1 Sigma Equations

1.1 Amplitude Equations

The (UHF) residual equations which determine the cluster amplitudes are written as following:

$$\sigma_i^a = \langle \Phi_i^a | \hat{\mathcal{H}} | 0 \rangle = \langle 0 | \{\hat{i}^\dagger \hat{a}\} \hat{H}_{\mathrm{N}} (1 + \hat{T}_1 + \hat{T}_2 + \hat{T}_1 \hat{T}_2 + \frac{1}{2!}\hat{T}_1^2 + \frac{1}{3!}\hat{T}_1^3) | 0 \rangle_{\mathrm{C}} \tag{1}$$

$$\begin{aligned} \sigma_{ij}^{ab} =& \langle \Phi_{ij}^{ab} | \hat{\mathcal{H}} | 0 \rangle \\ =& \langle 0 | \{\hat{i}^\dagger \hat{j}^\dagger \hat{b} \hat{a}\} \hat{H}_{\mathrm{N}} (1 + \hat{T}_1 + \hat{T}_2 + \hat{T}_1 \hat{T}_2 + \frac{1}{2!}\hat{T}_1^2 + \frac{1}{2!}\hat{T}_2^2 + \frac{1}{2!}\hat{T}_1^2 \hat{T}_2 + \frac{1}{3!}\hat{T}_1^3 + \frac{1}{4!}\hat{T}_1^4) | 0 \rangle_{\mathrm{C}} \end{aligned} \tag{2}$$

For the σ_i^a equation, the $e^{\hat{T}}$ operator expands up to (disconnected) triple excitations, due to the two-body natural of $\hat{H}_{\mathrm{N}}$ operator; and similarly the σ_{ij}^{ab} equation includes up to (disconnected) quadruple excitations.
As for the RHF residual equations, the singlet spin-traced operators E_i^a and e_{ij}^{ab} need to be used.