Iteration & Convergence:

Condition:

$$Flag < EPS(10^{-8})$$

$$e^{-\lambda N_{loop}}$$

$$Flag = \sum_{abij} (\bar{H}_{ij}^{ab})^2$$

$$Flag = |E_{corr}^{new} - E_{corr}^{old}|$$

Limitation for convergence:

Particle number	SP number	g_min	g_max
4	4*2	-1	8
4	8*2	-1	36

Iteration & Convergence:

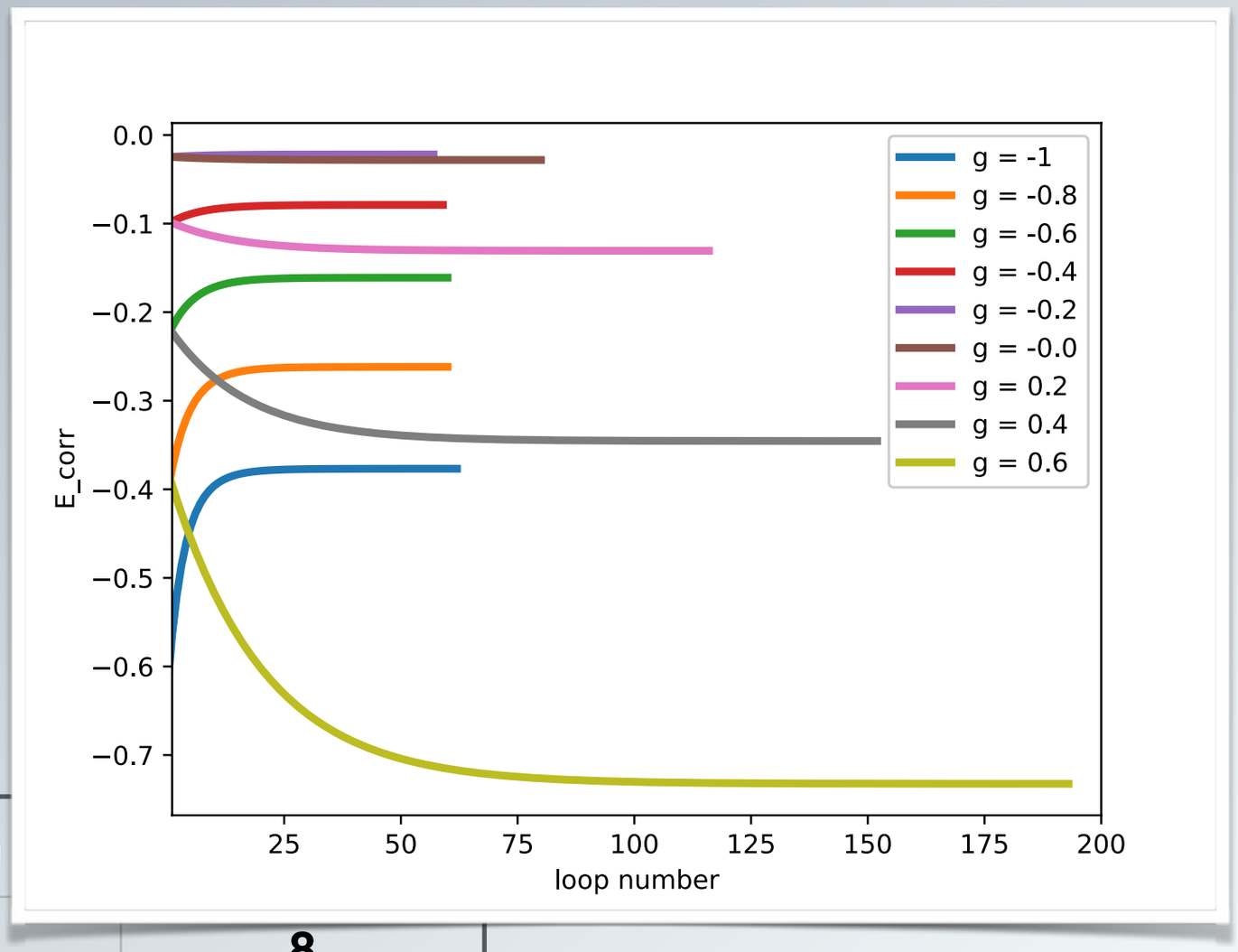
Condition:

$$Flag < EPS(10^{-8})$$

$$e^{-\lambda N_{loop}}$$

$$Flag = \sum_{abij} (\bar{H}_{ij}^{ab})^2$$

$$Flag = |E_{corr}^{new} - E_{corr}^{old}|$$



Limitation for convergence:

Particle number	SP number	g_min	
4	4*2	-1	8
4	8*2	-1	36

Iteration & Convergence:

Condition:

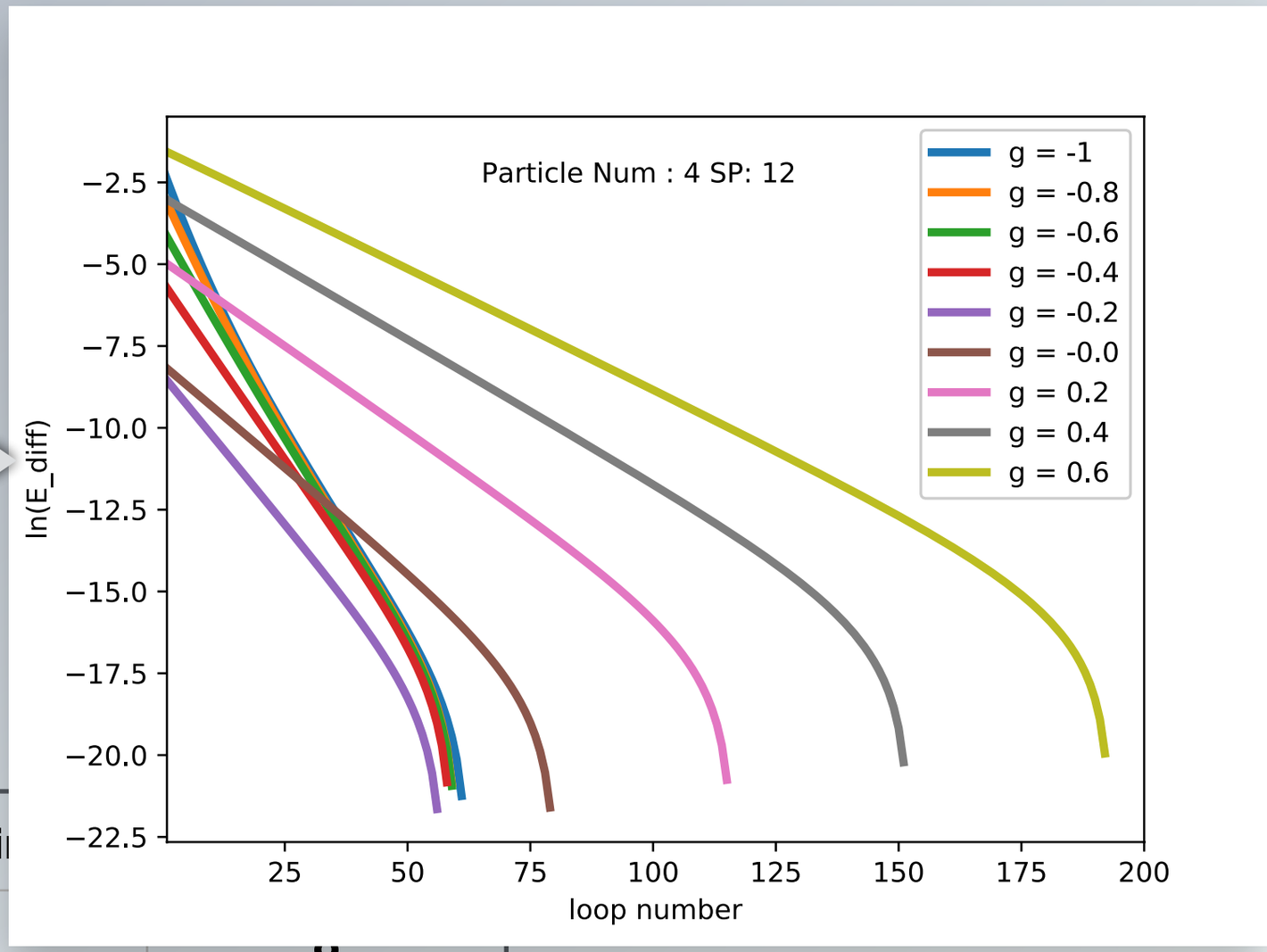
$$Flag < EPS(10^{-8})$$

$$e^{-\lambda N_{loop}}$$

$$Flag = \sum_{abij} (\bar{H}_{ij}^{ab})^2$$

$$Flag = |E_{corr}^{new} - E_{corr}^{old}|$$

$$log2(|E_{loop} - E_{final}|)$$



Limitation for convergence:

Particle number	SP number	g_mi	
4	4*2	-1	
4	8*2	-1	36

Iteration & Convergence:

Condition:

