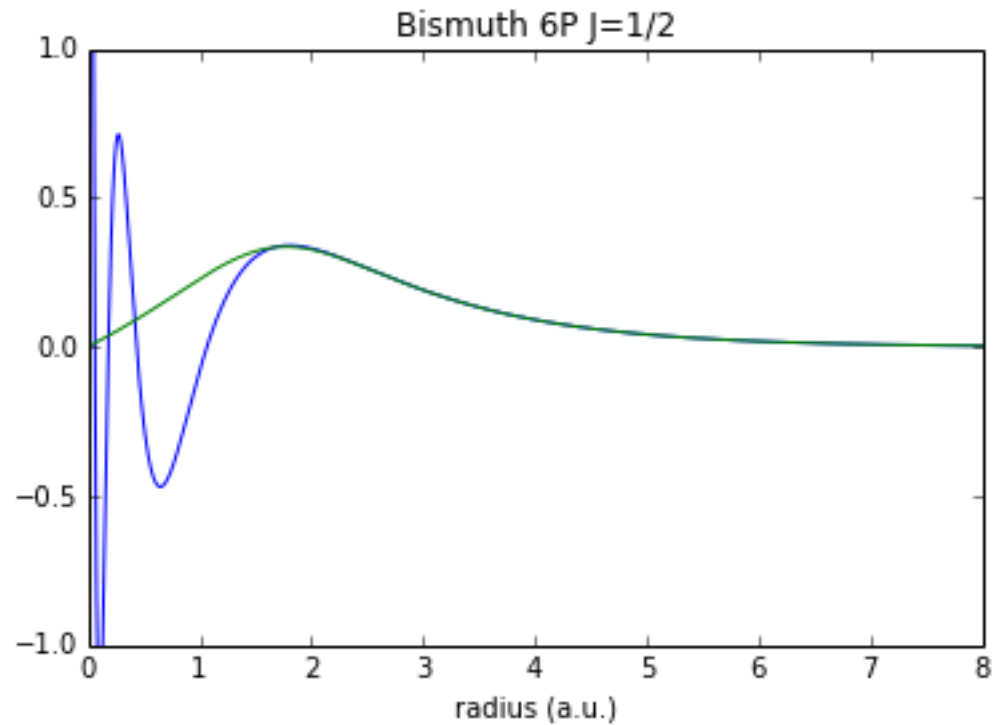
```
Out [42]:
         <matplotlib.text.Text at 0x109995550>
```

