Test generation of the local potential

```
[5]    import numpy as np
       import matplotlib.pyplot as plt

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

```
[6]    from pstudio import AE, set_output
       from pstudio.vloc import generate_vloc_RRKJ, generate_vloc_TM
       from pstudio.RRKJ import pseudize_RRKJ
       from pstudio.TM import pseudize_TM
       #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
```

```
[7]    rc = 1.54
```

```
vloc_rrkj = generate_vloc_RRKJ(ae.vtot, ae.rgd, rc, verbose=True)
vloc_tm = generate_vloc_TM(ae.vtot, ae.rgd, rc, verbose=True)
```

```
Local potential from RRKJ2 pseudization: rc=1.5382
AE norm within rc        : +3615080.371537
0-th AE derivative at rc: -0.834982
1-th AE derivative at rc: +1.100612
2-th AE derivative at rc: -2.053259
qi                  :   [1.32483843 3.19755673]
estimated cutoff : 5.11218 Ha

Local potential from RRKJ2+TM pseudization: rc=1.5382
AE norm within rc        : +3615080.371537
0-th AE derivative at rc: -0.834982
1-th AE derivative at rc: +1.100612
2-th AE derivative at rc: -2.053259
qi                  :   3.1415921460855087
estimated cutoff : 4.9348 Ha
```
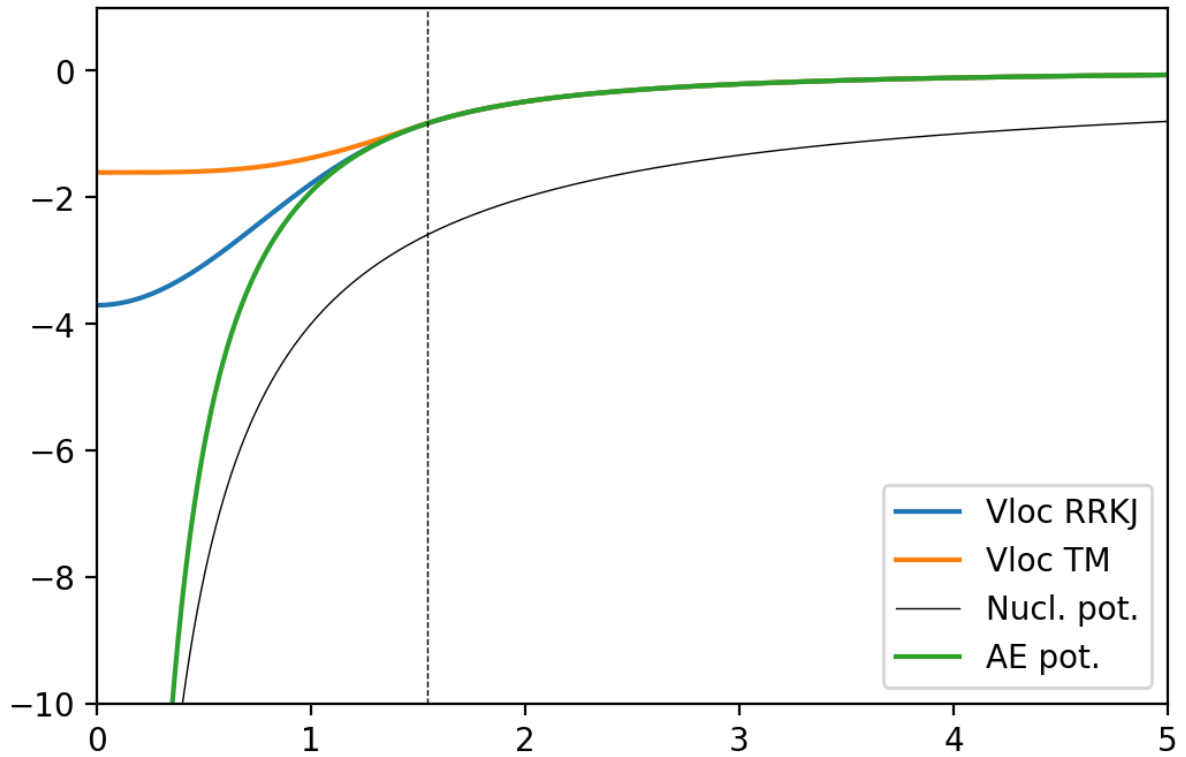
[8]
```python
r = ae.rgd.r
fig = plt.figure(figsize=(6,4), dpi=200)
plt.plot(r, vloc_rrkj, label='Vloc RRKJ')
plt.plot(r, vloc_tm, label='Vloc TM')
plt.plot(r, -4.0/r, color='black', linewidth=0.5, label='Nucl.
pot.')
plt.plot(r, ae.vtot, label='AE pot.')