$$Flag < EPS(10^{-8})$$

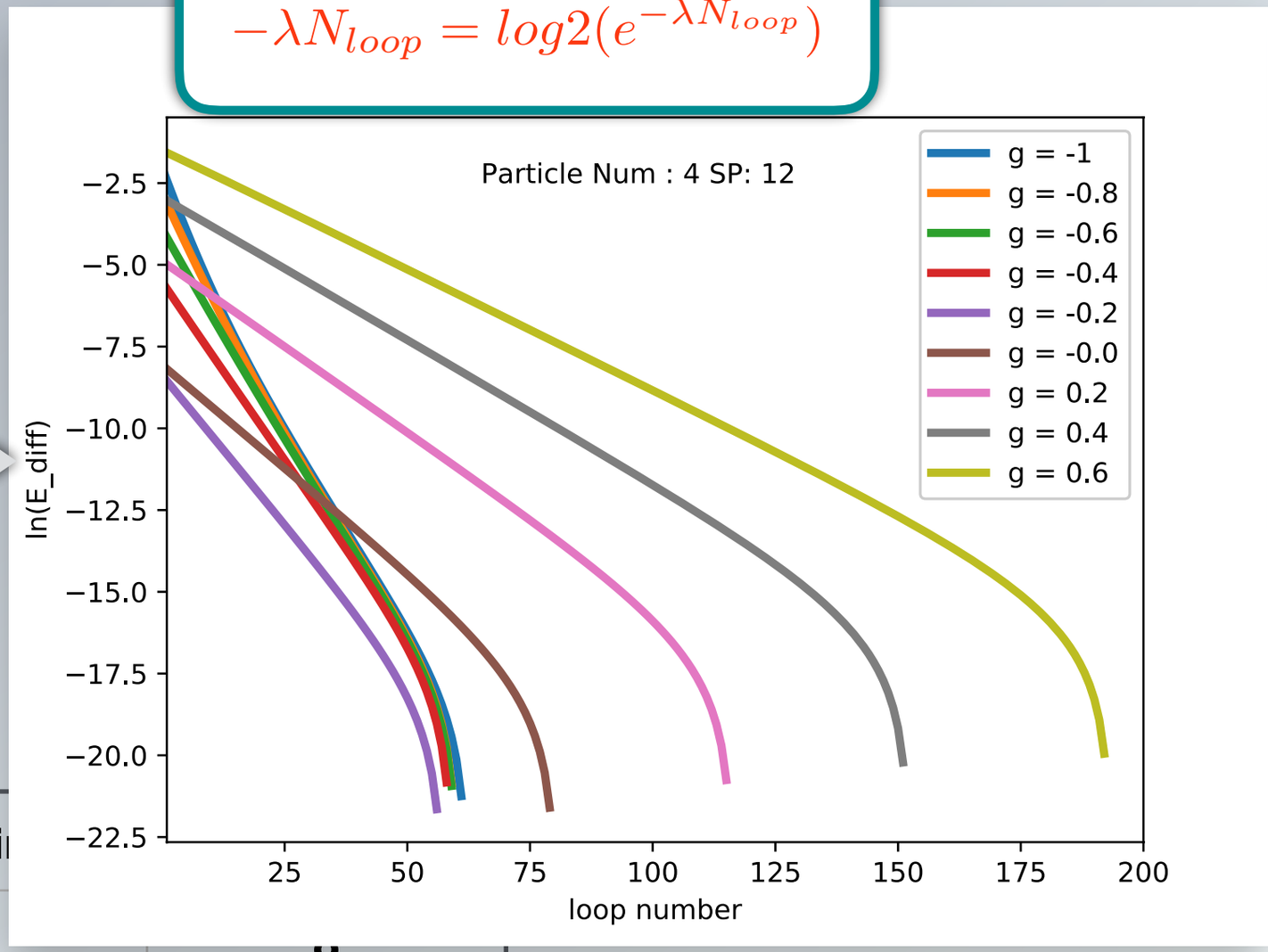
$$e^{-\lambda N_{loop}}$$

$$-\lambda N_{loop} = log2(e^{-\lambda N_{loop}})$$

$$Flag = \sum_{abij} (\bar{H}_{ij}^{ab})^2$$

$$Flag = |E_{corr}^{new} - E_{corr}^{old}|$$

$$log2(|E_{loop} - E_{final}|)$$



Limitation for convergence:

Particle number	SP number	g_mi	
4	4*2	-1	
4	8*2	-1	36

Iteration & Convergence:

Condition:

$$Flag < EPS(10^{-8})$$

$$e^{-\lambda N_{loop}}$$

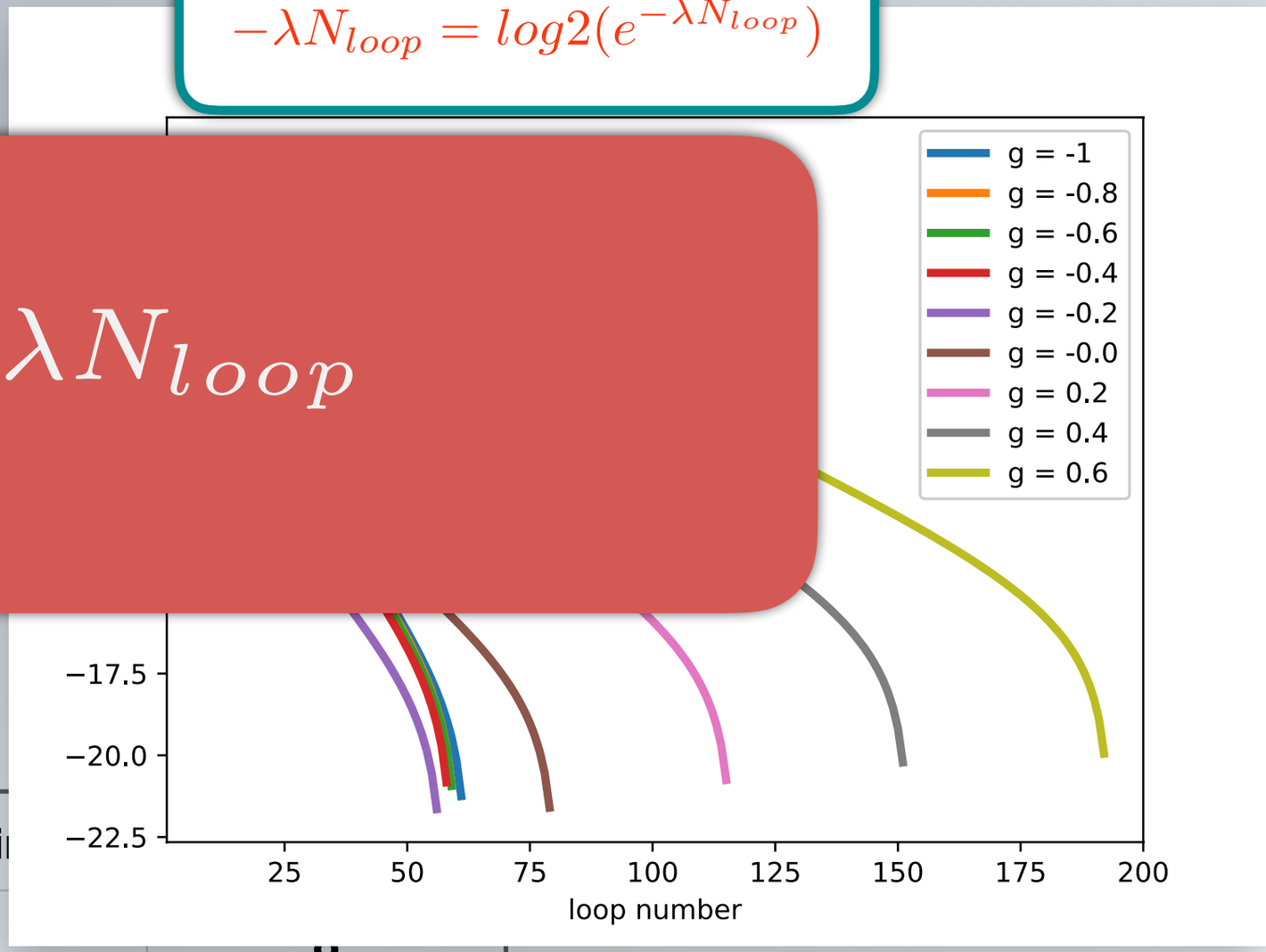
$$-\lambda N_{loop} = log2(e^{-\lambda N_{loop}})$$

