

Configuration Interaction Theory

$$\begin{array}{cccc} H_{11} & H_{12} & H_{13} & \dots \\ H_{21} & H_{22} & H_{23} & \dots \\ H_{31} & H_{32} & H_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{array} \xrightarrow[U^{-1}HU]{U^{-1} = U^+} \begin{array}{ccc} E_1 & & \\ & E_2 & \\ & & E_3 \\ & & \ddots \end{array}$$

If basis-1 is reference state,

$$E_C = E_1 - H_{11}$$

Coupled Cluster Theory

$$H = E_{HF} + H_N$$

$$H_N = \sum_{pq} f_{pq} \{a_p^\dagger a_q\} + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle \{a_p^\dagger a_q^\dagger a_s a_r\}$$

$$\langle \Phi_0 | H_N | \Phi_0 \rangle = 0 \quad \{a_a^\dagger a_b^\dagger a_i^\dagger a_j^\dagger a_c a_d a_k a_l\} = a_a^\dagger a_b^\dagger a_k a_l a_c a_d a_i^\dagger a_j^\dagger$$

$$|\Phi_0\rangle, |\Phi_i^a\rangle, |\Phi_{ij}^{ab}\rangle, \dots$$

$$\langle \Phi_i^a | H_N | \Phi_0 \rangle = H_i^a = \langle \Phi_0 | H_N | \Phi_i^a \rangle = H_a^i,$$

$$\langle \Phi_{ij}^{ab} | H_N | \Phi_0 \rangle = H_{ij}^{ab} = \langle \Phi_0 | H_N | \Phi_{ij}^{ab} \rangle = H_{ab}^{ij},$$

Coupled Cluster Theory

$$\begin{array}{ccc} 0 & H_a^i & H_{ab}^{ij} \\ H_i^a & \ddots & \\ H_{ij}^{ab} & & \ddots \end{array}$$

$$T = \sum_{ia} t_i^a a_a^\dagger a_i + \frac{1}{4} \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i$$



$$\overline{H} = e^{-T} H_N e^T$$

$$\begin{array}{ccc} E_c & \overline{H}_a^i & \overline{H}_{ab}^{ij} \\ 0 & \ddots & \\ 0 & & \ddots \end{array}$$

$$E_c = \sum_{ia} f_a^i t_i^a + \frac{1}{4} \sum_{ijab} \langle ij | V | ab \rangle t_{ij}^{ab} + \frac{1}{2} \sum_{ijab} \langle ij | V | ab \rangle t_i^a t_j^b$$



Coupled Cluster Theory

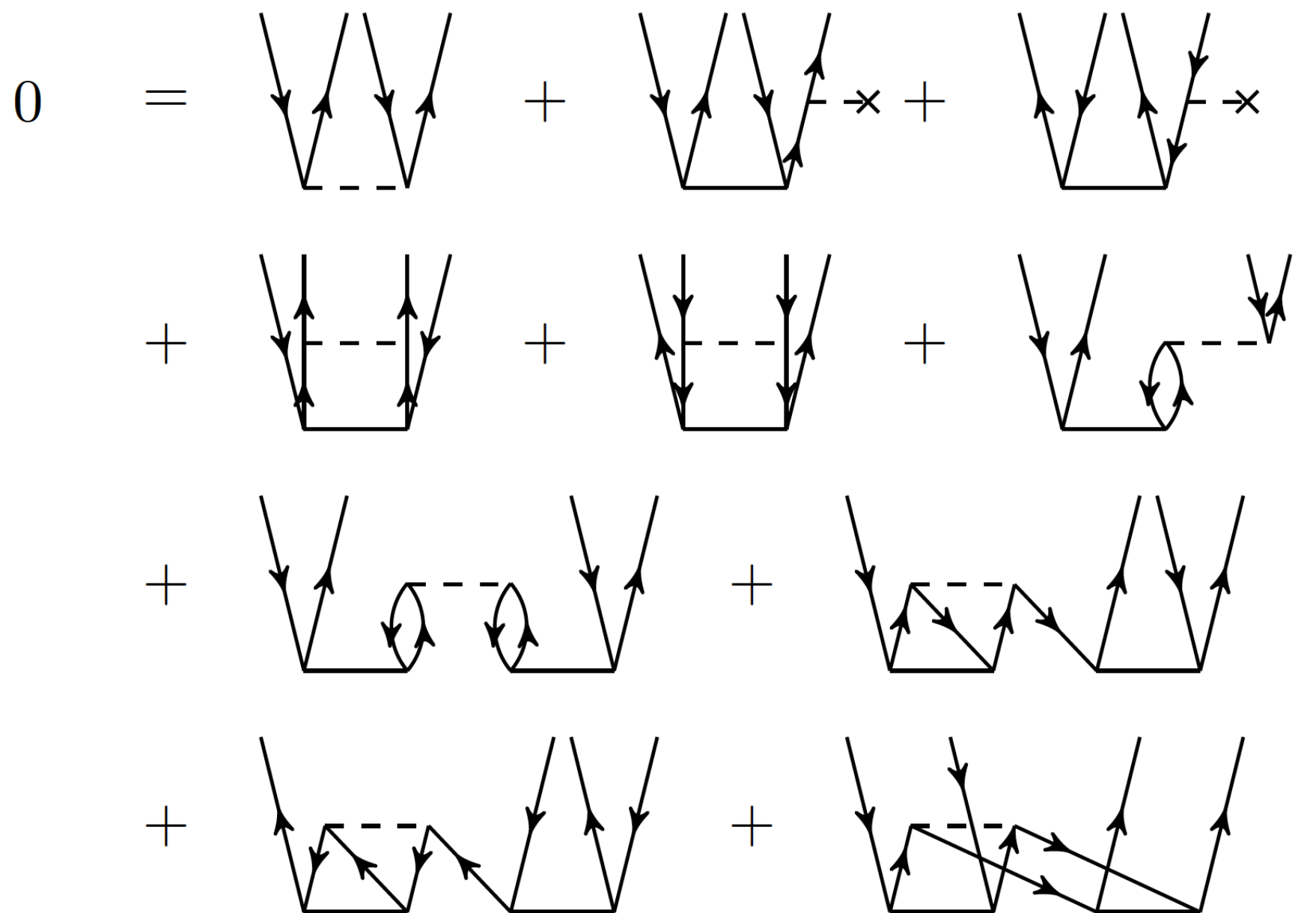
$$0 = \langle \Phi_{ij}^{ab} | e^{-T} H_N e^T | \Phi_0 \rangle = \langle \Phi_0 | a_i^\dagger a_j^\dagger a_b a_a e^{-T} H_N e^T | \Phi_0 \rangle$$

