

1. Prove 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.

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

3. Using equation 2, explain the following.

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

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

$$\frac{1}{4!} \langle \Phi_i^a | V_c T_1^4 | \Phi \rangle_C \quad \langle \Phi_{ijk}^{abc} | V_c | \Phi \rangle_C \quad \langle \Phi_{ijk}^{abc} | V_c T_1 | \Phi \rangle_C$$

¹For a slick alternative to the proof 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.