Bismuth 6S J=1/2
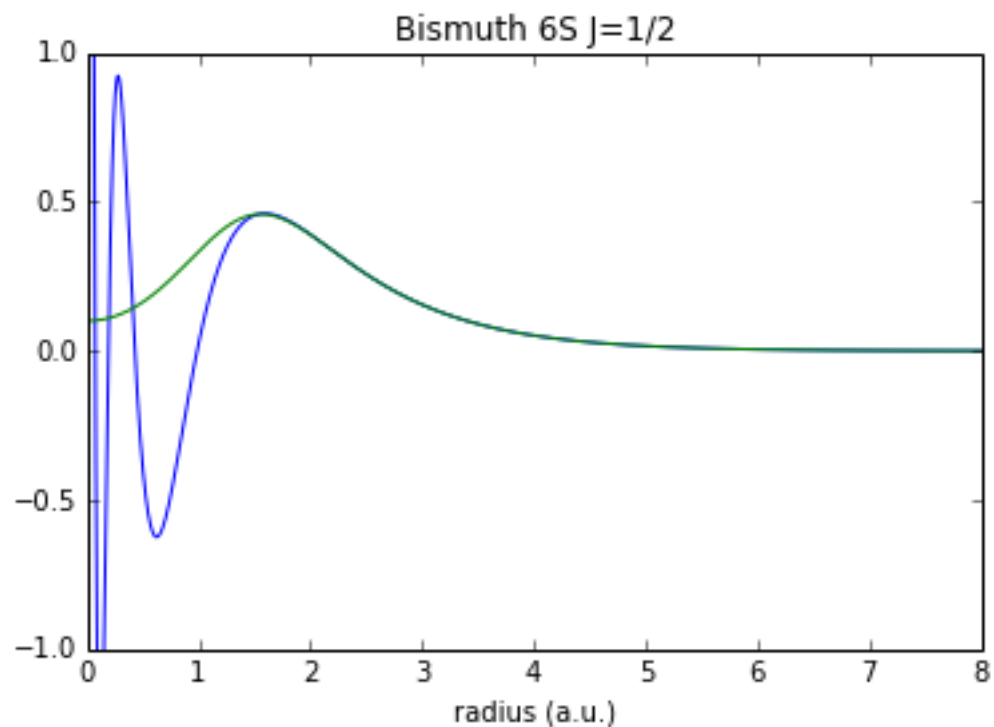
```
In [43]: biwfp1=dft_calc.post_process_read_ae('wf-6p0.5')
         biwfp2=dft_calc.post_process_read_pp('wf-6p0.5')

         plt.plot(biwfp1[:,0],biwfp1[:,1],biwfp2[:,0],biwfp2[:,1])
         plt.ylim([-1,1])
         plt.xlim([0,8])
         plt.title('Bismuth 6P J=1/2')
         plt.xlabel('radius (a.u.)')
```
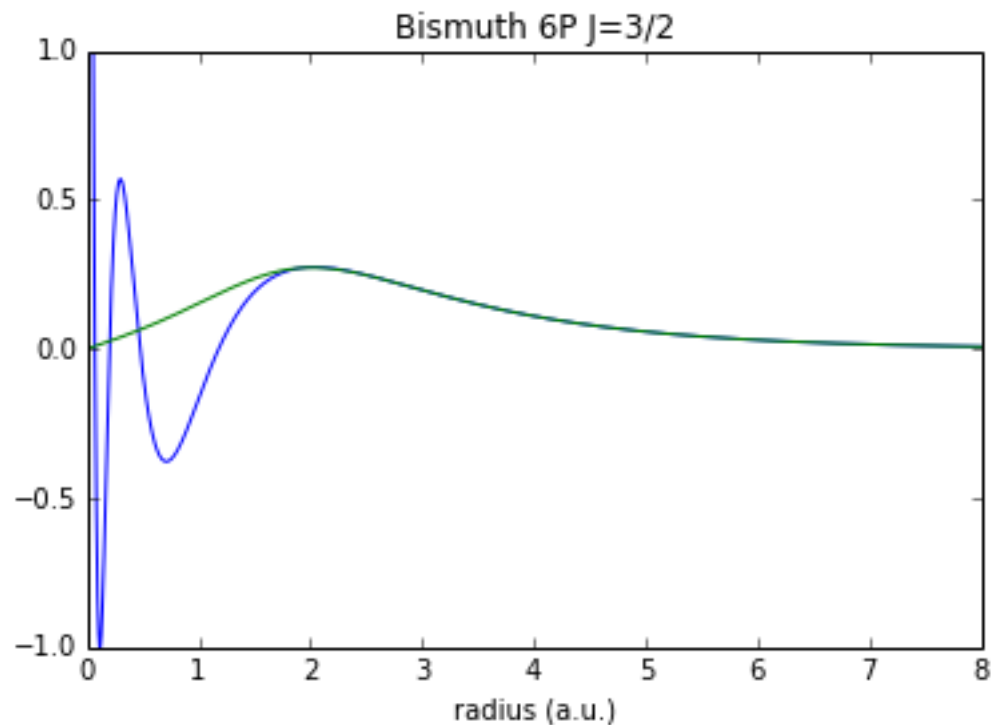
Out [43]:
        <matplotlib.text.Text at 0x109a93e90>

Bismuth 6P J=1/2

```
biwfp1b=dft_calc.post_process_read_ae('wf-6p1.5')
biwfp2b=dft_calc.post_process_read_pp('wf-6p1.5')

plt.plot(biwfp1b[:,0],biwfp1b[:,1],biwfp2b[:,0],biwfp2b[:,1])
plt.ylim([-1,1])
plt.xlim([0,8])
plt.title('Bismuth 6P J=3/2')
plt.xlabel('radius (a.u.)')
```