$$\begin{aligned} e^{-T} H_N e^T &= H_N + [H_N, T] + 1/2! [[H_N, T], T] \\ &\quad + 1/3! [[[H_N, T], T], T] + \dots \\ &= \dots + A_{ij}^{ab} a_a^\dagger a_b^\dagger a_i a_j + \dots \end{aligned}$$

$$0 = \langle \Phi_{ij}^{ab} | e^{-T} H_N e^T | \Phi_0 \rangle = A_{ij}^{ab}$$

Coupled Cluster Theory

$$0 = \langle \Phi_{ij}^{ab} | e^{-T} H_N e^T | \Phi_0 \rangle = \langle \Phi_0 | a_i^\dagger a_j^\dagger a_b a_a e^{-T} H_N e^T | \Phi_0 \rangle$$



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:



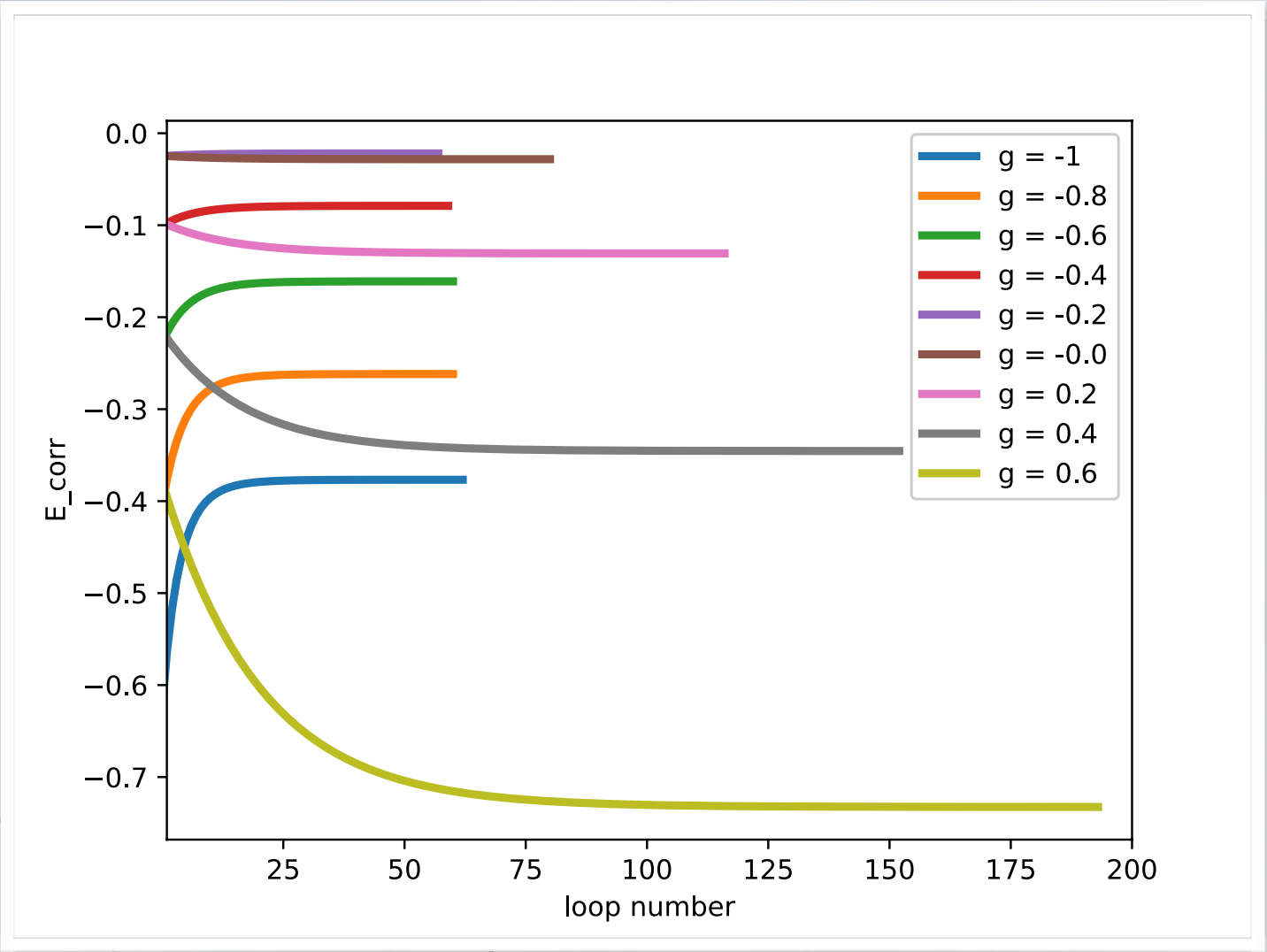
Condition:

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

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

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

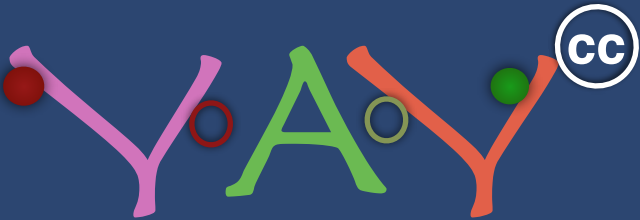
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Limitation for convergence:

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Iteration & Convergence:



Condition:

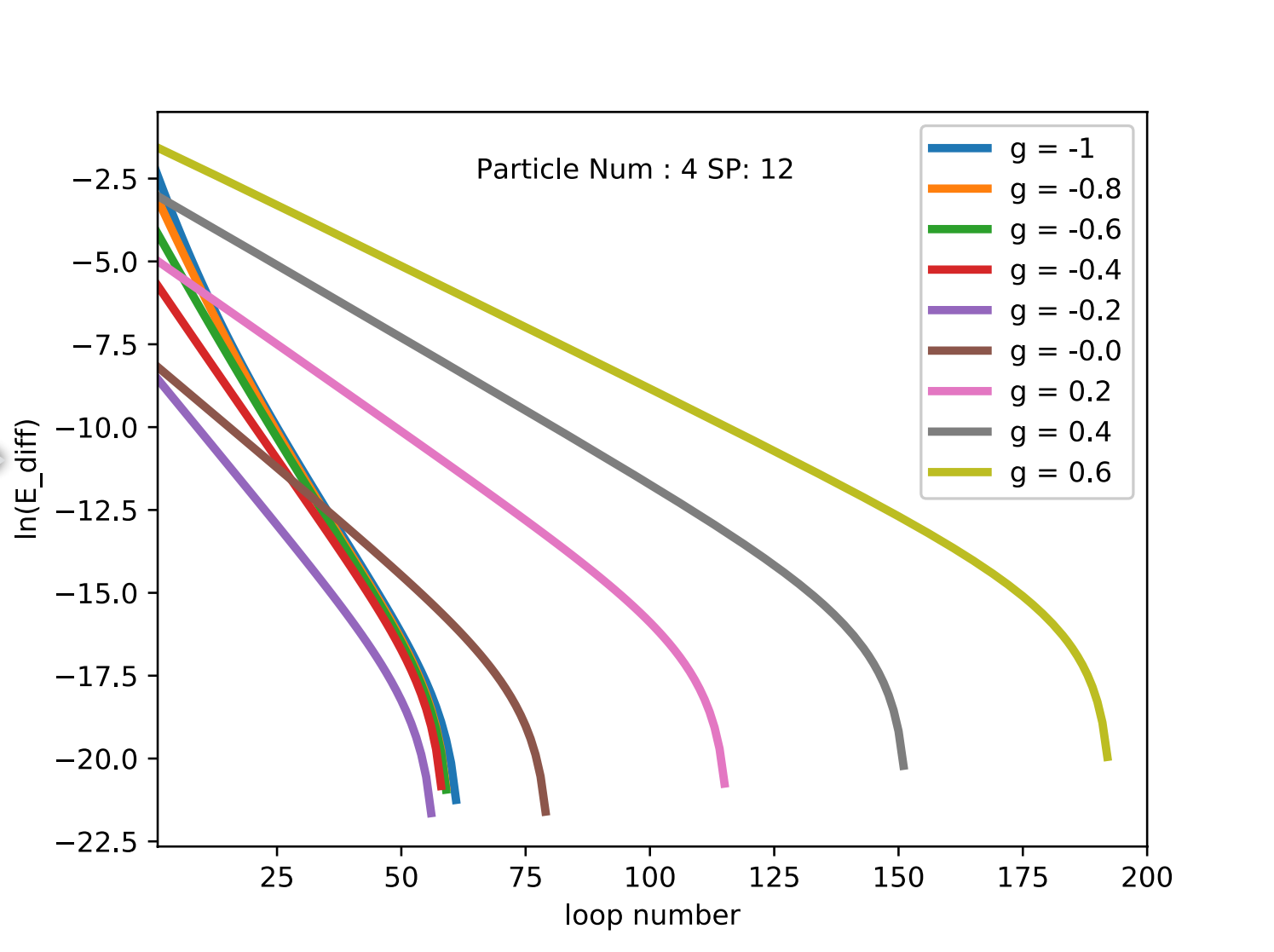
$$Flag < EPS(10^{-8})$$

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

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

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

$$\log_2(|E_{loop} - E_{final}|)$$



Limitation for convergence:

