

$$\langle - | a_j a_i a_p^\dagger a_q a_l a_k^\dagger | \rangle$$

$$H = \sum_{p,q=1}^n h_{pq} a_p^\dagger a_q \quad [a_p, a_q^\dagger] = \delta_{pq}$$

$$\langle \underbrace{-ij}_{pq} | \sum_{p,q} h_{pq} a_p^\dagger a_q | \underbrace{kl}_{pq} \rangle \quad \langle ij = \bar{i}\bar{j} \rangle^* \quad (a_j^\dagger a_i)^\dagger =$$

$$= (-1) \langle - | a_j a_p^\dagger a_i a_q a_l a_k^\dagger | \rangle$$

$$+ \delta_{pi} \langle - | a_j a_q a_l a_k^\dagger | \rangle$$

$$= (-1)^2 \langle - | a_p^\dagger a_j a_i a_q a_l a_k^\dagger | \rangle$$

$$+ \delta_{pj} (-1) \langle - | a_i a_q a_l a_k^\dagger | \rangle$$

$$+ \delta_{pi} \delta_{ql} \langle - | a_j a_k^\dagger | \rangle$$

$$+ (-1) \delta_{pi} \langle - | a_j a_q^\dagger a_q a_k^\dagger | \rangle$$

$$a_p a_q^\dagger + a_q^\dagger a_p = \delta_{pq}$$

$$a_p a_q^\dagger = \delta_{pq} - a_q^\dagger a_p$$

$$+ \delta_{pj} (-1) \left\langle \overline{a_i a_l^+ a_k^+} \right\rangle \Rightarrow 0$$

$$+ \delta_{pi} \delta_{ql} \left\langle a_j a_k^+ \right\rangle \quad (-1) \left\langle a_k^+ a_j \right\rangle$$

$$+ (-1) \delta_{pi} \left\langle a_j^+ a_l a_k^+ \right\rangle$$

$$= \delta_{pj} \left\langle \overline{a_i a_l^+ a_k^+} \right\rangle$$

$$+ (-1) \delta_{pj} \delta_{ql} \left\langle a_i a_k^+ \right\rangle$$

$$+ \delta_{pi} \delta_{ql} \delta_{jk}$$

$$+ (-1) \delta_{pi} \delta_{jl} \left\langle a_l a_k^+ \right\rangle$$

$$\# \delta_{pj} \delta_{il} \left\langle a_l a_k^+ \right\rangle \Rightarrow \delta_{pj} \delta_{il} \delta_{qk}$$

$$= - \delta_{pj} \delta_{ql} \delta_{ik} \quad \delta_{qk}$$

$$+ \delta_{pi} \delta_{ql} \delta_{jk}$$

$$- \delta_{pi} \delta_{jl} \delta_{qk}$$

$$+ \delta_{pj} \delta_{il} \delta_{qk}$$

$$\begin{aligned}
 & \langle ij | \left(\sum_{p,q} h_{pq} a_p^\dagger a_q \right) | kl \rangle \quad \begin{matrix} p=j \\ q=l \end{matrix} \\
 & = \sum_{p,q} h_{pq} \left(\begin{aligned} & - \delta_{pj} \delta_{ql} \delta_{ik} \\ & + \delta_{pi} \delta_{ql} \delta_{jk} \\ & - \delta_{pi} \delta_{jl} \delta_{qk} \\ & + \delta_{pj} \delta_{il} \delta_{qk} \end{aligned} \right)
 \end{aligned}$$

$$\begin{aligned}
 & = -h_{j,l} \delta_{jk} + h_{i,l} \delta_{jk} \\
 & \quad - h_{i,k} \delta_{qk} + h_{j,k} \delta_{il}
 \end{aligned}$$

$$O \left(\binom{n}{d}^3 \right)$$

Wick's Theorem: $O(r)$

$$\left\langle \begin{array}{c} \text{---} \\ | \quad | \quad | \\ \text{---} \end{array} a_j a_c a_p (a_q)^+ a_e^+ a_k^+ \right\rangle$$

$$(-1) \delta_{ip} \delta_{jl} \delta_{qk} \quad O(1)$$

$$(-1)^0 \delta_{jk} \delta_{ip} \delta_{ql}$$

$$(-1)^2 \delta_{jp} \delta_{il} \delta_{qk}$$

$$(-1) \delta_{jp} \delta_{ik} \delta_{ql}$$

Slater-Condon Rules

- Wikipedia

$$\left(\begin{array}{l} \boxed{\downarrow} \quad \downarrow \quad \downarrow \\ - \delta_{pj} \delta_{ql} \delta_{ik} \\ + \delta_{pi} \delta_{ql} \delta_{jk} \\ - \delta_{pi} \delta_{jl} \delta_{qk} \\ + \delta_{pj} \delta_{il} \delta_{qk} \end{array} \right)$$