Homework for Lecture 3.7 KM notation

1. Show algebraically that $\hat{P}_{(p/q/r)} = \hat{P}_{(p/qr)}\hat{P}_{(q/r)} = \hat{P}_{(pq/r)}\hat{P}_{(p/q)}$ and explain why these identities follow from the definition of the index antisymmetrizers.

2. Prove the following identities.

$$\tilde{a}^{p_1\cdots p_m}_{q_1\cdots q_m} = N[a^{p_1}_{q_1}\cdots a^{p_m}_{q_m}] \qquad N[a^{p_1\cdots p_m}_{q_1\cdots q_m}a^{r_1\cdots r_n}_{s_1\cdots s_n}] = N[a^{p_1}_{q_1}\cdots a^{p_m}_{q_m}a^{r_1}_{s_1}\cdots a^{r_n}_{s_n}] = \tilde{a}^{p_1\cdots p_m r_1\cdots r_n}_{q_1\cdots q_m s_1\cdots s_n}$$

   Furthermore, explain why these identities do not apply to contracted operators.

3. Explain why we cannot write:

$$\hat{P}^{(p/q)}_{(r/s)}\tilde{a}^p_r\tilde{a}^q_s$$

4. Put the Hamiltonian in Φ-Normal ordering using KM notation

5. Prove Slater's second rule using KM notation

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

6. Prove Slater's third rule using KM notation

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

7. Show that the Wick expansion of a triple excitation operator is:

$$a^{pqr}_{stu} = \tilde{a}^{pqr}_{stu} + \hat{P}^{(p/qr)}_{(s/tu)}\tilde{a}^{p^\circ qr}_{s^\circ tu} + \hat{P}^{(p/q/r)}_{(st/u)}\tilde{a}^{p^\circ q^{\circ\circ} r}_{s^\circ t^{\circ\circ} u} + \hat{P}^{(p/q/r)}\tilde{a}^{p^\circ q^{\circ\circ} r^{\circ\circ\circ}}_{s^\circ t^{\circ\circ} u^{\circ\circ\circ}}$$

8. Practice evaluating the following matrix elements using KM notation:

$$\langle\Phi^b_j|\Phi^a_i\rangle$$

$$\langle\Phi^b_j|H_c|\Phi^a_i\rangle$$

$$\langle\Phi^{cd}_{kl}|\Phi^{ab}_{ij}\rangle$$

$$\langle\Phi^{cd}_{kl}|H_c|\Phi^{ab}_{ij}\rangle$$

   The answers can be found in the last section of Andreas's "3q-1h-kutzelnigg-mukherjee.pdf" notes. Use it to check your results, but be sure you understand the work involved.