Out [44]:

```
<matplotlib.text.Text at 0x109a8e810>
```

Bismuth 6P J=3/2
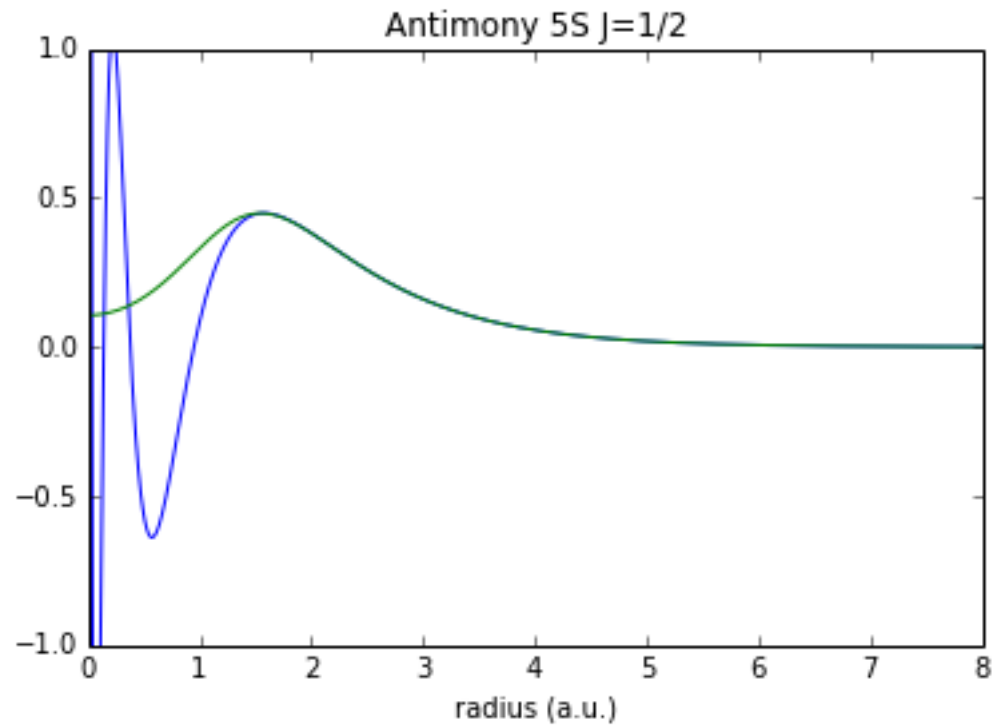
radius (a.u.)

In [44]:

In [45]:
```
#Antimony
os.chdir('/Users/shiangfang/Shiang DrobBox/Dropbox/Physics Research/Tim Kaxiras Group/

dft_job=job.job(subdir=False,job_manager_mode=False,write_post_process=False)
dft_calc=APE.calculator_APE(True,dft_job,None)
```

In [46]:
```
sbwfs1=dft_calc.post_process_read_ae('wf-5s0.5')
sbwfs2=dft_calc.post_process_read_pp('wf-5s0.5')

plt.plot(sbwfs1[:,0],sbwfs1[:,1],sbwfs2[:,0],sbwfs2[:,1])
plt.ylim([-1,1])
plt.xlim([0,8])
plt.title('Antimony 5S J=1/2')
plt.xlabel('radius (a.u.)')
```
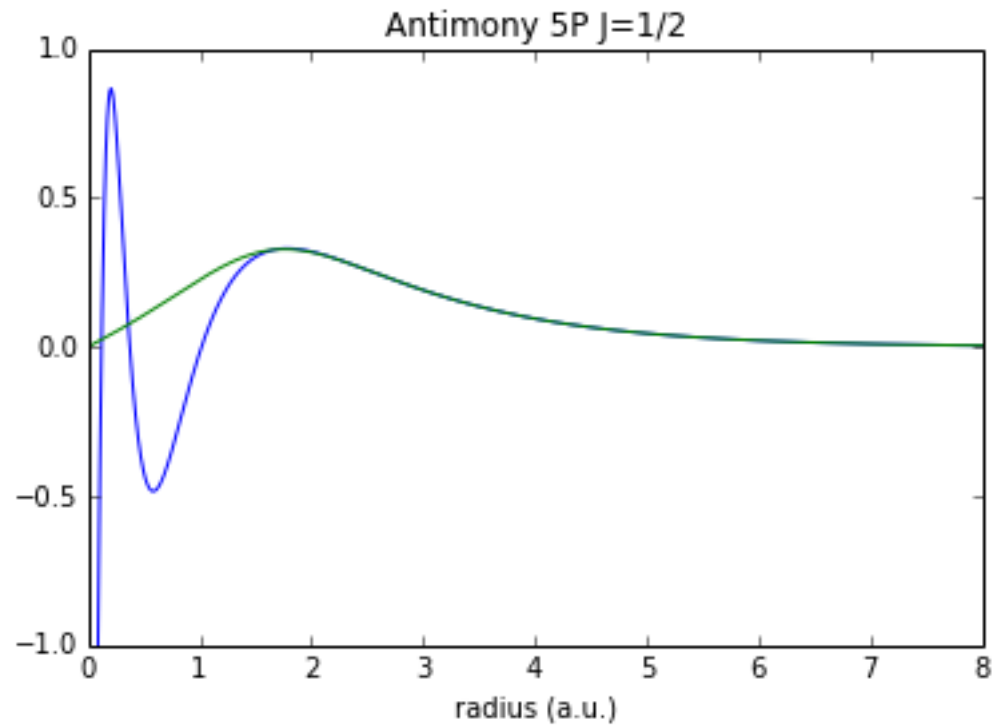
Out [46]:
```
<matplotlib.text.Text at 0x109bc7150>
```

