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.

Look at Lecture 3.6

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.

$$f_{pq} = h_{pq} + \sum_i \langle pi||qi\rangle$$

$\sum_{pq} f_{pq} N[a_p^\dagger a_q]$ is the Φ-normal ordered Fock operator, which is an effective one-electron operator that gives bare one-body contributions as well as mean-field one-body contributions from the two-body operator.

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.

$$H_N = H - \langle\Phi|H|\Phi\rangle$$

The Φ-normal ordered Hamiltonian is obtained by shifting the original Hamiltonian by the expectation value in the reference determinant, In other words, it is removing the energy contribution of the reference determinant. In our original mapping to the particle-hole formalism, we made the reference determinant a vacuum state. Thus, the Φ-normal ordered Hamiltonian, which is in the particle-hole formalism does not have any interaction with reference determinant. In the same way that in our original formalism,

$$\langle 0|H|0\rangle = 0$$

In the particle-hole formalism,

$$\langle\Phi|H_N|\Phi\rangle = 0$$

If we choose our reference determinant Φ to be the Hartree-Fock result, then shifting the Hamiltonian by the Hartree-Fock energy $E_{HF} = \langle\Phi|H|\Phi\rangle$ means we are really just defining a Hamiltonian that takes care of correlation effects.

$$H = \langle\Phi|H|\Phi\rangle + H_N = E_{HF} + H_c$$

The Φ-normal ordered Hamiltonian is thus equal to a correlation Hamiltonian H_c:

$$H_N = H_c$$

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

$$\sum_{pq} f_{pq} \langle \Phi_j^b | N[a_p^\dagger a_q] | \Phi_i^a \rangle = f_a \delta_{ij} - f_{ij} \delta_{ab}$$

$$\langle \Phi | H | \Phi_{ijk}^{abc} \rangle = 0$$

$$\langle \Phi | H | \Phi_j^b \rangle = h_{jb} + \sum_i \langle ji || bi \rangle$$

$$\langle \Phi_i^a | H | \Phi_i^a \rangle = \sum_k h_{kk} + \frac{1}{2} \sum_{kl} \langle kl || kl \rangle \text{, where k and l are indices occupied in} \Phi_i^a$$

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

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.

Wick's theorem gives a way to express any product of creation and annihilation operators in normal ordering. We can then take advantage of the properties of normal ordered products for quick evaluation of matrix elements. The generalized Wick's theorem states that we do not have to consider contractions between operators in the same normal-ordered group, and thus further reduces the number of terms we have to consider in a Wick expansion.

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

Particle-hole isomorphism the ability to map between particle and hole frameworks to arrive at the same result. In the particle-hole formalism, we work in the quasiparticle framework, switching from a particle framework to a hole framework only for the particle occupied spin-orbitals in our reference determinant. Under the quasiparticle framework, the reference determinant becomes our "vacuum state", and we do not have to consider the creation operators associated with the reference determinant as we had to in the original particle framework.

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

$\underbracket{a_p a_p^\dagger}$ is a contraction w.r.t. the true vacuum $|0\rangle$.

$$\underbracket{a_p a_p^\dagger} = \delta_{pp} = 1$$

A contraction w.r.t. the true vacuum gives the difference between the product $a_p a_p^\dagger$ and the normal ordered product $n[a_p a_p^\dagger]$.

[1]

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

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

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

$\overset{\sqcap}{a_p a_p^\dagger}$ is a contraction w.r.t. the Fermi vacuum $|\Phi\rangle$.

$$\underset{\sqcup}{a_p a_p^\dagger} = \eta_{pp}$$

A contraction w.r.t. the true vacuum gives the difference between the product $a_p a_p^\dagger$ and the Φ-normal ordered product $N[a_p a_p^\dagger]$

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

$N[a_p a_r^\dagger a_q^\dagger a_s]$ is a Φ-normal product w.r.t. the Fermi vacuum. In order to put it in Φ-normal ordering, we would have to know the occupation of the indices p, q, r, s.

$n[a_p a_r^\dagger a_q^\dagger a_s]$ is a normal product w.r.t. the true vacuum.

$$n[a_p a_r^\dagger a_q^\dagger a_s] = a_r^\dagger a_q^\dagger a_p a_s$$