$$Flag = \sum_{ab} (\bar{H}ab)2$$

$$Flag = |E$$

Follows:

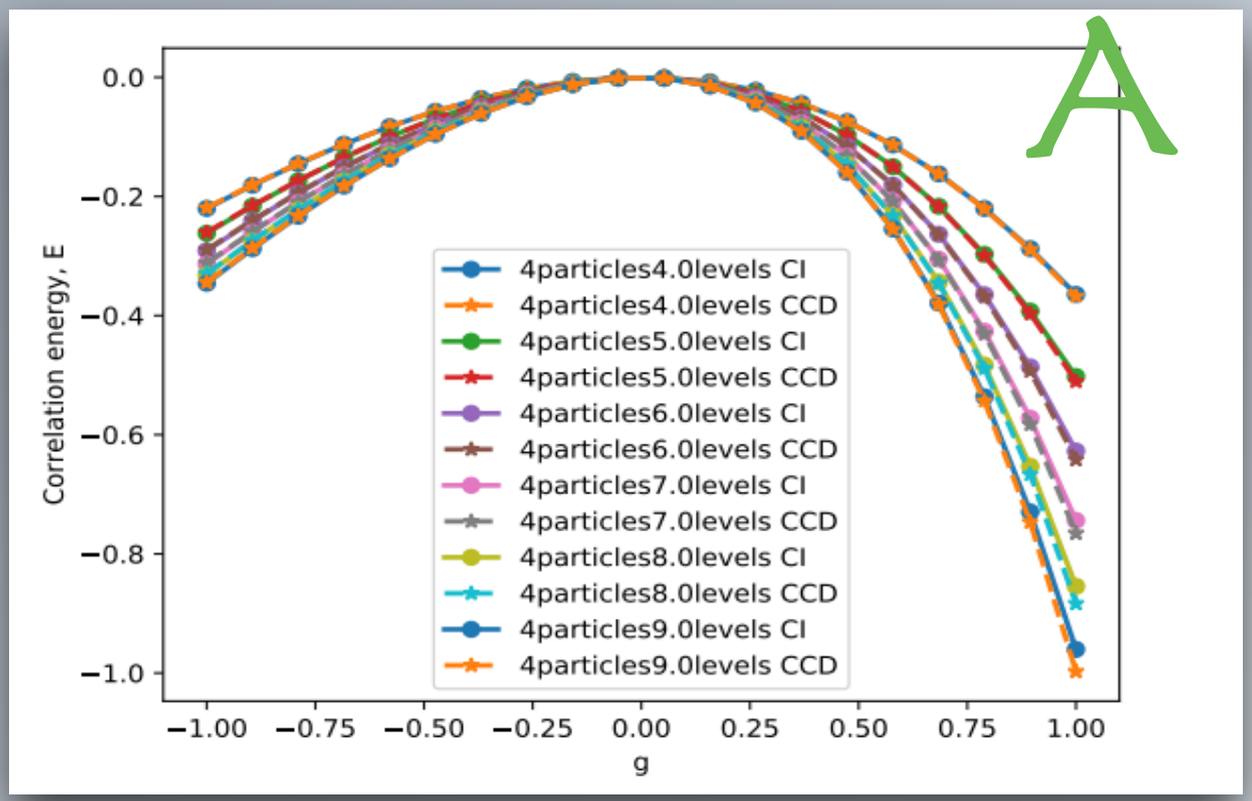
$$e^{-\lambda N_{loop}}$$