Antimony 5S J=1/2

```
In [47]:  sbwfp1=dft_calc.post_process_read_ae('wf-5p0.5')
          sbwfp2=dft_calc.post_process_read_pp('wf-5p0.5')

          plt.plot(sbwfp1[:,0],sbwfp1[:,1],sbwfp2[:,0],sbwfp2[:,1])
          plt.ylim([-1,1])
          plt.xlim([0,8])
          plt.title('Antimony 5P J=1/2')
          plt.xlabel('radius (a.u.)')
```
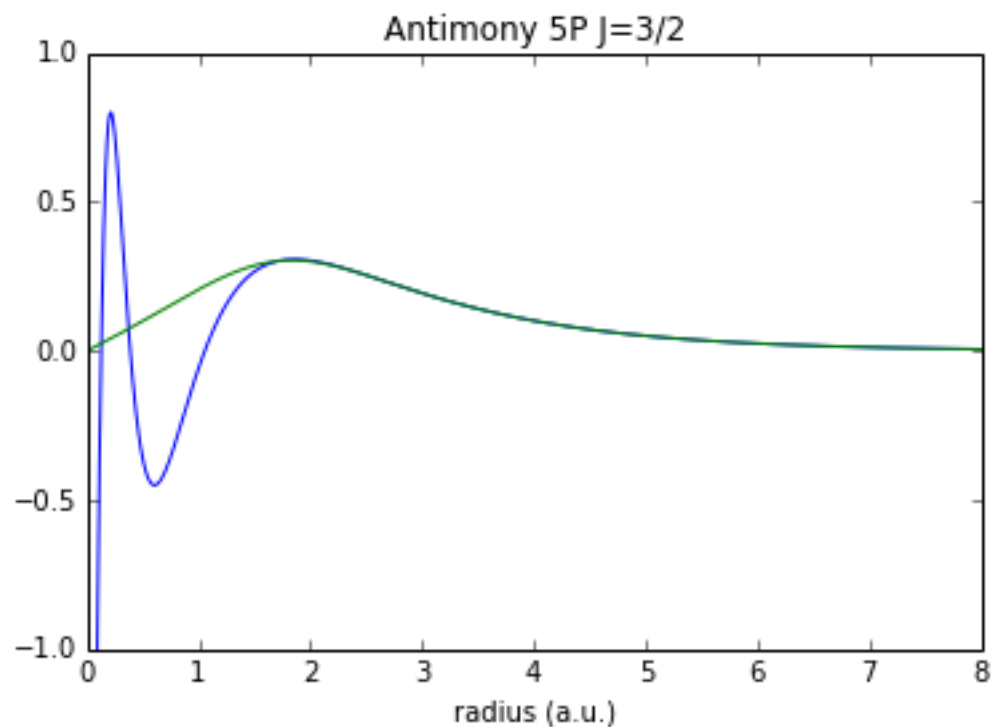
Out [47]:
        <matplotlib.text.Text at 0x109bf7a90>

Antimony 5P J=1/2

```
In [48]:  sbwfp1b=dft_calc.post_process_read_ae('wf-5p1.5')
          sbwfp2b=dft_calc.post_process_read_pp('wf-5p1.5')

          plt.plot(sbwfp1b[:,0],sbwfp1b[:,1],sbwfp2b[:,0],sbwfp2b[:,1])
          plt.ylim([-1,1])
          plt.xlim([0,8])
          plt.title('Antimony 5P J=3/2')
          plt.xlabel('radius (a.u.)')
```

