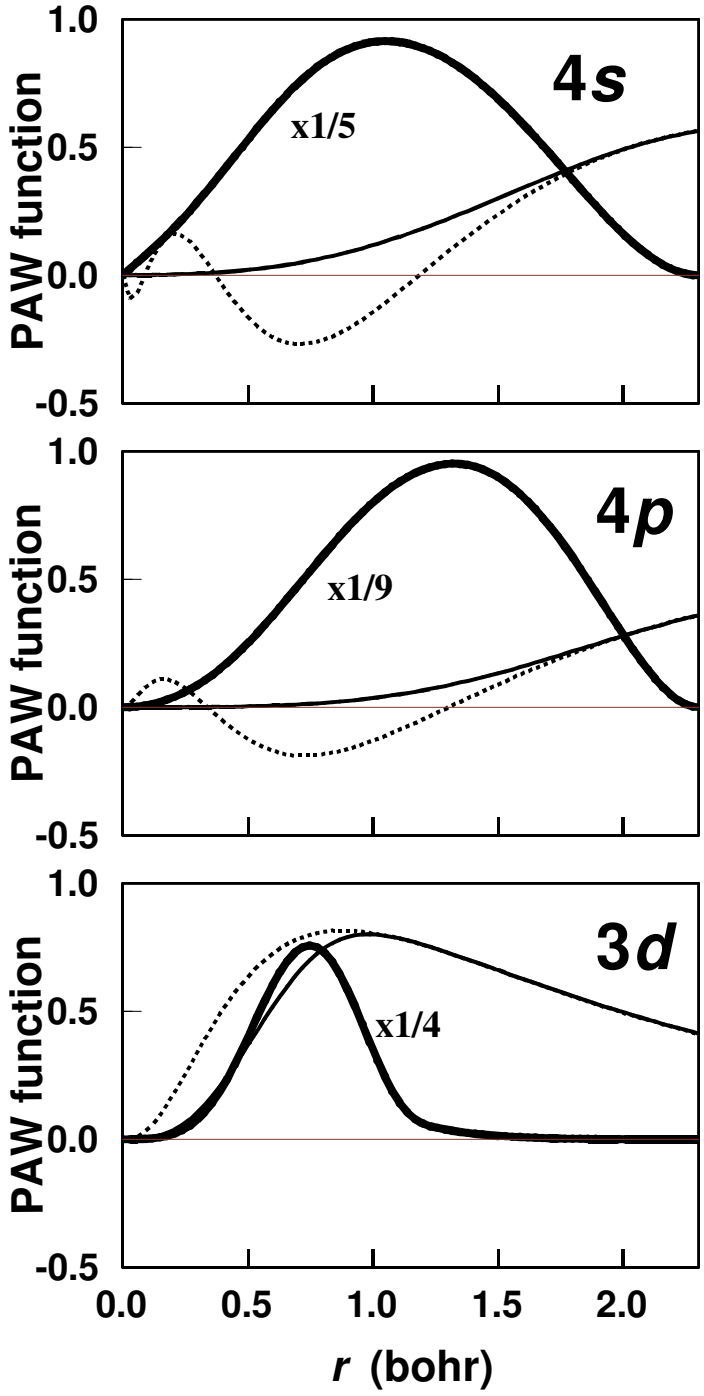
4s
x1/5
4p
x1/9
3d
x1/4
PAW function
1.0
0.5
0.0
-0.5
0.0
0.5
1.0
1.5
2.0
r (bohr)