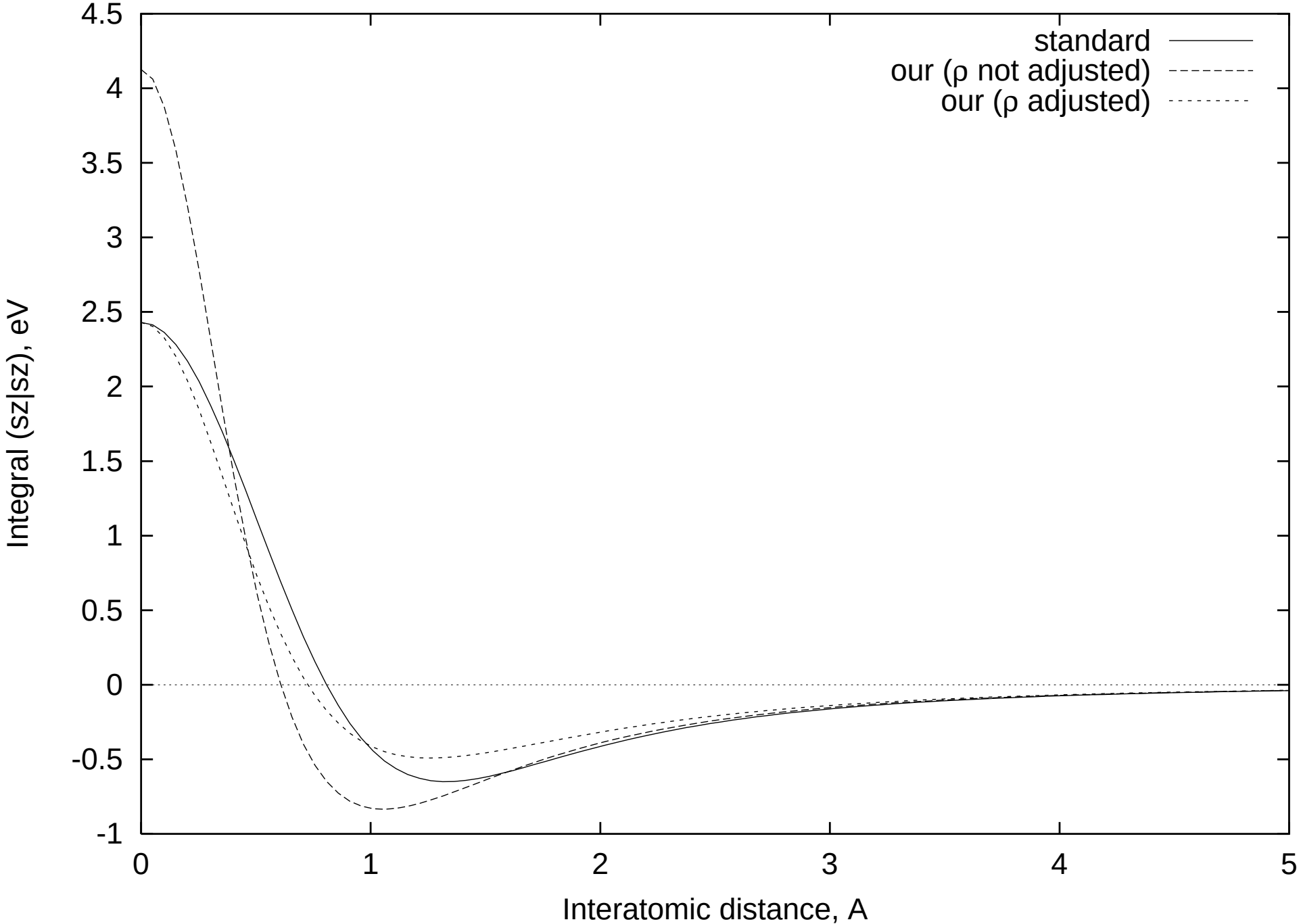
standard
our (ρ not adjusted)
our (ρ adjusted)
Integral (sz|sz), eV
Interatomic distance, A
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
-0.5
-1
0
1
2
3
4
5