

Appendix: Slater–Condon Rules

$$\mathcal{O}_1 = \sum_i h(i)$$

$$\mathcal{O}_2 = \sum_{i \rangle j} r_{ij}^{-1}$$

$$H = \mathcal{O}_1 + \mathcal{O}_2$$

$$\langle \Psi | \mathcal{O}_1 | \Psi \rangle = \sum_i h_{ii}$$

$$\langle \Psi | \mathcal{O}_2 | \Psi \rangle = \sum_{i \rangle j} [\langle ij | ij \rangle - \langle ij | ji \rangle]$$

$$\langle \Psi | H | \Psi \rangle = \sum_i \langle i | h | i \rangle + \sum_{i \rangle j} [\langle ij | ij \rangle - \langle ij | ji \rangle]$$

$$\langle \Psi_i^a | \mathcal{O}_1 | \Psi \rangle = \langle a | h | i \rangle = h_{ai}$$

$$\langle \Psi_i^a | \mathcal{O}_2 | \Psi \rangle = \sum_j [\langle aj | ij \rangle - \langle aj | ji \rangle]$$

$$\langle \Psi_i^a | H | \Psi \rangle = \langle a | h | i \rangle + \sum_j [\langle aj | ij \rangle - \langle aj | ji \rangle]$$

$$\langle \Psi_{ij}^{ab} | \mathcal{O}_2 | \Psi \rangle = \langle ab | ij \rangle - \langle ab | ji \rangle$$

$$\langle \Psi_{ij}^{ab} | H | \Psi \rangle = \langle ab | ij \rangle - \langle ab | ji \rangle$$