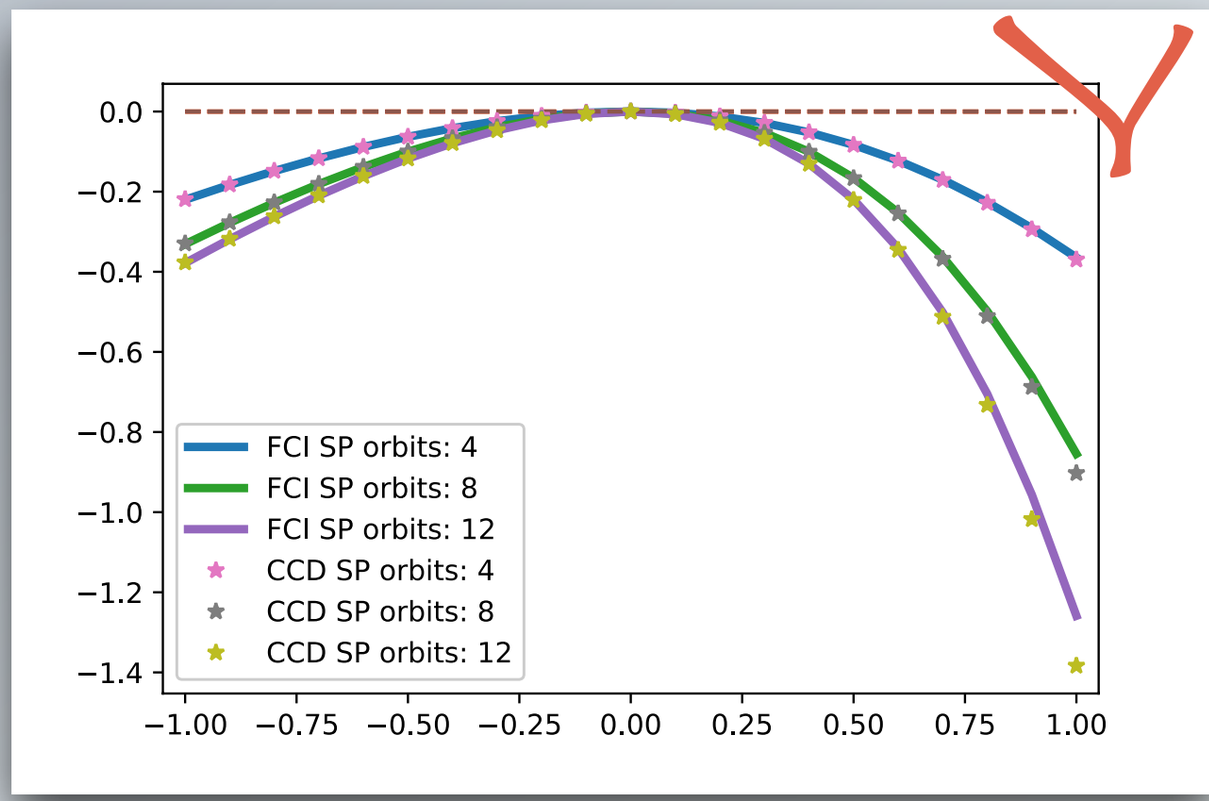


Limitation for convergence:

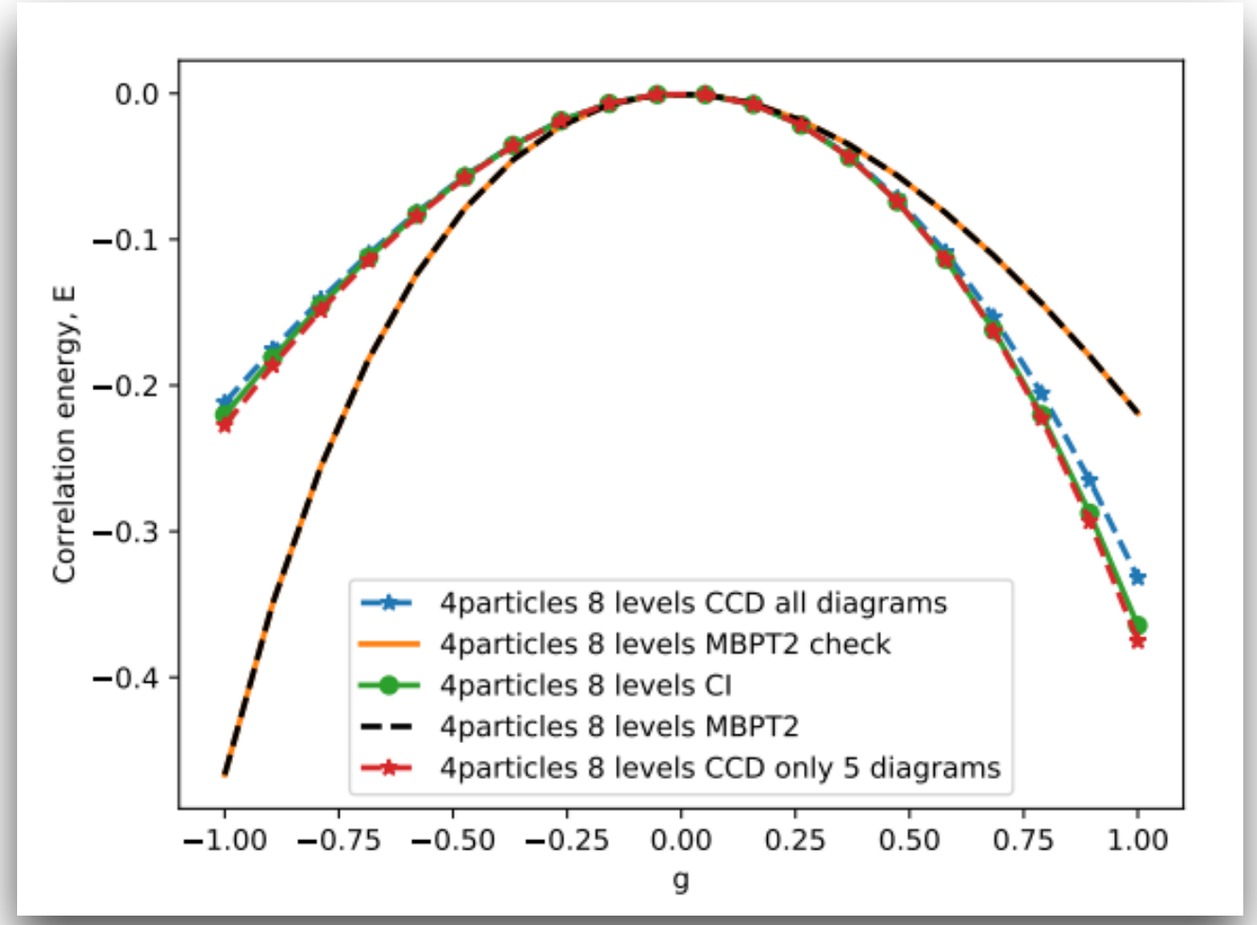
Particle number	SP number	g_mi	
4	4*2	-1	
4	8*2	-1	36