plt.axvline(rc, linestyle='dashed', color='black', linewidth=0.5)
plt.xlim(0,5)
plt.ylim(-10,1)
plt.legend()
plt.show()
```

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

       q, fq = ae.rgd.fft(vloc_rrkj)
       plt.plot(0.5*q*q, fq*fq, label='Vloc RRKJ')

       q, fq = ae.rgd.fft(vloc_tm)
       plt.plot(0.5*q*q, fq*fq, label='Vloc TM')

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

       plt.ylim(1e-3,10)
       plt.yscale('log')
       plt.ylabel('|V(q)|$^2$')

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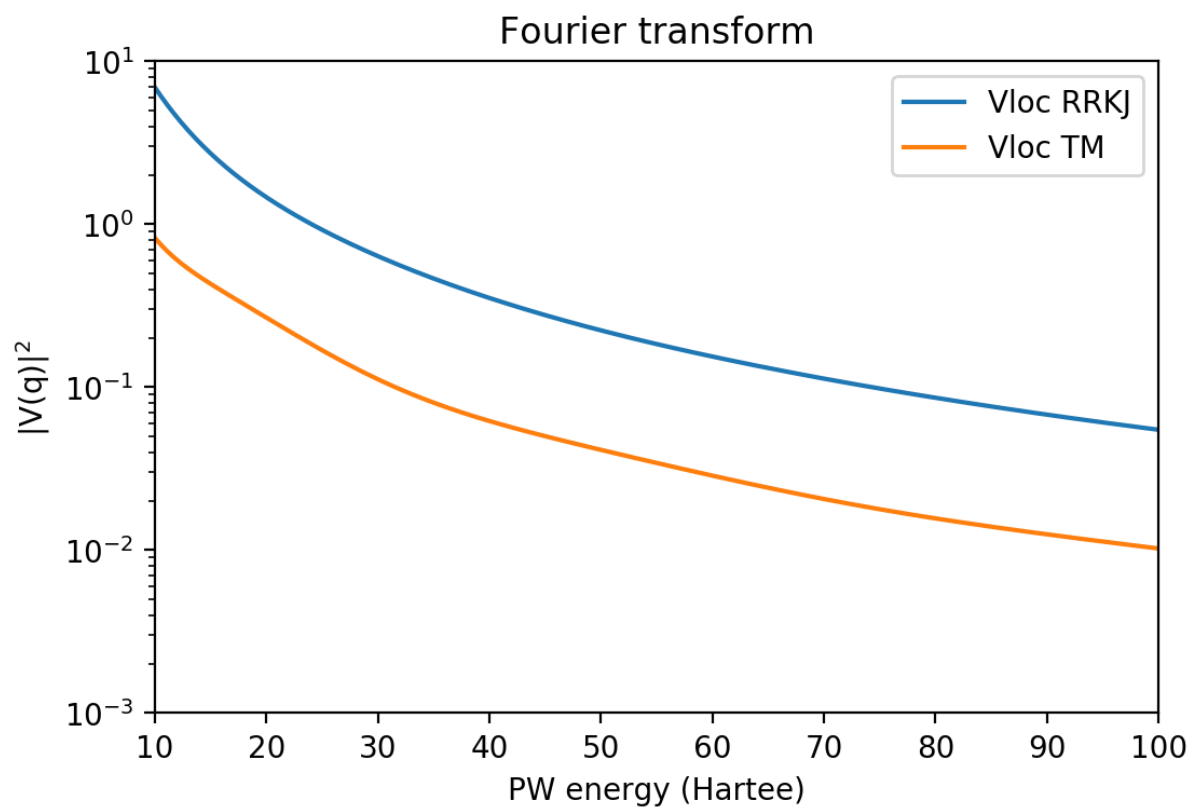
Fourier transform

[ ]

[ ]