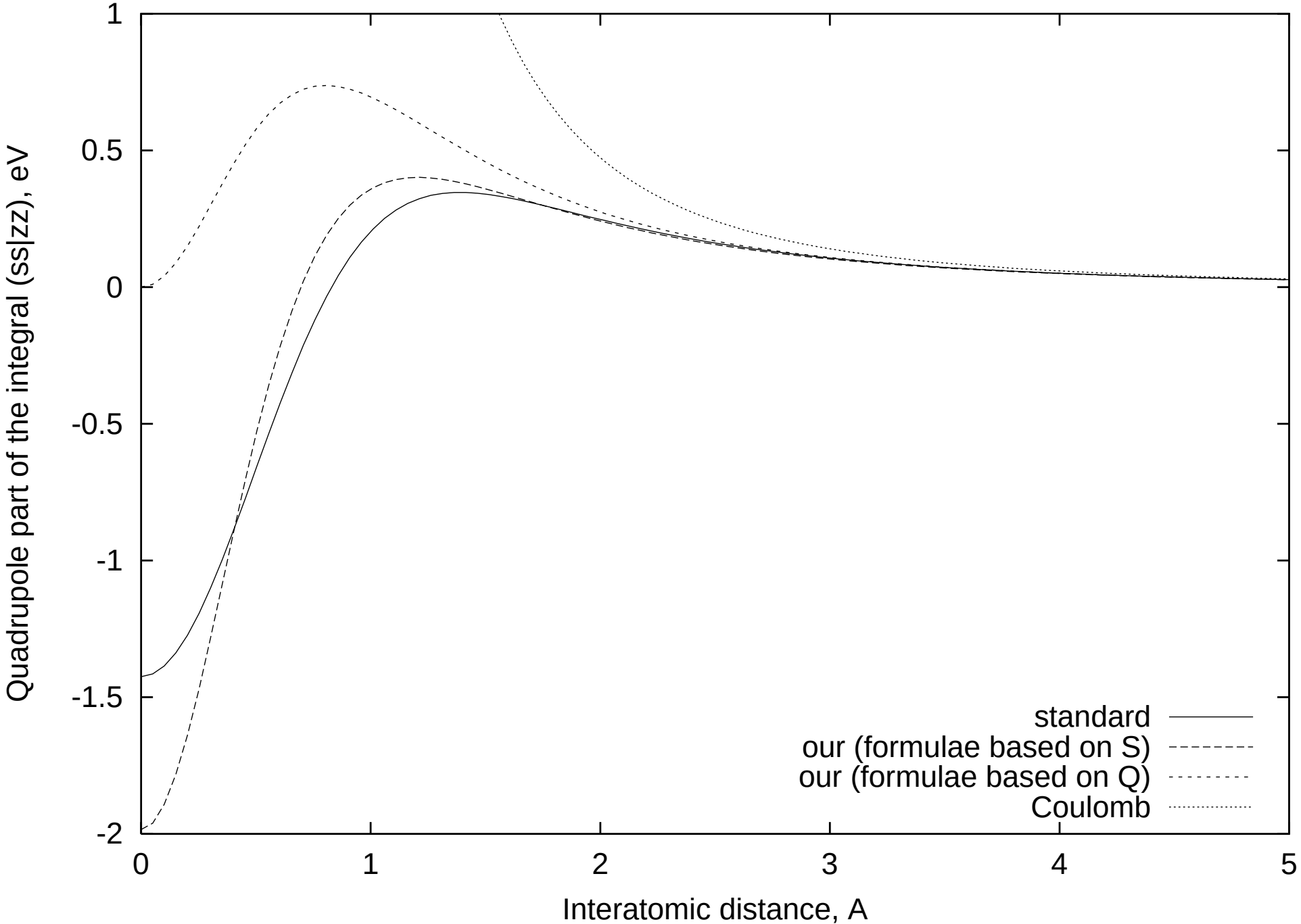
Quadrupole part of the integral (ss|zz), eV
Interatomic distance, A
1
0.5
0
-0.5
-1
-1.5
-2
0
1
2
3
4
5
standard
our (formulae based on S)
our (formulae based on Q)
Coulomb