1 UHF

2 RHF

2.1 Singlet Excitation Operators

Generally, the one- and two-body excitation operators are defined as:

$$E_q^p = \hat{p}_\alpha^\dagger \hat{q}_\alpha + \hat{p}_\beta^\dagger \hat{q}_\beta \tag{1}$$

$$e_{rs}^{pq} = \sum_{\sigma\tau} \hat{p}_\sigma^\dagger \hat{q}_\tau^\dagger \hat{s}_\tau \hat{r}_\sigma \tag{2}$$

By:

$$[\hat{p}^\dagger, \hat{q}]_+ = \hat{\delta}_{pq} \tag{3}$$

the two-body singlet excitation operator could be written as:

$$\begin{aligned}
e_{rs}^{pq} &= \sum_{\sigma\tau} \hat{p}_\sigma^\dagger \hat{q}_\tau^\dagger \hat{s}_\tau \hat{r}_\sigma \\
&= -\sum_{\sigma\tau} \hat{p}_\sigma^\dagger \hat{q}_\tau^\dagger \hat{r}_\sigma \hat{s}_\tau \\
&= -\sum_{\sigma\tau} \hat{p}_\sigma^\dagger (\delta_{qr}\delta_{\sigma\tau} - \hat{r}_\sigma \hat{q}_\tau^\dagger) \hat{s}_\tau \\
&= \sum_{\sigma\tau} \hat{p}_\sigma^\dagger \hat{r}_\sigma \hat{q}_\tau^\dagger \hat{s}_\tau - \sum_{\sigma\tau} \delta_{qr}\delta_{\sigma\tau} \hat{p}_\sigma^\dagger \hat{s}_\tau \\
&= \hat{p}_\alpha^\dagger \hat{r}_\alpha \hat{q}_\alpha^\dagger \hat{s}_\alpha + \hat{p}_\alpha^\dagger \hat{r}_\alpha \hat{q}_\beta^\dagger \hat{s}_\beta + \hat{p}_\beta^\dagger \hat{r}_\beta \hat{q}_\alpha^\dagger \hat{s}_\alpha + \hat{p}_\beta^\dagger \hat{r}_\beta \hat{q}_\beta^\dagger \hat{s}_\beta - \delta_{qr}(\hat{p}_\alpha^\dagger \hat{s}_\alpha + \hat{p}_\beta^\dagger \hat{s}_\beta) \\
&= E_r^p E_s^q - \delta_{qr} E_s^p
\end{aligned} \tag{4}$$

Note, conventionally, the indices for the two-body operator are written in Chemists' notation.

Considering the nature of excitation operators, the following expressions are often more useful:

$$E_i^a = \hat{a}_\alpha^\dagger \hat{i}_\alpha + \hat{a}_\beta^\dagger \hat{i}_\beta \tag{5}$$

$$e_{ij}^{ab} = \sum_{\sigma\tau} \hat{a}_\sigma^\dagger \hat{b}_\tau^\dagger \hat{j}_\tau \hat{i}_\sigma = E_i^a E_j^b \tag{6}$$