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

$$\begin{split} \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_r^p a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^{abc} | \Phi \rangle = \; ? & \langle \Phi | a_{rs}^{pq} a_{ijk}^$$

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

$$\frac{1}{m!} v_{p_1 \cdots p_m}^{q_1 \cdots q_m} a_{q_1 \cdots q_m}^{p_1 \cdots p_m} = (\frac{1}{m!})^2 \, \overline{v}_{p_1 \cdots p_m}^{q_1 \cdots q_m} a_{q_1 \cdots q_m}^{p_1 \cdots p_m}$$

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.

$$\tilde{a}_{q_{1}\cdots q_{m}}^{p_{1}\cdots p_{m}}=\mathbf{i}a_{q_{1}}^{p_{1}}\cdots a_{q_{m}}^{p_{m}}\mathbf{i} \qquad \qquad \mathbf{i}a_{q_{1}\cdots q_{m}}^{p_{1}\cdots p_{m}}a_{s_{1}\cdots s_{n}}^{r_{1}\cdots r_{n}}\mathbf{i}=\mathbf{i}a_{q_{1}}^{p_{1}}\cdots a_{q_{m}}^{p_{m}}a_{s_{1}}^{r_{1}}\cdots a_{s_{n}}^{r_{n}}\mathbf{i}=\tilde{a}_{q_{1}\cdots q_{m}s_{1}\cdots s_{n}}^{p_{1}\cdots p_{m}r_{1}\cdots r_{n}}\mathbf{i}=\mathbf{i}a_{q_{1}\cdots q_{m}s_{1}\cdots s_{n}}^{p_{m}}\mathbf{i}a_{s_{1}\cdots s_{n}}^{r_{1}\cdots r_{n}}\mathbf{i}=\mathbf{i}a_{q_{1}\cdots q_{m}s_{1}\cdots s_{n}}^{p_{m}}\mathbf{i}a_{s_{1}\cdots s_{n}}^{r_{1}\cdots r_{n}}\mathbf{i}a_{s_{1}\cdots s_{n}}^{r_{1}\cdots r_{n}}^{r_{1}\cdots r_{n}}\mathbf{i}a_{s_{1}\cdots s_{n}}^{r_{1}\cdots r_{n}}\mathbf{i}a_{s_{1}\cdots s_{n}}^{r_{1}\cdots r_{n}}\mathbf{i}a_{s_{1}\cdots s_{n}}^{r_{1}\cdots r_{n}}$$

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 Φ -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.