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

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

where

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

Diagram equations - Derivation

1. Contract $\hat{H}_N$ with $\hat{T}$ in all possible unique combinations that satisfy a given form. The diagram equation is the sum of all these diagrams.
2. Contract one $\hat{H}_N$ element with $0, 1$ or multiple $\hat{T}$ elements.
3. All $\hat{T}$ elements must have atleast one contraction with $\hat{H}_N$.
4. No contractions between $\hat{T}$ elements are allowed.
5. A single $\hat{T}$ element can contract with a single element of $\hat{H}_N$ in different ways.

Diagram rules

1. Label all lines.
2. Sum over all internal indices.
3. Extract matrix elements.
4. Extract cluster amplitudes with indices in the order left to right. Incoming lines are subscripts, while outgoing lines are superscripts. ($t_{\mathrm{in}}^{\mathrm{out}}$, $t_{\mathrm{lin,rin}}^{\mathrm{lout,rout}}$)
5. Calculate the phase: $(-1)^{\mathrm{holelines+loops}}$
6. Multiply by a factor of $\frac{1}{2}$ for each equivalent line and each ecuivalent vertex.
7. Antisymmetrize a pair of external particle/hole line that does not connect to the same operator.

CCSD $\hat{T}_1$ amplitude equation

$$0 = f_i^a + f_e^a t_i^e - f_i^m t_m^a + \langle ma|\hat{v}|ei\rangle t_m^e + f_e^m t_{im}^{ae} + \frac{1}{2}\langle am|\hat{v}|ef\rangle t_{im}^{ef} \quad -\frac{1}{2}\langle mn$$

CCSD $\hat{T}_2$ amplitude equation

$$0 = \langle ab|\hat{v}|ij\rangle + P(ij)\langle ab|\hat{v}|ej\rangle t_i^e - P(ab)\langle am|\hat{v}|ij\rangle t_m^b + P(ab) f_e^b t_{ij}^{ae} - P(ij$$