Out [48]:
        <matplotlib.text.Text at 0x10a12e410>

Antimony 5P J=3/2

In [49]:
```python
#Selenium
os.chdir('/Users/shiangfang/Shiang DrobBox/Dropbox/Physics Research/Tim Kaxiras Group/

dft_job=job.job(subdir=False,job_manager_mode=False,write_post_process=False)
dft_calc=APE.calculator_APE(True,dft_job,None)
```
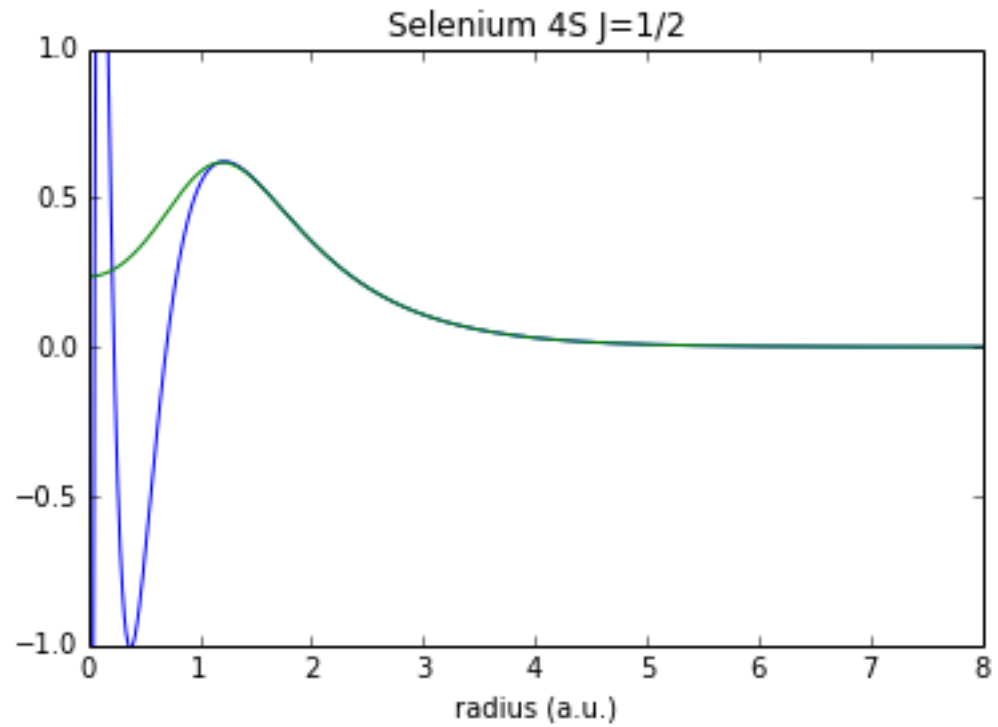
In [50]:
```python
sewfs1=dft_calc.post_process_read_ae('wf-4s0.5')
sewfs2=dft_calc.post_process_read_pp('wf-4s0.5')

plt.plot(sewfs1[:,0],sewfs1[:,1],sewfs2[:,0],sewfs2[:,1])
plt.ylim([-1,1])
plt.xlim([0,8])

plt.title('Selenium 4S J=1/2')
plt.xlabel('radius (a.u.)')
```
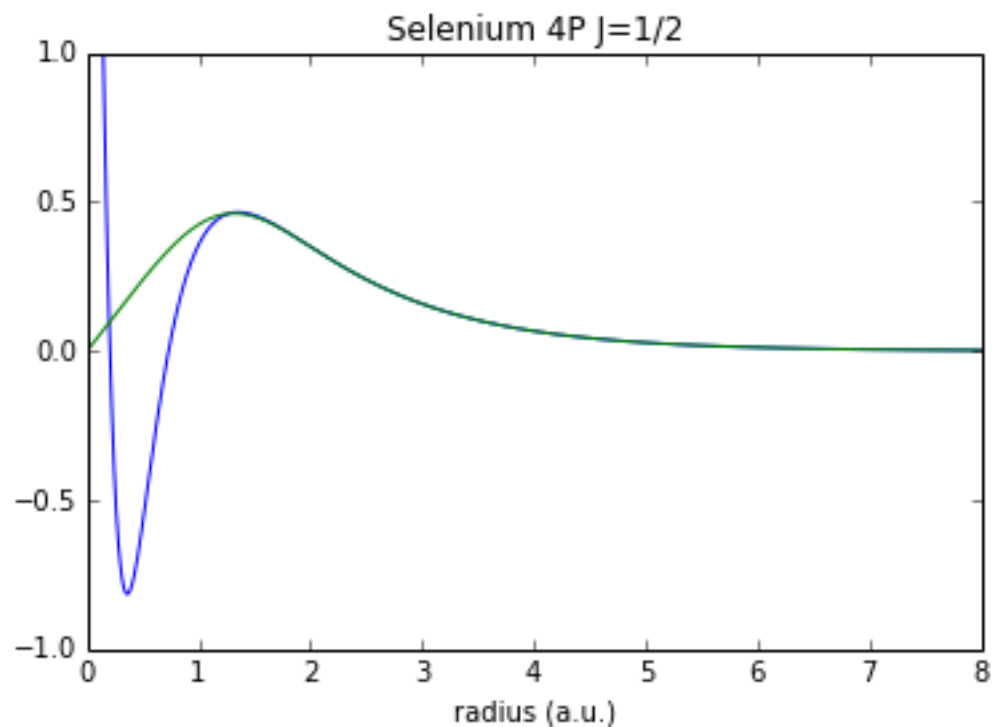
Out [50]:
```
<matplotlib.text.Text at 0x10a1c5d90>
```

