1. Answer each of the following in one sentence, using words only.

   (a) Define canonical Hartree-Fock orbitals.
   Answer: Hartree-Fock orbitals are "canonical" when the Lagrange multiplier matrix is diagonal.

   (b) Explain why the choice of Hartree-Fock orbitals is not unique.
   Answer: The Hartree-Fock energy and the orbital overlaps are invariant to a unitary transformation, so any unitary variation of the canonical orbitals satisfies the Hartree-Fock optimization conditions.

2. Expand $a_p a_q a_s^\dagger a_r^\dagger$ as a linear combination of strings which are in normal order. Identify the vacuum expectation value of this operator product.
Answer:

$$\begin{aligned}
a_p a_q a_s^\dagger a_r^\dagger &= \delta_{qs} a_p a_r^\dagger - a_p a_s^\dagger a_q a_r^\dagger \\
&= \delta_{qs}(\delta_{pr} - a_r^\dagger a_p) - (\delta_{ps} - a_s^\dagger a_p)(\delta_{qr} - a_r^\dagger a_q) \\
&= \delta_{qs}\delta_{pr} - \delta_{qs} a_r^\dagger a_p - \delta_{ps}\delta_{qr} + \delta_{ps} a_r^\dagger a_q + \delta_{qr} a_s^\dagger a_p - a_s^\dagger a_p a_r^\dagger a_q \\
&= \delta_{qs}\delta_{pr} - \delta_{qs} a_r^\dagger a_p - \delta_{ps}\delta_{qr} + \delta_{ps} a_r^\dagger a_q + \delta_{qr} a_s^\dagger a_p - \delta_{pr} a_s^\dagger a_q + a_s^\dagger a_r^\dagger a_p a_q \\
\langle \text{vac}| a_p a_q a_s^\dagger a_r^\dagger |\text{vac}\rangle &= \delta_{qs}\delta_{pr} - \delta_{ps}\delta_{qr}
\end{aligned}$$

3. Derive the Slater determinant expectation value of a two-electron operator in terms of two-electron integrals, showing your steps along the way. You may use second quantization methods (and your result from problem 2.) if you first expand the expectation value in terms of particle-hole operators.[1]

$$\tfrac{1}{2}\sum_{i\neq j}^{n} \langle \Phi | \hat{g}(i,j)\Phi\rangle = \,?$$

Answer:

$$\begin{aligned}
\frac{1}{2}\sum_{i\neq j}^{n} \langle \Phi | \hat{g}(i,j)\Phi\rangle &= \frac{n^2-n}{2}\langle \Phi|\hat{g}(1,2)\Phi\rangle && \text{Changing integration variables and using antisymmetry of } \Phi \\
&= \frac{\cancel{n^2-n}}{2}\frac{1}{\cancel{n(n-1)}}\sum_{pqrs}^{\infty}\langle pq|rs\rangle\langle a_q a_p \Phi | a_s a_r \Phi\rangle && \text{Using expansion from footnote in bra and ket} \\
&= \frac{1}{2}\sum_{pqrs}^{\infty}\langle pq|rs\rangle\langle \Phi | a_p^\dagger a_q^\dagger a_s a_r \Phi\rangle && \text{Definition of adjoint} \\
&= \frac{1}{2}\sum_{ijkl}^{n}\langle ij|kl\rangle\langle \widetilde{\text{vac}} | b_i b_j b_l^\dagger b_k^\dagger |\widetilde{\text{vac}}\rangle && \text{Particle-hole isomorphism} \\
&= \frac{1}{2}\sum_{ijkl}^{n}\langle ij|kl\rangle\left(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}\right) && \text{Result from problem 2.} \\
&= \frac{1}{2}\sum_{ij}^{n}\langle ij||ij\rangle
\end{aligned}$$

On the fourth line, we omit all other contributions to the quasiparticle expansion because either they don't have a balanced number of quasiparticle creation and annihilation operators or because they are in Φ-normal order.

[1] You may take the following expansion as given:

$$\Psi(1,2,3\ldots,n) = \frac{1}{\sqrt{n(n-1)}}\sum_{pq}^{\infty}\psi_p(1)\psi_q(2)(\hat{a}_q\hat{a}_p\Psi)(3,\ldots,n)$$