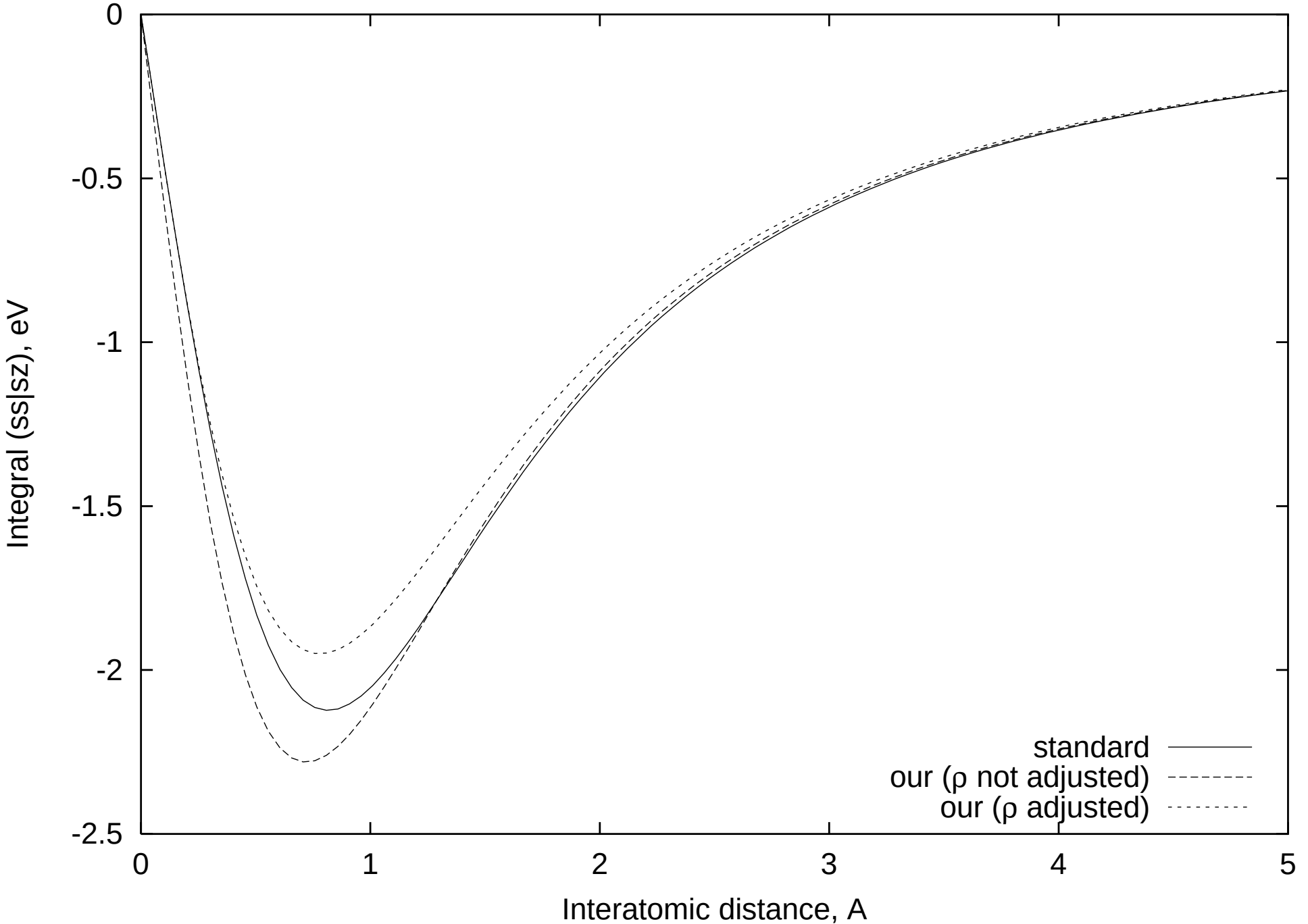
0
-0.5
-1
-1.5
-2
-2.5
Integral (ss|sz), eV
0
1
2
3
4
5
Interatomic distance, A
standard
our (ρ not adjusted)
our (ρ adjusted)