Selenium 4S J=1/2

```
sewfp1=dft_calc.post_process_read_ae('wf-4p0.5')
sewfp2=dft_calc.post_process_read_pp('wf-4p0.5')

plt.plot(sewfp1[:,0],sewfp1[:,1],sewfp2[:,0],sewfp2[:,1])
plt.ylim([-1,1])
plt.xlim([0,8])
plt.title('Selenium 4P J=1/2')
plt.xlabel('radius (a.u.)')
```
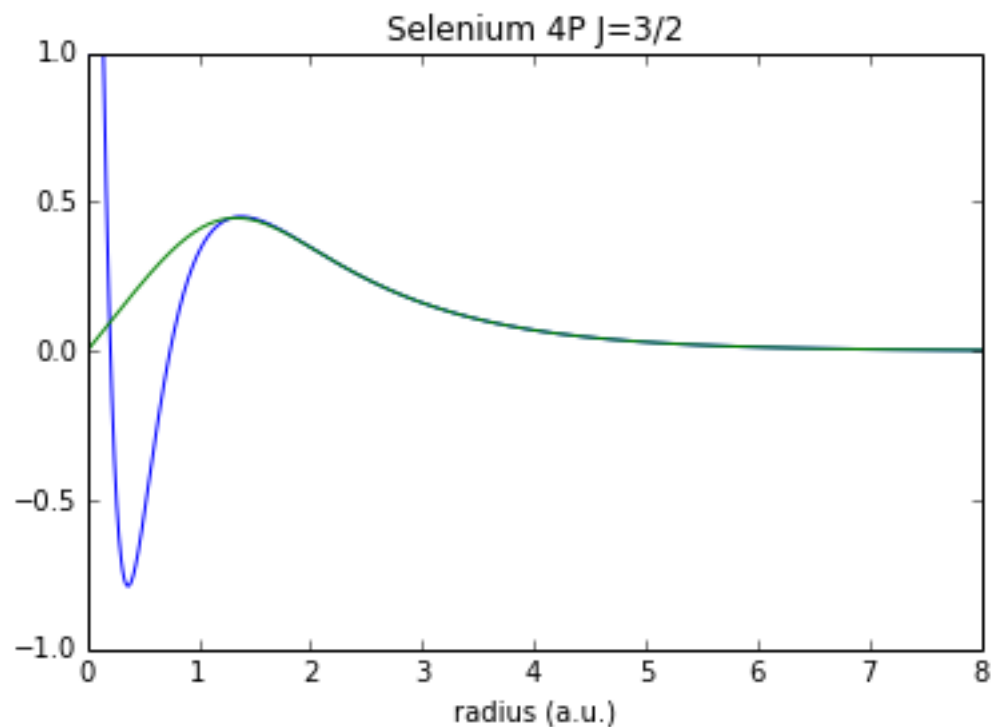
Out [51]:

```
<matplotlib.text.Text at 0x10a47a6d0>
```

Selenium 4P J=1/2

In [52]:
```python
sewfp1b=dft_calc.post_process_read_ae('wf-4p1.5')
sewfp2b=dft_calc.post_process_read_pp('wf-4p1.5')

plt.plot(sewfp1b[:,0],sewfp1b[:,1],sewfp2b[:,0],sewfp2b[:,1])
plt.ylim([-1,1])
plt.xlim([0,8])
plt.title('Selenium 4P J=3/2')
plt.xlabel('radius (a.u.)')
```

Out [52]:
```
<matplotlib.text.Text at 0x10a57c050>
```

Selenium 4P J=3/2

In [53]:
```
#Tellurium
os.chdir('/Users/shiangfang/Shiang DrobBox/Dropbox/Physics Research/Tim Kaxiras Group/

dft_job=job.job(subdir=False,job_manager_mode=False,write_post_process=False)
dft_calc=APE.calculator_APE(True,dft_job,None)
```

