

1. Explain why the maximum excitation level of the wavefunction increases by +2 with each order in perturbation theory.
2. Prove that the leading contribution to the k -tuples CI operator has order $\lceil k/2 \rceil$ in perturbation theory.
3. Write down the CISD energy and singles and doubles equations in terms of C_k operators. Identify the leading order of each term in perturbation theory with and without Brillouin's theorem.
4. Prove that CIS $\cdots m$ is correct to order $\lfloor m/2 \rfloor$ in the wavefunction and $2\lfloor m/2 \rfloor + 1$ in the energy.
5. Write down the CCSD energy and singles and doubles equations in terms of T_k operators. Identify the leading order of each term in perturbation theory with and without Brillouin's theorem.
6. Explain why the leading contribution to the k -tuples cluster operator has order $k - 1$.
7. Prove that CCS $\cdots m$ is correct to order $m - 1$ in the wavefunction and $m + \lfloor m/2 \rfloor$ in the energy.
8. "Derive" the [T] correction and evaluate it, showing both the diagrams and their algebraic interpretation.^{1 2} You may write your answer in terms of $^{[2]}t_{abc}^{ijk}$ amplitudes and evaluate those separately.

$$E_{[T]} = \langle \Phi | T_2^\dagger V_c T_3^{[2]} | \Phi \rangle \quad T_3^{[2]} = \left(\frac{1}{3!}\right)^2 \sum_{\substack{abc \\ ijk}} \tilde{a}_{ijk}^{abc} \langle \Phi_{ijk}^{abc} | R_0 V_c T_2 | \Phi \rangle \quad (1)$$

9. Prove that the left and right EOM-CC wave operators are given by

$$^k R = \exp(-T) (^k C_0 + ^k C) \quad ^k L = (^k C_0 + ^k C)^\dagger \exp(T) \quad (2)$$

where $^k C_0 + ^k C$ is the CI wave operator for the k^{th} state. Use this to show that we can determine excited state expectation values and transition matrix elements for an observable W as $\langle \Psi_k | W | \Psi_k \rangle = \langle \Phi | L_k \bar{W} R_k | \Phi \rangle$ and $\langle \Psi_k | W | \Psi_l \rangle = \langle \Phi | L_k \bar{W} R_l | \Phi \rangle$ where $\bar{W} \equiv \exp(-T) W \exp(T)$.

10. Evaluate the CCD lambda equations, showing both the diagrams and their interpretation.
13. Derive the $(m + 1)_\Lambda$ correction from the coupled-cluster Löwdin functional.
14. "Derive" the (T) correction as an approximation to $(T)_\Lambda$ correction and evaluate it.

$$E_{(T)} = E_{[T]} + \langle \Phi | T_1^\dagger V_c T_3^{[2]} | \Phi \rangle \quad (3)$$

¹"Derive" here means "give detailed motivation for".

²The operator Q_3 here simply projects onto the space of triply substituted determinants.