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Iteration & Convergence:



Condition:

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

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

$$-\lambda N_{loop} = \log_2(e^{-\lambda N_{loop}})$$

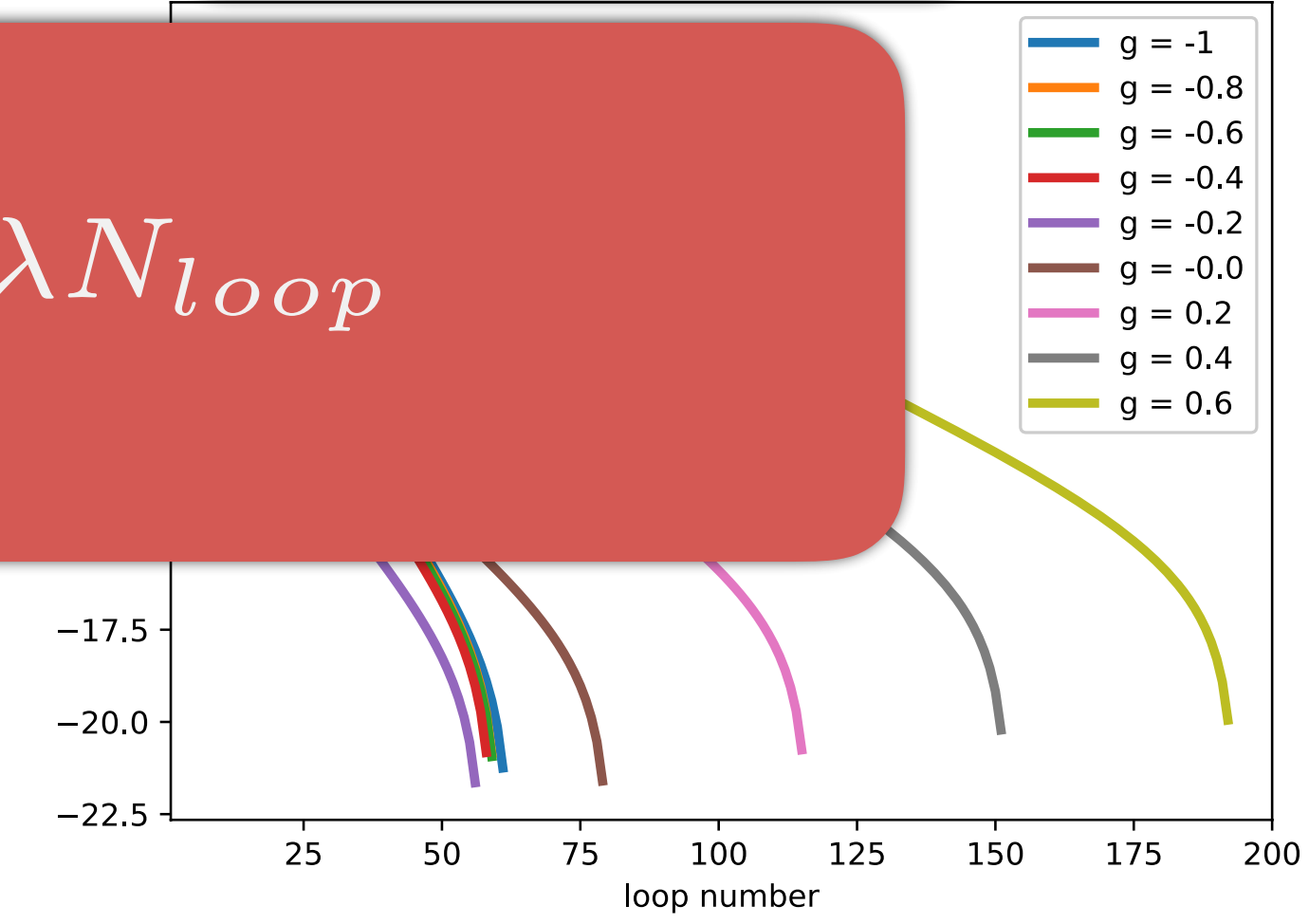
$$Flag = \sum_{ab} (\bar{r}_{ab})^2$$

$$Flag = |E$$

Follows:

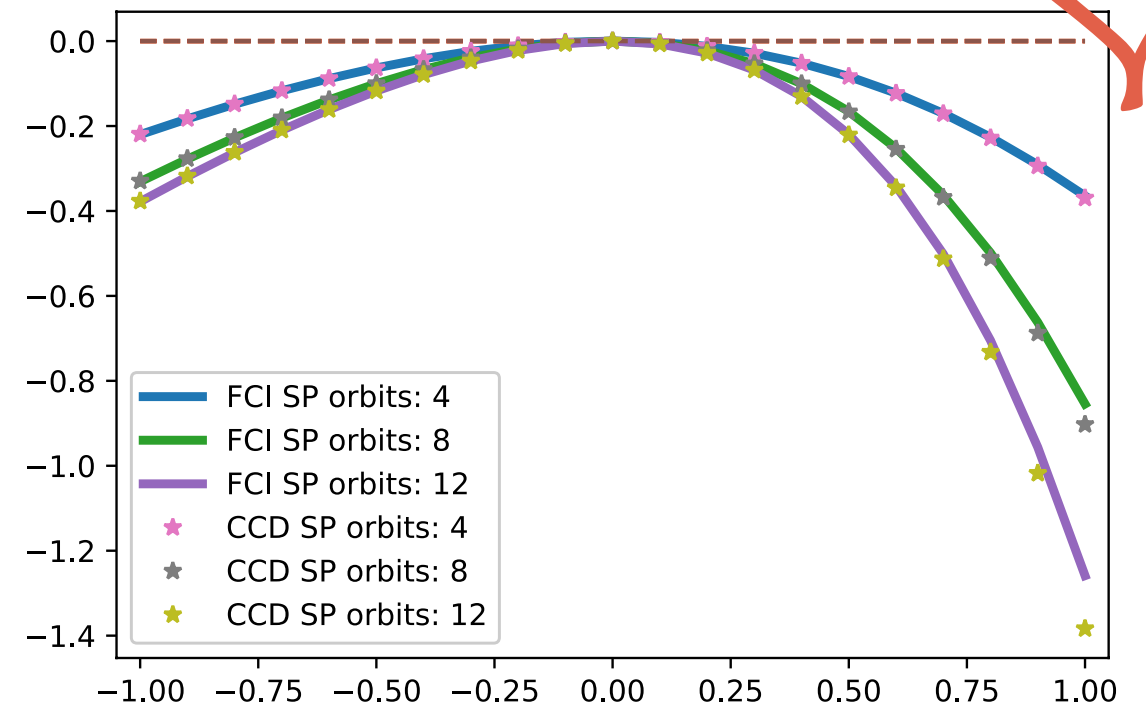
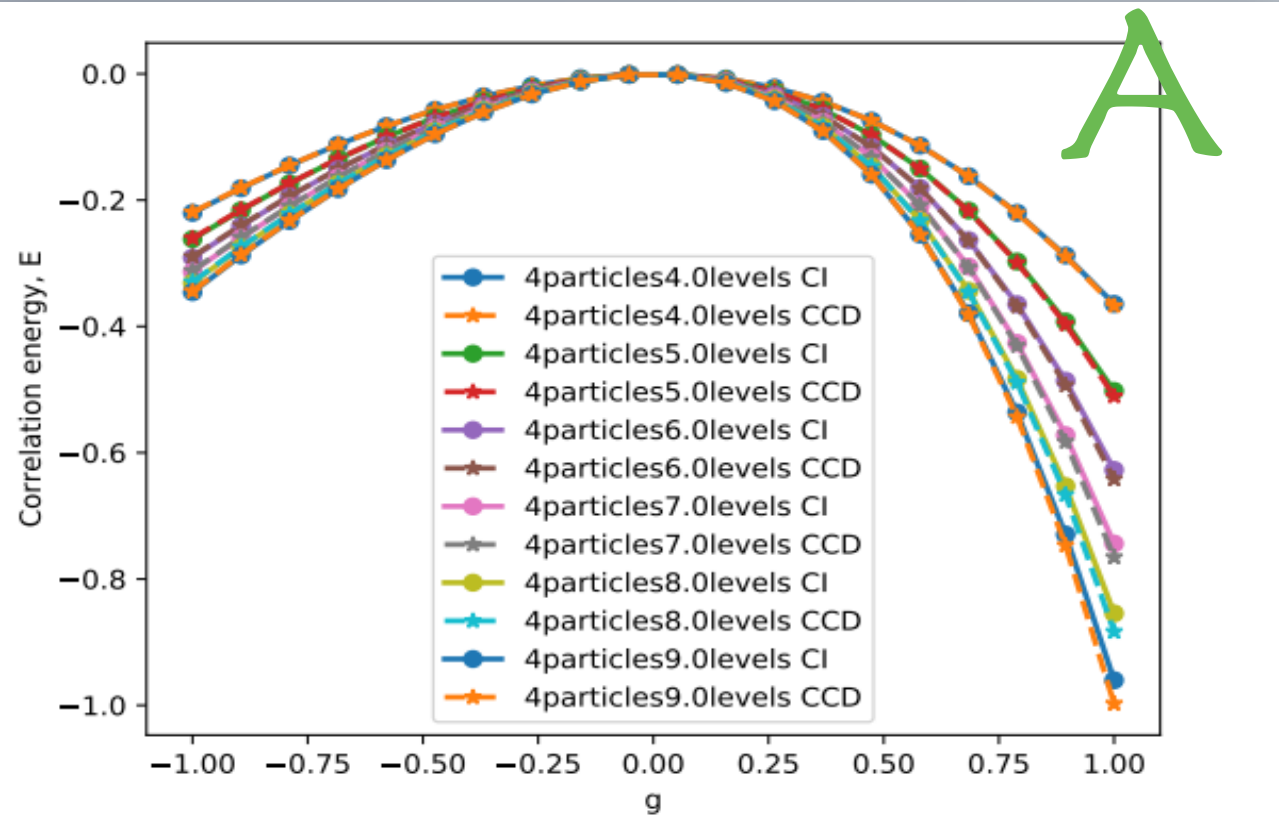
$$e^{-\lambda N_{loop}}$$

Limitation for convergence.