In [54]:
```
tewfs1=dft_calc.post_process_read_ae('wf-5s0.5')
tewfs2=dft_calc.post_process_read_pp('wf-5s0.5')

plt.plot(tewfs1[:,0],tewfs1[:,1],tewfs2[:,0],tewfs2[:,1])
plt.ylim([-1,1])
plt.xlim([0,8])
plt.title('Tellurium 5S J=1/2')
plt.xlabel('radius (a.u.)')
```
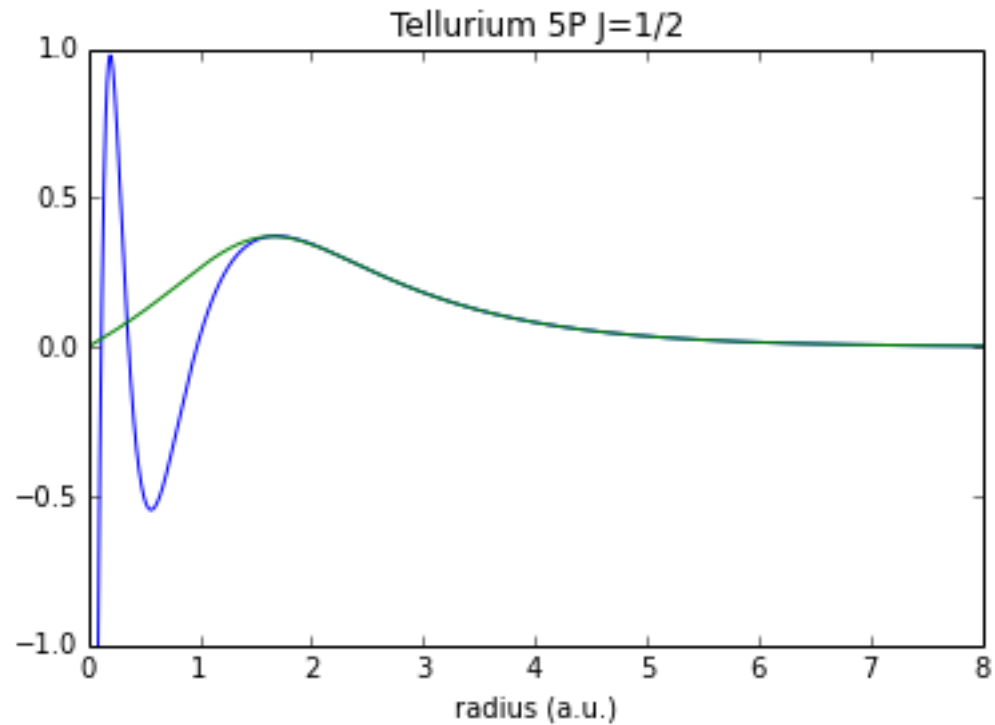
Out [54]:
```
<matplotlib.text.Text at 0x10a5ab950>
```
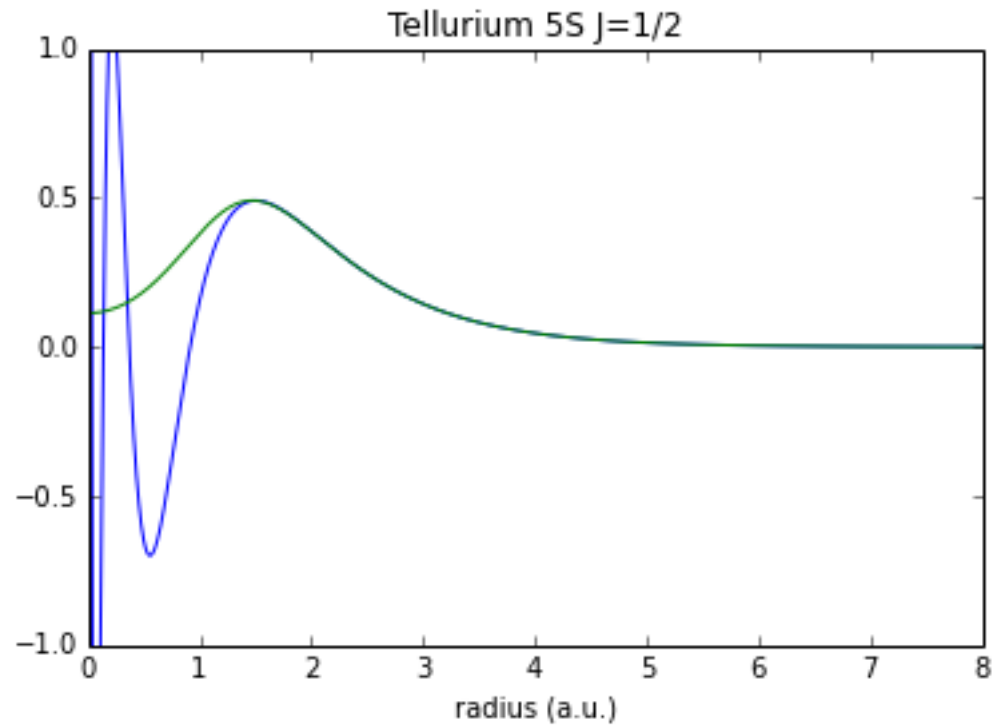
Tellurium 5S J=1/2

