Week 48: Coupled cluster theory and summary of course

Morten Hjorth-Jensen[1]

Department of Physics and Center for Computing in Science Education, University of Oslo, Norway[1]

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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

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

Two-body normal-ordered Hamiltonian

$$
\begin{aligned}
\hat{H} &= \sum_{pq} f_q^p \left\{a_p^\dagger a_q\right\} + \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} \\
&\quad + \mathrm{E}_0 \\
&= \hat{F}_N + \hat{V}_N + \mathrm{E}_0 = \hat{H}_N + \mathrm{E}_0,
\end{aligned}
$$

where

$$
\begin{aligned}
f_q^p &= \langle p|\hat{t}|q\rangle + \sum_i \langle pi|\hat{v}|qi\rangle \\
\langle pq||rs\rangle &= \langle pq|\hat{v}|rs\rangle \\
\mathrm{E}_0 &= \sum_i \langle i|\hat{t}|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|\hat{v}|ij\rangle.
\end{aligned}
$$