Homework for Lecture 6: Coupled Cluster

1. Write out the Hausdorff expansion for the CCSD case. You should get 15 terms containing at least one of H_{c}, T_1, and T_2.

2. Derive an expression for the CCSD correlation energy

$$\langle\Phi|(H_{\mathrm{c}}\exp(T))|\Phi\rangle_{\mathrm{C}} = E_{\mathrm{CCSD}}$$

   Hint: the only components of the Hausdorff expansion in question 1 which contribute are $H_{\mathrm{c}}T_1$, $H_{\mathrm{c}}T_2$, $\frac{1}{2}H_{\mathrm{c}}T_1^2$.

3. Pick 3 terms from the Hausdorff expansion in question 1 which did not contribute to the CCSD energy in question 2, and explain why in terms of excitation levels and/or because the term is disconnected.

4. Explain why the following terms vanish, either due excitation levels and/or because the term is disconnected.

$$\langle\Phi_i^a|V_{\mathrm{c}}T_2^2|\Phi\rangle$$

$$\langle\Phi_{ijk}^{abc}|V_{\mathrm{c}}T_2^2|\Phi\rangle$$

$$\langle\Phi_{ijk}^{abc}|V_{\mathrm{c}}T_1|\Phi\rangle$$