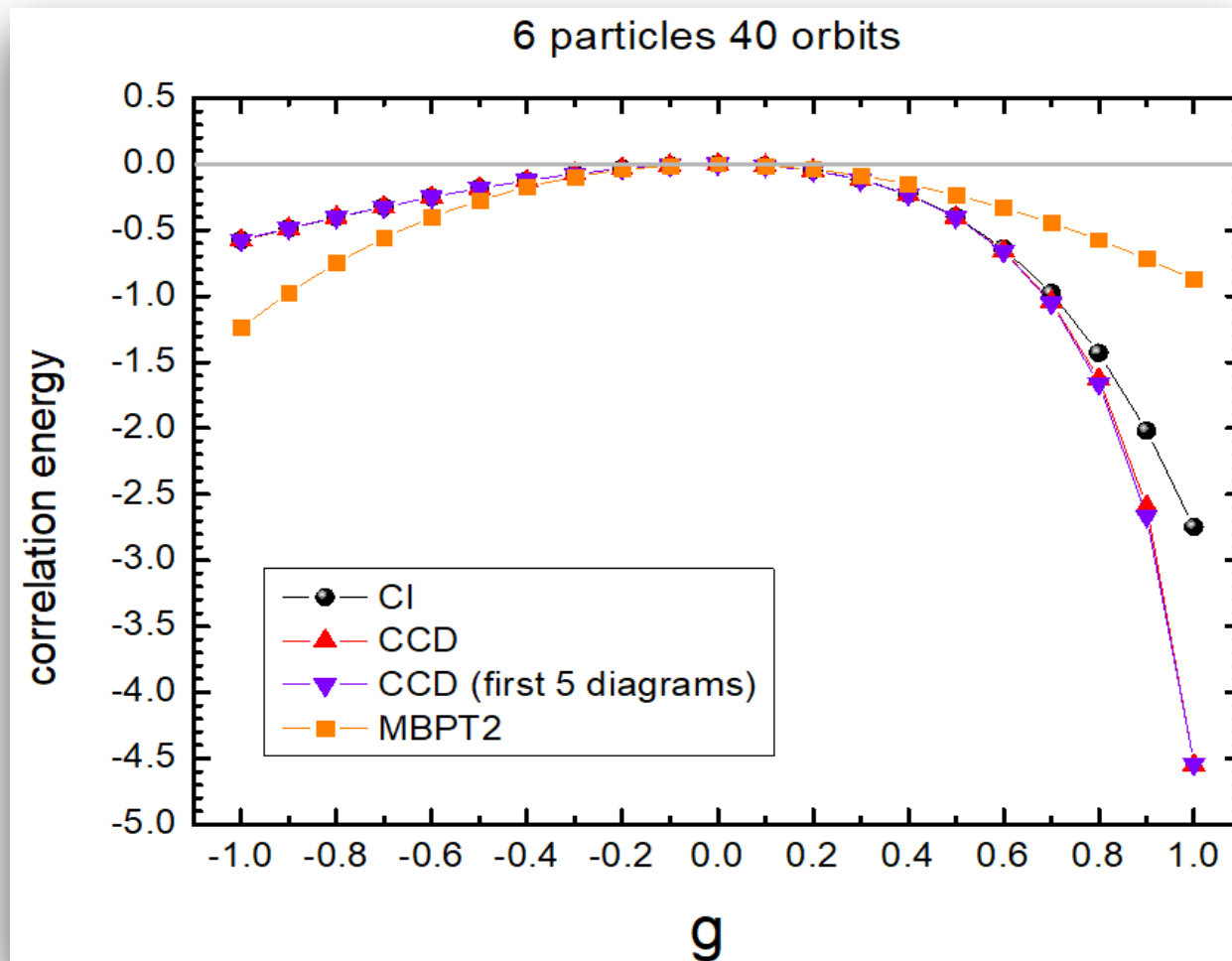
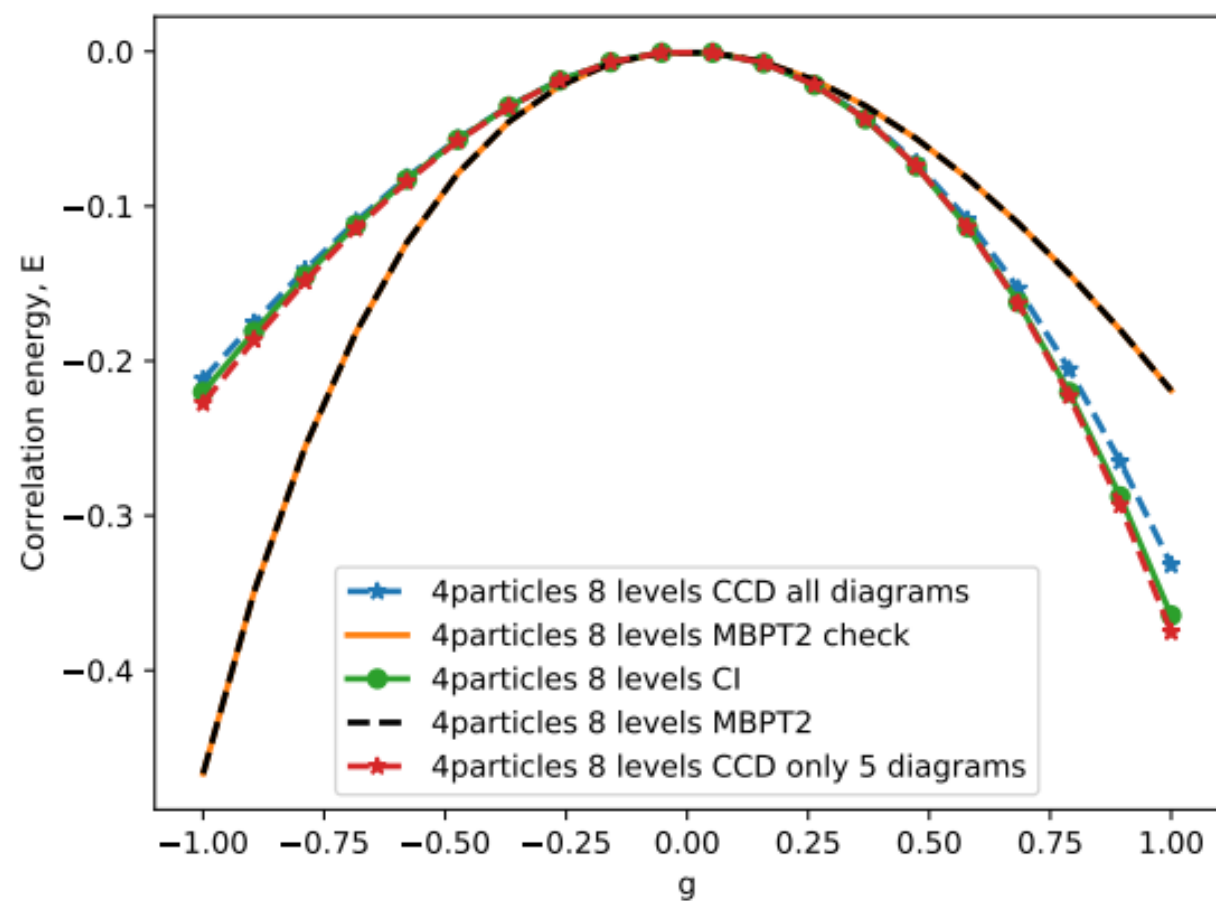


