

1. Answer each of the following in one sentence, using words only.
  - (a) Define canonical Hartree-Fock orbitals.
  - (b) Explain why the choice of Hartree-Fock orbitals is not unique.
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.
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.<sup>1</sup>

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

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<sup>1</sup>You may take the following expansion as given:

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