Homework for Lecture 3.3 Wick's Theorem

1. Show the following are true:
$$n[a_p a_q a_r^\dagger a_s a_t^\dagger a_u^\dagger] = -\delta_{pr}\delta_{qt}a_u^\dagger a_s$$
$$n[a_p a_q a_r^\dagger a_s a_t^\dagger a_u^\dagger] = \delta_{pr}\delta_{qt}\delta_{su}$$

2. Show that
$$a_p a_q^\dagger = n[a_p a_q^\dagger]$$

3. Show that $a_p a_q^\dagger a_r^\dagger = \delta_{pq}a_r^\dagger - \delta_{pr}a_q^\dagger + a_q^\dagger a_r^\dagger a_p$ can be rewritten as:
$$a_p a_q^\dagger a_r^\dagger = n[a_p a_q^\dagger a_r^\dagger] + n[a_p a_q^\dagger a_r^\dagger] + n[a_p a_q^\dagger a_r^\dagger]$$

4. Explicitly write out Wick's theorem for a general product of 3 operators, $x_1 x_2 x_3$. If you want more practice, try writing out Wick's theorem for a general product of 5 operators.

5. Explicitly write out Wick's theorem for a general product of 6 operators, $n[x_1 x_2 x_3]n[x_4 x_5 x_6]$ (use generalized Wick's theorem)

6. Evaluate
$$\langle \Phi_{pq} | \Phi_{rst} \rangle$$
using Wick's theorem. Compare the work with the work done for HW 3.2 Problem 1.

7. Evaluate
$$\langle \Phi_{pqr} | \Phi_{stu} \rangle$$
using Wick's theorem. (Hint: see Problem 5)

8. You showed in HW 3.1 Problem 4 that the overlap of a Slater determinant is a Slater determinant of overlaps for $\langle \Phi_{pq} | \Phi_{rs} \rangle$. Now, show this generally for a Slater determinant:
$$\langle \Phi_{p_1 \cdots p_N} | \Phi_{q_1 \cdots q_N} \rangle$$

9. For $\langle \Phi_{p_1 p_2 \cdots p_N} | H | \Phi_{q_1 q_2 \cdots q_N} \rangle$ which differ by one spin-orbital such that $p_1 \neq q_1, p_2 = q_2 \cdots p_N = q_N$, show that
$$\langle \Phi_{p_1 p_2 \cdots p_N} | H | \Phi_{q_1 q_2 \cdots q_N} \rangle = h_{p_1 q_1} + \sum_{k=2}^{N} \langle p_1 p_k || q_1 p_k \rangle$$
This is an example of Slater's second rule

10. For $\langle \Phi_{p_1 p_2 \cdots p_N} | H | \Phi_{q_1 q_2 \cdots q_N} \rangle$ which differ by two spin-orbitals such that $p_1 \neq q_1, p_2 \neq q_2, p_3 = q_3 \cdots p_N = q_N$, show that
$$\langle \Phi_{p_1 p_2 \cdots p_N} | H | \Phi_{q_1 q_2 \cdots q_N} \rangle = \langle p_1 p_2 || q_1 p_2 \rangle$$
This is an example of Slater's third rule

11. Apply Slater's first rule to explicit write out (i.e. without summation symbols) all terms for
$$\langle \Phi_{pqr} | H | \Phi_{stu} \rangle$$
(Hint: There should be six terms total)