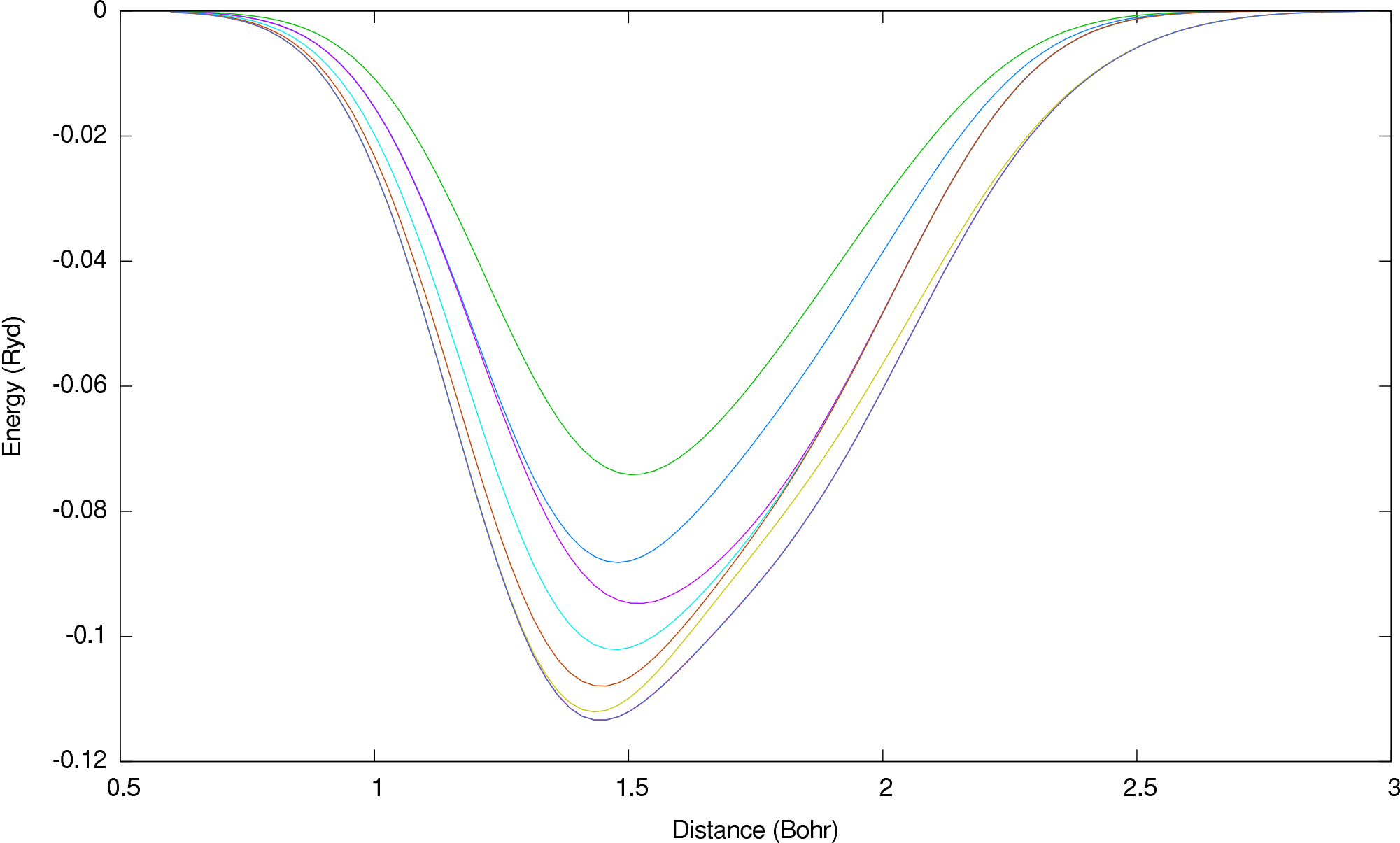
0
-0.02
-0.04
-0.06
-0.08
-0.1
-0.12
Energy (Ryd)
0.5
1
1.5
2
2.5
3
Distance (Bohr)