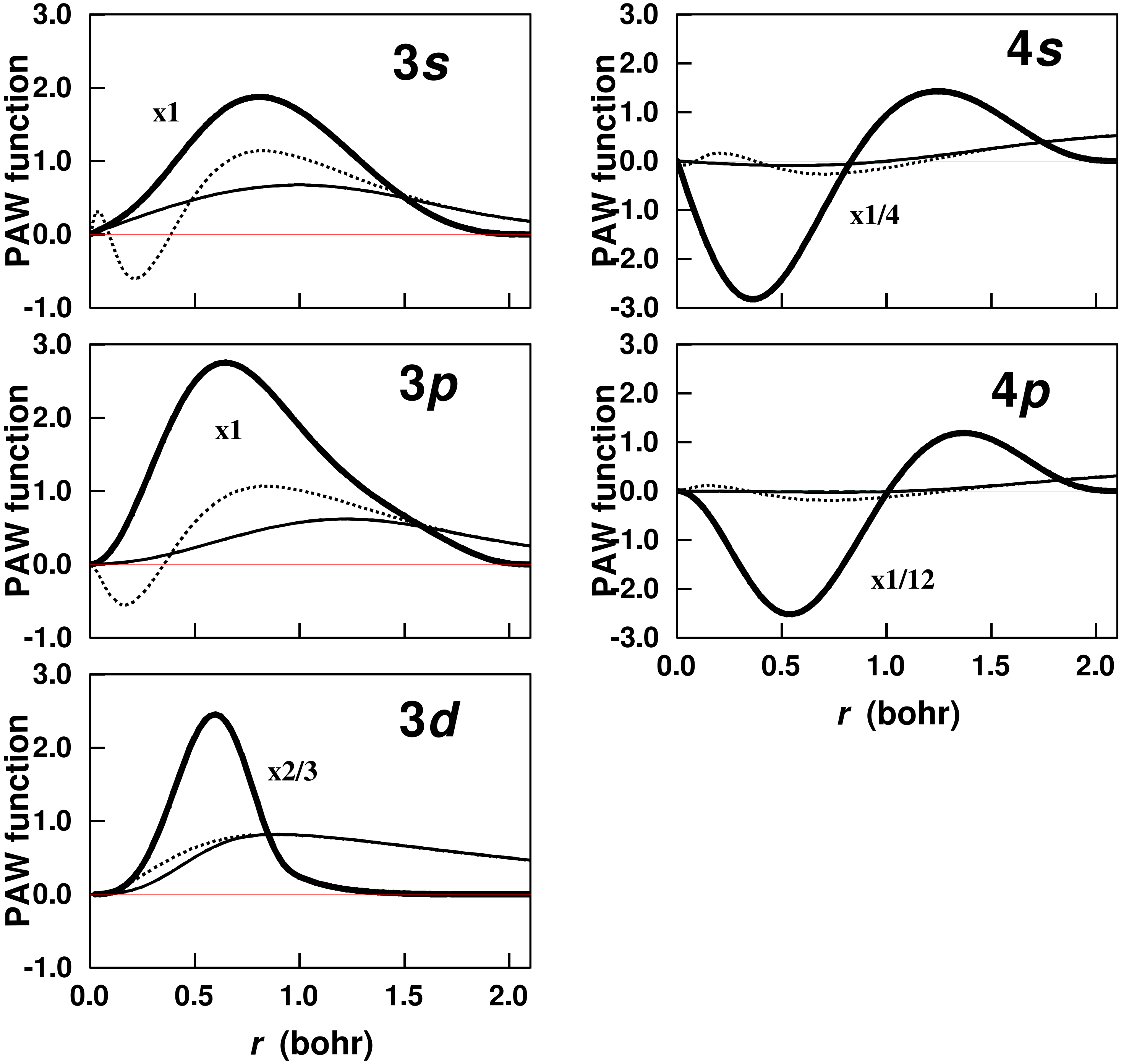
3s
x1
4s
x1/4
3p
x1
4p
x1/12
3d
x2/3
PAW function
r (bohr)
3.0
2.0
1.0
0.0
-1.0
-2.0
-3.0
0.0
0.5
1.0
1.5
2.0