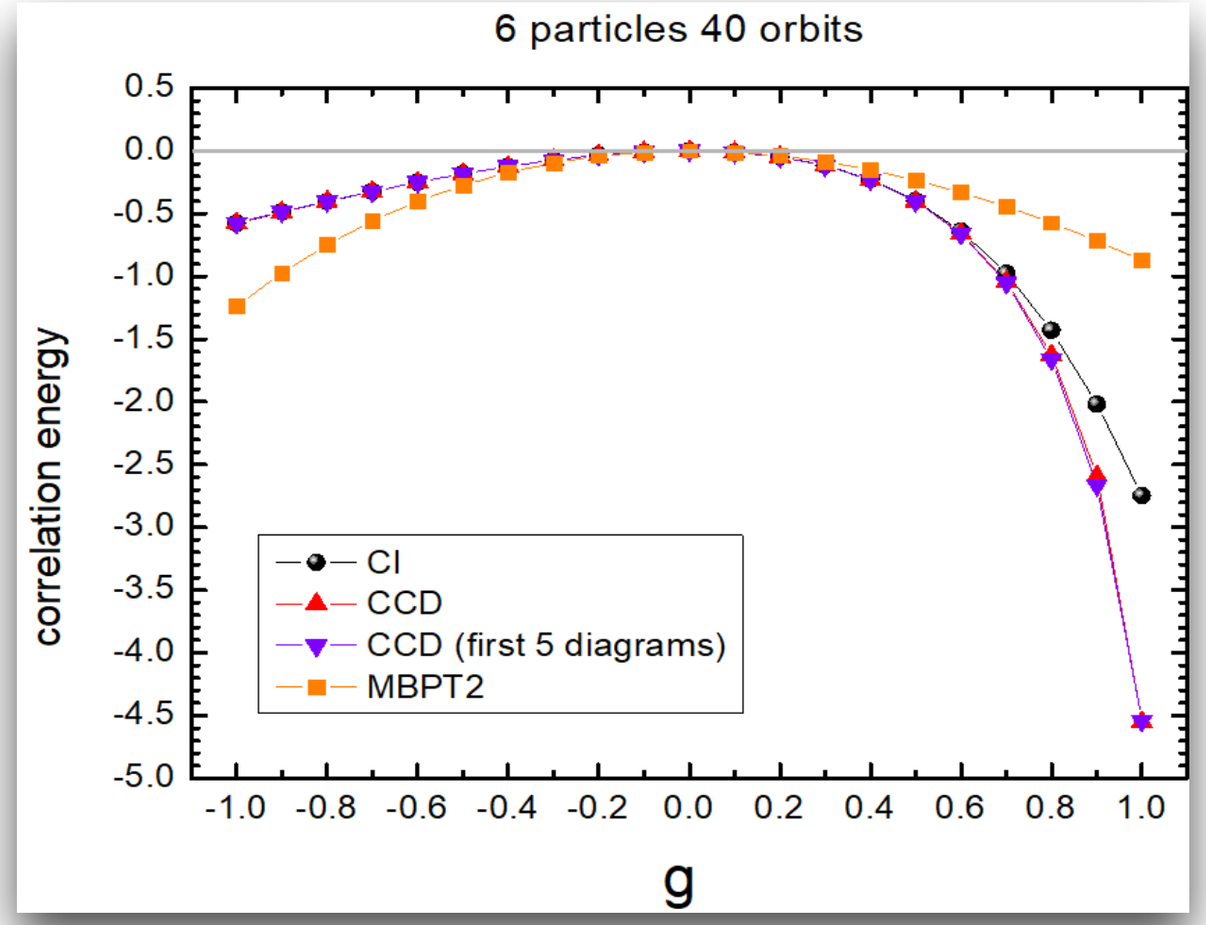
Comparison :


A
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
Correlation energy, E
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
g
4particles4.0levels CI
4particles4.0levels CCD
4particles5.0levels CI
4particles5.0levels CCD
4particles6.0levels CI
4particles6.0levels CCD
4particles7.0levels CI
4particles7.0levels CCD
4particles8.0levels CI
4particles8.0levels CCD
4particles9.0levels CI
4particles9.0levels CCD


Y
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
−1.2
−1.4
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
FCI SP orbits: 4
FCI SP orbits: 8
FCI SP orbits: 12
CCD SP orbits: 4
CCD SP orbits: 8
CCD SP orbits: 12

