

Week 48: Coupled cluster theory and summary of course

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Week 48, November 25-29, 2024

1. Thursday:

- 1.1 Short repetition from last week
- 1.2 How to write your own coupled-cluster theory code, pairing model example
- 1.3 Coupled cluster theory, singles and doubles excitations, diagrammatic expansion

2. Friday:

- 2.1 Coupled cluster theory for singles and doubles excitations using a diagrammatic derivation
- 2.2 Summary of course and discussion of final oral exam

3. Lecture material: Lecture notes and Shavitt and Bartlett chapters 9 and 10. See also slides at

<https://github.com/ManyBodyPhysics/FYS4480/blob/master/doc/pub/week48/pdf/cc.pdf>

CCSD with twobody Hamiltonian

Truncating the cluster operator \hat{T} at the $n = 2$ level, defines CCSD approximation to the Coupled Cluster wavefunction. The coupled cluster wavefunction is now given by

$$|\Psi_{CC}\rangle = e^{\hat{T}_1 + \hat{T}_2} |\Phi_0\rangle,$$

where

$$\begin{aligned}\hat{T}_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\ \hat{T}_2 &= \frac{1}{4} \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i.\end{aligned}$$

Two-body normal-ordered Hamiltonian

$$\begin{aligned}\hat{H} &= \sum_{pq} \langle p | \hat{f} | q \rangle \{ a_p^\dagger a_q \} + \frac{1}{4} \sum_{pqrs} \langle pq | \hat{v} | rs \rangle \{ a_p^\dagger a_q^\dagger a_s a_r \} \\ &\quad + E_0 \\ &= \hat{F}_N + \hat{V}_N + E_0 = \hat{H}_N + E_0,\end{aligned}$$

where

$$\begin{aligned}\langle p | \hat{f} | q \rangle &= \langle p | \hat{h}_0 | q \rangle + \sum_i \langle pi | \hat{v} | qi \rangle \\ E_0 &= \sum_i \langle i | \hat{h}_0 | i \rangle + \frac{1}{2} \sum_{ij} \langle ij | \hat{v} | ij \rangle.\end{aligned}$$