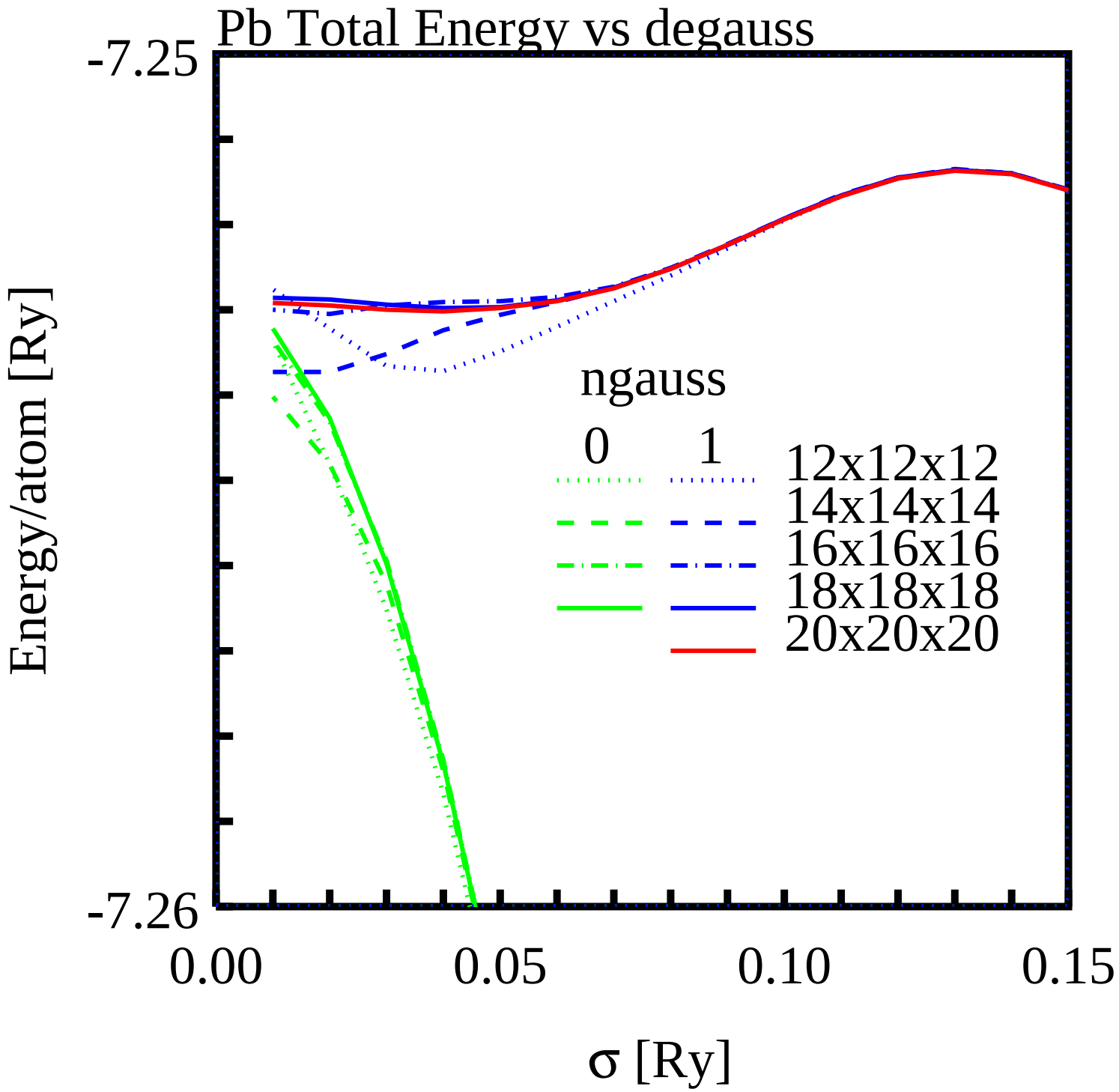
Pb Total Energy vs degauss
-7.25
-7.26
Energy/atom [Ry]
0.00
0.05
0.10
0.15
σ [Ry]
ngauss
0
1
12x12x12
14x14x14
16x16x16
18x18x18
20x20x20