Particle number	SP number	g_min	g_max
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Comparison :



Results



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

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

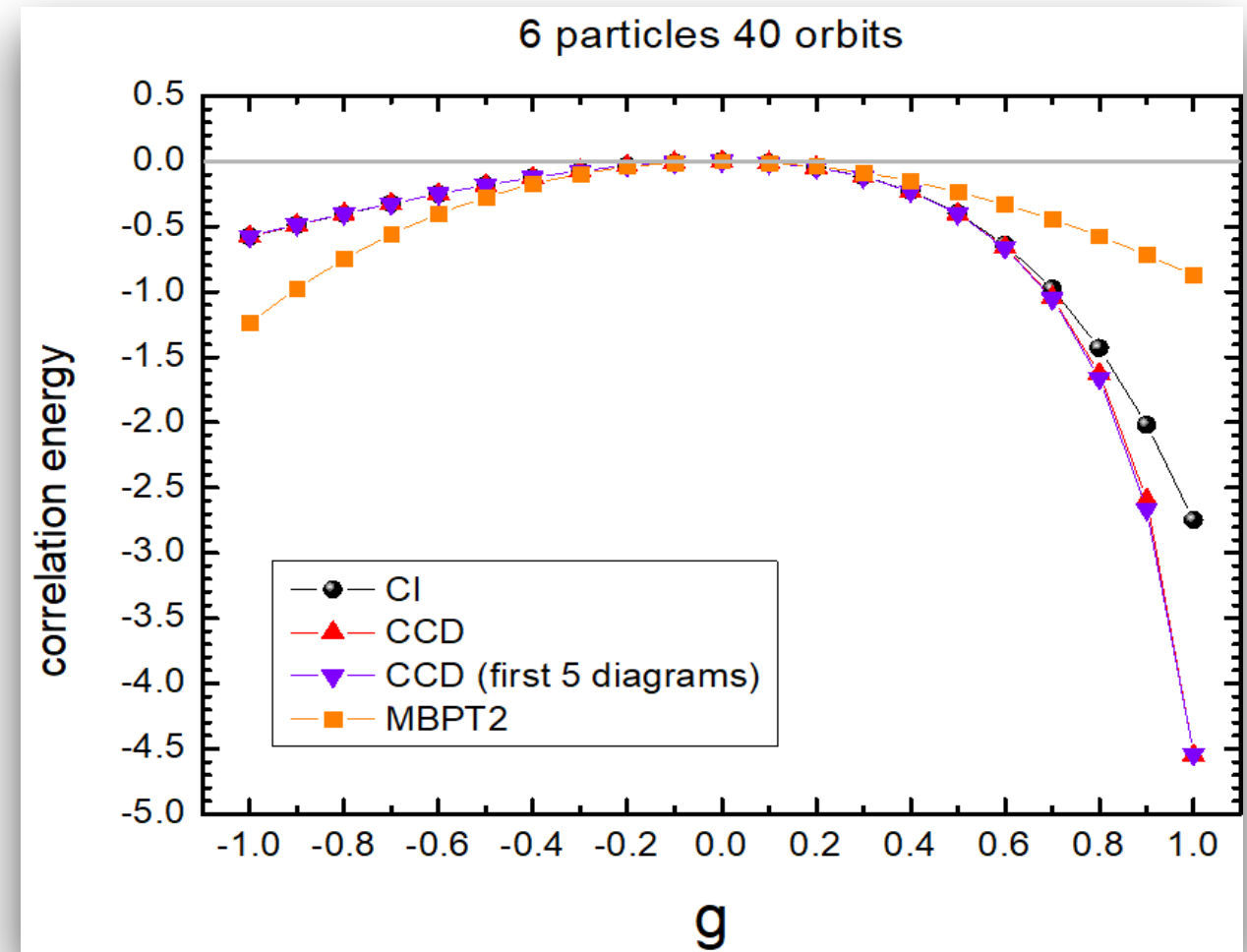
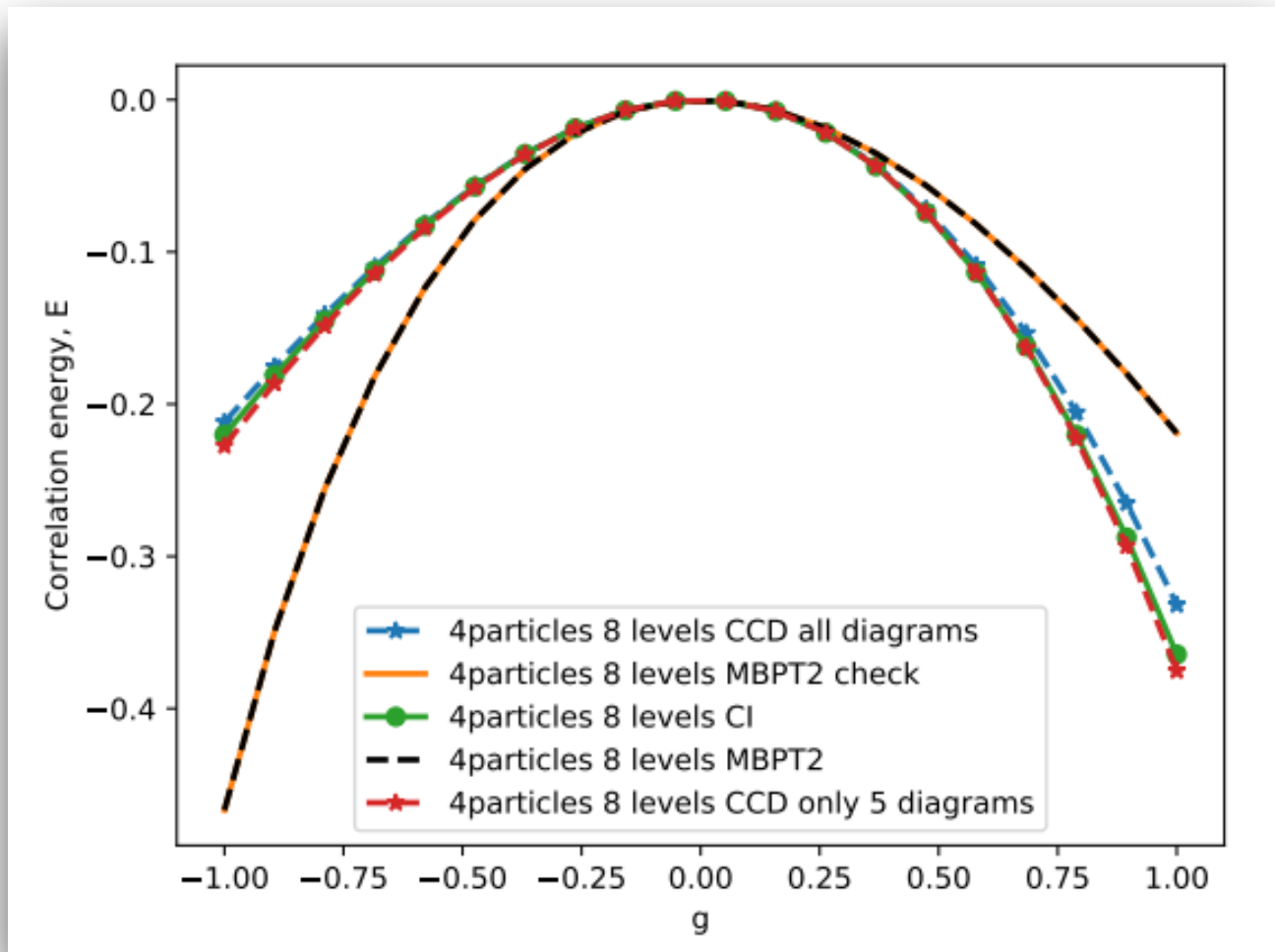
Results



$$\begin{aligned} 0 = & \left[\text{Diagram 1} + \text{Diagram 2} \times + \text{Diagram 3} \times \right] \\ & + \left[\text{Diagram 4} + \text{Diagram 5} \right] + \text{Diagram 6} \\ & + \text{Diagram 7} + \text{Diagram 8} \\ & + \text{Diagram 9} + \text{Diagram 10} \end{aligned}$$

The diagrams are Feynman diagrams representing various particle interactions. Diagrams 1, 2, and 3 are enclosed in a red box. Diagrams 4 and 5 are also enclosed in a red box. Diagram 6 is enclosed in a red box. Diagrams 7, 8, 9, and 10 are not enclosed in a red box.

Results



Thank you!

Group No.5

YIYUAN CHENG

ADAM VERNON

YUANZHUO MA

