Homework for Lecture 3.2

1. Evaluate
$$\langle \Phi_{pq} | \Phi_{rst} \rangle$$

2. Show that the first Slater's rule using the second quantization formalism:
$$\langle \Phi | \hat{H} | \Phi \rangle = h_{ii} + \frac{1}{2} \sum_{ij} \langle ij || ij \rangle$$
holds for Φ_{p_1} and $\Phi_{p_1 p_2}$

3. (Optional, if you need more practice) Show that the second Slater's rule using the second quantization formalism:
$$\langle \Phi | \hat{H} | \Phi_i^a \rangle = h_{ia} + \frac{1}{2} \sum_{j} \langle ij || aj \rangle$$
where $|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi\rangle$ holds for Φ_{p_1} and $\Phi_{p_1 p_2}$

4. Work through the derivation of the one-electron and two-electron operators in the second quantization formalism yourself and make sure you understand what is going on

5. Show that normal vs antisymmetrized forms of the two-electron operator are equivalent. Bonus: show that the antisymmetrized form for a general k-body operator is equivalent to its normal form

6. Show that $\hat{h}(\mathbf{r_i})\phi_p(\mathbf{r_i}) = \sum_q \langle q|\hat{h}|p\rangle \, \phi_q(\mathbf{r_i})$ (Hint: rewrite in terms of bra-ket notation, and write ϕ_a as $|a\rangle$)

7. (Optional) Show that $\hat{g}(\mathbf{r_i}, \mathbf{r_j})\phi_{p_i}(\mathbf{r_i})\phi_{p_j}(\mathbf{r_j}) = \sum_{pq} \langle pq|\hat{h}|p_i p_j\rangle \, \phi_p(\mathbf{r_i})\phi_q(\mathbf{r_i})$

8. (Optional) Show that
$$a_r a_s \prod a^\dagger |0\rangle = \sum_{i<j}^{N} (-1)^{i+j} \delta_{rp_i} \delta_{sp_j} \prod{}^{p_i p_j} a^\dagger |0\rangle + \sum_{i>j}^{N} (-1)^{i+j-1} \delta_{rp_i} \delta_{sp_j} \prod{}^{p_i p_j} a^\dagger |0\rangle$$
by applying Equation 5 twice