

1. Derive the Hausdorff expansion.¹

$$e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \frac{1}{3!}[X, [X, [X, Y]]] + \dots \quad (1)$$

2. Prove the following.

$$[H_c, T] = \overline{\mathfrak{H}_c T} \mathfrak{H} \quad [[H_c, T], T] = \overline{\mathfrak{H}_c T T} \mathfrak{H} \quad [[[[H_c, T], T], T], T] = \overline{\mathfrak{H}_c T T T T} \mathfrak{H} \quad \dots \quad (2)$$

3. Using equation 2, explain the following.

$$[\cdot, T]^n(H_c) = \overline{\mathfrak{H}_c T T T T} \mathfrak{H} \text{ for } n \geq 4 \quad (3)$$

4. Prove that the determinant basis consists of eigenfunctions of the diagonal Fock operator.

$$H_0 \Phi_{i_1 \dots i_k}^{a_1 \dots a_k} = \mathcal{E}_{i_1 \dots i_k}^{a_1 \dots a_k} \Phi_{i_1 \dots i_k}^{a_1 \dots a_k} \quad H_0 \equiv f_p^p \tilde{a}_p^p \quad \mathcal{E}_{i_1 \dots i_k}^{a_1 \dots a_k} \equiv \sum_{r=1}^k f_{a_r}^{a_r} - \sum_{r=1}^k f_{i_r}^{i_r} \quad (4)$$

5. Use equations 2 and 4 to write the coupled-cluster amplitude equation $\langle \Phi_{ij\dots}^{ab\dots} | \overline{H}_c | \Phi \rangle = 0$ as follows.

$$t_{ab\dots}^{ij\dots} = (\mathcal{E}_{ab\dots}^{ij\dots})^{-1} \langle \Phi_{ab\dots}^{ij\dots} | V_c \exp(T) | \Phi \rangle_C \quad V_c \equiv H_c - H_0 \quad (5)$$

6. Explain why the following terms vanish.³

$$\frac{1}{2} \langle \Phi_i^a | V_c T_2^2 | \Phi \rangle_C \quad \langle \Phi_{ijk}^{abc} | V_c | \Phi \rangle_C \quad \langle \Phi_{ijk}^{abc} | V_c T_1 | \Phi \rangle_C$$

¹For an alternative to the direct, somewhat bullheaded proof shown in the notes look at the solution to Exercise 3.1.6 in Helgaker's big purple book, but note that you should give a proper proof by induction.²

²See https://en.wikipedia.org/wiki/Mathematical_induction.

³Hint: Use arguments about the excitation levels of their operators.