Results

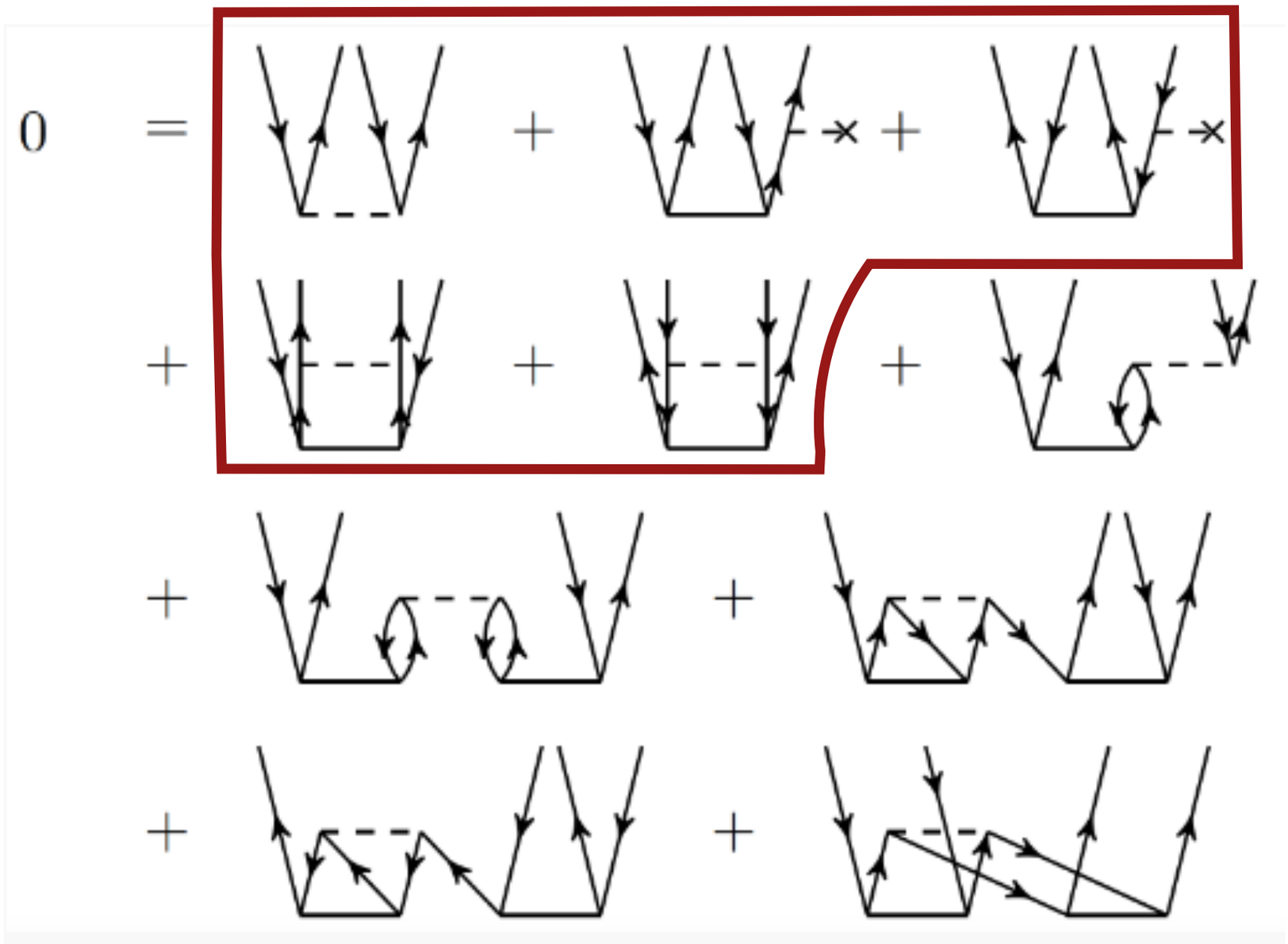




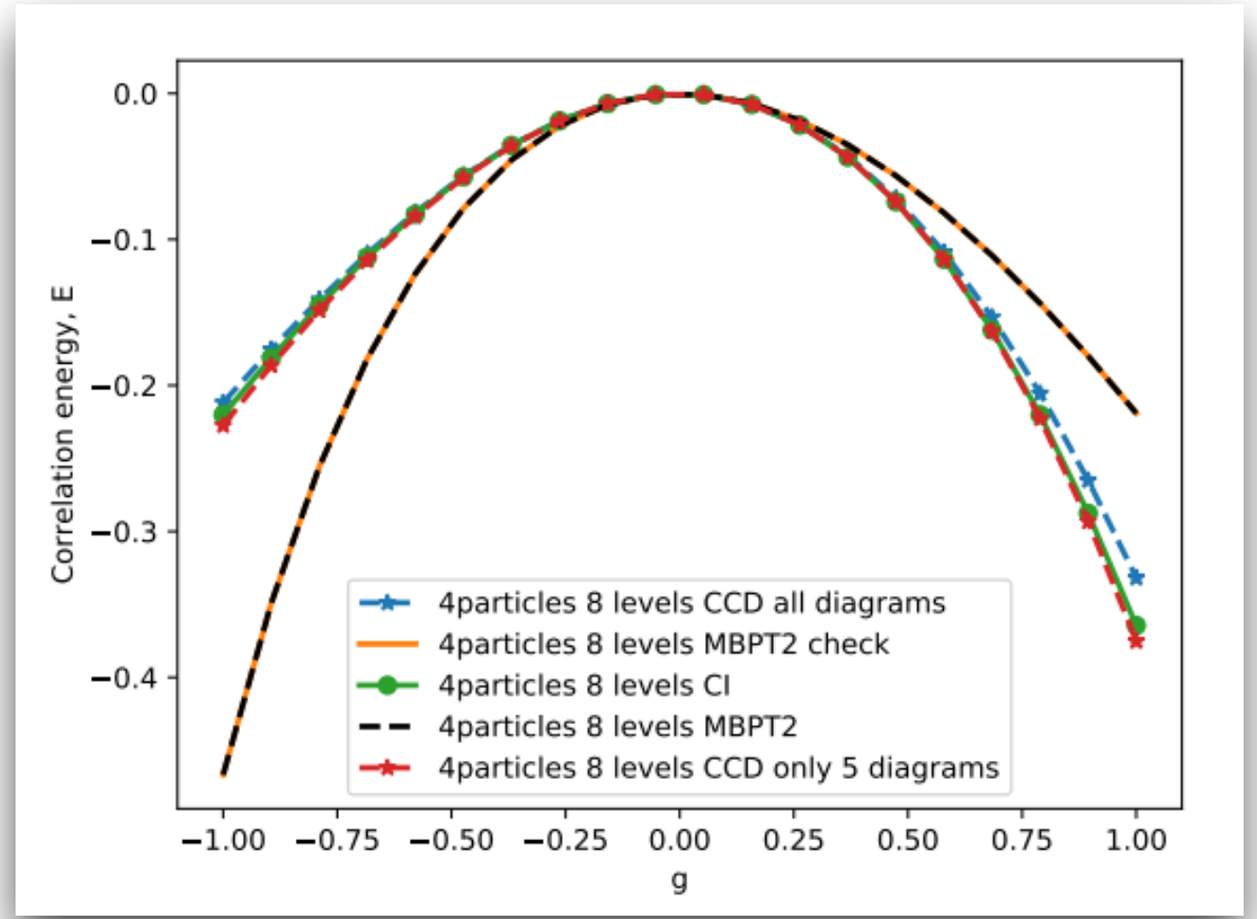
$$\Delta E^{(0)}_{\mathrm{CCD}} = \frac{1}{4}\sum_{abij}\langle ij|\hat{v}|ab\rangle (t^{ab}_{ij})^{(0)} = \frac{1}{4}\sum_{abij}\frac{\langle ij|\hat{v}|ab\rangle\langle ab|\hat{v}|ij\rangle}{(\epsilon_i+\epsilon_j-\epsilon_a-\epsilon_b)}.$$

