

1. Derive the expansion of  $H_e$  in terms of  $\Phi$ -normal excitations using KM notation with index antisymmetrizers.
2. Evaluate the following expectation values by Wick's theorem, using KM notation.

$$\begin{aligned} \langle \Phi | a_q^p | \Phi \rangle &= ? & \langle \Phi | a_q^p a_i^a | \Phi \rangle &= ? & \langle \Phi | a_q^p a_{ij}^{ab} | \Phi \rangle &= ? & \langle \Phi | a_q^p a_{ijk}^{abc} | \Phi \rangle &= ? \\ \langle \Phi | a_{rs}^{pq} | \Phi \rangle &= ? & \langle \Phi | a_{rs}^{pq} a_i^a | \Phi \rangle &= ? & \langle \Phi | a_{rs}^{pq} a_{ij}^{ab} | \Phi \rangle &= ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle &= ? \end{aligned}$$

Substitute your results into  $\langle \Phi | H_e | \Phi \rangle$ ,  $\langle \Phi | H_e | \Phi_i^a \rangle$ ,  $\langle \Phi | H_e | \Phi_{ij}^{ab} \rangle$ , and  $\langle \Phi | H_e | \Phi_{ijk}^{abc} \rangle$  to get the Slater rules.

3. Show that

$$\frac{1}{m!} v_{p_1 \dots p_m}^{q_1 \dots q_m} a_{q_1 \dots q_m}^{p_1 \dots p_m} = \left(\frac{1}{m!}\right)^2 \bar{v}_{p_1 \dots p_m}^{q_1 \dots q_m} a_{q_1 \dots q_m}^{p_1 \dots p_m}$$

which proves that any  $m$ -electron operator can be represented with an antisymmetrized interaction tensor. This generalizes the expression for electron repulsion in terms of antisymmetrized two-electron integrals.

4. Prove the following identities.

$$\tilde{a}_{q_1 \dots q_m}^{p_1 \dots p_m} = \text{:} a_{q_1}^{p_1} \dots a_{q_m}^{p_m} \text{:} \quad \text{:} a_{q_1 \dots q_m}^{p_1 \dots p_m} a_{s_1 \dots s_n}^{r_1 \dots r_n} \text{:} = \text{:} a_{q_1}^{p_1} \dots a_{q_m}^{p_m} a_{s_1}^{r_1} \dots a_{s_n}^{r_n} \text{:} = \tilde{a}_{q_1 \dots q_m s_1 \dots s_n}^{p_1 \dots p_m r_1 \dots r_n}$$

Furthermore, explain how the presence of a contraction line restricts which rearrangements are possible, and how this is remedied by the use of dot notation.

5. 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.
6. Show that the following identity holds for any four-index tensor  $t_{rs}^{pq}$ , whether antisymmetric or not.

$$\bar{g}_{pq}^{rs} \hat{P}_{(r/s)}^{(p/q)} t_{rs}^{pq} = 4 \bar{g}_{pq}^{rs} t_{rs}^{pq}$$

7. Show that the following identity holds for any  $w^{pqr}$  if  $v_{pqr}$  is antisymmetric.

$$v_{pqr} \hat{P}^{(p/qr)} w^{pqr} = 3 v_{pqr} w^{pqr}$$

8. Derive the Wick expansion of  $a_{stu}^{pqr}$  in terms of  $\Phi$ -normal excitations, using index antisymmetrizers to generate the full expansion from the unique contraction patterns.
9. Derive the CIS equations in KM notation.
10. Derive the CID equations in KM notation.