Question 1a (9 pts). Starting from:

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} \langle pq|rs\rangle \, a_p^\dagger a_q^\dagger a_s a_r$$

Derive the Φ-normal ordered Hamiltonian:

$$H_N = \sum_{pq} f_{pq} N[a_p^\dagger a_q] + \frac{1}{2} \sum_{pqrs} \langle pq|rs\rangle \, N[a_p^\dagger a_q^\dagger a_s a_r]$$

Be sure to explicitly show your work.

Question 1b (3 pts). Explicitly define f_{pq} and qualitatively explain what the term $\sum_{pq} f_{pq} N[a_p^\dagger a_q]$ is.

Question 1c (3 pts). Qualitatively explain how the Φ-normal ordered Hamiltonian H_N differs from the standard Hamiltonian H. Be sure to address the significance of $H - H_N$ in the context of particle-hole isomorphism. Also be sure to address why $H_N = H_c$, where H_c is the correlation Hamiltonian if we choose the reference determinant to be the Hartree-Fock result.

Question 2 (6 pts). Evaluate the following matrix elements (you may use Slater's rules when applicable)[1]:

$$\sum_{pq} f_{pq} \langle \Phi_j^b | N[a_p^\dagger a_q] | \Phi_i^a \rangle$$

$$\langle \Phi | H | \Phi_{ijk}^{abc} \rangle$$

$$\langle \Phi | H | \Phi_j^b \rangle$$

$$\langle \Phi_i^a | H | \Phi_i^a \rangle$$

$$\langle \Phi_i^a | H | \Phi_{ijk}^{abc} \rangle$$

Question 3 (3 pts). Qualitatively explain the purpose of Wick's Theorem in 1-2 sentences. Then, explain why the generalized Wick's theorem is useful in 1-2 sentences.

Question 4 (2 pts). Qualitatively explain particle-hole isomorphism and why it is useful in 2-3 sentences.

Question 5 (3 pts). Qualitatively explain the difference between $\underbracket{a_p a_p^\dagger}$ and $\overbracket{a_p a_p^\dagger}$. Be sure to address:

- the type of contraction involved in each term
- the result in each case
- the qualitative meaning of the result

Question 6 (2 pts). Explain the difference between $N[a_p a_r^\dagger a_q^\dagger a_s]$ and $n[a_p a_r^\dagger a_q^\dagger a_s]$. Be sure to address:

- which formalism each term belongs to
- the result in each case

[1]

$$\langle \Phi | H | \Phi \rangle = \sum_i h_{ii} + \frac{1}{2} \sum_{ij} \langle ij||ij\rangle$$

$$\langle \Phi | H | \Phi_i^a \rangle = h_{ia} + \sum_j \langle ij||aj\rangle$$

$$\langle \Phi | H | \Phi_{ij}^{ab} \rangle = \langle ij||ab\rangle$$