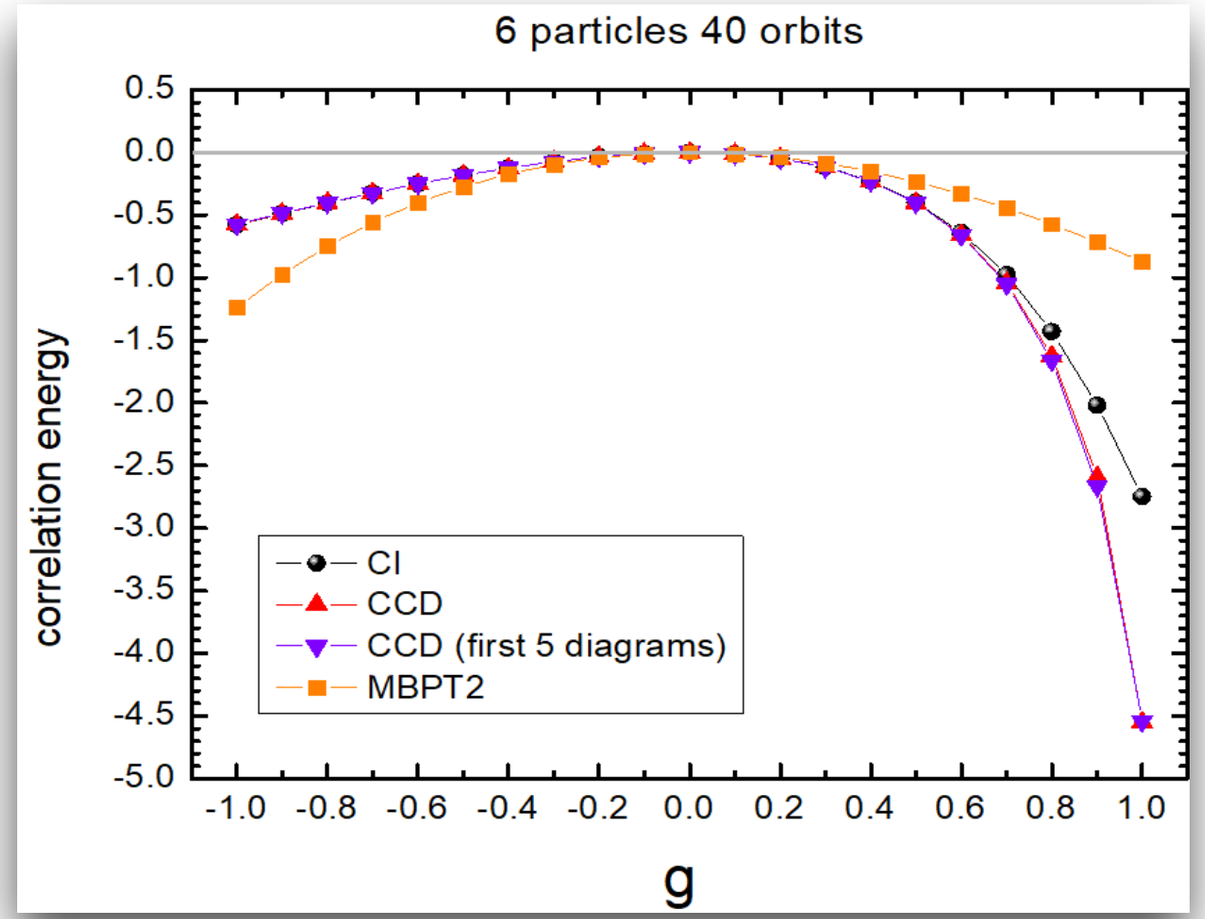
$$\Delta E_{MBPT2} = -\frac{g^2}{4}\left(\frac{1}{4+g}+\frac{1}{6+g}+\frac{1}{2+g}+\frac{1}{4+g}\right).$$

Results



Results


0.0
−0.1
−0.2
−0.3
−0.4
Correlation energy, E
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
g
4particles 8 levels CCD all diagrams
4particles 8 levels MBPT2 check
4particles 8 levels CI
4particles 8 levels MBPT2
4particles 8 levels CCD only 5 diagrams


6 particles 40 orbits
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
-3.0
-3.5
-4.0
-4.5
-5.0
correlation energy
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
0.2
0.4
0.6
0.8
1.0
g
CI
CCD
CCD (first 5 diagrams)
MBPT2

Thank you!

Group No.5

Yiyuan Cheng Adam Vernon Yuanzhuo Ma