In [55]:
```
tewfp1=dft_calc.post_process_read_ae('wf-5p0.5')
tewfp2=dft_calc.post_process_read_pp('wf-5p0.5')

plt.plot(tewfp1[:,0],tewfp1[:,1],tewfp2[:,0],tewfp2[:,1])
plt.ylim([-1,1])
plt.xlim([0,8])
plt.title('Tellurium 5P J=1/2')
plt.xlabel('radius (a.u.)')
```

Out [55]:
```
<matplotlib.text.Text at 0x10a5dd290>
```

Tellurium 5P J=1/2

In [56]:
```python
tewfp1b=dft_calc.post_process_read_ae('wf-5p1.5')
tewfp2b=dft_calc.post_process_read_pp('wf-5p1.5')

plt.plot(tewfp1b[:,0],tewfp1b[:,1],tewfp2b[:,0],tewfp2b[:,1])
plt.ylim([-1,1])
plt.xlim([0,8])
plt.title('Tellurium 5P J=3/2')
plt.xlabel('radius (a.u.)')
```
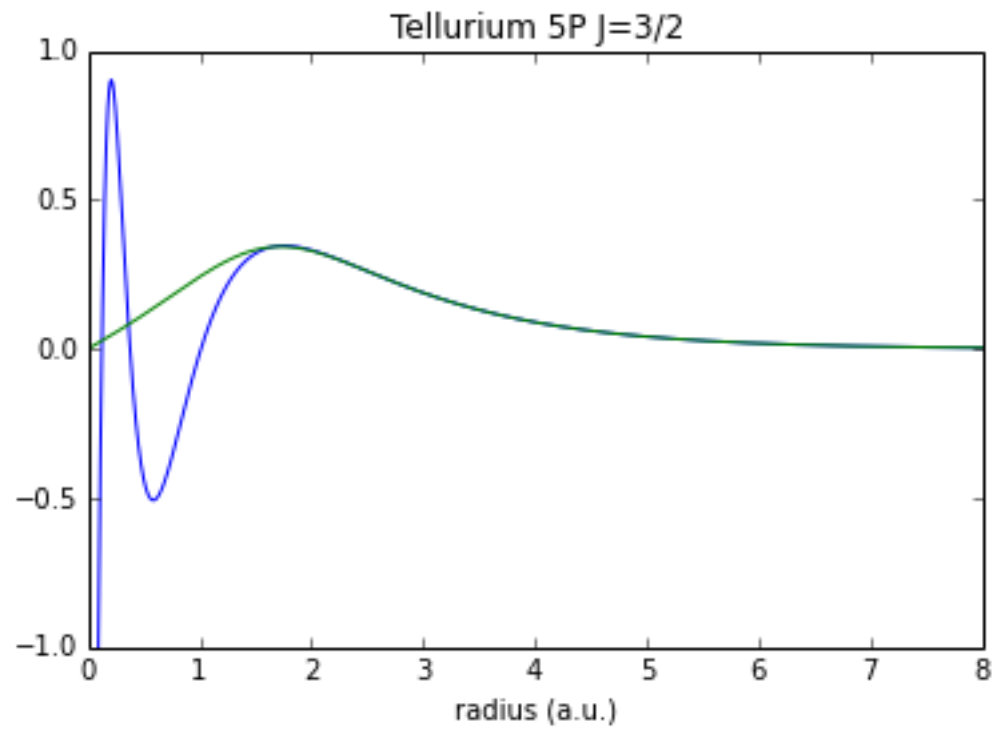
Out [56]:
```
<matplotlib.text.Text at 0x10b21ab90>
```

Tellurium 5P J=3/2

In [53]:

In [53]:

In [53]:

In []: