1. Prove the following identity.

$$\tilde{a}^{p_1\cdots p_m}_{q_1\cdots q_m} = (\tfrac{1}{m!})^2\, \overline{\delta}^{q'_1\cdots q'_m}_{p'_1\cdots p'_m}\, \tilde{a}^{p'_1\cdots p'_m}_{q'_1\cdots q'_m} \qquad\qquad \overline{\delta}^{q'_1\cdots q'_m}_{p'_1\cdots p'_m} \equiv \hat{P}^{(p_1/\cdots/p_m)}_{(q_1/\cdots/q_m)} \delta^{p_1}_{p'_1}\cdots\delta^{p_m}_{p'_m}\delta^{q'_1}_{q_1}\cdots\delta^{q'_m}_{q_m} \tag{1}$$

2. Derive each of the following rules in your own words.
   (a) Each set of k equivalent internal lines[1] or equivalent subgraphs contributes a factor of $k!$ to the degeneracy.
   (b) Each open cycle contributes $(-)^{h_i} a^p_q$ to the normal-ordered product, where p and q label the free ends.
   (c) Each closed loop contributes $(-)^{h_i+1}$ to the overall sign, where h_i is the number of hole contractions.
   (d) The overall sign of a closed graph is $(-)^{h+l}$, where h and l denote the total number of hole lines and loops.
   (e) For each bare excitation operator in a coefficient graph, the coefficient lines contribute an antisymmetrizer $\hat{P}^{(P_1/\cdots/P_h)}_{(Q_1/\cdots/Q_k)}$ where the P_i's and Q_i's label subsets of equivalent creation and annihilation lines, respectively.

3. Assuming Lemma 4.1 holds true, prove Wick's Theorem for Graphs (WTG) in your own words.

4. Expand the full electronic Hamiltonian H in terms of Φ-normal-ordered operators using WTG.

5. Using KM notation, split the Einstein summations in H_c into summations over occupied and virtual indices. After combining like terms in your expansion, translate each one into a graph.

6. Derive the CIS Hamiltonian matrix as a coefficient graph using WTG.

7. Derive the CID energy and coefficient equations using WTG.

8. Derive the CCD energy and coefficient ("amplitude") equations using WTG.

9. Compare the CID and CCD equations, and explain the cancellation of unlinked terms in the CCD amplitude equation.

10. Show that the CCD amplitude equation can be written as

$$t^{ij}_{ab} = (\mathcal{E}^{ij}_{ab})^{-1} \langle \Phi^{ab}_{ij} | (H_\mathrm{c} - f^p_p \tilde{a}^p_p) \exp(T_2) | \Phi \rangle_\mathrm{L} \qquad\qquad \mathcal{E}^{ij}_{ab} \equiv f^i_i + f^j_j - f^a_a - f^b_b \tag{2}$$

    for a general, possibly non-canonical, reference determinant. Write this equation in graphical form using resolvent lines.

11. If Φ is an excellent approximation to the wavefunction the coupled-cluster amplitudes will be very small, leading to $T_2 \approx 0 \implies \exp(T_2) \approx 1$. This is the so-called *first-order approximation* of equation 2. Write down graphical and algebraic expressions for these *first-order amplitudes*, ${}^{(1)}t^{ij}_{ab}$, assuming Φ is a canonical Hartree-Fock reference function. Substitute these amplitudes into the CCD energy expression to derive the *second-order energy*, $E^{(2)}_c$. This is the MP2 energy expression.[2]

12. If the T_2 amplitudes are small but not negligible, we can improve upon the first-order approximation using $\exp(T_2) \approx 1 + T_2$, which is known as linearized CCD or "CEPA_0".[3] Write down the CEPA_0 amplitude equation in graphical form.

13. Whereas the MP2 energy can be determined in a single step, the CEPA_0 and CCD equations require iterative solution. Typically, this is achieved by starting from a guess of $T_2 \approx 0$ and repeatedly substituting the amplitudes into the right-hand side of equation 2 until self-consistency is reached.[4]

$$^{[n+1]}t^{ij}_{ab} = (\mathcal{E}^{ij}_{ab})^{-1} \langle \Phi^{ab}_{ij} | (H_\mathrm{c} - f^p_p \tilde{a}^p_p) \exp(^{[n]}T_2) | \Phi \rangle_\mathrm{L} \qquad\qquad ^{[0]}t^{ij}_{ab} \equiv 0 \tag{3}$$

    Write down graphical and algebraic expressions for the first- and second-iteration CEPA_0 amplitudes, as well as the corresponding energies. This procedure can be carried out indefinitely, which shows that the exact CEPA_0 and CCD amplitudes contain contributions to infinite order in perturbation theory.

[1] If rule 2e is used, this excludes coefficient lines. Otherwise, replace rule 2e with the full antisymmetrizer.
[2] MP2 stands for "second-order Møller-Plesset perturbation theory".
[3] CEPA stands for "coupled electron-pair approximation".
[4] The numbers in square brackets refer to the iteration.